IN THE UNITED STATES DISTRICT COURT
FOR THE EASTERN DISTRICT OF NORTH CAROLINA
Civil Action No.: 7:23-CV-00897

IN RE:	)	
	)	PLAINTIFFS' MEMORANDUM IN OPPOSITION TO DEFENDANT'S MOTION TO EXCLUDE THE OPINION TESTIMONY OF R. JEFFREY DAVIS AND NORMAN L. JONES, PH.D
CAMP LEJEUNE WATER LITIGATION	)	
	)	
This Pleading Relates to:	)	
	)	
ALL CASES.	)	
	)	

TABLE OF CONTENTS

I. INTRODUCTION

Pursuant to Local Rules 7.1(f) and 7.2, Plaintiffs' Leadership Group (PLG) submits this response in opposition to the Government's Motion to Exclude Opinion Testimony of Mr. R. Jeffrey Davis and Dr. Norman L. Jones. DE-356. The Government has brought a motion under *Daubert* and Fed. R. Evid. 702 with no argument concerning the experts' qualifications, the relevance of their testimony, or the reliability of a post-audit analysis. Instead, the Government seeks to discredit expert conclusions not by truly challenging the methodology used, but by imposing an inapplicable standard of document review that ignores the basis of Dr. Jones and Mr. Davis's opinions and the empirical nature of the work. The Government's criticisms go to the weight of Dr. Jones and Mr. Davis's testimony, not its admissibility, and the Court should deny the motion.

II. STATEMENT OF RELEVANT FACTS

Following the selection of twenty-five Track 1 plaintiffs for trial, the Court entered scheduling orders for expert discovery and motion practice across three phases: (1) Water Contamination (Phase 1); (2) general causation (Phase 2); and (3) specific causation, damages, and residual issues (Phase 3). DE-270; DE-312. Phase 1 is dedicated to establishing the contaminant concentration levels in finished water at Camp Lejeune from 1953 to 1987, which the parties agree involves presenting evidence on "the contamination sources, the fate and transport of the contaminants within the groundwater underlying Camp Lejeune, the supply of water through wells to the various treatment plants at Camp Lejeune, and the distribution of the water from the treatment plants to relevant areas of Camp Lejeune during this time frame." DE-329.

To establish the contaminant concentration levels in finished water at Camp Lejeune from 1953 to 1987, the PLG is relying on the groundwater flow and contaminant fate and transport models developed by the Agency for Toxic Substances and Disease Registry (ATSDR) to simulate monthly mean contaminant concentration levels in water delivered to the Tarawa Terrace, Hadnot Point, and Holcomb Boulevard areas of the base. In support of these models, and to rebut criticisms raised by the Government's experts, the PLG disclosed six experts in the fields of engineering, hydrogeology, mathematical modeling, and physiochemical processes.[1] Dr. Jones and Mr. Davis were retained to perform a post-audit goodness-of-fit assessment of ATSDR's groundwater flow and contaminant transport model for Tarawa Terrace using site remediation data collected after ATSDR built its model. DOJ Ex. 3, Jones and Davis Report (DE-357-4) at 1-1–1-2; DOJ Ex. 4, Jones and Davis Rebuttal Report (DE-357-5) at 2-1; DOJ Ex. 5, Jones Dep. (DE-357-6) at 113:10-15. This involved extending ATSDR's MODFLOW and MT3DMS models for Tarawa Terrace from 1995 to 2008 and comparing the outputs to actual PCE concentrations observed at monitoring wells during that period. DOJ Ex. 3, Jones and Davis Report (DE-357-4) at vi.

A post-audit tests a model's accuracy.[2] It is a technical exercise and a technique used by modelers to quantitatively and qualitatively assess the degree of correspondence between a model's simulated values and observation data.[3] It is an optional step in what is considered a standard protocol for developing and applying groundwater flow and contaminant fate and

[1] The PLG's experts for Phase 1 are Morris Maslia, P.E.; Mustafa Aral, Ph.D.; Norman Jones, Ph.D.; R. Jeffrey Davis, P.E.; Leonard Konikow, Ph.D.; and David Sabatini, Ph.D.
[2] Ex. 1, Excerpt from Hill and Tiedman, Effective Groundwater Model Calibration (2007), at 262.
[3] Ex. 1, Excerpt from Hill and Tiedman, Effective Groundwater Model Calibration (2007), at 338 ("Model accuracy can be evaluated by comparing simulated predictions with existing data intentionally omitted from model calibration or new data. . . Tests against new data are sometimes called postaudits."); Ex. 2, ASTM International D5490-93: Standard Guide for Comparing Ground-Water Flow Model Simulations to Site-Specific Information (2002), at 1.

transport models.[4] The "degree of correspondence" between simulated and observed values reflects model accuracy and it is assessed visually through graphs and by calculating summary statistics such as the mean absolute error.[5]

Consistent with industry practice and guidelines on evaluating models,[6] Dr. Jones and Mr. Davis's methodology for the post-audit of the Tarawa Terrace model consisted of:

- Reviewing pertinent Tarawa Terrace chapter reports;
- Converting ATSDR's original MODFLOW and MT3DMS models to newer versions (MODFLOW 2000 and MT3DMS v5.3);
- Extending the original model's simulation period from 1995 to 2008 by incorporating updated rainfall-recharge data from nearby weather stations and remediation well pumping rates;
- Quantitatively evaluating the original model's accuracy using summary statistics (mean error and mean absolute error), scatter plots, and time series plots of simulated versus observed PCE concentrations; and

---

[4] *See* Ex. 3, Excerpt from Anderson and Woessner, Applied Groundwater Modeling: Simulation of Flow and Advective Transport (2015), at CL_PLG-EXPERT_ARAL_0000000077, CL_PLG-EXPERT_ARAL_0000000083-86; Ex. 4, Anderson, The Role of The Postaudit in Model Validation, Advances in Water Resources 15 (1992) 167-173, at 168; Ex. 5, ASTM International D5447-17: Standard Guide for Application of a Groundwater Flow Model to a Site-Specific Problem (2017), at 2.

[5] Ex. 6, Reilly and Harbaugh, Guidelines for Evaluating Ground-Water Flow Models, U.S. Geological Survey, Scientific Investigations Report 2004-5038 (2004), at 23 ("There are different quantitative measures that investigators use to show the accuracy of the calibration of a ground-water flow model. Some of these are: the mean error, the mean absolute error, and the root mean squared error.") (citation omitted); Ex. 2, ASTM International D5490-93: Standard Guide for Comparing Ground-Water Flow Model Simulations to Site-Specific Information (2002), at 2 ("Quantitative and qualitative comparisons are both essential. Both should be used to evaluate the degree of correspondence between a ground-water flow model simulation and site-specific information.").

[6] *See, e.g.*, Ex. 2, ASTM International D5490-93: Standard Guide for Comparing Ground-Water Flow Model Simulations to Site-Specific Information (2002).

- Qualitatively assessing the spatial distribution and migration of the PCE plume across model layers and at monitoring wells.

DOJ Ex. 5, Jones Dep. (DE-357-6) at 85:2-10, 87:18-88:24; DOJ Ex. 3, Jones and Davis Report (DE-357-4) at 2-1, 3-1 to 3-2, 4-1 to 4-2, 5-1 to 5-4; Ex. 7, Jones & Davis Rainfall Imputation Addendum.

Dr. Jones and Mr. Davis's opening report details each step of their post-audit analysis, identifies the underlying data and model input files used (i.e., ATSDR's calibrated model input files), and explains in detail how the residual errors and scatter plots were calculated and what they show in terms of the original model's ability to simulate PCE concentrations in monitoring wells. DOJ Ex. 3, Jones and Davis Report (DE-357-4); Ex. 8, Jones and Davis Revised Materials Considered List. Dr. Jones and Mr. Davis also produced their native post-audit model files, allowing the Government's experts to reproduce and test their work, which they did. DOJ Ex. 4, Jones and Davis Rebuttal Report (DE-357-5) at 3-10 to 3-13; Ex. 9, Nov. 5, 2024 PLG Expert Files Production Letter.

As is evident from their reports,[7] Dr. Jones and Mr. Davis were hired to conduct a post-audit – not to provide an opinion of ATSDR's work based on a review of the chapter reports. Their role in this case is to offer testimony on the post-audit, including what the post-audit results convey

[7] Dr. Jones and Mr. Davis's rebuttal report explains their role in this litigation:

> In 2024, we were tasked with performing a post-audit of the Tarawa Terrace flow and transport models. The objective of the post-audit was to extend the range of the groundwater flow and transport models from 1995 to 2008 and compare the output of the transport model with concentrations sampled at monitoring wells in Tarawa Terrace during the 1995–2008 period to assess the performance of the model as an interpretive and predictive tool. This comparison involved both a quantitative analysis of simulated versus observed concentrations and a qualitative analysis of the shape and migration of the simulated PCE plume over that period.

DOJ Ex. 4, Jones and Davis Rebuttal Report (DE-357-5) at 2-1.

about how reliable the underlying ATSDR flow and transport model is.[8] PLG's other experts, including Morris Maslia and Dr. Leonard Konikow, reviewed all chapter reports and are prepared to offer opinions on them. Dr. Jones explained in deposition that, following a high-level review of all nine chapters, they focused on the chapters that were necessary and appropriate to perform the post-audit:

> . . . Chapter A is kind of a comprehensive summary, as I understand it, of all of the work that was done, including what was put in those other chapters. And so felt like I had a reasonably good exposure to the overall methods and processes that were used and then described in more detail in those chapters.
>
> But for the purpose of the post-audit which we were hired to do, certainly the most important chapters would be A, C, and F.
>
> **Q.** Why are A, C, and F the most important chapters for the post-audit you were hired to do?
>
> **A.** Because A is a -- is a comprehensive summary, a detailed summary of the entire modeling project. It was very helpful in getting an overview of all of the work that was done
>
> Chapter C provided a very detailed description of the construction and calibration of the MODFLOW flow model.
>
> And Chapter F was a very detailed description of the construction and calibration, uncertainty analysis associated with the contaminant transport model.
>
> And we were asked to, in -- in conducting the post-audit, to -- to perform simulations using both the flow and transport model. So they were clearly the most relevant chapters for our work.

DOJ Ex. 5, Jones Dep. (DE-357-6) at 87:18-88:24. *See also*, *id.* at 86:6-10, 89:2-6, 90:16-20.

[8] DOJ Ex. 3, Jones and Davis Report (DE-357-4) at vi ("The audit extends the original model's simulation period from 1995 to 2008 and assesses the accuracy of its predictions by comparing simulated PCE concentrations to actual concentrations measured at monitoring wells during this extended period.").

The first, Chapter A, is a comprehensive, 100-page discussion of ATSDR's historical reconstruction analysis for Tarawa Terrace. Ex. 10, ATSDR Tarawa Terrace Report Chapter A. It includes:

- The models used and the data and sequence in which the data were applied to each model. *Id.* at A12-A14.
- The model calibration process and results of related statistical analyses. *Id.* at A22-A26.
- The calibrated model parameters and their values. *Id.* at 29.
- Simulation results and results of related statistical analyses. *Id.* at A32-A39
- Degradation by-product analysis and results. *Id.* at A41-A46.
- Details and results of sensitivity analyses, probabilistic analyses, and tracer study. *Id.* at A47-67.

Chapters C and F are the chapters dedicated to the ATSDR's methodology for developing and applying its groundwater flow (MODFLOW, Chapter C) and PCE fate and transport (MT3DMS, Chapter F) models – which is the sole focus of Dr. Jones and Mr. Davis's post-audit.[9] DOJ Ex. 3, Jones and Davis Report (DE-357-4) at vi ("This post-audit report evaluates the performance of groundwater flow and transport models developed for the Tarawa Terrace region of Camp Lejeune by the Agency for Toxic Substances and Disease Registry (ATSDR)."). The remaining chapters address elements of the ATSDR's study that either did not concern the models evaluated in the post-audit (e.g., Chapter G on the development of TechFlowMP for degradation by-products) or were sufficiently covered in Chapter A. DOJ Ex. 5, Jones Dep. (DE-357-6) at 87:18-25.

Based on the results of the post-audit, their experience and expertise in the fields of hydrogeology and groundwater modeling, and their review of pertinent ATSDR chapter reports, Dr. Jones and Mr. Davis are prepared to offer the opinions stated in their report: (1) that the Tarawa

[9] *See generally* Ex. 11, ATSDR Tarawa Terrace Report Chapter C: Simulation of Groundwater Flow; Ex. 12, ATSDR Tarawa Terrace Report Chapter F: Simulation of the Fate and Transport of Tetrachloroethylene (PCE).

Terrace flow and transport model was developed using sound methods, and (2) the model is a reliable tool for understanding contaminant migration in the Tarawa Terrace region of Camp Lejeune. DOJ Ex. 3, Jones and Davis Report (DE-357-4) at 6-1.

III. LEGAL STANDARD

The admissibility of expert testimony is governed by Rule 702 of the Federal Rules of Evidence. Rule 702 allows a witness qualified by knowledge, skill, experience, training, or education to testify if the witness's "testimony is based on sufficient facts or data," the witness's "testimony is the product of reliable principles and methods," and the "opinion reflects a reliable application of the principles and methods to the facts of the case." *See* Fed. R. Evid. 702(a)-(d). This Court and the Fourth Circuit has "distilled Rule 702's requirements into three crucial inquiries: (1) whether the proposed expert witness is qualified; (2) whether the proposed testimony is relevant; and (3) whether the proposed testimony is reliable." *Dew*, 2024 WL 4349883, at *2 (citing *Kumho Tire Co., Ltd. v. Carmichael*, 526 U.S. 137, 141 (1990)); *Daubert v. Merrell Dow Pharms, Inc*., 509 U.S. 579, 589 (1993); *United States v. Forrest*, 429 F.3d 73, 80 (4th Cir. 2005).

While there is no definitive checklist or test to assess reliability, factors that often guide the court's reliability analysis include: (1) whether a theory or technique can be (or has been) tested; (2) whether it has been subjected to peer review and publication; (3) its potential rate of error; (4) whether standards exist to control the technique's operation; and (5) the degree of acceptance of the methodology within the relevant scientific community. *Daubert*, 509 U.S. at 593-94; *Kumho Tire Co., Ltd. v. Carmichael*, 526 U.S. 137, 138 (1999); *Nix v. Chemours Co. FC*, No. 7:17-CV-189-D, 7:17-CV-197-D, 7:17-CV-201-D, 2023 WL 6471690, at *7 (E.D.N.C. Oct. 4, 2023). Ultimately, in determining "whether proffered testimony is sufficiently reliable, the court has broad latitude to consider whatever factors bearing on validity that the court finds to be useful; the particular factors will depend upon the unique circumstances of the expert testimony involved."

Westberry v. Gislaved Gummi AB, 178 F.3d 257, 261 (4th Cir. 1999). "'[R]ejection of expert testimony is the exception rather than the rule.'" *Gillis v. Murphy-Brown, LLC,* No. 7:14-CV-185-BR, 2018 WL 5284607, at *2 (E.D.N.C. Oct. 24, 2018) (quoting Fed. R. Evid. 702 Advisory Comm. Notes (2000 Amendments) and noting that opinions should not be excluded "merely because they are impeachable").

IV. ARGUMENT

As is set out in detail in both their opening and rebuttal reports, Dr. Jones and Mr. Davis have a very specific role in this case: to test the reliability of the Tarawa Terrace flow and transport model via a post-audit analysis. The Government now moves to exclude their conclusion—that the post-audit demonstrates the model is sound and reliable—not based on the reliability of the post-audit methodology, its acceptance in the scientific community, the experts' application of it, or their interpretation of the results, but solely because they believe Dr. Jones and Mr. Davis should have spent more time reading certain documents. The Government does not point to any industry standard or authority to support its position and, importantly, it does not identify a single let alone critical "fact or data" in these other ATSDR chapters it believes was not covered in the chapters Dr. Jones and Mr. Davis reviewed. Instead, a review of the record demonstrates that Dr. Jones and Mr. Davis's opinions regarding the reliability and soundness of the flow and transport model meet Rule 702's admissibility requirements. Any criticisms the Government has about the documents reviewed is a subject for cross examination, not a basis for exclusion. The Court should deny the motion.

The Government does not challenge Dr. Jones and Mr. Davis's qualifications or the relevance of their testimony; however, because the PLG must demonstrate the proffered testimony meets Rule 702's admissibility requirements by a preponderance of the evidence, Plaintiffs will address each element in turn. Fed. R. Evid. 702; *see also*, *Dew v. E.I. du Pont de Nemours and Company*, No. 5:18-CV-73-D, 2024 WL 4349883, at *2 (E.D.N.C. Sept. 30, 2024) (unpublished).

A. Dr. Jones and Mr. Davis are Qualified to Offer Opinions Regarding the Reliability and Soundness of ATSDR's Tarawa Terrace Model.

The first step in the Court's Rule 702 admissibility inquiry is to determine if the expert is qualified to testify. Qualification can be based on "knowledge, skill, experience, training, or education" and should be assessed "in reference to the matter to which the witness seeks to testify." Dew, 2024 WL 4349883, at *3 (citing *Daubert*, 509 U.S. at 591–93). The Government does not challenge Dr. Jones and Mr. Davis's qualifications; however, even if it did, the record demonstrates that both are amply qualified to testify about the design, application, and evaluation of groundwater flow and contaminant fate and transport models.

Dr. Norman Jones has over three decades of experience in civil and environmental engineering. He has a Ph.D. in civil engineering from the University of Texas and currently serves as a professor and Chair of the Department of Civil and Construction Engineering at Brigham Young University, where he has taught courses on computer programming, soil mechanics, and groundwater flow and transport modeling. DOJ Ex. 3, Jones and Davis Report (DE-357-4) at 8-1 to 8-2, Report Exhibit 2. Dr. Jones is the original developer of the Groundwater Modeling System (GMS) software, "which is a graphical user interface for MODFLOW and MT3DMS and is used by thousands of organizations all over the world." *Id.* He has also authored 179 technical publications, including 88 peer-reviewed journal articles, and received awards from both the American Society of Civil Engineers and the National Groundwater Association for his work. *Id.* The Court should find Dr. Jones qualified to testify.

Mr. R. Jeffrey Davis is a licensed professional engineer and certified ground water professional (CGWP) with nearly 30 years of experience in civil and environmental engineering, hydrogeology, groundwater fate and transport modeling, and software and model development. DOJ Ex. 3, Jones and Davis Report (DE-357-4) at 8-1. He has both undergraduate and graduate degrees from Brigham Young University in civil engineering and currently serves on the board of directors for the National Ground Water Association (NGWA). *Id.* Mr. Davis has worked on hundreds of groundwater modeling projects for a wide range of industries, including agriculture, mining, oil and gas, and hydraulic fracturing, and has served as an expert witness in groundwater contamination litigation. DOJ Ex. 2, Davis Dep. (DE-357-3) at 54:6-10; DOJ Ex. 3, Jones and Davis Report (DE-357-4) at 8-1, Report Exhibit 1. He is also regularly invited to participate on panels discussing groundwater, water supply, and water contamination issues. *Id.* Like Dr. Jones, Mr. Davis is qualified to testify.

B. Dr. Jones and Mr. Davis's Opinions Regarding the Reliability and Soundness of ATSDR's Tarawa Terrace Model are Relevant.

The second step in the Court's Rule 702 admissibility inquiry is to determine if the testimony is relevant. To be relevant, the proposed expert testimony must "help the trier of fact to understand the evidence or to determine a fact in issue." Fed. R. Evid. 702(a). "A key 'aspect of relevancy ... is whether expert testimony proffered in the case is sufficiently tied to the facts of the case that it will aid the jury in resolving a factual dispute.'" *United States v. Ferncreek Cardiology*, P.A., No. 5:17-CV-616-FL, at *6 (E.D.N.C., Mar. 20, 2025) (quoting *Daubert*, 509 U.S. at 591).

The Government does not challenge the relevance of Dr. Jones and Mr. Davis's testimony regarding the reliability and soundness of ATSDR's MODFLOW and MT3DMS models for Tarawa Terrace. More important, this testimony will help the Court both understand evidence in this case and resolve factual disputes. As this Court has recognized, "this case is about water," and the "court must understand the chemicals in the water at Camp Lejeune during the operative period." DE-247 at 2. The PLG relies on the results of ATSDR's Tarawa Terrace model to establish

PCE concentrations in that area of the base and the Government is challenging its admissibly on the grounds that it is "unreliable and scientifically invalid." DE-368 at 16. Dr. Jones and Mr. Davis's post-audit analysis relates to the reliability of the model and will undoubtedly help the Court to understand and resolve this issue. Therefore, the Court should find the testimony relevant.

C. Dr. Jones and Mr. Davis's Opinions Regarding the Reliability and Soundness of ATSDR's Tarawa Terrace Model are Reliable and Properly Supported.

The Government's motion focuses on the reliability of Dr. Jones and Mr. Davis's opinions regarding the accuracy and soundness of the model, arguing primarily that the opinions are not based on sufficient facts and data and sometimes that they failed to employ a reliable methodology. The Government's argument misses the mark for two reasons. First, it ignores that the post-audit is the primary basis for their opinion and fails to discuss the post-audit methodology entirely. Second, it fails to present any evidence that Dr. Jones and Mr. Davis's quantitative and qualitative analysis of the extended ATSDR model was missing facts and data.

1. Dr. Jones and Mr. Davis's opinions are based primarily on their post-audit, the reliability of which the Government does not challenge.

The Government's motion misses the boat entirely by ignoring the post-audit itself. As is evident from their reports, Dr. Jones and Mr. Davis were hired to conduct a post-audit – not to provide an opinion of ATSDR's work based on a review of the chapter reports.[10] And the Government makes no argument that the methodology of the post-audit is unreliable under the *Daubert* factors or otherwise. Instead, relying on a single answer taken out of context in deposition, the Government contends that Dr. Jones and Mr. Davis's "opinion testimony regarding the accuracy and soundness of ATSDR's methodology is based *solely* on their reading of a small

---

[10] Ex DOJ Ex. 3, Jones and Davis Report (DE-357-4) at vi; DOJ Ex. 4, Jones and Davis Rebuttal Report (DE-357-5) at 2-1.

subset of ATSDR's reports." DE 357 at 7 (emphasis added). That is false. Dr. Jones and Mr. Davis never "disclaimed that their post-audit was the basis for their opinion that the ATSDR model was reliable," which is why the Government does not include a citation to the record for that assertion. Quite the opposite, Mr. Davis identified the post-audit as a way in which they evaluated ATSDR's methodology and as a basis for opinions regarding the model's reliability throughout his deposition. *See* DOJ Ex. 2, Davis Dep. (DE-357-3) at 269:24-270:5, 281:2-22, 282:14-19, 282:20-283:6.

The reality is that Dr. Jones and Mr. Davis's opinion testimony regarding the reliability and soundness of ATSDR's methodology is based primarily on their post-audit,[11] the reliability of which the Government does not challenge. But even if the Government had challenged the reliability of the post-audit methodology—which it does not—consideration of the *Daubert* factors supports reliability of these opinions.

A post-audit is an accepted method used "to test prediction accuracy." Ex. , Excerpt from Hill and Tiedman, Effective Groundwater Model Calibration (2007), at 262. The technique has been subject to peer review, and there are industry guidelines that inform the assessment's application, which Dr. Jones and Mr. Davis adhered to.[12] Indeed, comparing a model's simulated

---

[11] This is evident in their reports—*see, e.g.*, DOJ Ex. 4, Jones and Davis Rebuttal Report (DE-357-5) at 1-1 (identifying the post-audit as a basis for their opinions)—and in their deposition testimony. *See, e.g.*, DOJ Ex. 2, Davis Dep. (DE-357-3) at 258:7-9 (stating the post-audit strengthened the validity of the model), 279:1-3 (explaining that based on the post-audit, it is his opinion the model effectively modeled month-by-month concentrations), 281:2-22 (confirming that based on the post-audit, it is his opinion the model is reliable for determining the migration of the PCE contamination); 281:23-282:19 (explaining that based on the results of the post-audit, it is his opinion that the model can reliably determine monthly PCE concentrations); DOJ Ex. 5, Jones Dep. (DE-357-6) at 116:18-117:13 (explaining that the results of the post-audit supported the accuracy and soundness of the model).

[12] *See, e.g.*, Ex. 13, Konikow, Predictive Accuracy of a Ground-Water Model – Lessons from a Postaudit. Ground Water, 24 (1986) 173-1984; Ex. 4, Anderson and Woessner, The Role of the

values to field observed values to evaluate a model's accuracy is discussed in textbooks and is a common practice in the scientific community.[13] Dr. Jones and Mr. Davis's technique is carefully documented and can and has been tested by the Government's experts.[14] They have also calculated and identified the mean error (48 micrograms per liter) for their post-audit results—meaning the average difference between the extended model's simulated PCE concentration and the measured PCE concentration was only 48 μg/L.[15] This demonstrates a well-balanced fit and supports the reliability of the post-audit results. DOJ Ex. 4, Jones and Davis Rebuttal Report (DE-357-5), at 3-5. Based on the record, the Court should find that the post-audit satisfies every *Daubert* factor.

In arguing that Dr. Jones and Mr. Davis did not test ATSDR's methods, the Government again falls short. DE 357 at 11. The post-audit itself is a test of the ATSDR's model – it tests how accurate the model predictions are by running the model for thirteen additional years and comparing the model results to the measured remediation results. The argument that Dr. Jones and Mr. Davis failed to evaluate the input parameters underlying the ATSDR model and simply used input parameters from the PLG is similarly misguided. DE 357 at 11-13. The input parameters Dr. Jones and Mr. Davis used were not selected by the PLG – the model input files used for the post-

Postaudit in Model Validation. Advances in Water Resources 15 (1992) 167-173; Ex. 2, ASTM International D5490-93: Standard Guide for Comparing Ground-Water Flow Model Simulations to Site-Specific Information (2002), at 1; DOJ Ex. 5, Jones Dep. (DE-357-6) at 232:20-233:4 (Dr. Jones testifying that he has performed post-audits comparing a model's simulated values to field observed values to evaluate the model's accuracy countless times).

[13] Ex. 6, Reilly and Harbaugh, Guidelines for Evaluating Ground-Water Flow Models, U.S. Geological Survey, Scientific Investigations Report 2004-5038 (2004), at 23; Ex. 3, Excerpt from Anderson and Woessner, Applied Groundwater Modeling: Simulation of Flow and Advective Transport (2015), at CL_PLG-EXPERT_ARAL_0000000452-459.

[14] DOJ Ex. 4, Jones and Davis Rebuttal Report (DE-357-5) at 3-10 to 3-13.

[15] DOJ Ex. 4, Jones and Davis Rebuttal Report (DE-357-5) at 3-5. Dr. Jones also calculated and provided the geometric bias for the post-audit results in deposition. DOJ Ex. 5, Jones Dep. (DE-357-6) at 283:1-10 (2.1 for all observations, and only 1.2 when limited to observations above 5 micrograms per liter).

audit were the ATSDR's original model input files produced by the Government in this litigation. The input parameters included in those files are the parameters from the original model. *See* Ex. 8, Jones and Davis Revised Materials Considered List at 6-7 (identifying the ATSDR model input files, materials 99-123, by bates number). Using the same input parameters ensures the post-audit is testing ATSDR's actual model, not a different model.

The Government's reliance on *Sommerville v. Union Carbide Corp.*, No. 2:19-CV-00878, 2024 WL 1204094 (S.D. W. Va. Mar. 20, 2024) further highlights its misconceptions about the nature and function of the post-audit. *Sommerville* did not involve an expert tasked with *testing* an existing model. It involved an expert who *built* an air dispersion model to prove exposure levels using, among other problematic and inappropriate data, "patently unreliable" worst-case emissions estimates reported in regulatory documents, non-representative meteorological data, and inaccurate operating scenarios. *Id.* at 11-19. The *Sommerville* expert's failure to make any attempt to assess the appropriateness of the data he put into his model is not "analogous" to the recognized technical exercise Dr. Jones and Mr. Davis performed in this case.

A proper post-audit that assesses a model's accuracy by comparing the simulated values to additional observation data requires the modeler to use the original model, including the original input parameters.[16] When done this way, the degree of correspondence between simulated and observed values found via the post-audit reflects the appropriateness of the model's input parameters and assumptions. If there was no correspondence between simulated and observed values, that would indicate flaws in the original model. However, as Dr. Jones explained in

[16] *See* DOJ Ex. 5, Jones Dep. (DE-357-6) at 273:1-9 ("the model inputs would be extended over a new period. We would not change anything in the original models, other than extending it, and then run the simulations and compare the predicted results of the extended model with any new field observed value data that were available, is the general process.).

deposition, the post-audit showed good agreement between the two, which is evidence that the original model is a reliable tool developed using sound methods. DOJ Ex. 5, Jones Dep. (DE-357-6) at 113:10-117:13. The post-audit results supporting their opinions regarding the reliability and soundness of the model are presented in a series of tables, plots, and graphs included with the report, none of which the Government contests or even discusses.[17] Significantly, the Government does not contest Dr. Jones and Mr. Davis's opinion that the post-audit results demonstrate that the ATSDR's model "reasonably captured the key behaviors of the PCE plume." DOJ Ex. 3, Jones and Davis Report (DE-357-4) at 6-1.

2. The Government fails to present any evidence that Dr. Jones and Mr. Davis's quantitative and qualitative analyses of the extended ATSDR model were missing facts and data.

The Government's primary criticism regarding Dr. Jones and Mr. Davis's opinions concerns the documents they reviewed to perform their post-audit. Without identifying any supportive industry practice or a single "fact or data" it believes is missing from Dr. Jones and Mr. Davis's extended model, the Government asks this Court to supplant the judgment of two engineers with a combined sixty years of flow and transport modeling experience with that of its lawyers. The Court should reject the invitation. Disagreements over the universe of documents reviewed is a subject for cross examination, not exclusion. *SAS Institute, Inc. v. World Programming Ltd.*, 125 F.Supp.3d 579, 590 (E.D.N.C. 2015), aff'd 874 F.3d 370 (4th Cir. 2017).

To support its position, the Government cites *E.E.O.C. v. Freeman*, 778 F.3d 463 (4th Cir. 2015) and *Yates v. Ford Motor Co.*, 113 F.Supp.3d 841, 858–860 (E.D.N.C. 2015) – two cases with facts that are in no way analogous to the circumstances here. In *Freeman*, the Fourth Circuit

---

[17] *See* Ex DOJ Ex. 3, Jones and Davis Report (DE-357-4) Figures and Tables appendix. DOJ Ex. 4, Jones and Davis Rebuttal Report (DE-357-5), Appendix A, presents updated versions of this data.

upheld the district court's decision to exclude an expert's statistical analysis based on the "alarming number of errors and analytical fallacies in Murphy's reports, making it impossible to rely on any of his conclusions" and the "'mind-boggling' number of errors and unexplained discrepancies" in the expert's database. 778 F.3d 463, 466-67. The expert excluded "hundreds, if not thousands" of datapoints in his statistical analysis, failed to code data correctly, and managed to introduce new errors in each attempt to revise his report. *Id.* Here, the Government's motion does not identify any data missing from Dr. Jones and Mr. Davis's extended model, it does not discuss a single error let alone critical errors in their statistical analysis, nor does it identify any "facts and data" pertinent to the post-audit that Dr. Jones and Mr. Davis did not encounter in Chapters A, C, and F of the ATSDR report.[18] Dr. Jones explained in deposition his reasoning for focusing on Chapters A, C, and F of ATSDR's Tarawa Terrace model, and testified that those chapters provided good exposure to the methods and processes used. DOJ Ex. 5, Jones Dep. (DE-357-6) at 87:18-89:6. The Court should not substitute its or the Government's judgment "for that of the expert as to what is sufficient evidence to inform his experiential conclusion." *SAS Institute, Inc. v. World Programming Ltd.*, 125 F. Supp.3d 579, 590.

The Government's reliance on *Yates v. Ford Motor Co.*, 113 F.Supp.3d 841, 858–860 (E.D.N.C. 2015) for its argument that Dr. Jones and Mr. Davis should have discussed the NRC Report and the Navy's 2008 letter in their report is similarly misplaced. *Yates* concerned the reliability of a plaintiff's general and specific causation expert opinions in a case involving exposure to asbestos. There, one of the plaintiff's causation experts with an opinion based in part

[18] The operative results of Dr. Jones and Mr. Davis's quantitative and qualitative analysis is in their rebuttal report. DOJ Ex. 4, Jones and Davis Rebuttal Report (DE-357-5). The Government's expert identified minor errors in Dr. Jones and Mr. Davis's opening report, all of which were corrected and addressed in their rebuttal report served January 14, 2025. The Government's motion does not identify or discuss a single remaining error.

on an assessment of epidemiological studies failed to provide a credible explanation as to why he excluded approximately 30 epidemiological studies that found no association between brake work and mesothelioma. *Id.* at 857-860.

Here, the NRC Report and the Navy's letter are merely critiques of ATSDR's work – they do not provide additional facts or data, and they are not "contrary scientific literature" similar to the peer-reviewed published epidemiological studies the *Yates* court determined plaintiff's causation expert should have considered. The NRC Report, for example, is an incomplete review of the ATSDR's model,[19] and it contains numerous errors and inaccuracies regarding the hydrogeology of Camp Lejeune and the specifics of ATSDR's modeling work. Ex. 15, Expert Report of Morris Maslia at 101-02 & App. M (ATSDR Response to NRC Report). More importantly, the Government does not present any evidence demonstrating that the NRC report and Navy letter and the critiques in them are the type of facts and data an engineer would rely on to extend a model and prepare a quantitative and qualitative assessment of its performance. *See* Fed. R. Evid. 703. Given the nature and function of a post-audit, there is no conceivable role for these documents to play in Dr. Jones and Mr. Davis's report. Even if there was, their import is a subject for cross examination. *See Bresler v. Wilmington Trust Company*, 855 F.3d 178, 195 (4th Cir. 2017) ("questions regarding the factual underpinnings of the [expert witness'] opinion affect the weight and credibility of the witness' assessment, 'not its admissibility.'") (quoting *Structural Polymer Grp. v. Zoltek Corp.*, 543 F.3d 987, 997 (8th Cir. 2008)); Fed. R. Evid. 702 Advisory Comm. Notes (2023 Amendments) ("[I]if the court finds it more likely than not that an expert has

[19] Ex. 14, 2/18/2009 Clement email to Maslia, at ATSDR_WATERMODELING_01-0000891040. For example, Dr. Clement did not review Chapter I regarding sensitivity and uncertainty analyses performed for Tarawa Terrace before releasing the NRC Report. *Id.*

a sufficient basis to support an opinion, the fact that the expert has not read every single study that exists will raise a question of weight and not admissibility.")

Contrary to the Government's assertion, *SAS Institute, Inc. v. World Programming Ltd.* is instructive. In *SAS*, the defendant criticized the plaintiff's computer science expert for failing to base his opinion on a larger universe of data, which should have also included an independent investigation of certain software. In rejecting the defendant's reliance on *E.E.O.C. v. Freeman*, the court's analysis demonstrates there is no draconian rule that all relevant evidence must be considered. Instead, it depends on the nature of the testimony and whether the expert provided a reasoned basis for the evidence's exclusion. 125 F. Supp.3d at 590 (citing *Cooper v. Smith & Nephew, Inc.*, 259 F.3d 194 (4th Cir. 2001)). Materials considered by an expert are reviewed with the understanding that the court should not substitute its judgment for that of the expert as to what is sufficient evidence to inform conclusions based on experience. *SAS Institute, Inc.*, 125 F. Supp.3d at 590.

In this case, Dr. Jones and Mr. Davis's opinions regarding the reliability and soundness of the ATSDR's model are based on the results of a technical exercise and informed by their extensive experience developing, applying, and evaluating groundwater flow and contaminant transport models. Dr. Jones provided a reasoned basis as to why they focused on Chapters A, C, and F of the ATSDR reports, and performed only a high-level review of the other chapters. Further, despite questioning both experts about the general concerns raised in the NRC report and the Navy's letter, the Government fails to identify any specific "fact and data" in either document that it contends contradicts an opinion based primarily on a post-audit analysis. Viewed holistically, the record demonstrates that Dr. Jones and Mr. Davis's opinions regarding the reliability and soundness of the model are sufficiently supported by the results of their post-audit. The Court should find the testimony reliable and, in turn, admissible.

V. CONCLUSION

For the foregoing reasons, the PLG respectfully requests the Court to deny Defendant's motion to exclude opinion testimony from Dr. Jones and Mr. Davis regarding the reliability and soundness of ATSDR's model for Tarawa Terrace.

[Signature page to follow.]

DATED this 4th day of June 2025.

/s/ J. Edward Bell, III

J. Edward Bell, III (admitted *pro hac vice*)
Bell Legal Group, LLC
219 Ridge St.
Georgetown, SC 29440
Telephone: (843) 546-2408
jeb@belllegalgroup.com

Lead Counsel for Plaintiffs

/s/ Zina Bash

Zina Bash (admitted *pro hac vice*)
Keller Postman LLC
111 Congress Avenue, Suite 500
Austin, TX 78701
Telephone: 956-345-9462
zina.bash@kellerpostman.com

Co-Lead Counsel for Plaintiffs and Government Liaison Counsel

/s/ Elizabeth J. Cabraser

Elizabeth J. Cabraser (admitted *pro hac vice*)
Lieff Cabraser Heimann & Bernstein, LLP
275 Battery Street, 29th Floor
San Francisco, CA 94111
Telephone: (415) 956-1000
ecabraser@lchb.com

Co-Lead Counsel for Plaintiffs

/s/ W. Michael Dowling

W. Michael Dowling (NC Bar No. 42790)
The Dowling Firm PLLC
Post Office Box 27843
Raleigh, North Carolina 27611
Telephone: (919) 529-3351
mike@dowlingfirm.com

Co-Lead Counsel for Plaintiffs

/s/ Robin L. Greenwald

Robin L. Greenwald (admitted *pro hac vice*)
Weitz & Luxenberg, P.C.
700 Broadway
New York, NY 10003
Telephone: 212-558-5802
rgreenwald@weitzlux.com

Co-Lead Counsel for Plaintiffs

/s/ James A. Roberts, III

James A. Roberts, III
Lewis & Roberts, PLLC
3700 Glenwood Ave., Ste. 410
Raleigh, NC 27612
Telephone: (919) 981-0191
jar@lewis-roberts.com

Co-Lead Counsel for Plaintiffs

/s/ Mona Lisa Wallace

Mona Lisa Wallace (N.C. Bar No.: 009021)
Wallace & Graham, P.A.
525 North Main Street
Salisbury, North Carolina 28144
Tel: 704-633-5244
mwallace@wallacegraham.com

Co-Lead Counsel for Plaintiffs

CERTIFICATE OF SERVICE

I, J. Edward Bell, III, hereby certify that the foregoing document was electronically filed on the Court's CM/ECF system on this date, and that all counsel of record will be served with notice of the said filing via the CM/ECF system.

This the 4th day of June 2025.

*/s/ J. Edward Bell, III*________________

J. Edward Bell, III

IN THE UNITED STATES DISTRICT COURT
FOR THE EASTERN DISTRICT OF NORTH CAROLINA
SOUTHERN DIVISION
Civil Action No.: 7:23-CV-897

IN RE:	)
	)
CAMP LEJEUNE WATER LITIGATION	)
	)
This Pleading Relates to:	)
	)
ALL CASES.	)
	)
	)

TABLE OF EXHIBITS
IN SUPPORT OF PLAINTIFFS' MEMORANDUM IN OPPOSITION TO DEFENDANT'S MOTION TO EXCLUDE THE OPINION TESTIMONY OF R. JEFFREY DAVIS AND NORMAN L. JONES, PH.D

Ex. 1 – Excerpt from Hill and Tiedman, Effective Groundwater Model Calibration (2007)

Ex. 2 – ASTM International D5490-93: Standard Guide for Comparing Ground-Water Flow Model Simulations to Site-Specific Information (2002)

Ex. 3 – Excerpt from Anderson and Woessner, Applied Groundwater Modeling: Simulation of Flow and Advective Transport (2015)

Ex. 4 – Anderson and Woessner, The Role of The Postaudit in Model Validation, Advances in Water Resources 15 (1992)

Ex. 5 – ASTM International D5447-17: Standard Guide for Application of a Numerical Groundwater Flow Model to a Site-Specific Problem (2017)

Ex. 6 – Reilly and Harbaugh, Guidelines for Evaluating Ground-Water Flow Models (2004)

Ex. 7 – Jones and Davis Rainfall Imputation Addendum

Ex. 8 – Jones and Davis Revised Materials Considered List

Ex. 9 – November 5, 2024 PLG Expert Files Production Letter

Ex. 10 – ATSDR Tarawa Terrace Report Chapter A: Summary of Findings

Ex. 11 – ATSDR Tarawa Terrace Report Chapter C: Simulation of Groundwater Flow

Ex. 12 – ATSDR Tarawa Terrace Report Chapter F: Simulation of the Fate and Transport of Tetrachloroethylene (PCE)

Ex. 13 – Konikow, Predictive Accuracy of a Ground-Water Model – Lessons from a Postaudit (1986)

Ex. 14 – February 18, 2009 Clement email to Maslia

Ex. 15 – Expert Report of Morris Maslia PE

EXHIBIT 1

EFFECTIVE GROUNDWATER MODEL CALIBRATION

With Analysis of Data, Sensitivities, Predictions, and Uncertainty

MARY C. HILL
CLAIRE R. TIEDEMAN

BICENTENNIAL 1807 WILEY 2007 BICENTENNIAL

WILEY-INTERSCIENCE
A JOHN WILEY & SONS, INC., PUBLICATION

EFFECTIVE GROUNDWATER MODEL CALIBRATION

1807 WILEY 2007
BICENTENNIAL

The Wiley Bicentennial–Knowledge for Generations

Each generation has its unique needs and aspirations. When Charles Wiley first opened his small printing shop in lower Manhattan in 1807, it was a generation of boundless potential searching for an identity. And we were there, helping to define a new American literary tradition. Over half a century later, in the midst of the Second Industrial Revolution, it was a generation focused on building the future. Once again, we were there, supplying the critical scientific, technical, and engineering knowledge that helped frame the world. Throughout the 20th Century, and into the new millennium, nations began to reach out beyond their own borders and a new international community was born. Wiley was there, expanding its operations around the world to enable a global exchange of ideas, opinions, and know-how.

For 200 years, Wiley has been an integral part of each generation's journey, enabling the flow of information and understanding necessary to meet their needs and fulfill their aspirations. Today, bold new technologies are changing the way we live and learn. Wiley will be there, providing you the must-have knowledge you need to imagine new worlds, new possibilities, and new opportunities.

Generations come and go, but you can always count on Wiley to provide you the knowledge you need, when and where you need it!

William J. Pesce

William J. Pesce
President and Chief Executive Officer

Peter Booth Wiley

Peter Booth Wiley
Chairman of the Board

EFFECTIVE GROUNDWATER MODEL CALIBRATION

With Analysis of Data, Sensitivities, Predictions, and Uncertainty

MARY C. HILL
CLAIRE R. TIEDEMAN

WILEY-INTERSCIENCE
A JOHN WILEY & SONS, INC., PUBLICATION

Published 2007 by John Wiley & Sons, Inc., Hoboken, New Jersey.
Published simultaneously in Canada.

For general information on our other products and services or for technical support, please contact our Customer Care Department within the United States at 877-762-2974, outside the United States at 317-572-3993 or fax 317-572-4002.

Wiley also publishes its books in a variety of electronic formats. Some content that appears in print may not be available in electronic formats. For more information about Wiley products, visit our web site at www.wiley.com.

Library of Congress Cataloging-in-Publication Data:

Hill, Mary C. (Mary Catherine)
Effective groundwater model calibration: with analysis of data, sensitivities, predictions, and uncertainty/Mary C. Hill, Claire R. Tiedeman.
p. cm.
Includes index.
ISBN-13: 978-0-471-77636-9 (cloth)
ISBN-10: 0-471-77636-X (cloth)
1. Groundwater- -Mathematical models. 2. Hydrologic models. I. Tiedeman, Claire R. II. Title.
GB1001.72.M35H55 2006
551.4901′5118- -dc22 2005036657

Printed in the United States of America

10 9 8 7 6 5 4 3 2 1

We dedicate this book to the groundwater modelers and software developers of the U.S. Geological Survey. These men and women devote their careers to providing sound scientific analyses for policy makers and to enabling others in the government and the private sector to do the same. We are honored to be their colleagues.

We also dedicate this book to the United States taxpayers, to whom we are ultimately accountable. They have supported our educations, salaries, field work and students. We hope our efforts have improved the understanding and management of their groundwater resources.

With love, we also dedicate this book to our husbands and families.

CONTENTS

10

GUIDELINES FOR EFFECTIVE MODELING

This chapter introduces and summarizes a set of guidelines for effective modeling of natural and engineered systems. These guidelines show how data, models, and the methods presented in Chapters 3 through 9 can be used together to gain insight into the simulated system, and to successfully attain goals related to calibrating and evaluating the simulated system. The guidelines are summarized in Table 10.1 and are explained in Chapters 11 through 14. The guidelines are organized into four topics: (a) Guidelines 1 through 8 for model development (presented in Chapter 11), (b) Guidelines 9 and 10 for model testing (Chapter 12), (c) Guidelines 11 and 12 for evaluating potential new data (Chapter 13), and (d) Guidelines 13 and 14 for evaluating prediction uncertainty (Chapter 14).

In Figure 1.1, the terms "system information" and "observations" are used for what are sometimes called "soft" and "hard" data, respectively. For a groundwater system, the system information includes hydrologic and hydrogeologic data; observations include hydraulic heads, streamflow gains and losses, and concentrations used directly or used interpretively to define advective-travel observations. In the guidelines, the terms "system information" and "observations" are used instead of "hard" and "soft" data because we believe they describe the data more clearly. For example, prior information generally is derived from system information, but because it appears in the regression objective function in the same manner as observations, it is sometimes classified as hard data. Using the terms system information and observations reduces the confusion.

Effective Groundwater Model Calibration: With Analysis of Data, Sensitivities, Predictions, and Uncertainty. By Mary C. Hill and Claire R. Tiedeman
Published 2007 by John Wiley & Sons, Inc.

TABLE 10.1 Guidelines for Effective Development and Use of Models

Guideline[a]	Description and Suggested Actions[b]
Preliminary Steps (*Not covered by the guidelines. See, for example, Anderson and Woessner, 1992*)	
Define purpose	Design the model to meet the modeling objectives.
Develop conceptual models	Select processes and system characteristics. Identify ways to attain a tractable model and aspects that are uncertain.
Choose code	Use modular codes that allow easy inclusion and exclusion of processes.
Model Development Guidelines (*Chapter 11*)	
1. Apply the principle of parsimony	• Start simple and add complexity as warranted by the hydrology and hydrogeology, the inability of the model to reproduce observations, and the complexity that can be supported by the available observations.
2. Use a broad range of system information (soft data) to constrain the problem	• Identify spatial and temporal structure. Use it to represent the system well using few parameters. • Do not add features or parameters to improve model fit if they contradict system information. • Possibly use geographic information systems (GIS) and 3D database and visualization methods to organize, analyze, interpret, and present data.
3. Maintain a well-posed, comprehensive regression problem	• Maintain a well-posed regression: define few parameters. • Maintain a comprehensive model: represent many aspects with parameters. • To be both well-posed and comprehensive, seek simple models that represent important system dynamics. • Detect ill-posed regressions with *css* and *pcc*.
4. Include many kinds of data as observations (hard data) in the regression	• Add different kinds of observations; this can be critical to obtaining a reasonably accurate model. In groundwater flow model calibration, it is very important to include information about flows. • Use *opr* to evaluate which observations dominate the predictions.
5. Use prior information carefully	• Begin with no prior information to investigate the observations. • Insensitive parameters (e.g., small *css*): include with prior information or exclude to reduce run time. Include for Guidelines 11–14. • Sensitive parameters: do not use prior information to make unrealistic optimized parameter values realistic. See Guideline 10.
6. Assign weights that reflect errors	• Assign weights that equal $1/\sigma_i^2$.
7. Encourage convergence by making the model more accurate and evaluating the observations	• If nonlinear regression does not converge (can occur even when *css*, *pss*, and so on indicate observations are sufficient to estimate the parameters), work to make the model represent the system more accurately and make sure observations are interpreted correctly.

(*Continued*)

TABLE 10.1 *Continued*

Guideline[a]	Description and Suggested Actions[b]
	• Use model fit, *dss*, *css*, *pss*, and system information to determine what to change.
8. Consider alternative models	• Develop alternative models using deterministic or stochastic methods. • Judge models based on better fit and more realistic parameter estimates.
	Model Testing Guidelines (*Chapter 12*)
9. Evaluate model fit	• Use standard error, AIC_c, and other statistics from Chapter 6 to assess overall model fit. • Use weighted and unweighted residuals to assess details of model fit.
10. Evaluate optimized parameter values	• Unreasonable estimated parameter values can indicate model error. • Perhaps combine parameters with overlapping confidence intervals, divide parameters with large *css*.
	Potential New Data Guidelines (*Chapter 13*)
11. Identify new data to improve simulated processes, features, and properties	• Use fit-independent statistics *dss*, *css*, *pcc*, *leverage* to identify potential important new observations. • Use *css* and *pcc* to identify parameters for which existing and potential observations contain substantial information. Consider representing the associated system characteristics using additional estimated parameters.
12. Identify new data to improve predictions	• Identify observations and parameters important to predictions using fit-independent statistics *dss*, *css*, *pss*, *pcc*, *ppr*, *opr*.
	Prediction Uncertainty Guidelines (*Chapter 14*)
13. Evaluate prediction uncertainty and accuracy using deterministic methods	• Use regression to determine whether predicted values of interest (such as regulatory guidelines) contradict the observations. • Use postaudits to test prediction accuracy.
14. Quantify prediction uncertainty using statistical methods	• Use statistical inference—linear and nonlinear. Includes uncertainty intervals. • Use designed and random sampling—omit poor-fit realizations. • Include parameters not estimated by regression, perhaps with prior information. • Consider alternative models by including the probability of each.

[a]The guidelines generally are used iteratively, not just once in sequence.
[b]*dss*, *css*, *pss*, dimensionless, composite, and prediction scaled sensitivities, respectively; *pcc*, parameter correlation coefficients; *ppr*, parameter–prediction statistic; *opr*, observation–prediction statistic; 3D, three-dimensional; σ_i^2 is the best approximation of the observation error variance. See text for discussion of weight matrices. Fit-independent statistics are italicized.

This chapter explains the purpose of the guidelines, discusses them in the context of previous work and other modeling approaches, and provides suggestions for effectively implementing them during modeling.

10.1 PURPOSE OF THE GUIDELINES

An entire modeling protocol is presented by Anderson and Woessner (1992, pp. 4–9), which spans the modeling procedure from defining the purpose of the model and selecting a code, through predictive analysis and postaudits. The guidelines presented in Chapters 10 to 14 fit into that protocol, enhancing the sensitivity analysis, calibration, prediction, and uncertainty evaluation phases. The guidelines also emphasize investigation of different conceptual models. The guidelines do not address the preliminary steps of the protocol. For example, there are no guidelines for the important steps of defining the modeling objectives and selecting or programming a code with the appropriate capabilities.

The guidelines are closely tied to the modeling process represented in Figure 1.1. As discussed in Chapter 1, Section 1.1, Figure 1.1 shows how the model, with its defined parameters, quantitatively links the system information and the observations to the predictions of interest and measures of prediction uncertainty. Figure 1.1 emphasizes the direct links the model provides between the triad composed of *observations*, *parameters*, and *predictions*. The methods and statistics presented in Chapters 3 through 8 take advantage of these links. Selected statistics that connect each element of the triad are listed in Table 10.2. The guidelines show how modelers can use these links and associated methods and statistics advantageously during model development, testing, and evaluation of predictions and their uncertainty.

TABLE 10.2 Statistics[a] from Chapters 4, 7, and 8 that Indicate the Importance of Observations to Parameters, Parameters to Predictions, or Observations (Through the Parameters) to Predictions

Observations–Parameters	Parameters–Predictions (Chapter 8)
dss, css, pcc, leverage (Chapter 4) Parameter standard deviations, coefficients of variation, confidence intervals, DFBETAS, Cook's *D* (Chapter 7)	*pss, ppr*
Observations–Parameters–Predictions (Chapter 8)	
opr Prediction standard deviations, coefficients of variation, confidence intervals. Cross-validation, jackknifing, bootstrapping (only mentioned briefly in the text).	

[a] *dss*, *css*, *pss*, dimensionless, composite, and prediction scaled sensitivity, respectively; *pcc*, parameter correlation coefficient; *ppr*, parameter–prediction statistic; *opr*, observation–prediction statistic. Fit-independent statistics are italicized.

In the context of the entire modeling process shown in Figure 1.1, the ideas suggested in the guidelines are aimed at facilitating effective use of the system information and the observations to constrain the model and at making the model and model development more transparent. The goal is to produce a model that represents the simulated system more accurately, compared to modeling procedures that use these data less effectively, and to encourage clear testing.

10.2 RELATION TO PREVIOUS WORK

The guidelines are presented in the context of groundwater modeling problems but are applicable to other fields. Many aspects of the approach have had a long history in a variety of fields. The idea of parsimony—starting simple and building complexity slowly—is emphasized in Guideline 1 and has been discussed by Popper (1982), Cooley et al. (1986), Constable et al. (1987), Backus (1988), Cooley and Naff (1990), and Parker (1994). The importance of conceptual models is discussed by many authors, including Bredehoeft (2003, 2005). Most of the graphical analyses of Guideline 8 were suggested for application to groundwater problems by Cooley and Naff (1990) as derived from Draper and Smith (1981). Very similar approaches were tested using simple and complex synthetic test cases in Poeter and Hill (1996, 1997) and in Hill et al. (1998). Alternative guidelines have been presented by Refsgaard and Henrikson (2004). Hill et al. (2004) provide a review.

From the perspective of stochastic inverse methods (e.g., Kitanidis, 1997), many aspects of the approach presented here can be applied directly. This is accomplished by considering the parameters of the stochastic model to be analogous to the parameters discussed in this work, and calculating sensitivities appropriately.

Alternatively, the approach presented here can be thought of as a strategy to approximate mean, or effective, values. Stochastic methods generally require that the mean of any spatially distributed quantity, such as hydraulic conductivity, be constant, a simple function, or known. Unfortunately, geologic media often defy these limitations. A model developed using the guidelines presented here can be used to evaluate whether the mean is constant, and, if not, to provide an estimate of what could be a very complex spatial distribution, often with sharp contrasts. Once large-scale variations are established, stochastic methods can be used to assess the influence of small-scale variations. To date, methods to characterize large- and small-scale variations mostly have been considered separately, and integration is sorely needed. One goal of such work can be thought of as identifying the aspects of a given problem that can most profitably be regarded as deterministic, and the aspects that can be most profitably be regarded as stochastic, given the information available (perhaps using the ideas in Guidelines 2 and 4) and the objectives of the work (such as the predictions considered in Guideline 12).

10.3 SUGGESTIONS FOR EFFECTIVE IMPLEMENTATION

Although the guidelines are presented roughly in the order along which most studies proceed, flexible application is important to their success. We encourage modelers to

TABLE 10.3 Common Questions, Useful Statistics and Graphs, and Related Figures, Tables, and Guidelines[a]

Questions	Statistic or Graph	Figures (**F**) or Tables (**T**)	Guideline
Evaluate Information that Observations Provide on Parameters			
Which of the defined parameters can be estimated? What types of additional parameters can be estimated	*css*	**F**: 4.3, 7.5, 9.11, 9.18, 11.3 **T**: 5.5	1, 2, 3, 5, 11
	leverage	**F**: 7.2; **T**: 13.1	
	DFBETAS	**T**: 7.3	
Can the defined parameters be estimated uniquely?	*pcc*	**F**: 4.2, 5.4, 9.5, 11.4 **T**: 4.2, 4.3	3
Which observations contain the most information?	*dss*	**F**: 8.1, 13.1; **T**: 4.1, 7.5, 13.1	3, 4, 11
	Cook's *D*	**F**: 15.6; **T**: 7.2	
	one-percent-scaled sensitivities	**F**: 4.4, 9.6–9.10	
Evaluate Model Fit			
Are the observations correctly interpreted, simulated, and weighted?	Extreme values of residuals and weighted residuals	**F**: 6.8	9
What is the overall fit for all observations and for each type of observation?	Standard error, fitted error statistics, AIC_c, BIC	**F**: 6.6, 9.13, 11.6	9
How is the fit to individual observations? Are the weighted residuals random?	Weighted residuals vs. [weighted] simulated values	**F**: 6.1, 6.2, 6.7, 9.14, 11.7, 15.3	9
	Graphs using independent variables	**F**: 6.9, 9.15, 12.2, 12.3, 15.4, 15.5	
	Runs test	**F**: 6.4, 6.10, 9.16, 12.4	
Are the weighted residuals normally distributed?	Normal probability graphs	**F**: 6.5, 6.11, 6.14, 9.17	—
	R^2_N	**F**: 6.12, 9.17	

(*Continued*)

TABLE 10.3 *Continued*

Questions	Statistic or Graph	Figures (**F**) or Tables (**T**)	Guideline
How can misfit be obscured? (Question is included to discourage use of this graph.)	[Weighted] observed vs. [weighted] simulated values	**F**: 6.3, 6.7, 9.14, 15.3	9
	Evaluate Estimated Parameter Values		
Are the parameter estimates reasonable?	Estimated parameter values, confidence intervals, reasonable ranges	**F**: 7.4, 7.7, 7.8, 7.19, 12.5, 15.15 **T**: 7.9	
Are the parameter estimates unique?	*pcc*	**T**: 7.4, 7.6, 7.8, 9.7	10
	Evaluate Predictions		
How accurate are the predictions?	Check for bias using model fit and estimated parameter values	As for model fit and estimated parameters	13
How precise are the predictions?	Confidence intervals, Monte Carlo	**F**: 8.15, 8.16, 9.23, 14.1	14
How reliable are the predictions?	Accuracy and precision → reliability	As for previous two questions	
What parameters are most important to the predictions?	*css*, *pss*, *pcc*	**F**: 8.1, 8.8, 9.22, 15.8 **T**: 8.4, 8.5, 9.8	12
	ppr	**F**: 8.9, 15.8	
What observations are most important to the predictions?	*dss*, *css*, *pss*, *pcc*	**F**: 8.1, 8.11; **T**: 8.7	12
	opr	**F**: 8.10, 8.12, 8.13, 15.9, 15.10	

[a] *dss*, *css*, *pss*, dimensionless, composite, and prediction scaled sensitivities, respectively; *pcc*, parameter correlation coefficients; *ppr*, parameter–prediction statistic; *opr*, observation–prediction statistic; [weighted], could be unweighted instead. Fit-independent statistics are italicized.

follow the guidelines out of order if warranted by the individual modeling situation, or to revisit some of the guidelines during the course of model development, calibration, and evaluation. For example, analyses of prediction uncertainty discussed in Guideline 14 often are useful in guiding data collection, which is the topic of Guidelines 11 and 12.

Sun (1994, p. 210) recognized the need for flexible application of modeling steps. He noted that there is an inherent difficulty associated with the optimal design of data collection for nonlinear problems: the solution for the optimal design depends on the values of the unknown parameters, which in turn depend on the data. In addition, new data may cause the conceptual model to evolve and may challenge previous conceptual models and result in changes to many aspects of the model, including the optimized parameter values. Sun (1994) presents some elegant methods of addressing this problem that are generally very computationally intensive. The methods presented in this book tend to be simpler and less computationally intensive, while still being useful in many situations. The methods presented here may be used alone or may serve as preliminary steps to a more computationally intensive evaluation.

The guidelines do not suggest formally considering the predictions or using the model to evaluate potential new data until Guidelines 11 and 12. This is because it is expected that a reasonably accurate model is needed for a quantitative evaluation of predictions. The placement of predictions in the guidelines is not intended to diminish the importance of considering prediction issues throughout data collection and model development. Indeed, as predictions differ from observations significantly in terms of location, depth, time, type, or system stresses, it becomes increasingly important to simulate the predictions as calibration proceeds, as emphasized in Figure 1.1. This allows the modeler to understand how the assumptions and simplifications being made during model calibration affect the predictions. However, the results need to be considered cautiously until the model is reasonably accurate, which is the reason for the order of the guidelines. In addition, ethics require that the model not be designed to obtain desired predictions. If assessing predictions during calibration in any way endangers the integrity of the model, delay the simulation of predictions until the end of model development.

Many statistical and graphical analyses related to inverse modeling methods were presented in Chapters 3 to 8. In the guidelines, additional examples of using these statistics and graphs are presented. To aid cross-referencing, Table 10.3 lists most of the statistics and graphs discussed in Chapters 3 to 8 and shows the figures and guidelines in which they are presented and discussed in Chapters 11 to 14. These are presented in the context of typical questions that arise during model sensitivity analysis, calibration, and evaluation.

As the methods described in this work are used in the context of the guidelines, modelers may devise new methods or apply these to new situations. Thoughtful innovation is welcome and essential in this immature field.

11

GUIDELINES 1 THROUGH 8— MODEL DEVELOPMENT

Eight guidelines focus on model development: (1) follow the principle of parsimony in all model development endeavors; (2) use system information effectively; (3) use as few parameters as possible to represent as many important aspects of the system as possible; (4) include observations that cover a broad range of system dynamics; (5) use prior information when appropriate; (6) specify weighting that represents errors; (7) encourage convergence of the regression by using results from failed regressions to guide model improvements; and (8) consider alternative conceptual models.

GUIDELINE 1: APPLY THE PRINCIPLE OF PARSIMONY

> The methods of science depend on our attempts to describe the world with simple theories. Theories that are complex become unstable, even if they happen to be true. Science may be described as the art of oversimplification: the art of discerning what we may with advantage omit.
>
> —Popper (1982)

The principle of parsimony calls for keeping the model as simple as possible while accounting for the system processes and characteristics that are evident in the observations and are important to the predictions, and while respecting all system information. In many fields, including groundwater hydrology, the known

Effective Groundwater Model Calibration: With Analysis of Data, Sensitivities, Predictions, and Uncertainty. By Mary C. Hill and Claire R. Tiedeman
Published 2007 by John Wiley & Sons, Inc.

complexities of the simulated systems often seem overwhelming, and applying parsimony in model development can require substantial restraint.

Of greatest concern are two- or three-dimensional spatial fields that also may vary in time. Literally an infinite number of parameters could be defined. In numerical models, the possible number of parameters is finite because of the discretization of the numerical grid or mesh, but it is still far more than can be supported using observations of the simulated system, and probably more than is useful.

G1.1 Problem

Keeping a model simple is important because though more complex models generally fit the observations more closely compared to simpler models, they can have greater prediction error. For example, consider the situation shown in Figure 11.1*a*,*b*, where the true model is linear. A more complicated model (Figure 11.1*b*) clearly produces a better fit to the observations, but much of the improved fit is achieved by matching the observation error rather than the system processes. In this example the predictions are less accurate in the more complicated model than in the simpler model. Figure 11.1*c* displays the general situation, in which there is a trade-off between model fit and prediction accuracy with respect to the number of parameters. All model-fit statistics used for model discrimination include a penalty as the number of parameters increases to account for this effect; see Chapter 6, Section 6.3.2.

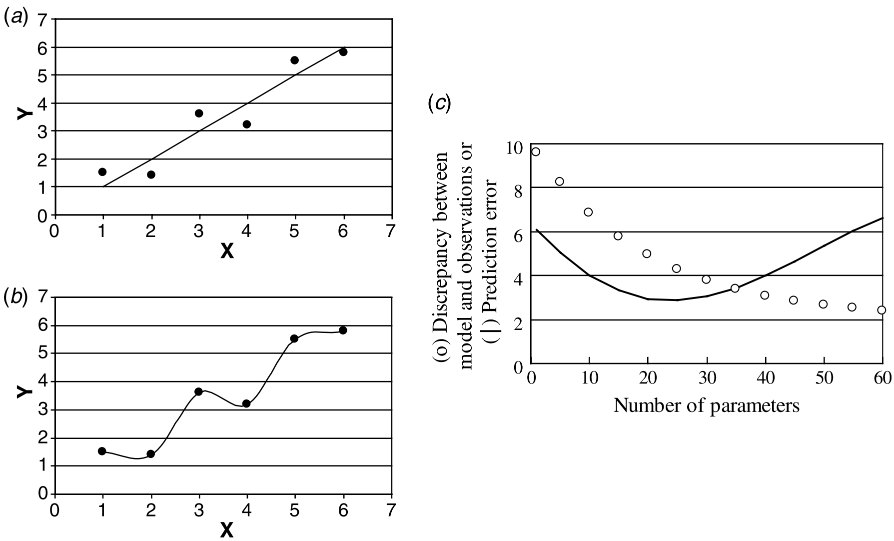


FIGURE 11.1 (*a*) Data with a true linear model. (*b*) The same data with an overly complex model with little predictive capability. (*c*) Schematic graph showing conceptually the trade-off between model fit to observations and prediction accuracy with an increasing number of parameters.

In practice, we do not know many of the characteristics of the underlying model. We do not know, therefore, when we are using observations advantageously to characterize the processes of concern, and when we are fitting errors and are probably degrading the predictive capabilities of the model. Guideline 1 suggests approaching this problem from the left in Figure 11.1*c*—that is, by starting with simple models and building complexity carefully. By starting with a simple model, the modeler can more easily understand the effect that added complexity, such as additional simulated processes or using more parameters to represent system features, has on model fit, optimal parameter estimates, predicted values, and prediction uncertainty. This helps keep the behavior of the model as a whole in perspective, compared to narrowly focusing on a small portion of the spatial or temporal domain of the model. This "big picture" view is consistent with the sparse data available for characterizing many systems. In many cases, it also is consistent with the detail needed to obtain useful predictions.

There has been an active discussion in the Earth science literature about the advantages and disadvantages of using models with different levels of complexity. For example, Parker (1994) and Smith et al. (1999) address these issues with regard to a geophysical investigation and suggest the utility of simple models; Murray (2002, 2003), Bras et al. (2003), and Harry (2003) discuss general numerical modeling issues, the first two with an emphasis on geomorphic modeling; de Marsily et al. (2005) stress the importance of detailed hydraulic-conductivity structure in simulations of groundwater transport (an issue also mentioned in Chapter 9, Section 9.2.3); Hill (2006) and Gomez-Hernandez (2006) debate simplicity and complexity of groundwater models. Yeh and Sun (1990) suggest a stepwise approach. Oreskes (2000) discusses the paradox of complex models and the importance of refutability and transparency. Refutability means the model is constructed such that different assumptions can be tested; transparency means the model dynamics are understandable. Both refutability and transparency suffer as a model becomes more complicated, and this loss needs to be weighed against perceived advantages gained. One goal of the guidelines is to increase refutability and transparency.

G1.2 Constructive Approaches

Applying the principle of parsimony to all aspects of model development is important. For example, only include the processes needed for the system being simulated. The most useful models are designed modularly so that different combinations of processes can easily be included to test their relevance and unused capabilities do not interfere by increasing execution time or computer storage, or affecting simulated values. This approach also allows execution time to be managed efficiently, as noted in Chapter 15, Section 15.1.

To represent a system adequately with relatively few parameters, as suggested in Guideline 1, the model and parameters need to be defined carefully to capture the important processes and system features. When considering changes that decrease the complexity of a model, it is important to test whether system information and/or observations contradict the changes and the importance of the changes to the predictions. The remaining model development guidelines suggest how to obtain a parsimonious, useful model.

The remainder of this section investigates two difficulties commonly encountered that need to be managed well to obtain a useful model. The first is nonlinearities of the forward model and the second is variability of system properties. Both are presented in the context of groundwater models, but the basic ideas are directly applicable to other fields.

Managing Forward Model Nonlinearities Part of managing execution time efficiently is managing forward model nonlinearities efficiently. Replacing nonlinear forward problems with linear approximations as much as possible can dramatically reduce execution time. If designed wisely, this can be achieved without substantially diminishing model accuracy. Basically this comes down to managing the nonlinearity to best serve the purpose of the model.

In groundwater flow simulations, for example, unconfined and convertible layers (as they are called in MODFLOW96 and MODFLOW-2000, respectively) can be replaced by confined layers with approximate defined thicknesses during model calibration. Using confined layers is always good practice for steady-state simulations because in the final calibrated model the saturated thicknesses are expected to conform to observed hydraulic heads. Allowing saturated thicknesses to vary as the parameters vary during calibration can be a numerical nightmare and produces no advantage. The result will be about the same regardless of whether confined layers are used during calibration; we suggest choosing the easier option and spending the effort on more worthwhile endeavors. A sensible approach is to maintain saturated thicknesses that are consistent with the observed heads and, therefore, the expected simulated heads in the final calibrated model. This can save a tremendous amount of time and aggravation.

The approach also can be useful in transient simulations depending on how much de-watering or saturation occur over time. It is important to consider the proportion of the pumped strata that becomes dewatered, which may not be the same as the proportion of a pumped model layer. For example, if a well intersects permeable material that is 50 m thick and is represented by ten 5-m thick model layers, it is the proportion of the 50-m thickness that needs to be considered.

Once a model is close to being calibrated, two options can be pursued.

First, the importance of the linear approximation can be evaluated. It is easy to evaluate the model inaccuracy that results from defining layers as confined with approximate specified thickness instead of as unconfined or convertible. This involves simply comparing a forward simulation that includes the water table and the convertible layers to a forward simulation with approximate layer thicknesses and confined layers.

Second, if needed, there are several options for integrating the nonlinearity into the simulation. For example, the top of the system can be updated using the topmost simulated hydraulic heads iteratively until little change occurs between iterations. Also, the water table can be explicitly simulated using, for example, the wet/dry capability of MODFLOW.

The likely consequence of using confined layers can be evaluated by considering the effect of dewatering on the transmissivity (hydraulic conductivity times saturated thickness) versus the effect of the possible range of hydraulic-conductivity values. For example, dewatering half the saturated thickness of a model layer or hydrogeologic unit reduces transmissivity by a factor of two, whereas possible variation in hydraulic conductivity for the layer easily can be an order of magnitude or more. In this situation, it would be reasonable to set the thickness and define model layers as confined, at least for preliminary regression runs. As noted, the model layers can then be represented as unconfined or convertible layers for final regression runs.

Managing Variability Often the variability of data is the driving force behind increasing model complexity. Scheibe and Chien (2003), however, present a study that suggests that increased model complexity is not always advantageous. They investigated an extensive groundwater data set using numerical simulations with transport predictions and different levels of detail used in representing the hydraulic-conductivity (K) field. The data are used to construct predictive models that were not calibrated. Scheibe and Chien (2003) draw the following conclusion important to Guideline 1: “model conditioning to local (effectively point support) data, even hundreds of such data, provides little benefit for prediction and may even provide misleading results. One would expect that conditioning data would improve predictions overall and decrease model uncertainty (narrow the range of variations in predicted behavior). However, the average summary performance metric for the simulations conditioned to borehole flowmeter measurements of K . . . was not significantly improved over the homogeneous base case.”

However, Scheibe and Chien (2003) also found that conditioning on larger-scale hydraulic-conductivity data, consisting of estimates based on geophysical tomography, did significantly improve the predictions. Thus, this study found that adding very detailed complexity on the basis of local-scale measurements was not beneficial to predictive analyses, but that adding less detailed complexity was beneficial. These conclusions were possible because the investigators started with a very simple model, which served as a base case for objectively assessing whether or not the additional complexities were advantageous.

GUIDELINE 2: USE A BROAD RANGE OF SYSTEM INFORMATION TO CONSTRAIN THE PROBLEM

In most scientific and engineering modeling studies, there is system information that is related to model inputs. Effective use of this information in building conceptual models of the system can mean the difference between a model that represents the system well and one that does not. This applies whether or not the model is constructed in a parsimonious manner. In developing the parsimonious models encouraged by these guidelines, we try to use system information to define simplifications and approximations that produce a model with just enough of the right detail, and no more (paraphrasing Albert Einstein). The goal, of course, is for the resulting model to be as useful as possible, which requires as much transparency and refutability as possible (see Guideline 1).

G2.1 Data Assimilation

Guidelines 2 and 4, when taken together, emphasize what is sometimes referred to as data assimilation or data fusion. Examples of approaches for incorporating different types of system information in groundwater flow and transport model development are reported by Rubin et al. (1992), McKenna and Poeter (1995), Poeter and McKenna (1995), Eppstein and Dougherty (1996), Woodbury and Ulrych (2000), Barrash and Clemo (2002), and Chen and Rubin (2003). Many of these studies provide site-specific applications of the methods. A general framework for hydrologic data assimilation that is not limited to groundwater systems is described by McLaughlin (2002). Koltermann and Gorelick (1996) divide approaches of using field data to construct groundwater models into three categories: structure imitating, process imitating, and descriptive. It is becoming common to use diverse types of data in model construction, and methods for integrating these data have much potential for further development.

G2.2 Using System Information

System information can be used to define model structure, including the choice of processes to simulate, or to directly provide information on parameter values through determination of reasonable ranges (Chapter 7, Section 7.6), parameter limits (Chapter 5, Section 5.5), or prior information (Chapter 3, Sections 3.1 and 3.4.1). Here we focus on using system information to constrain the structure of groundwater models. This reflects the problem-specific nature of using system information to constrain model structure. We expect that providing concrete approaches for a specific field will be more useful than a general presentation.

If a groundwater model is to have any credibility, the simulated hydraulic-conductivity distribution needs to be consistent with the known hydrology and hydrogeology. Most groundwater investigations consider relatively shallow systems for which substantial surficial and subsurface information can be determined. This is in contrast to many fields of geophysics and other Earth sciences in which the great depths of interest preclude substantially constraining the calibration with known geology. Indeed, Carerra et al. (2005) state the following in relation to groundwater models: “when available, geologic information about parameter variability is so compelling (in the sense that it can be included deterministically) that it overcomes the advantages of conventional geostatistics.”

For groundwater systems, hydrogeologic data often indicate that faults, fractures, and/or depositional processes have produced sharp contrasts in the hydraulic-conductivity distribution. These contrasts sometimes need to be explicitly represented in the model to simulate the system accurately. While zones of constant value provide an unrealistically uniform distribution of hydraulic conductivity within the zone, they are very useful when large-scale contrasts overwhelm the importance of smaller scale features. Even when smaller scale features are important, they often need to be characterized within the structure provided by such zones. At large or small scales, depositional conditions may suggest a gradual refining or coarsening in horizontal or vertical directions such that interpolation methods instead of zonation are most useful. When many interpolation points are used, as in pilot point methods, advantages of zonation can sometimes be captured. Representing hydraulic-conductivity variations is also discussed in Chapter 9, Section 9.2.3. D'Agnese et al. (1997, 1999) provide a good example of analyzing three-dimensional hydrologic and hydrogeologic data to construct a groundwater flow model of a complex system. This system is discussed in Chapter 15.

Commonly, the information used to constrain a problem as described in this guideline also is used to support the prior information on parameters discussed in Guideline 5. For example, the results of aquifer tests may be used to determine that two hydrogeologic units have similar hydraulic-conductivity values and probably can be combined to form one parameter in the regression. This information may be an important constraint on the problem. Later, the same results might be used to determine a prior information value for the combined or individual hydrogeologic units.

G2.3 Data Management

Evaluating, integrating, and using different types of system information for model development can require sophisticated data management capabilities. The level of sophistication required depends on the complexity of the system investigated. For example, in groundwater models, the system hydrogeology might be represented as homogeneous, as layered, or as a complex heterogeneous distribution. Homogeneous models require a simple data management structure, layered models generally require standard GIS (geographic information systems) capabilities, and more complex representations could require sophisticated methods found mostly in either fairly expensive software packages such as GMS (Environmental Modeling Systems, 2006) or more expensive software packages such as StratWorks 3D (Landmark, 2006), Earthvision (Dynamic Graphics, 2006), and GOCAD (Earth Decision, 2006). D'Agnese et al. (1999) and associated publications describe the software used to develop a complex groundwater flow model of the regional Death Valley groundwater system, and part of their discussion is presented in Chapter 15. Examples applied to glacial sediments are presented by Frind et al. (2002) and Ross et al. (2005). Many aspects of their approaches are directly applicable to studies of other types of systems.

For fully three-dimensional systems, the methods available for data organization and analysis are not very mature and can be very expensive. Recent and continuing advances in computer capabilities and standardization of technology related to sophisticated visualization and databases are likely to result in greatly improved methods in the coming years.

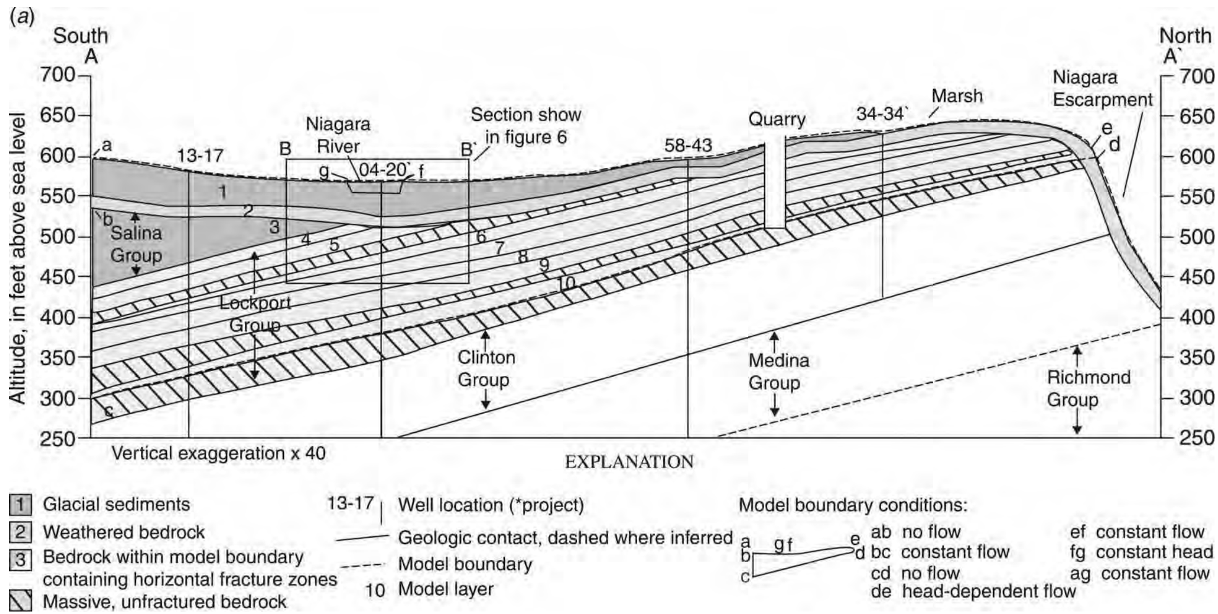


FIGURE 11.2 Hydrogeology of a fractured dolomite near Niagara Falls, New York. (*a*) Generalized section showing extent of model layers and model boundary conditions. (*b*) Relationships among stratigraphy, regional water-bearing zones, and model layers. Use of proposed nomenclature for the Lockport Group does not constitute formal acceptance by the U.S. Geological Survey. (From Yager, 1996, Figures 2 and 5.)

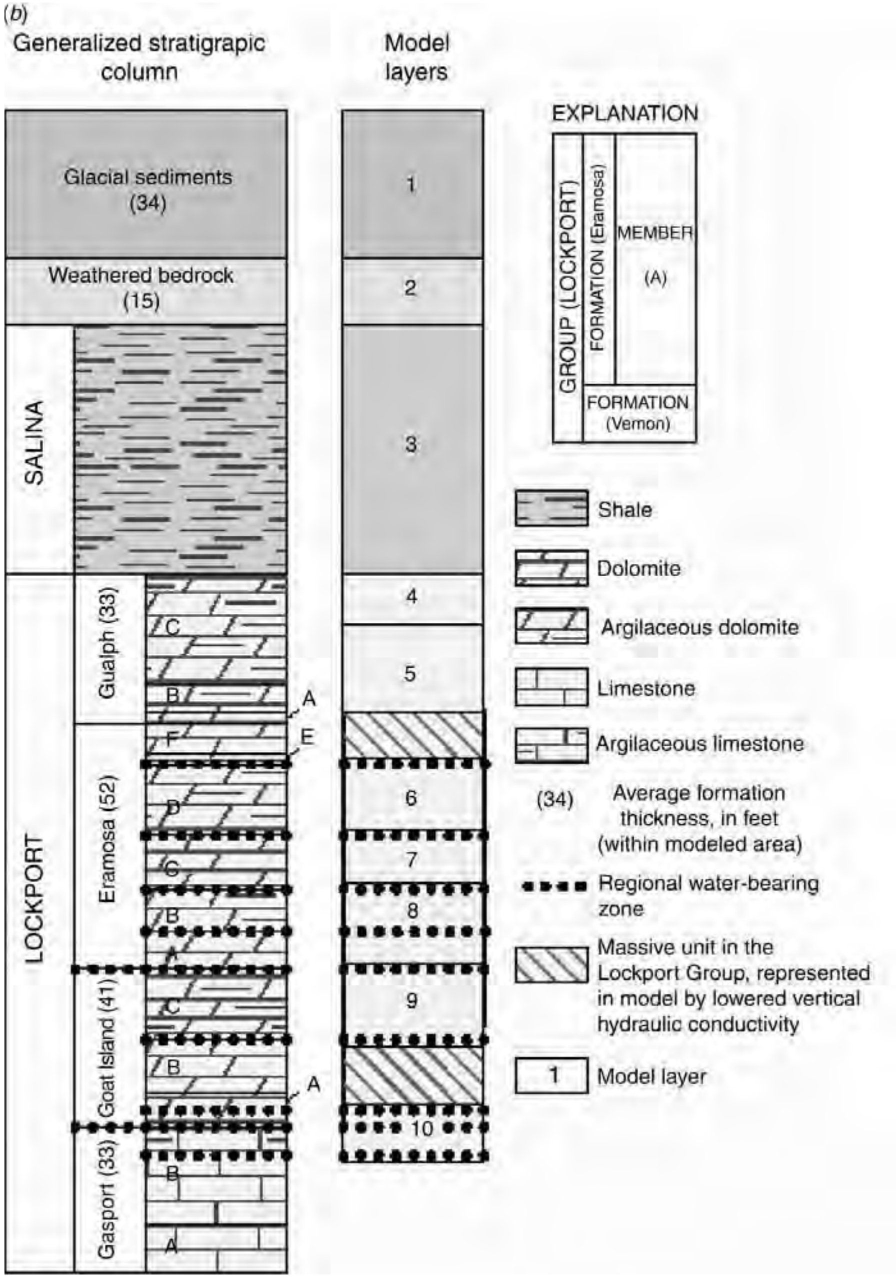


FIGURE 11.2 *Continued.*

Generally, the constraints imposed by the system information are never enough to fully characterize the system. Computational methods have been proposed for identifying the structure of a model and can be useful as long as the system data are respected, such as geologic and hydrogeologic information for groundwater systems. Parameter structure identification methods are presented by Tsai et al. (2003a,b), who also provide a comprehensive review of past work on this topic applied to groundwater models. A continuing challenge is the integration of these methods with the constraints imposed by the system information.

G2.4 Application: Characterizing a Fractured Dolomite Aquifer

Yager (1996) simulated a groundwater flow system near Niagara Falls, New York, that is dominated by fractured dolomite (Figure 11.2). Definition of parameters for this system appeared problematic until a simple and powerful relation was derived from aquifer-test results available as part of the system information. Two factors contributed to the simplification.

1. The dominant regional fractures in the dolomite are roughly horizontal and along bedding planes. Fractures between these planes are dominated by vertical flow.
2. Transmissivities calculated for different aquifer tests were approximately proportional to the number of bedding-plane fractures intersected by the pumped well.

These two factors led to the assumption that each fracture has equal transmissivity, so that model-layer transmissivity is proportional to the known number of fractures in each layer. This relationship allows the entire heterogeneous horizontal hydraulic-conductivity distribution to be realistically represented using a single hydraulic-conductivity parameter and multiplication arrays that indicate the number of fractures in each model layer. Multiplication arrays are available in MODFLOW-2000 and possibly other models.

GUIDELINE 3: MAINTAIN A WELL-POSED, COMPREHENSIVE REGRESSION PROBLEM

The first part of this guideline suggests that the regression problem be well posed. For the purposes of these guidelines, a regression is well posed if it converges to an optimal set of reasonable parameter values given reasonable starting parameter values. In Earth systems, available observations are commonly sparse, so the requirement of maintaining a well-posed regression usually produces rather simple models with relatively few estimated parameters. Thought of in another way, only this simple level of model complexity can be supported by the observations, and the regression is providing an assessment of the information contained in the data. Thus, determining the greatest possible level of model complexity while maintaining a well-posed regression can be considered an objective analysis of the information provided by the observations. Prior information and regularization can be used to support additional complexity (see Guideline 5). However, it is important to model transparency for the modeler to know and to communicate to others what complexity is supported by the observations, what is supported by other types of information, and what is pure speculation.

The second part of this guideline suggests that the regression problem be comprehensive. This means characterizing as many aspects of a given system as possible using defined parameters. Being comprehensive is important for two reasons.

1. Preconceived notions about various aspects of the system only can be quantitatively tested against the observations by defining parameters, calculating sensitivities, and attempting estimation by regression. Such testing and resultant reevaluation of system characteristics is a key advantage of using regression methods, as discussed, for example, by Poeter and Hill (1997).
2. Many methods evaluate model uncertainty using the parameter variance–covariance matrix. As more aspects of the system are represented by defined parameters, more aspects are represented in the uncertainty evaluation using these methods.

The two parts of this guideline represent a fundamental tension faced by modelers of most natural systems. For most modelers, a comprehensive regression problem is easier to achieve than a well-posed regression problem. That is, it is easier to add complexity than to be simple, even if a simple design could be found that represents the system well.

A number of the statistics discussed in this book and listed in Table 10.2 can be used to encourage a well-posed problem. In the initial stages of model development, it can be advantageous to use fit-independent statistics. Sections G3.1 and G3.2 discuss the utility of two of the most useful fit-independent statistics: composite scaled sensitivities (*css*), presented in Chapter 4, and parameter correlation coefficients (*pcc*), presented in Chapters 4 and 7. Dimensionless scaled sensitivities (*dss*) also are useful, particularly for better understanding *css* values.

G3.1 Examples

The *css* and *pcc*, along with the system information discussed in Guideline 2, can be used to define parameters and to decide which parameters to estimate using regression. The *css* and *pcc* are well suited for this purpose because they are fit-independent, as discussed in Chapter 4. This means that they depend only on the observation sensitivities and weights; they are independent of the model fit to observed values. When evaluated at the starting parameter values, these fit-independent statistics can be used to determine what sets of parameters are likely to be estimated successfully given a model and a set of observations.

Composite Scaled Sensitivities (css) Composite scaled sensitivities were used to help achieve a well-posed regression for the three-layer model of the Death

Valley regional groundwater flow system (DVRFS) (see Chapter 15). The bar chart of *css* for the initial, uncalibrated model used by D'Agnese et al. (1997, 1999) (Figure 11.3*a*) indicates that the K4 and RCH parameters are likely to be easily estimated by regression, whereas the ANIV1 and ETM parameters are not likely to be

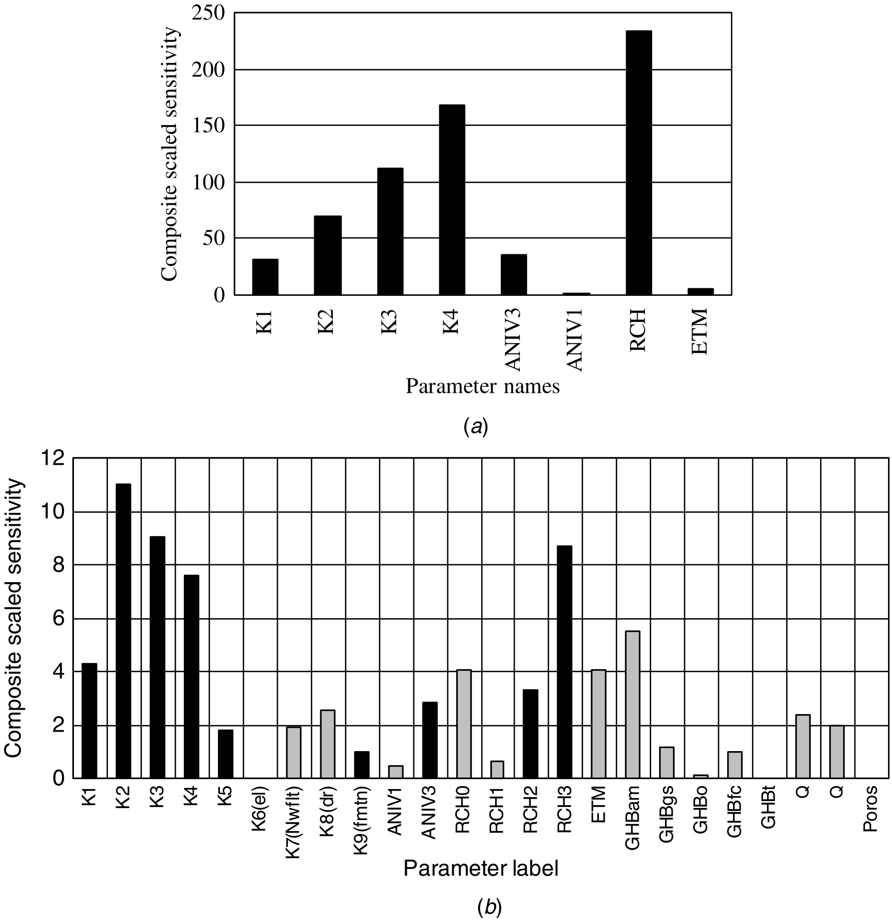


FIGURE 11.3 Composite scaled sensitivities for parameters of the DVRFS model of D'Agnese et al. (1997, 1999) for (*a*) the initial model and (*b*) the final model. In (*b*), parameters estimated by regression have black bars; parameters defined but not estimated by regression have gray bars. Parameters represent the following: K*, hydraulic conductivity; ANIV*, vertical anisotropy; RCH*, areal recharge; ETM, maximum evapotranspiration parameter; GHB*, conductance of head-dependent boundaries used to represent springs; Q, pumping (the two Q parameters apply to different areas); POROS, effective porosity. The observations provide no information for POROS, but this parameter is important to the transport predictions of interest. Together these parameters define all aspects of the system except the lateral and bottom boundary conditions.

easily estimated. In general, the available observations appear to contain substantial information about the K (hydraulic conductivity) and RCH (areal recharge) parameters, and less information about the ANIV (vertical anisotropy) and ETM (maximum evapotranspiration) parameters. Composite scaled sensitivities were calculated often during the calibration of this model and were used to determine what new parameters to introduce and whether previously excluded parameters should be included.

The *css* for the final model are shown in Figure 11.3*b*. Note that there are additional K and RCH parameters, and that most of these were estimated by regression. This is consistent with the initial evaluation showing that the data contained substantial information for these types of parameters. An important aspect of this analysis is that the basic conclusions from the initial and final evaluations are the same, despite the model nonlinearity and the substantial model and parameter-value changes made during calibration. This stability is typical and makes this method useful. If problems are too nonlinear to be stable, the utility of the composite scaled sensitivity method is diminished and possibly absent altogether.

Chapter 4, Section 4.3.4 states that if any parameters have *css* values that are less than one-percent of the largest *css* values, problems with convergence can be expected in regression. In Figure 11.3*b*, there are a few parameters with very small values, and these were not estimated. There are others with larger values that were not estimated for other reasons. For example, consider the one new type of parameter, GHB*, which are the hydraulic conductivity of the head-dependent boundary conditions used to represent groundwater supported springs. None of the GHB parameters were estimated in the regression for the final model because they tended to produce a good match solely to the flow of the spring or set of springs at which they were applied. This was evident because the dimensionless scaled sensitivities for each of these parameters generally were large for only one observation. Any error in the spring-flow measurements would have been fit by the model through adjustment of the GHB parameters. The values of the GHB parameters were determined primarily on the basis of hydrogeologic arguments and a few preliminary regression results.

Recall that the *pcc* indicate whether the estimated parameter values are likely to be unique. For the parameters of Figure 11.3*b*, all *pcc* were less than 0.95, suggesting that the estimates are unique. These simulations used a parsimonious model and the sensitivity-equation sensitivities of MODFLOWP (Hill, 1992) and MODFLOW-2000 (Hill et al., 2000), so potential problems with *pcc* accuracy, discussed in Chapter 4, Section 4.4.2, were not expected.

***Parameter Correlation Coefficients* (*pcc*)** Anderman et al. (1996) and Anderman and Hill (1998) used *pcc* to investigate what types of observations were needed to achieve a well-posed regression for a model of groundwater flow in a shallow aquifer on Cape Cod, Massachusetts. The system had a lake and a well-monitored sewage plume. Three different sets of observation data were considered: (1) hydraulic heads

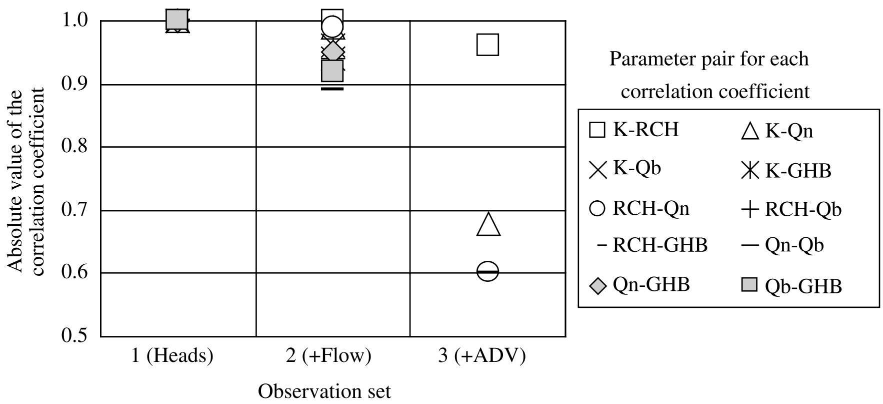


FIGURE 11.4 Parameter correlation coefficients for five parameters for three data sets from the Cape Cod sewage plume model as reported by Anderman et al. (1996), evaluated for the final parameter values. For values close to 1.00, parameter estimates are likely to be nonunique. For values less than 0.95, unique values are expected. The five parameters are K, hydraulic conductivity; RCH, areal recharge; Qb, sewage discharge sand-bed flux; Qn, northern boundary flux; GHB, conductance of the lake bottom. For data set 3, correlations not shown are $<|0.5|$. (From Anderman and Hill, 1998.)

only, (2) hydraulic heads and a lake seepage value, and (3) hydraulic heads, lake seepage, and an advective-transport observation derived from the monitored concentrations of the sewage plume. Figure 11.4 shows the *pcc* calculated at final parameter values for five model parameters, for each of the three observation data sets. This figure clearly shows that with only hydraulic heads (data set 1), all parameters are completely correlated (the absolute values of all correlation coefficients equal 1.00), so that any parameter estimates found by the regression are not unique. Adding one lake seepage measurement (data set 2) reduced correlations somewhat, but correlations remain very large. Only the observation set with the advective-travel observation (data set 3) could uniquely estimate all of the parameters.

G3.2 Effects of Nonlinearity on the *css* and *pcc*

As discussed above and in Chapter 4, Section 4.4, the utility of many of the statistics presented in this book can be affected by model nonlinearity. Some (like *pcc*) also are affected by even slightly inaccurate sensitivities. Here, we consider *css* and *pcc* because the authors have the most experience with these statistics; the discussion can largely be extended to other statistics. In general, difficulties with nonlinearity and inaccurate sensitivities occur when the conclusions drawn from the statistics are in error. The most common problems, their consequences, and suggested resolutions are displayed in Table 11.1.

TABLE 11.1 Consequences and Suggested Actions When Nonlinearity and Inaccurate Sensitivities Plague Parameter Correlation Coefficients and Nonlinearity Plagues Composite Scaled Sensitivities

Problem	Effect	Consequences	Actions
		Parameter Correlation Coefficients	
Nonlinearity	Correlation coefficients calculated using different sets of parameter values result in very different conclusions about whether the observations contain enough information to estimate parameters uniquely. (See Figure 4.2.)	Incorrect conclusions might be drawn about whether the observations are adequate to estimate the defined parameters uniquely.	In nonlinear systems, correlation coefficients can vary substantially for different sets of parameter values. The primary concern is whether the optimized values are unique.[a] That is, are any parameters extremely correlated at the optimized parameter values? If the answer is inconclusive because of problems with nonlinearity or inaccurate sensitivities, consider further tests: (a) Check whether the estimates and objective-function values are similar[b] in regressions with different starting values. (b) Reduce problems related to small *css* by combining parameters.[c] (c) If correlation is suspected, change the parameter values substantially in a way that reflects the suspected correlation. If the resulting objective-function value is similar,[b] extreme correlation is confirmed. Note: Parameter correlation cannot be detected by the progress or convergence of a single regression. (See Exercise 5.1b.)
Inaccurate calculated sensitivities (most problematic if *css* is small)[c]	Extremely correlated parameters do not have correlation coefficients equal to 1.00 or −1.00, as needed to detect correlation.		

	Composite Scaled Sensitivities (*css*)		
Nonlinearity	*css* values calculated using different sets of reasonable parameter values result in very different conclusions about whether the observations contain enough information to estimate certain parameters.	(a) Judgments about the feasibility of estimating a parameter may be in error.	(a) Judgments about likely success or failure of estimation are preliminary. If results are not as expected (e.g., parameters with relatively large *css* cannot be estimated), recalculate *css* for updated sets of reasonable parameter values.
		(b) Parameterizations and other aspects of model structure designed using *css* values results in unexpected model performance. For example, a system characteristic changes from being important to unimportant when the parameterization is changed.	(b) Keep evaluating *css* as the model evolves. If problems persist, try to figure out why. Appropriate strategies depend on the situation. In nonlinear systems, parameter changes can fundamentally modify system dynamics. Use model fit to observations, understanding of the mathematical model, and the system information to evaluate the system dynamics for the different parameter values and pameterizations. If the problems continue to occur for plausible parameter values and system dynamics, consider using a global search technique (Chapter 5, Section 5.2).

[a]The focus here is nonuniqueness caused by parameter correlation, but further test (a) checks for local minima.
[b]"Similar" for parameter values means differences are small relative to the calculated parameter standard deviations (see Exercise 7.1e). "Similar" for objective-function values means within a few percent.
[c]This is discussed in Chapter 4, Section 4.4.2.

GUIDELINE 4: INCLUDE MANY KINDS OF DATA AS OBSERVATIONS IN THE REGRESSION

Guideline 4 stresses the importance of using as many kinds of observations as possible. Guidelines 2 and 4, when taken together, emphasize data assimilation. References on data assimilation are listed in Section G2.1.

Different systems offer different observation possibilities. For example, in groundwater flow problems it is important to augment commonly available hydraulic-head observations with flow observations. Flows often constrain solutions much more than do hydraulic heads, which tend to be easier to match. Using observations that reflect the rate and/or direction of groundwater flow, therefore, tends to promote the development of more accurate models. In many settings, measurements of groundwater flow are difficult to obtain. Often concentrations of contaminants are used. Groundwater age dates and geochemical measurements are alternative types of data that also can provide valuable information on flow rates and directions (see Section G4.4). Many studies have shown that regression results improve when transport observations are included in regression models of flow and/or transport, compared to use of only hydraulic heads and flows. Studies illustrating this finding are cited in Chapter 9, Section 9.2.5.

The observations that can be used with MODFLOW-2000, UCODE_2005, and PEST are described in Chapter 2, Table 2.1. Detailed analyses of the importance of different observation types are presented by, for example, Anderman et al. (1996), Poeter and Hill (1997), and in this book.

Three issues about observations are discussed next: the use of interpolated observations, clustered observations, and observations that are inconsistent with model construction. Lastly, three applications are presented.

G4.1 Interpolated "Observations"

In some circumstances, it is appealing to use interpolated values to increase the number of "observations" available for the regression. Interpolated values are obtained by interpolating the actual observations. If interpolated "observations" are used, then the errors of the interpolated "observations" are correlated with each other and with the errors in the actual observations. Thus, the weight matrix needs to be full (see Chapter 3 and Guideline 6). In groundwater examples, Clifton and Neuman (1982), Neuman (1982), Neuman and Jacobson (1984), and Carrera and Neuman (1986) kriged hydraulic-head measurements to generate interpolated hydraulic heads and used them as observations in the regression. When kriging is used, the associated kriging variances and variogram can be used to calculate the variance–covariance matrix on hydraulic-head observation errors that is needed to calculate the full weight matrix for the observations.

The disadvantage of interpolation methods is that the interpolated "observations" generally are not consistent with the processes governing the simulated system. For example, Cooley and Sinclair (1976) show that for groundwater systems, interpolated hydraulic heads are not necessarily based on the physics of groundwater flow. Thus, the interpolated values are expected to respect the underlying processes represented in the model only to the extent that (1) they are constrained by the actual observations and (2) the actual processes happen to be represented well by the chosen interpolation scheme. The problems associated with item (2) can be severe if there are abrupt spatial variations in aquifer properties. Abrupt spatial variations can result in regions of steep and flat gradients that are only partially captured by the actual observations and, therefore, by the interpolation. This could cause the "observed" hydraulic-head distribution to be unrealistically smooth. Alternatively, it could cause a steep gradient evident in some of the actual observations to be unrealistically extrapolated.

These problems can be avoided if the observations are used directly in the regression. Then, the processes built into the model do the "interpolation," and lack of fit focuses attention on the quality of the observations and the model, which is where the focus of model calibration needs to be.

G4.2 Clustered Observations

In many circumstances data are clustered in limited areas or within short time intervals. For example, in groundwater systems, wells are often clustered in areas of high hydraulic conductivity where yields are highest and/or near population centers served by groundwater. As a result of the clustering of wells, hydraulic-head observations tend to be clustered spatially. Also, hydraulic-head observations are often limited to recent times, long after the start of substantial pumping.

There are two problems in regression related to clustered observations.

First, the presence of a large number of observations may make it difficult to evaluate whether the model is reproducing basic system characteristics represented by the observations. If the system characteristics are well represented by a subset of the observations, it can be productive to use the subset in at least the initial stages of regression. Alternatively, the observations can be averaged over defined areas or times. The error used to weight an averaged observation would not necessarily be much smaller than the error of the individual observations, because many components of error are caused by effects that averaging does not eliminate.

Second, clustered data can be problematic if they dominate regression methods such that observations are ignored elsewhere in the system or at other times. This would produce poor fit to sparse observations. If poor model fit occurs where observations are sparse, the possibility that clustering is the problem can be tested by grossly increasing the weights on some of the sparsely distributed observations in some regression runs. If this does not significantly improve the fit to those observations, then clustered data probably are not the problem. Instead, problems such as conceptual model error should be considered—that is, some aspect of model construction may be preventing any set of parameter values from producing a match at the location(s) in question. This is discussed in Section G4.3.

Data clustering is not a major problem in many groundwater models because most of the data clusters are hydraulic heads in areas of high hydraulic conductivity where significant quantities of water are pumped. In these areas, sensitivities of hydraulic heads to most parameters tend to be relatively small and the clustered wells will not adversely affect the regression.

G4.3 Observations that Are Inconsistent with Model Construction

Model simplifications and assumptions can result in observation data that reflect processes that are impossible to simulate using the constructed model. This can occur by design or can be unintended.

Situations that occur by design include those discussed for transient groundwater models in Chapter 9, Section 9.1.2. Consequences of designed inconsistencies depend on how the inconsistency is expected to affect model fit. If the omitted processes are expected to create a bias, such that the observations are consistently higher or lower than values simulated by an accurate model, the observations need to be adjusted to eliminate the bias. If the omitted processes are not expected to create a bias, so that the observations may be higher or lower than values simulated by an accurate model, the observation weights need to be adjusted to reflect the expected error introduced by omitting the processes.

Unintended inconsistencies can be more difficult. An example is presented by Hvilshøj and Jensen (2000) in which an analytic solution for a dipole test in a well was inconsistent with measured heads. This was resolved by simulating the test with a heterogeneous numerical model. If matching observations is troublesome or estimated parameter values are unrealistic, try to identify contributing model inconsistencies.

First, inspect the model for characteristics that could prohibit fitting the observation(s) in question using reasonable parameter values. In groundwater models when the problem is with fitting hydraulic heads, check for nearby head-dependent boundaries or specified heads. When the problem is with fitting flows, think about how the model simulates flow approaching or leaving the location in question. Compare the simulated flow paths involved to the flow paths conceptualized based on field information to ensure there are no unintentional simulated barriers or sources of water. Also, consider if there are any processes that occur in the true system and affect the observed values but that the model does not simulate.

Second, the existence, and sometimes the cause, of model inconsistencies can be identified by assigning the observation(s) in question enormous weight(s) (equivalent to a tiny variance, standard deviation, or coefficient of variation) and proceeding with a regression run. There are two possibilities.

1. *The fit to observation(s) does not improve*. This is a clear indication of inconsistency between the model and the observation(s). The model is constructed in such a way that the observation cannot be matched. Consider the options presented in the preceding paragraph.
2. *The fit to observation(s) improves*. Two results need to be checked.
   (a) *Model fit to other observations*. If the fit to the observation(s) is achieved by making the fit to other observations much worse, note what other observations those are. Determine if the original difficulty in fitting the observation(s) was because of other inconsistent observations, and resolve any inconsistencies.

(b) *Optimized parameter values*. If the fit to the observation(s) is achieved with clearly unrealistic parameter values, evaluate the associated simulated features, such as the geometry of hydrogeologic units in groundwater models. Is the simulated geometry or some other aspect of the features possibly in error?

G4.4 Applications: Using Different Types of Observations to Calibrate Groundwater Flow and Transport Models

Imaginative modelers continually explore, including testing new types of observations in the development of environmental models. Here, we describe several examples from the groundwater literature in which innovative types of observations were included. Generally, the use of such observations requires the use of a universal inverse code such as UCODE_2005 or PEST.

Age and Geochemistry Observations It can be especially difficult to obtain measurements of flows to or from groundwater systems in arid environments, where the water-table elevation is often far below surface-water bodies. To overcome the lack of flow data when calibrating a regional flow model of the Middle Rio Grande Basin aquifer system in central New Mexico, Sanford et al. (2004a,b) used an extensive set of carbon-14 and other geochemical data to estimate hydraulic-conductivity and recharge parameters.

Carbon-14 measurements were used to infer age dates, which in the regression were compared to simulated ages calculated by backward particle tracking with MODPATH (Pollock, 1994).

Geochemistry data were used to infer whether or not groundwater originated from the Rio Grande River. These data were used in the regression by defining nine hydrochemical zones. In each zone, an observation was defined as the percentage of groundwater that originated in the river, which was determined using geochemistry samples collected from all wells in the zone. The corresponding simulated percentage of water in the zone that originated in the river was calculated by backtracking a large number of particles from model layer 2 to any recharge location, and calculating the percentage of these particles that were tracked back to the river. The advantage of defining the observations in this way is that they were then continuous instead of discrete numbers, so that sensitivities could be calculated and the observations fit into readily available regression methods.

Use of these two data sets in addition to hydraulic-head data allowed estimation of 59 model parameters with no large correlation coefficients for any parameter pairs. The regression also produced recharge estimates that were more consistent with independent data than were recharge values estimated by previous groundwater models of the basin that used very few flow data.

Temperature Observations If groundwater flow is sufficient for advective heat transport to occur, then groundwater temperature data can provide information about parameters that govern groundwater flow.

Manning and Ingebritsen (1999) describe several studies in which temperature data were used to develop models of heat transport in relatively deep groundwater flow systems through, for example, sedimentary basins and mountainous terrain. Although most of the studies cited did not use formal inverse modeling techniques, they illustrate the substantial benefit of temperature data for constraining crustal permeability estimates in numerical models.

Anderson (2005) recently reviewed the use of heat as a tracer in groundwater systems and cites numerous studies in which temperature data are used to constrain hydraulic-conductivity estimates. For example, temperature measurements have been widely used in recent years in unsaturated zone models to constrain estimates of the vertical hydraulic conductivity of streambeds (e.g., Burow et al., 2005; Niswonger et al., 2005). This constraint leads to more accurate estimates of the flux between streams and groundwater systems. Only a small number of studies have incorporated temperature observations in a formal inverse modeling context; two such studies are described next.

Woodbury and Smith (1988) demonstrate the advantages of temperature data to estimating parameters of a cross-sectional model of groundwater flow and heat transport through and beneath a large landslide. They showed that when only hydraulic-head data were used for calibration, the estimated recharge and hydraulic-conductivity parameters were perfectly correlated. With temperature observations, these parameters could be uniquely estimated, as could additional parameters such as thermal conductivity and basal heat flux. The latter parameters had a fairly high degree of uncertainty, but the estimates were consistent with results from other studies.

Bravo et al. (2002) simulated groundwater flow and heat transport through a wetland system characterized by a fluvial sedimentary layer underlain by sandstone. Subsurface temperatures varied on a daily and seasonal basis. Application of inverse modeling to a flow and heat transport model using both head and temperature observations yielded parameter estimates with much smaller uncertainty and produced fewer problems with convergence of the regression procedure, compared to calibration of a flow model using only hydraulic-head observations.

GUIDELINE 5: USE PRIOR INFORMATION CAREFULLY

Prior information allows measurements related to defined parameters to be included in the regression (see Eq. (3.1)). The measurements involved are a subset of the system information of Guideline 2 and are related to model input.

G5.1 Use of Prior Information Compared with Observations

It can be argued that prior information should be treated differently than observations for two reasons. First, experience has shown that in many systems observations often can be measured more accurately than prior information. Second, the relationship between observed and simulated values is usually more direct than is the relationship between prior information and model parameter values. Often both problems result from what could be called scale issues: local variability makes it difficult to measure many model input quantities at a scale that is consistent with the model input. Resulting measurements can be grossly in error relative to what is appropriate in the model.

To the extent that measurements of the model input values represented by parameters are accurate as well as applicable to the scale of the model, model calibration may become unnecessary or less important. This book addresses problems in which model calibration is important, which implies that the measurements related to model inputs are inadequate in some way.

We suggest that for problems in which observations are more accurate and well understood, they be emphasized more than prior information that is less accurate and poorly understood. For systems with accurate measurements that directly relate to some or all of the parameters, the prior information might be more strongly emphasized and perhaps used in a manner closer to that suggested here for the observation data. In the applications described below, geophysical data are used in that way.

To encourage understanding of the information that is directly available from the observations alone, Guideline 5 suggests initially omitting from the regression any prior information on parameters. Two reasons generally motivate the subsequent inclusion of prior information.

First, if the parameter is insensitive, as indicated by a small composite scaled sensitivity (*css*), regression that includes the parameter often will not converge. Problematic parameters can be identified as those with the largest fractional changes calculated by Eq. (5.7), which are printed by most nonlinear regression programs (e.g., see Exercise 5.2b). Two options generally exist for dealing with these problematic parameters: (1) specify prior information for the parameter or (2) set the parameter value so that it is not changed during the regression.

In the regression, specifying prior information on an insensitive parameter usually results in a parameter estimate that is close to the specified prior value. Thus, the estimated parameter value generally is equal to or close to the prior information value regardless of which option is chosen. Model execution time is less when the parameter value is set, because this eliminates the need to calculate sensitivities for the parameter. Thus, option (2) often works well for model calibration. This will continue to be a good option as long as the parameter remains insensitive. Sensitivities can be checked by occasionally calculating *css* for all defined parameters.

Other groundwater studies, in which prior information was used either because of insensitive parameters or to explore its effect on parameter or prediction uncertainty, include those by Parker and Islam (2000), Christensen and Cooley (1999), Heidari and Ranjithan (1998), Christensen (1997), Bentley (1997), and Cooley (1983a).

The second common reason for using prior information occurs when a parameter value estimated by the regression is unreasonable. This problem is discussed in

Chapter 5, Section 5.5. As noted there, the most productive response to this problem depends on the amount of information the observations provide on the parameter in question.

1. If little information is provided, the problem falls into the category of insensitive parameters. Detection and resolution of such problems are discussed above.
2. If substantial information is provided, the unrealistic estimated parameter value may indicate problems with the model or the data, as discussed in Chapter 7, Section 7.6 and Guideline 10 in Chapter 12. These problems need to be resolved to achieve an accurate model.

In both of these situations, imposition of prior information during model calibration is not the best way to proceed.

Weiss and Smith (1998) also suggest cautious use of prior information and present methods of identifying parameters for which specification of prior information would be most beneficial. Their methods are based on analyzing attributes of scaled objective-function surfaces and parameter confidence regions. One method identifies parameters for which imposition of prior information will most stabilize the regression in terms of making it better posed. This method is likely to produce similar results as would be obtained by analyzing composite scaled sensitivities to determine parameters about which the observations provide little information.

G5.2 Highly Parameterized Models

In some situations, a modeler purposely defines more parameters than can be directly supported by the data, to represent potential variability in system properties. When very large numbers of parameters are defined, the model is considered highly parameterized. To obtain a tractable regression problem, such models require the use of prior information; the associated weights generally result in it being classified as regularization (see Guideline 6). The regularization is used to penalize parameter distributions that violate certain requirements. Commonly, the requirement is simply that the parameter values be close to specified values. This approach was considered in a simple way by Hill et al. (1998), and in more sophisticated ways by Valstar et al. (2004), among others. Alternatively, neighboring estimated parameter values that differ from one another are penalized so that high frequency variations are discouraged. Resulting distributions tend to be smooth. This is one of the approaches presented by Tikhonov and Arsenin (1977) and has been used extensively (e.g., Eppstein and Dougherty, 1996; Moore and Doherty, 2005, 2006). This approach is available through the regularization capability of PEST (Doherty, 1994, 2005).

Thus, parsimonious and highly parameterized models are two end-member approaches to obtaining tractable regression problems for complex groundwater systems. Parsimonious models are the focus of much of this book, though the methods presented have potential utility for highly parameterized models as well.

For example, parameter correlations can be revealed using single parameters multiplying the highly parameterized fields. Extreme correlations would suggest that though the variability produced by the highly parameterized model may be important, the overall mean depends on the value of other parameters. Thus, despite a good fit to observations, the model may poorly simulate results sensitive to the values of the individual system properties. The issue of scale discussed in Chapter 9, Section 9.2.3 also is relevant. Parsimonious methods are not necessarily limited to characterizing large-scale variations (e.g., Carle et al., 1998). Highly parameterized models generally represent variability at the scale of the grid or, in the case, for example, of pilot points, at a larger scale. Methods for sub-grid scale effects exist (e.g. Anderman and Hill, 2001; Rubin et al., 2003), but, to the authors' knowledge, have not yet been used in highly parameterized models.

G5.3 Applications: Geophysical Data

For models of groundwater systems, geophysical data are commonly used to define model layer thickness and define parameterizations as discussed in Guideline 2. A few investigations have used geophysical data more directly; selected studies are listed in Table 11.2. Most commonly, the geophysical data are used to support prior information, which is why geophysical data are included here under Guideline 5. However, in some of these studies the geophysical data is classified as a type of observation because equations relating the geophysical data to hydraulic conductivity are included as a model equation.

GUIDELINE 6: ASSIGN WEIGHTS THAT REFLECT ERRORS

Chapter 3, Section 3.1 of this book shows how weights and weight matrices appear in the objective functions minimized in nonlinear regression; Section 3.3.3 presents the purpose and theoretical requirements of weighting; and Section 3.4.2 suggests that, except for limited testing, it is useful to define weights that equal one divided by the variance of the errors in observations and prior information, or a weight matrix that equals the inverse of the variance–covariance matrix of errors.

Under Guideline 6, we first show how weights can be determined using common field data and assumptions and we then discuss selected issues related to weighting. The discussion reveals the importance of assigning weighting in a way that respects its intended role in the regression. Seven points emphasized in the discussion are:

1. The strategy of defining weighting based on likely error is supported by theory, has a strong intuitive appeal, and provides practical advantages. A chief advantage is that the strategy provides a formal mechanism for including an analysis of errors in model development.

TABLE 11.2 Selected Investigations Showing the Use of Geophysical Data as Observations or to Support Prior Information in Groundwater Model Calibrations

Reference	System	Parameter Estimation Method[a]	Geophysical Data		Observed and Prior Values[b]	Parameters Estimated[b]	Results
			Type[b]	Method of Including in Model Calibration[b]			
Rubin et al. (1992) Copty et al. (1993)	2D groundwater flow; synthetic	Geostatistical inversion ML	τ	Function relates SVL to K. Processing τ to obtain SVL is independent of groundwater model calibration.	Hydraulic head, K	Mean and covariance of log K probability distribution function	Including τ data produced a much more accurate K field.
Hyndman et al. (1994)	2D groundwater flow, solute transport; synthetic	NLR	τ	Coinversion of τ, solute arrival time, and concentrations.	Solute arrival time, concentrations, τ	K, dispersivity, SSL field used to delineate K zones	Combining seismic and tracer data can provide high-resolution estimates of aquifer zonation and properties.
Hyndman et al. (1996)	3D groundwater flow, solute transport; Kesterson, CA	NLR	τ	Used two steps with feedback: delineate K zones, estimate parameters.	Solute arrival time, drawdown, τ		
Hyndman et al. (2000)		NLR	τ	Process τ to yield SSL. Generate SSL fields. Function relates SSL to K.	Concentrations, drawdown, τ	Dispersivity, SLK	

Dam and Christensen (2003)	2D groundwater flow; synthetic	NLR	ER	Function relates ER to K. Processing to obtain ER data is independent of groundwater model calibration.	Hydraulic head, prior K, prior ER	ER, K, ERK	With ER data, a greater number of more accurate K parameters were estimated, compared with no ER data.
Day-Lewis et al. (2006)	3D groundwater flow, solute transport; Mirror Lake, NH	NLR	Radar	Postcalibration evaluation of alternative models.	Solute arrival times, concentrations, drawdown	K, effective porosity, dispersivity	Used radar data to resolve alternative conceptual models that were nonunique based on groundwater model calibration.

[a]ML, maximum likelihood; NLR, weighted least-squares nonlinear regression (in most circumstances these are equivalent; see Appendix A).
[b]τ, seismic travel time; ER, electrical resistivity; K, hydraulic conductivity; SVL, seismic velocity; SSL, seismic slowness; ERK, parameters relating electrical resistivity to K; SLK, parameters relating seismic slowness to K.

2. Additional insight into model fit can be achieved if the weighting relates directly to observation error instead of relating to it proportionately, as required by theory.
3. Theoretical considerations and available data can be used to determine weighting that is adequate, partly because regression results are not very sensitive to modest variations in weighting. The requirement that the weights reasonably represent observation error provides a sufficiently restrictive framework for determining weights.
4. The terminology used by different parameter-estimation methods causes part of the confusion that plagues weighting.
5. Some kinds of model errors can be included in determining weighting as long as the expected value of each error represented by the weighting equals zero.
6. Large weights on selected observations or prior information can be useful to the following interrelated goals: (a) ensuring the data are not being ignored, (b) determining whether a plausible solution exists with a given model construction, and (c) identifying model construction errors. This is related to the analyses proposed in Sections G4.2 and G4.3.
7. For uncertainty analyses to be meaningful, all observations and prior information need to be weighted based on likely errors.

G6.1 Determine Weights

Substantial guidance for determining weights is provided by the idea that weights need to equal one divided by the variance of the observation error and that weight matrices need to equal the inverse of the error variance–covariance matrix. Even if alternate weighting is chosen, it is important to evaluate errors in observations and prior information as discussed here to ensure the data are used appropriately. Using this strategy to determine the weights provides a formal mechanism for including analysis of errors in model development.

For problems with one kind of observation (e.g., all hydraulic heads) measured and simulated with errors of apparently equal variance, it is common to set all weights equal to 1.0. For example, see the Theis problem of Figure 5.3. The calculated standard error of the regression (defined after Eq. (6.1)) can be compared to the expected standard deviation of the errors to evaluate the likely model error (see Chapter 6, Section 6.3.2).

For commonly used diagonal weight matrices, the weight is defined to be equal to one divided by the variance of the errors, σ_i^2, as discussed in Chapter 3, Section 3.4.2. More readily understood quantities are σ_i, the standard deviation, and σ_i/y_i or σ_i/y_i', the coefficient of variation, where y_i is an observed value or prior estimate and y_i' is an equivalent simulated value. Variances are readily calculated from these quantities.

For full weight matrices, the weighting equals the inverse of the variance–covariance matrix of the observation errors.

For any observation, errors result from many processes. Determining the statistic (the variance, standard deviation, or coefficient of variation) used to calculate the weight requires quantifying as many of the major error sources as possible. In this section, we first consider quantifying a single component of error, then many components of error, and finally errors for observations that are sums of or differences between measurements when the errors are independent, additive, and normally distributed. Chapter 3, Section 3.3.3 discussed situations in which these assumptions may not apply.

Quantify One Component of Error: An Observation Well Example The statistics used to calculate observation weights can often be determined using readily available information about likely errors and a simple statistical framework. For example, consider the common situation in groundwater modeling of error in the elevation of an observation well used to determine head measurements at the well.

The data on the well are as follows: the well elevation was determined by an altimeter and is thought to be accurate to within 3 ft. To estimate the variance of the error, this statement needs to be quantified. For example, the statement that "the probability is 95 percent that the true elevation is within 3 ft of the measured elevation" might apply. If, in addition, the errors are assumed to be normally distributed, a table of areas under the standard normal curve (Table D.1 in Appendix D) can be used to determine the desired statistics. This process is outlined in Table 11.3.

For some data and/or instrument types, error studies have been conducted. For example, for determining elevations from U.S. Geological Survey (USGS)

TABLE 11.3 Steps Needed to Determine a Standard Deviation that Can Be Used by MODFLOW-2000 and UCODE_2005 to Calculate a Weight

Step	Description	Example
1.	*Quantify the statement about measurement accuracy; include a significance level.*	"The probability is 95 percent that the true elevation is within 3 ft of the measured elevation." The significance level is 5 percent ($5 = 100 - 95$)
2.	*Determine the critical value.* For normally distributed errors, use areas under the standard normal curve (Table D.1) to obtain the critical value.	A significance level of 5 percent has a critical value of 1.96.
3.	*Construct a confidence interval* on the measured value, y_i, using the critical value and standard deviation of the error. Equate it to the confidence interval expressed in the statement developed in step 1.	Confidence interval $= y_i \pm 1.96 \times s_{y_i}$ $= y_i \pm 3$ ft Thus, $1.96 \times s_{y_i} = 3$ ft
4.	*Solve for* s_{y_i}.	$s_{y_i} = 1.53$.

topographic maps, the USGS (1980, p. 6) states that on these maps, "not more than ten percent of the elevations tested shall be in error more than one-half the contour interval." This statement indicates that a 90-percent confidence interval for this error equals plus and minus one-half the contour interval. Assuming that the error is normally distributed, a 90-percent interval is constructed by adding and subtracting 1.65 times the standard deviation of the measurement error. Thus, the standard deviation of the measurement error can be calculated as one-half the contour interval divided by 1.65, or (contour interval)$/(2 \times 1.65)$. The value of 1.65 was obtained from Table D.1 as described in Table 11.3.

Errors can also be evaluated by modeling the sampling process. For example, Schäfer et al. (2003) use what they call virtual aquifers to evaluate solute concentrations measured at wells in heterogeneous materials.

Many situations are not as definitive as the examples above. Difficulties in determining weighting are discussed in Section G6.2.

Accumulate All Error Components Generally, for any observation there are many sources of error. For example, possible errors for hydraulic heads in the simulation of a groundwater system include:

1. Error in measuring the water level in the well.
2. Error in determining the elevation of the well. (For drawdowns, this cancels out.)
3. Aspects of well construction. If we could drill 100 wells in the same place, different gravel packs, screen settings, grouting, and so on would produce variations in the measured water levels. Unfortunately, such repeated sampling is not practical, so these variations are not well characterized. Errors related to well construction are likely to be greatest in dynamic situations such as during an aquifer test.

There are other errors in placing the well in the context of the model:

4. Errors in placement horizontally.
5. Errors in placement vertically.

There are errors that can be classified as model errors in that they could be corrected with a finer grid or time step, but can be included in the weighting if they have a mean of zero. These include:

6. Incorrect placement of hydrogeologic units caused by grid size.
7. Unrepresented temporal variations in recharge, pumping, and so on (see Chapter 9, Section 9.1.2).
8. Unrepresented flow fields, such as typically local flow fields in a regional flow model (see Section G6.2).
9. Unrepresented flow fields, such as regional flow omitted from a site model.

Often the errors can be considered independent and normally distributed. In this situation, the variance of the sum of the errors equals the sum of the variances. That is, $\sigma^2_{\text{total}} = \sigma^2_1 + \sigma^2_2 + \cdots$. Only variances are additive; standard deviations and coefficients of variation cannot be added. This is because the standard deviation (from which the coefficient of variation is calculated) is defined as the square root of the variance, and the square root of the sum of two quantities does not equal the sum of the square roots of the two quantities. An example of accounting for a number of different types of error for transient head observations in a groundwater model is presented in Chapter 15, Section 15.2.1.

Weights for Observations that Are Sums of or Differences Between Measurements Observations can be sums of or differences between measured values. For example, consider streamflow measurements between two streamflow gauging stations. In groundwater modeling, the difference between two flow measurements often is used as an observation in the regression. These observations are called streamflow gains or losses.

Consider a situation in which the upstream and downstream flow measurements are 3.0 ft^3/s and 2.5 ft^3/s, so that there is a 0.5 ft^3/s loss in streamflow between the two measurement sites, and in which the following assumptions apply:

1. The measurements are each thought to be accurate to within 5 percent (using the error analysis of Carter and Anderson, 1963).
2. There is a 90-percent probability that the first measurement is within 0.15 ft^3/s (5 percent) of the true value, and a 95-percent chance that the second measurement is within 0.125 ft^3/s (5 percent) of the true value.
3. The errors in the two measurements are independent and are normally distributed.

The procedure for calculating the coefficient of variation of the streamflow loss is as follows:

1. Calculate the standard deviation of the first measurement using the method described in Table 11.3.

$$1.65\, s_{q_1} = 0.15\,\text{ft}^3/\text{s}, \quad \text{so } s_{q_1} = 0.091.$$

2. Calculate the standard deviation of the second measurement in the same manner.

$$1.96\, s_{q_2} = 0.125\,\text{ft}^3/\text{s}, \quad \text{so } s_{q_2} = 0.064.$$

3. Square the standard deviations to calculate variances.

$$s^2_{q1} = 0.0083(\text{ft}^3/\text{s})^2 \quad \text{and} \quad s^2_{q_2} = 0.0041\,(\text{ft}^3/\text{s})^2.$$

4. Calculate the variance of the 0.5-ft^3/s streamflow loss (the difference between the two flows) by adding the variances.

$$s^2_{q_1} + s^2_{q_2} = 0.0124\,(\text{ft}^3/\text{s})^2.$$

5. Take the square root of the variance to obtain the standard deviation of measurement error.

$$[0.0124(\mathrm{ft}^3/\mathrm{s})^2]^{1/2} = 0.111\,\mathrm{ft}^3/\mathrm{s}.$$

6. Calculate the coefficient of variation of the loss by dividing the standard deviation by the loss.

$$c.v. = (0.111\,\mathrm{ft}^3/\mathrm{s})/(0.5\,\mathrm{ft}^3/\mathrm{s}) = 0.22, \quad \text{or 22 percent.}$$

In UCODE_2005 and MODFLOW-2000, a variance, standard deviation, or coefficient of variation can be specified by the user for each observation. The choice generally is based on achieving statistical values that are most meaningful to the modeler. For many types of flow observations, coefficients of variation are often most meaningful.

Determine Covariances for Weight Matrices Some circumstances clearly produce correlations between errors of different observations. For example, consider three streamflow measurements, $q1$, $q2$, and $q3$, along the length of a stream, and three associated measurement error variances, σ_1^2, σ_2^2, and σ_3^2. Gains or losses are calculated by subtracting each measurement from the next downstream measurement. For the three measurements, this results in two gain/loss observations, $q2 - q1$ and $q3 - q2$ and, from the preceding discussion, error variances $\sigma_1^2 + \sigma_2^2$ and $\sigma_2^2 + \sigma_1^2$. The errors in the two differences are not statistically independent, because the error in $q2$ is included in both differences. Hill (1992, p. 43) reported that in this circumstance the covariance between the two differences equals $-\sigma_2^2$. Christensen et al. (1998) extended this result to measurements along branching streams and indicate that the covariance equals -1 times the sum of the variances of the flows shared by any two gain/loss observations. Covariances can be included in UCODE_2005 or MODFLOW-2000. In some situations, inclusion of off-diagonal covariance terms in the weight matrix have had a negligible effect on estimated parameters (unpublished results by the first author of this book and S. Christensen, 1996, Aarhus University, oral communication). In others they have been important (Bentley, 1997).

It is not known how large the covariances need to be before a diagonal weight matrix produces significant errors in parameter estimates or measures of uncertainty. Additional work and definitive publications would be useful. In some situations, correlated errors can be accommodated by differencing, as discussed in Chapter 9, Section 9.1.2 in the context of temporal observations.

G6.2 Issues of Weighting in Nonlinear Regression

The following common issues are considered: difficulties in determining the weights, confusion about the term weighting, measurement error versus model error, the utility and difficulty of using exaggerated weights, the importance of weighting strategy in detecting model error and overfitting, and weighting system information on parameter values.

Difficulties in Determining the Weights In practice, it is generally impossible to identify all errors that contribute to an observation. In addition, the variances, standard deviations, and coefficients of variation calculated using the methods discussed in this guideline are clearly approximate. Thus, determining proper weighting can seem problematic and has discouraged some from using regression methods.

Yet, it is rarely difficult to determine weighting that adequately represents errors for use in regression. If one poses different levels of potential error, almost always some can clearly be identified as realistic while others are not realistic. Indeed, posing a range of values generally reveals a believable range of error. Such evaluations can be used to create statements for step 1 of Table 11.3, and the statistics can then be determined using steps 1 through 4. While the resulting statistics are not rigidly defined, such an analysis generally is able to determine the weights well enough. This is because regression results generally are not sensitive to moderate variation in the weighting: nearly identical results are typically obtained given weighting within a range that reasonably represents the likely observation error. If the weighting is changed beyond reasonable ranges, large variations in regression results can occur, causing the regression to lose meaning and become arbitrary.

In applications of multiobjective optimization, which was discussed in Chapter 3, Section 3.2.3 and Chapter 5, Section 5.3, alternative weighting schemes are considered. In those methods, the weighting changes as multipliers on the different objective functions change. An example in which only four weightings are considered is presented by Ghandi et al. (2002a), who used head, concentration, and interwell flow data to calibrate a transport model of a groundwater recirculation system used for in situ bioremediation. As for most applications of multiobjective optimization, the weighting strategy differed from that suggested in this book in that none of the observation weights were based on likely errors, and they may have varied over a larger range than would have been supported by an analysis of errors. Even so, the four strategies only resulted in moderately different estimates of some parameters. The authors selected the final weighting strategy on the basis of its ability to produce a good overall fit to all three data types. Because no analysis of observation error is presented, the relationship between the weighting and the errors cannot be evaluated.

Confusion About Terminology Confusion about weighting occurs for many reasons. One reason is that very different definitions for the terms "weights" and "weighting" are used in different parameter-estimation methods. In this book we use these terms only to describe a term in the objective function (Eq. (3.1)). However, other authors have used these terms very differently. For example, Yeh et al. (1996) use terms "weights" and "weighting" to describe quantities that reflect the smoothness of the parameter field (through the spatial variance–covariance matrix of, typically, hydraulic conductivity) and the sensitivities. Other methods may have no formal mechanism for accommodating expected data errors, a role suggested for weights in this book. To avoid confusion about the role of weights in different parameter-estimation methods, careful reading and writing are important. This will help all modelers clearly understand the function of weights and weighting in any application of any method.

Measurement Error and Model Error Model errors are defined here as any errors that could be eliminated by changes in the model given greater computer capacity, more time, or more complete information about the groundwater flow system even if the information is not attainable given present technology. Model errors are caused by, for example, inaccurate interpolation of simulated equivalents to observations, inability of the model to represent some processes, fluctuations in properties that are smaller than the grid size, and parameterizations that limit the spatial or temporal variability of parameters. As noted in Chapter 1, parameterization is needed to attain a tractable problem, but it does produce model errors. Dealing with this conflict is the topic of Guideline 3.

Here we consider whether the observation errors accounted for by weighting should include only measurement errors, or whether some types of model error can be included as well. While this point can be, and is, argued extensively, a useful definition is:

Observation error is error related to any aspect of the observation not accounted for by the model considered, for which the expected value is zero.

Unambiguous types of measurement errors are those associated with the measuring device and the spatial location of the measurement. Ambiguous contributions include, for example, heads measured in wells that only partially penetrate the numerical layer to which they are assigned, or temporally averaged head measurements or single measurements that are clearly affected by transient effects used in a steady-state model. These are more ambiguous because the model could be modified to better accommodate the measurements. Despite such ambiguities, the above definition for observation error works well in practice, because it produces sufficiently accurate weighting, and, as mentioned above, the regression often is not highly sensitive to moderate changes in the weighting.

For example, in a groundwater model of the Madison aquifer in the northern Great Plains, USA, Cooley et al. (1986, p. 1764) anticipated that the small error with which the hydraulic head in shallow wells could be measured would produce accurate observations at these points, and thus assigned them large weights. During calibration it was determined that "the model fit no better at these points than elsewhere" (Cooley et al., 1986, p. 1772). Apparently, heads in the shallow wells were affected by shallow, local flow systems not represented by the regional-scale model, and this situation produced residuals that were as large as those associated with inaccurately measured heads in deep wells. Decreasing the weights (increasing the variances) for observations from shallow wells to account for the model not simulating the shallow flow dynamics produced better results.

If weights are determined based on observation errors that include measurement errors and possibly some model errors, the standard error of the regression is significantly greater than 1.0 (as determined using the methods described in Chapter 6, Section 6.3.2), and the fitted error statistics (see Section 6.3.2) are too large to be accounted for by measurement error, it is likely that model error is involved in the misfit. If the weighted residuals are randomly distributed, it is possible that unaccounted for model errors have zero means and a variance–covariance matrix that is proportional to the variance–covariance matrix of the observation errors. In this situation, the large value of the calculated error variance produces a variance–covariance matrix on the parameters of Eq. (7.1) that appropriately accounts for the unaccounted for model errors.

Using Large Weights It can be useful to assign large weights to selected observations or prior information, as discussed in Sections G4.2 and G4.3. Figure 5.4 and Exercise 5.1b showed how a regression could become better posed by increasing the weighting on an observation to place more emphasis on it than is warranted given likely observation errors. This is frequently done to establish the existence of a solution (Backus, 1988), especially for observations that provide unique information. Such observations may be identified from an understanding of the simulated processes, or because statistics such as scaled sensitivities or measures of leverage or influence are distinctive. Examples include observations that are a different measurement type or that are collected at a different location or time.

For example, in groundwater flow modeling there are typically many hydraulic-head observations but very few flow observations (such as streamflow gains and losses, or spring flows). There is a perception that the small number of special observations (here, flows) will not be properly accounted for in the regression, and thus there is often an inclination to assign larger weights than are consistent with likely errors in these observations. The concern is heightened if predictions of interest are closely related to the few special observations.

However, the possibility that keeping large weights throughout both model calibration and uncertainty analysis might diminish the accuracy of the model, predictions, and/or measures of uncertainty is suggested by the theoretical requirements of weighting and needs to be considered.

To investigate this issue, consider a simple problem in which linear regression is applied in a situation known to be characterized by a linear model. Figure 11.5 shows that of 10 observations only one is located in the range of relatively large x values for which predictions are of interest. The important question is whether the accuracy of the predictions can be improved by increasing the weighting of the special observation. It is apparent from Figure 11.5 that the answer is no, because the other data are clearly relevant to predictions at larger values of x, given that a linear model is valid. Increasing the weighting of the observation with large x would produce a model that closely matches the error of that measurement, but is likely to degrade the accuracy of the resulting calibrated model.

The one observation for large x in Figure 11.5 is analogous, for example, to the few flow observations in a groundwater system, because in both cases these observations have sensitivities that are special in some way. For this linear regression problem, the sensitivity of each data point with respect to the intercept parameter equals 1.0, and the sensitivity to the slope parameter equals the x value

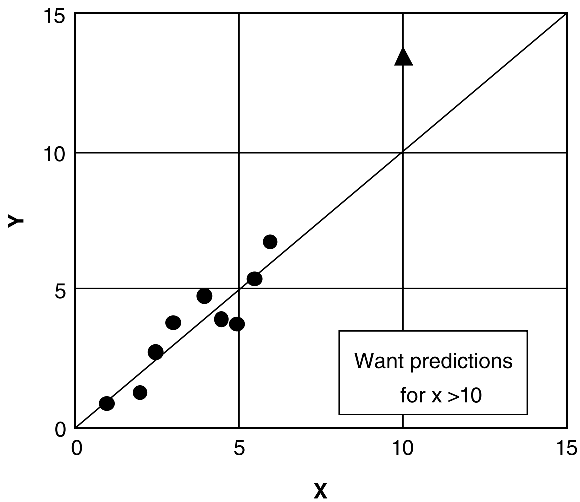


FIGURE 11.5 The true model of $y = 0.0 + 1.0x$, and possible observations to be used in linear regression. The data represented by dots are clustered and have x values that are distinctly different from that of the data point represented by the triangle.

of the observation (i.e., for the model $y = a + bx$, $\partial y/\partial a = 1.0$, and $\partial y/\partial b = x$). Thus, for the special observation, the sensitivity to the slope parameter is larger than that for the other observations. In groundwater systems, flow data provide special information, which is expressed by sensitivities that often reduce correlations among parameters, and thus produce a regression better able to uniquely estimate parameter values. Also, errors in flow data tend to have very different sources and magnitudes than errors in head data, as well as different units (e.g., m^3/day versus m).

To more closely examine this issue, consider the results of Exercise 5.1a and define a prediction of interest as the advective-transport distance toward the river from the center of the top layer after 10 years. The true predicted value is 1737 m. Objective-function surfaces for the parameter-estimation problem are shown in Figure 5.4. With hydraulic-head observations alone (Figure 5.4*a*), the objective-function surface is composed of parallel lines, and no minimum exists.

Addition of the flow observation using weighting that realistically represents the observation error produces the objective function in Figure 5.4*b*; imposing a large weight that assumes an unrealistically small observation error produces the objective function of Figure 5.4*c*. Increasing the weighting of this observation obviously produces a better-defined minimum and might be justified if the existence of a plausible solution is being explored, but the consequences need to be considered. As shown in Table 11.4, for this simple model the parameter estimates and the advective-transport prediction are very similar for the two different weightings. The regression with the large, unrealistic weight on the flow observation produced a slightly more accurate prediction. However, in general, this accuracy could either improve or deteriorate, depending on the actual error in the flow observation.

TABLE 11.4 Selected Regression Results Using Weighting of the Flow Observation Resulting from Reasonable (10 percent) and Unrealistically Small (1 percent) Coefficients of Variation

Flow Coefficient of Variation	Parameter Estimate		Prediction (Distance Traveled Toward River in 10 years) (m)	Confidence Interval[b] (m) on the Prediction	Interval Includes True Value of 1737 m?
	K_MULT	RCH_MULT			
10 percent	1.16	0.89	1017	71; 1964	Yes
1 percent	1.18	0.91	1036	940; 1131	No

[a]A smaller coefficient of variation produces a larger weight.
[b]Ninety-five percent linear confidence intervals constructed assuming a normal probability distribution.

The most significant consequence of using an unrealistic weight is related to the confidence intervals on the predictions (Table 11.4). With the unrealistically small coefficient of variation of 1 percent, the small prediction confidence interval does not reflect a realistic level of prediction uncertainty, as indicated by its omission of the true predicted value by a wide margin. In contrast, with a more reasonable coefficient of variation of 10 percent, the interval is more realistic and contains the true predicted value. This results from the unrealistic weight being included in the calculation of the parameter variance–covariance matrix (Eq. (7.1)) and the effects being propagated to the standard deviation on the prediction using Eq. (8.1).

In more complex situations, unrealistic weightings may produce different estimates and predictions compared to when realistic weights are used, but there is no assurance that the different values will be more accurate. In addition, the consequences for uncertainty analysis are likely to be similar to those shown here for the simple two-parameter model. Ultimately, exaggerated weighting cannot be expected to produce more accurate models; that goal can only be achieved by better data and/or better use of data. This book focuses on the latter.

Detecting Model Error and Overfitting Specifying weighting that equals the inverse of the variance–covariance matrix of the observation errors establishes a context for detecting model error and for identifying fits that are too good (as shown in Figure 11.1*b*). This analysis uses common measures of model fit and is discussed in Chapter 6, Section 6.3.2 and considered later in Guideline 8. This analysis is useful and is often overlooked, so a summary of the analysis is included here.

If the model fit is consistent with the assigned weighting, then the calculated error variance and the standard error of regression will be close to 1.0. Larger values (common in practice) indicate that the model fits the data more poorly than is consistent with the weighting. For example, if the standard error is 5.0, the model fit is, on average, five times worse than is consistent with the expected observation error. Possible sources of the additional error are neglected measurement error or model error. If model error is suspected, but no bias is evident in the weighted residuals, the error may be accumulated from small contributions, and model predictions and measures of uncertainty may still be useful (Hill et al., 1998) (see Chapter 6, Section 6.3.2).

The calculated error variance and the standard error of regression also can be less than 1.0. This is not common in practice but may occur if too many model parameters are estimated. The value of the standard error might not increase as the number of parameters increases if prior information is added for each added parameter value. Small values of the standard error indicate that the model fits the observations better than expected based on the analysis of observation errors. Thus, for example, if the standard error is 0.1 and the confidence interval on the value (Eq. (6.2)) does not include 1.0, then the model fit is, on average, 10 times better than is consistent with the preliminary analysis of observation error. In this situation, the expected errors and the model fit should be closely examined for evidence that the model is fitting errors rather than system processes. Overfitting can be more easily identified if the observation errors have been carefully evaluated. This can be accomplished when weighting is defined as suggested here.

Defining weights on the basis of an analysis of errors encourages comparison of the weighting to theoretical ideals. If nonideal weighting is used to achieve regression results, the nonideal weighting can be compared to likely errors. For example, if an observation has a weighted residual that is distinctly larger than other weighted residuals in absolute value, reducing the weight (by increasing the variance, standard deviation, or coefficient of variation) can make the weighted residual more comparable to other weighted residuals. Indeed, robust regression automatically makes such adjustments to the weights (Huber, 1981). However, it is important to evaluate whether the final statistics believably represent the error. If manual adjustment or robust regression methods result in variances, standard deviations, or coefficients of variation that seem to represent an unrealistic level of error, evaluate the magnitude of the associated unweighted residual for indications of important model error or observation bias. Clearly, resolving these two problems is more likely to yield an accurate model than hiding the problem by reducing the weight (increasing the value of the statistic).

The example above and comments in Chapter 6, Section 6.3.2 suggest that the relatively simple idea of making the weights equal to one over the variance of the error or making the weight matrix equal to the inverse of the error variance–covariance matrix has proved to be very useful. It respects the statistical theory, provides a framework for identifying model error and/or measurement bias, and contributes to using the standard error of regression as a measure of model error. That is quite an accomplishment for a simple idea!

Weighting System Information on Parameter Values The discussion above focused on observations but is directly applicable to weighting prior information. Errors in system information often result from scale issues; see, for example, Beckie and Harvey (2002).

Weighting on prior information can be determined by, for example, constructing a 95-percent confidence interval on the basis of the likely range of parameter values, using independent field data or knowledge about hydrologic or geologic processes related to the quantities represented by the parameters. Two issues of special importance to prior information are the use of large weights and resulting "regularization," and the use of log-transformed parameters. While observations can be log-transformed, as mentioned in Chapter 3, Section 3.3.3, it is not very common. Thus, the effects of log-transformations on weighting are discussed here in the context of system information.

If the weighting realistically represents the uncertainty, the system information on parameter values included in the regression is called prior information and fits into the framework of either classical statistics or Bayesian statistics (the latter being the framework from which the term "prior information" originates). Sometimes, however, larger weights (smaller statistics) are assigned to the system information to achieve a stable regression, in which case the term "regularization" needs to be used instead of prior information (Backus, 1988). Setting parameter values to constants that are not changed by the regression can be thought of as an extreme case of regularization. When regularization is used, confidence intervals on parameters and predictions tend to underestimate actual uncertainty, as demonstrated in Table 11.4. Thus, it is very important in practice to appropriately classify prior information and regularization.

Prior information and regularization can be imposed on individual parameter values, or on characteristics of a parameter distribution, such as smoothness, as discussed in Chapter 1, Section 1.3.2 and Section G5.1. Extreme examples of the latter are (1) requiring that the model input value be constant over a region, a volume, or a specific type of material wherever it exists, or (2) requiring a specific interpolation scheme.

The capability of defining many parameters is implemented in PEST as its regularization capability. An example is presented by Doherty (2003). PEST is programmed to allow the user to specify the desired fit to observations and then adjust the weighting to achieve that fit. As suggested by Doherty (2003), users need to take care that the model fit specified is not less than expected observation errors. In addition, the resulting weighting of the observations and regularization need to be checked to determine if the weights are supportable based on hydrogeologic data. If not, it is important to modify the weighting before proceeding with uncertainty analysis.

The second issue unique to prior information occurs when the associated parameter is log-transformed. In this situation, the statistic used to weight the prior information generally needs to relate to the log of the parameter value. The methods discussed above for quantifying errors are directly applicable, but an extra step often is needed because usually it is easier to establish a range of plausible values for native than for transformed values. Thus, if the prior estimate for a hydraulic conductivity is 1×10^{-5} m/s, and the true value is expected to fall between 1×10^{-6} and 1×10^{-4} m/s with a certainty of about 95 percent, a 95-percent confidence interval for the native value has approximate limits of 1×10^{-6} to 1×10^{-4} m/s. Taking the log (base 10) of these values produces limits of -6 and -4 about a prior estimate of -5. If it is assumed that the uncertainty in the hydraulic conductivity can be approximated by a log-normal distribution, the log-transformed value is normally distributed. The methods described above can be used to determine that the standard deviation relevant to the log-transformed parameter equals 0.51. This value would be specified as the statistic used to calculate the weight for the prior estimate.

GUIDELINE 7: ENCOURAGE CONVERGENCE BY MAKING THE MODEL MORE ACCURATE AND EVALUATING THE OBSERVATIONS

Nonlinear regression models of complex systems often do not converge despite using the ideas suggested in Guideline 3 to maintain a well-posed problem. The major reasons for convergence problems are insensitive parameters, nonlinearity of the forward model with respect to estimated parameters, and inconsistencies between the processes important to the observations and simulated processes caused by poor representation of the system by the model and/or misinterpretation of data. These causes are listed in Table 11.5. Parameter correlation is

TABLE 11.5 Possible Actions to Encourage Convergence and Obtain an Accurate Model

General Comments

Identify the parameters associated with the largest values of *max-calculated-change*. This information is provided by the computer codes used in this book, as shown in Figure 5.5, and possible actions are as follows.

The Three Main Problems that Plague Convergence and Possible Solutions [a]

Insensitivity

If *css* for any parameter is less than 1 percent of the largest *css*, consider ideas presented in Guideline 3. These include:

(a) Specify the parameter values with small *css*.[b]
(b) Check problematic parameters. Consider combining existing parameters or redesigning the parameterization. Consider the suggestions in Guideline 2 about creative use of system information.

Nonlinearity

Evaluate simulated results for parameter values from intermediate parameter-estimation iterations. Look for evidence of nonlinearity. Consider weighted residuals that are largest in absolute value, observations omitted because simulated equivalents could not be obtained, and whether parameter values are realistic. If forward model nonlinearities are problematic, consider using a linear approximation, as suggested in Guideline 1.

Inconsistencies

Check the representation of the parameters. Check dominant observations identified using *dss*, DFBETAS, and leverage statistics.
Evaluate observations, prior information, and their simulated equivalents.

(*Continued*)

TABLE 11.5 *Continued*

All

Consider reducing the amount by which parameters are allowed to change within one parameter-estimation iteration—called *max-allowed-change* in Chapter 5, Section 5.1.3 before Eq. (5.7). Alternatively, consider using the trust-region approach available in UCODE_2005 or other methods.

Diagnosing Problems that Plague Convergence

Regression Performance	Problem[c]
(1) In the first parameter-estimation iteration, values of sensitive parameters move far from their starting values.	Inconsistencies. If evaluation indicates no inconsistencies, move starting parameter values closer to those from the first iteration, after first checking model fit.
(2) *max-calculated-change* remains large in absolute value and is either consistently positive or consistently negative.	Insensitivity.
(3) *max-calculated-change* goes through a repeated sequence in which it is reduced in size over several iterations only to dramatically increase.	Nonlinearity and/or insensitivity.
(4) *max-calculated-change* oscillates between large positive and negative values (as in Figure 5.5).	Insensitivity of one or more parameters.

[a]The solution of obtaining more data on insensitive parameters is not listed. Potential data acquisition efforts often are most advantageously considered in the context of predictions, as discussed in Guidelines 11 and 12 in Chapter 13.

[b]If parameter values are specified to alleviate convergence problems, calculate their *css* and *pcc* in later regression runs. If possible, estimate the parameters using regression. Generally, specified parameters need to be included to assess uncertainty. See Chapters 7 and 8.

[c]The problems are listed with the performance to which they are most likely to apply. However, consider all problems and actions listed to address convergence problems.

Note: *css*, composite scaled sensitivity; *dss*, dimensionless scaled sensitivity; *pcc*, parameter correlation coefficient.

not likely to result in lack of convergence of a single regression, as shown in Exercise 5.1b and discussed in Guideline 3. Similar results are expected for local minima.

Convergence is usually improved as the model becomes a better representation of the system that produced the observations being matched by the regression. This means that, generally, the goal of achieving convergence with a valid regression and the goal of achieving a model that accurately represents major processes are identical.

Information available from regressions that fail to converge provide substantial insight. This insight can be obtained by careful consideration of dimensionless, one-percent, and composite scaled sensitivities; parameter correlation coefficients;

weighted and unweighted residuals; parameter values; parameter updates calculated by the regression; and other information from the regression. These items can be used to detect inaccuracies in model construction. Review of Tables 10.1 and 10.2 and the questions of Table 10.3 may help to suggest useful approaches.

In addition, evaluation of regression performance can be useful, as suggested in Exercise 5.2b. The *max-calculated-change* defined after Eq. (5.7) is the largest calculated fractional change, in absolute value, for any parameter in one parameter-estimation iteration and is reported for each iteration. Generally, *max-calculated-change* must be less than a user-defined criterion for the regression to converge (see Chapter 5, Section 5.1.3). When it does not diminish sufficiently, the regression is said to not converge. Possibilities include, but are not limited to: *max-calculated-change* remains large in absolute value and is either consistently positive or consistently negative; *max-calculated-change* goes through a repeated sequence in which it is reduced in size over several iterations only to dramatically increase; *max-calculated-change* oscillates between large positive and negative values (as in Figure 5.5).

These possibilities are listed in Table 11.5. They are related to the three likely causes of nonconvergence mentioned above in this guideline and in the first part of Table 11.5. Suggested causes and solutions are listed. There is no suggestion to change observation weighting, which is tempting but rarely helpful in this circumstance and can be very time-consuming. Also, when the regression performs in the four ways listed in the second part of Table 11.5, increasing the number of parameter-estimation iterations is rarely helpful for achieving convergence.

GUIDELINE 8: CONSIDER ALTERNATIVE MODELS

There is always more than one possible representation of natural systems, because there are different possible interpretations of the incomplete data about the systems. Guideline 8 encourages considering as many alternative models as possible and offers strategies for designing, organizing, and comparing them.

Formal parameter-estimation methods that produce optimal parameter values are essential to use when considering alternative models if results are to be at all definitive. If parameter values are determined using a clear process such as optimization, model fit and other model attributes can be compared without speculation about whether conclusions would be different if only this parameter value was a bit higher or that one a bit lower.

Commonly, to begin the modeling process, one model is constructed using Guidelines 1 through 7. During development of this model, model fit and parameter values are evaluated at various stages using Guidelines 9 and 10 in Chapter 12. In addition, predicted quantities are evaluated, and their relationships to model calibration issues are considered, as discussed in Guideline 13 in Chapter 14. This process is an example of how the guidelines are not always used sequentially. Guideline 8 is positioned to emphasize that alternative models are fundamental to the study of any natural system.

G8.1 Develop Alternative Models

Alternative model evaluation often indicates that many plausible models exist. Considered another way, the data are insufficient to further limit the possible alternatives. Development of alternative models can be motivated by many different circumstances, including different equally plausible interpretations of incomplete system information (Guideline 2) and difficulties with initial models of the system, such as problems with model fit or optimal parameter values (Guidelines 9 and 10 in Chapter 12).

Alternative models typically differ in their representation of the characteristics and properties of the simulated system and/or in their simulated processes. Commonly, they have the same set of observations, and this is required by some methods of analysis.

The mechanisms for developing alternative models fall into three categories: deterministic, stochastic, or a combination of these two. These approaches are discussed below.

Deterministic methods of developing alternative models generally use different conceptual models. For example, in groundwater systems it is common that different interpretations of geologic processes yield different hydrogeologic framework models. Different choices of included processes are also usually determined from a deterministic decision process: for example, including the effects of temperature or subsidence on groundwater flow. Deterministic development of alternative conceptual models often is facilitated for complex three-dimensional problems by using the data organization, visualization, and analysis tools discussed in Chapter 15 for the Death Valley regional groundwater flow system.

Stochastic methods for developing alternative models usually identify one aspect of the system that is expected to dominate simulated results of interest (e.g., predictions) and randomly generate model input realizations. Each realization is then used in the model to produce simulated results. The model input may be a single number; or it may be many numbers that define a spatial and/or temporal field of—using groundwater model examples—hydraulic conductivity and areal recharge. The model input might also be numbers that define the spatial distribution of a system property, but not the actual values. For example, Poeter and McKenna (1995) present an innovative method in which alternative models are developed using indicator kriging to generate different zonation arrays that are used in the model to define the hydraulic-conductivity distribution. Hydraulic-conductivity values for each zonation are then estimated by regression. This example is discussed in Guideline 14 in Chapter 14. The transition-probability method of Carle et al. (1998) and the indicator simulation method of Gomez-Hernandez (2006) also are designed to generate many realizations of a three-dimensional field.

For field systems, methods of developing alternative models that depend on both deterministic and stochastic contributions are likely to be very useful. This includes generating stochastic distributions within a deterministic structure. For example, in a groundwater model the alternative structures may be different interpretations of large-scale hydrogeologic units; stochastic methods might be used to generate alternative models of the interior variability of selected units and/or selected parts of the system.

G8.2 Discriminate Between Models

Models that are more likely to be accurate tend to have three attributes: lower values of overall fit statistics (Chapter 6 and Guideline 9); weighted residuals that are more randomly distributed (Chapter 6 and Guideline 9); and more realistic optimal parameter values (Chapter 7 and Guideline 10).

Often these criteria are used to identify a single most likely model and all subsequent simulations of predictions and other analyses are pursued with this one model. However, for most natural systems, one model generally is insufficient to represent the variety of defensible ideas about how the system works, and many alternative models should be evaluated. In this context, these criteria are used to identify strengths and weaknesses of the developed models.

The first attribute of more accurate models is a better match to observed data, as indicated by smaller values of the calculated error variance (Eq. (6.1)), the standard error of the regression (the square root of Eq. (6.1)), fitted error statistics (Chapter 6, Section 6.3.2), AIC_c and BIC statistics (Eqs. (6.3) and (6.4)), or the maximum likelihood criteria (Eq. (3.3)). These measures are printed by UCODE_2005 and MODFLOW-2000. The UCODE_2005 and MMA (Multi-Model Analysis; Poeter and Hill, in press) computer codes report additional statistics, such as Kashyap's measure (Medina and Carrera, 1996).

Figure 11.6 shows a graph of AIC_c and BIC statistics and the sum of squared, weighted residuals for five models of the Maggia Valley in southern Switzerland. The models differed in that the hydraulic-conductivity distribution was represented with between one and six parameters defined using geologic mapping of fluvial deposits. As is typical, the sum of squared, weighted residuals diminishes or is unchanged as parameters are added. The AIC_c and BIC statistics are smallest for the model with three hydraulic-conductivity parameters, which suggests that, of the models considered, this one is preferable.

The second attribute of better models is that weighted residuals (defined in Chapter 3, Section 3.4.3) are more randomly distributed. This attribute generally is determined using the graphs and related statistics discussed in Chapter 6, Section 6.4 and Guideline 9 in Chapter 12. Graphs of weighted residuals against weighted simulated values are shown for two models of the same system in Figure 11.7. The weighted simulated values have been adjusted because the coefficients of variation for the weighting are calculated using the observed values, as discussed in Chapter 6, Section 6.4.2. The weighted residuals from model CAL0 tend to be larger than those of CAL3, as indicated by the greater spread about the 0.0 weighted-residual line. In this example, the weighting on the streamflow gains and lake loss was modified within reasonable limits during the course of model development to achieve statistically consistent weighted residuals (Hill et al., 1998, Table 1). A consequence is that the spread of weighted residuals for flows in model CAL3 does not necessarily indicate a closer fit between simulated and observed flows, compared to model CAL0. However, the smaller spread for hydraulic heads in model CAL3

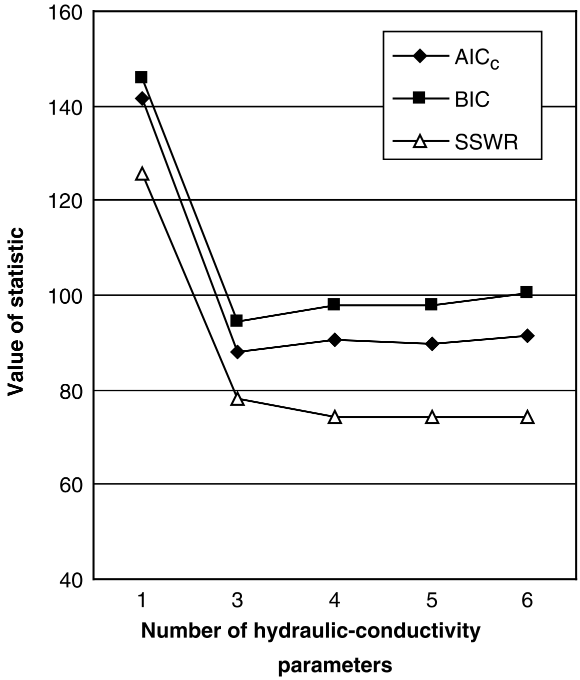


FIGURE 11.6 AIC_c and BIC statistics and the sum of squared, weighted residuals (SSWR), defined in Chapter 3, calculated for five models of the Maggia Valley in southern Switzerland. (From data presented by Foglia et al., in press).

does indicate a better fit, as also is evident in Figure 11.7. The two sets of weighted residuals of Figure 11.7 are both reasonably random, although the dominance of positive CAL0 residuals in Figure 11.7*a* for weighted simulated values between 15 and 30 may indicate some model bias.

In analyzing the distribution of weighted residuals when comparing alternative models, it also is important to consider additional types of figures that display the observations, simulated values, residuals, and weighted residuals, as discussed in Chapter 6, Section 6.4 and Guideline 9 in Chapter 12.

The third attribute of better models is that optimal parameter values tend to be more reasonable. Evaluating the optimal estimates and confidence intervals is discussed in Chapter 7, in Guideline 10 in Chapter 12, and in Guideline 14 in Chapter 14.

For the complex synthetic system considered by Hill et al. (1998), analyses of the optimal parameter estimates resulted in elimination of model CAL0 as a viable model. In the calibrated CAL0 model, one hydraulic-conductivity estimate was unreasonable, and the confidence interval on the parameter excluded all reasonable values. Analyses of optimal parameter estimates showed that all of the other alternative models were viable, and that none could be considered clearly better than the others on the basis of analyzing these estimates.

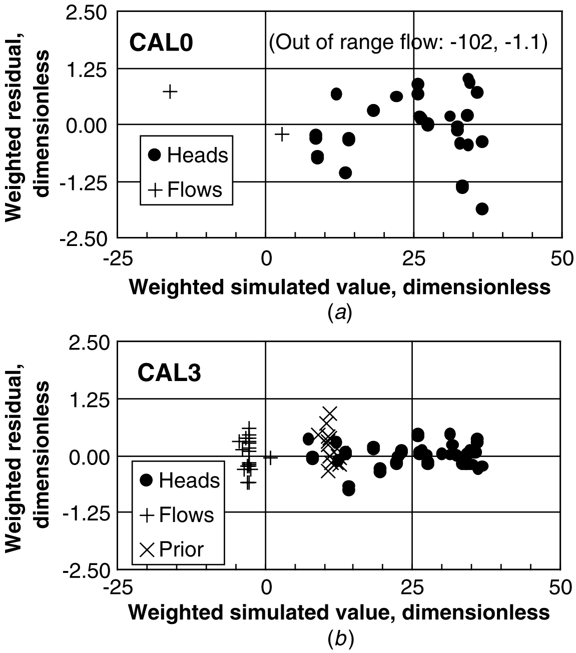


FIGURE 11.7 Weighted residuals versus weighted simulated values for models (*a*) CAL0 (with 34 heads and 3 flows) and (*b*) CAL3 (with 54 heads, 19 flows, and 16 prior) of Hill et al. (1998).

G8.3 Simulate Predictions with Alternative Models

There is general agreement that predictions need to be evaluated using alternative models, but there is disagreement about what alternative models should be included. Some suggest that all models developed should be included in any analysis of predictions (e.g., Burnham and Anderson, 2004; Poeter and Anderson, 2004), while others suggest a more selective approach. The argument for including all models is that those that do not fit the observations well, as indicated by large values of one or more of the measures of overall fit listed in Section G8.2, are given little credence in the analysis, and leaving them in allows all underlying conceptual models to be represented. The argument for a more selective approach is that results from clearly unreasonable models can be confusing to resource managers and the public.

The presentation of predictions from alternative models is important because usually this communicates the most important result of a typically substantial investment by a government, commercial, or nonprofit entity. Ideally, the presentation reveals the predictions, measures of prediction uncertainty, and possibly a separate indicator of model plausibility.

Measures of prediction uncertainty can be calculated using the methods described in Chapter 8, Sections 8.4 and 8.5. Quantifying prediction uncertainty using alternative models is discussed in Chapter 8, Section 8.6 and Guideline 14 in Chapter 14.

G8.4 Application

Here we discuss three alternative models presented by Tiedeman et al. (1997, 1998a). The models represent a regional groundwater flow system in fractured crystalline rock near Mirror Lake, New Hampshire. In each of the models, two model layers represent surficial glacial deposits, and three layers represent fractured crystalline bedrock. The three alternative models differ in their representation of the bedrock hydraulic conductivity, as shown in Figure 11.8. In model A, the bedrock hydraulic conductivity is homogeneous; in model B, it varies with depth; and in model D, it varies with land-surface elevation. Model C is not discussed here. The variations each have a hydrogeologic rationale. For example, consider weathering processes, where weathering of the fractured crystalline rock is expected to

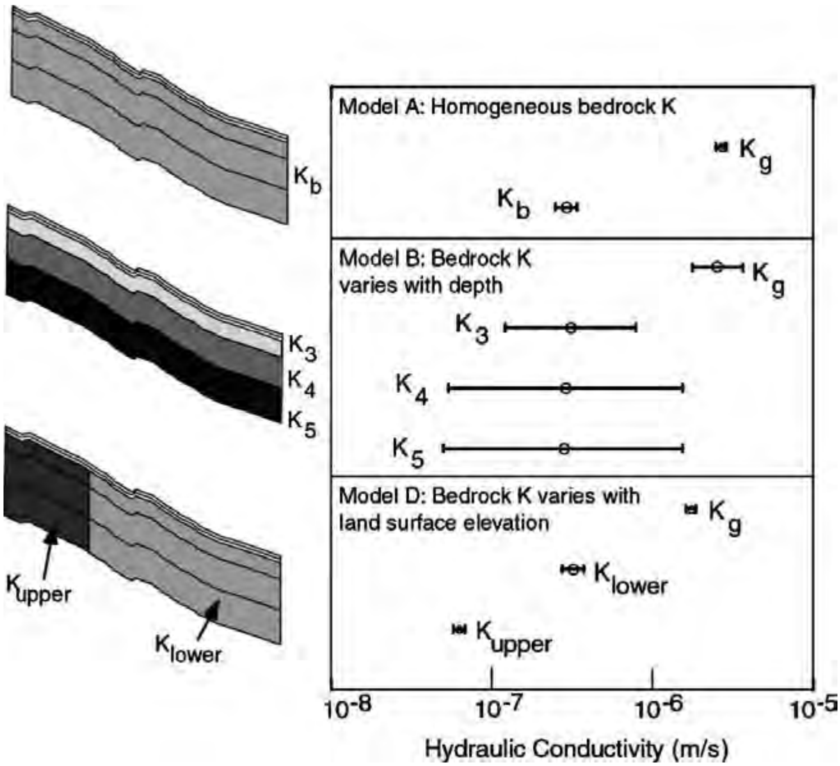


FIGURE 11.8 Representations of bedrock hydraulic conductivity along a hillside cross section (vertical exaggeration approximately 5:1), parameter estimates, and linear individual 95-percent confidence intervals for alternative models A, B, and D of a regional groundwater flow system in fractured crystalline rock near Mirror Lake, New Hampshire. K_g is the hydraulic conductivity of surficial glacial deposits; other K parameters are hydraulic conductivities of the bedrock, as shown on the left for each alternative model. (Adapted from Tiedeman et al., 1997, 1998a.)

increase hydraulic conductivity. Homogeneity (model A) suggests little weathering; model B suggests weathering concentrated at the surface and evenly distributed throughout the area, and model D suggests weathering concentrated in the lower elevations.

Each model was calibrated by nonlinear regression using three flow observations. The number of hydraulic-head observations was 90 for models A and B and 91 for model D. The additional head observation lies in the upper elevations of the system and displays a fairly shallow water level. Only one such observation is available, and it is not known if the water level detected at this well represents the regional water table. As a result, all models were tested with and without this observation; it is only included in the results shown here for model D. Models A and B, which lack any change in hydraulic conductivity with elevation, cannot simultaneously match this observation and head observations at lower elevations. The importance of this depends on the validity of the high-elevation head observation, which is unclear. The optimal hydraulic-conductivity estimates and linear confidence intervals produced by the three models are shown in Figure 11.8.

In model B, the parameter estimates for the hydraulic conductivity of each bedrock model layer (K_3, K_4, and K_5) are nearly the same as the estimate of homogeneous bedrock hydraulic conductivity (K_b) in model A. The confidence intervals for K_3, K_4, and K_5 are each significantly larger than that for K_b. These results suggest that the observations do not support the hypothesis that hydraulic conductivity varies with depth. The model fit to the observations is almost identical in models A and B (the standard error of regression, s, equals 3.0 in both models), which also supports the conclusion that model B is not an improved representation of the flow system compared to model A. Further discussion considers only models A and D.

In model D, the estimate of K_{lower} is about the same as that of K_b in model A, but the estimate of K_{upper} is substantially smaller, and the confidence intervals for K_{lower} and K_{upper} are relatively small and do not overlap, suggesting that the calibration observations support the hypothesis that conductivity varies with elevation. However, the standard error of regression for model D of 3.4 is somewhat larger than that for model A, primarily because model D produces a poorer match to the three flow observations.

Models A and D appear to represent conceptual models that are reasonably well supported by the observations. Additional hydraulic-head data at the upper elevations are needed to better delineate the regional water table. If collected, these data could then help discriminate between the two models. Because models A and D are both plausible, predictions of the regional water budget and of the three-dimensional groundwater basin are simulated for both models (Tiedeman et al., 1997, 1998a).

12

GUIDELINES 9 AND 10—MODEL TESTING

A basic attribute of nonlinear regression methods is that, given a well-posed problem, parameter values are calculated that produce the best fit between simulated and observed values. The model can then be evaluated without speculation about whether a different set of parameter values would produce a better model fit.

A primary purpose of evaluating model fit is to detect ways in which the model incorrectly represents the real system. This incorrect representation is commonly referred to as model error. Model error that causes systematic problems with model fit is denoted model bias. Two common problems are strong indicators of model error: (1) the model does a poor job of matching observations in that the lack of fit is large and/or the weighted residuals are not randomly distributed in time, in space, and/or relative to simulated values and (2) the optimized parameter values are unrealistic and confidence intervals on the optimized values do not include reasonable values. The fundamental premise is displayed in Figure 12.1. Model fit issues are discussed in Guideline 9; estimated parameter-value issues are discussed in Guideline 10.

Effective Groundwater Model Calibration: With Analysis of Data, Sensitivities, Predictions, and Uncertainty. By Mary C. Hill and Claire R. Tiedeman
Published 2007 by John Wiley & Sons, Inc.

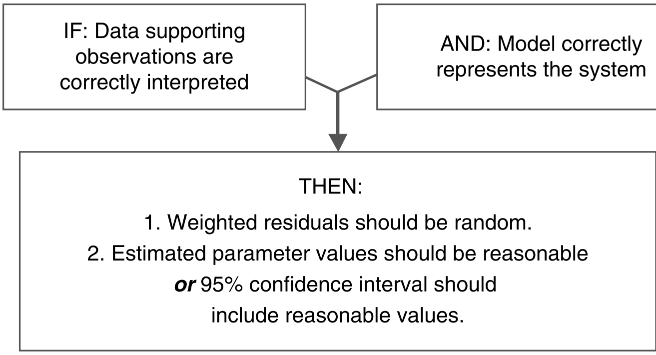


FIGURE 12.1 Premise underlying much of the analysis of model fit and estimated parameter values suggested in Guidelines 9 and 10. If 1 and/or 2 are not true, a better model can be obtained by reevaluating the observations and the model.

GUIDELINE 9: EVALUATE MODEL FIT

The match to observations can be evaluated using the methods described in Chapter 6. The evaluation generally involves the following: (1) determine model fit, including both overall fit and variation in fit among individual observations and (2) diagnose the cause of poor model fit. Evaluations of model fit have been presented in many publications, including Cooley et al. (1986), Yager (1993, 1996), D'Agnese et al. (1997), Tiedeman et al. (1998a,b), Hill et al. (1998), and other studies cited in Chapter 15.

G9.1 Determine Model Fit

Overall measures of model fit were discussed in Chapter 6, Section 6.3; graphical measures are discussed in Section 6.4. Here, we present additional example analyses of model fit.

Weighted residuals have the advantage of indicating model fit in the context of expected observation error (Guideline 6). Model misfit is often more useful when presented in this context. This is especially true if observation errors are proportional to the observed or simulated value and this value varies over many orders of magnitude. In such situations, unweighted residuals can be very misleading. Examples include flow observations in surface-water models and concentration observations in any type of transport model. On the other hand, weighted residuals can be confusing because they are dimensionless. Often it is useful to include maps and other figures of both weighted and unweighted residuals in reports. The discussion of these figures can then indicate whether any large unweighted residuals are actually less problematic than their magnitudes suggest, because of observation error. Figures constructed using unweighted and weighted residuals from a model of the Death Valley regional flow system are presented in Chapter 15.

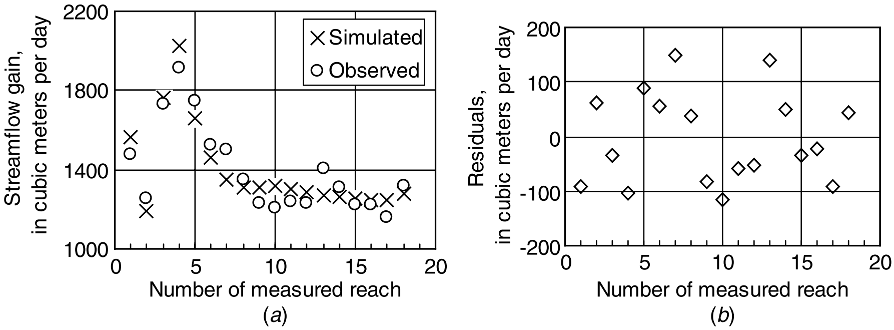


FIGURE 12.2 (*a*) Observed and simulated streamflow gains for model CAL3 of Hill et al. (1998). (*b*) Streamflow gain residuals, equal to the observed minus the simulated values.

Two graphs that illustrate model fit are presented in Figure 12.2. Figure 12.2*a* shows observed and simulated streamflow gains along the length of a river. Figure 12.2*b* shows the related residuals, which are a good indication of model fit if the observed gains are all similarly reliable. Although the two figures present identical information about model fit, each display is useful in a unique way. Figure 12.2*a* places the model fit in the context of the observed quantity. Figure 12.2*b* more clearly displays the variation of misfit with the number of the measured reach.

Figure 12.3 shows an example of weighted residuals displayed on a map of a groundwater model domain. This type of figure is effective for assessing the details of model fit and the spatial randomness of the weighted residuals. Figure 12.3 shows that the weighted residuals are generally small and appear to be randomly distributed in the southern part of the domain. However, in the northern part, weighted residuals are larger and clusters of residuals with similar signs are present, illustrating some bias in the model fit. In this model, the subsurface hydrogeology in the north was not as well characterized as that in the central and southern part of the region, which helped explain this bias (Sanford et al., 2004a).

Identifying trends (lack of randomness) by visual inspection is not always reliable and is made more difficult by the small sample size typical of many regression problems. Often it is useful to evaluate randomness using formal methods to avoid false identification of trends and to identify trends that are difficult to detect. One such method is the runs test, as discussed in Chapter 6, Section 6.4.4. The runs test statistics are calculated using Eq. (6.16) and (6.17).

MODFLOW-2000 and UCODE_2005 each calculate a runs statistic that evaluates the randomness of the weighted residuals with respect to the order in which the observations are listed in the model input files. This statistic can be used to quickly and roughly assess whether the spatial randomness of the weighted residuals is improving as changes are made in the model during the calibration process, which can be advantageous when it is time-consuming to produce maps of weighted residuals such as those shown in Figure 12.3. For example, if water-level observations are listed in the model input file in order from north to south, and initially

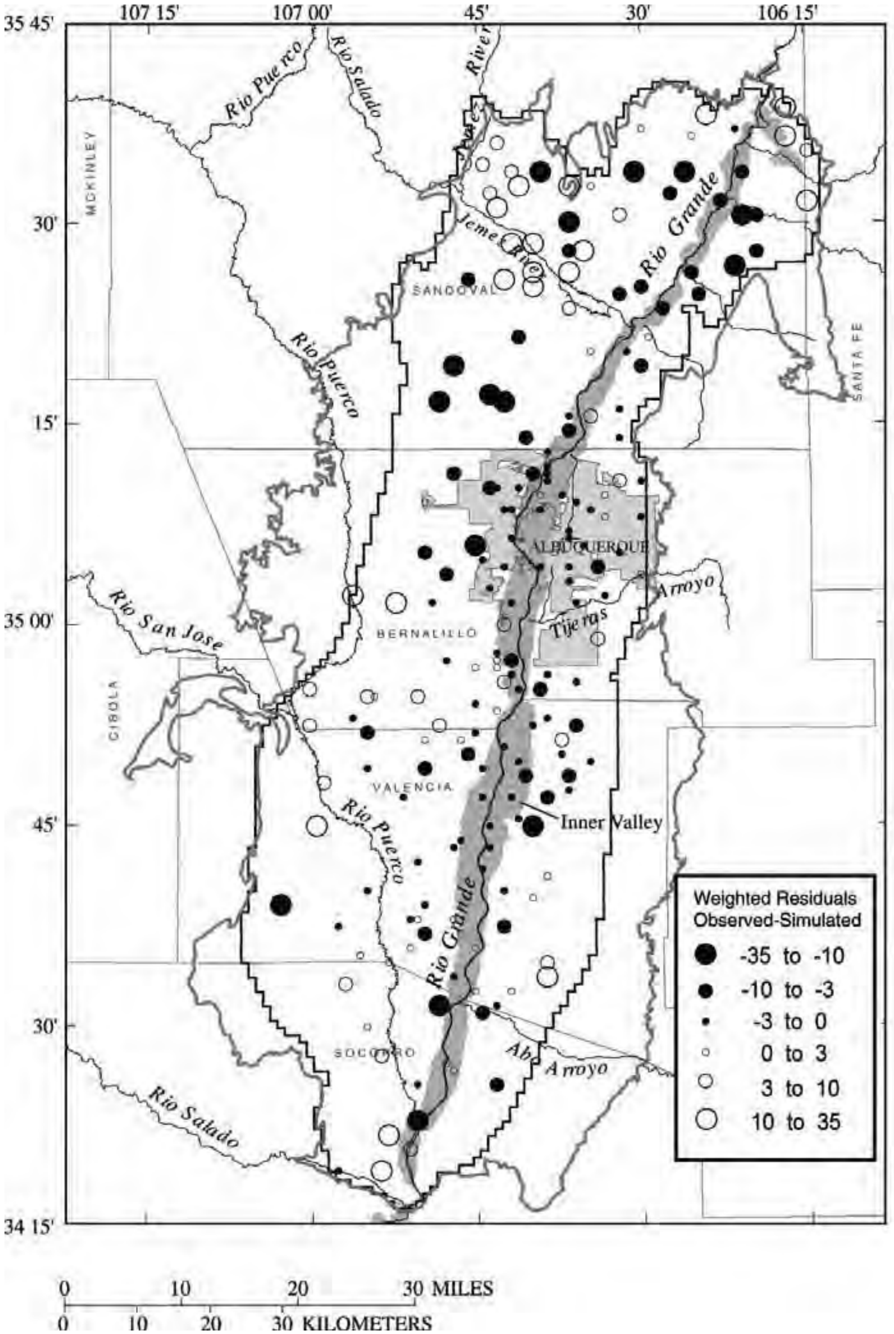


FIGURE 12.3 Distribution of weighted hydraulic-head residuals in a model of steady-state predevelopment groundwater flow in the Middle Rio Grande Basin, New Mexico. (From Sanford et al., 2004a.)

the model fit is such that simulated water levels are consistently too large in the north and too small in the south, then the runs statistic will indicate too few runs (a large negative value). As the model is refined and additional regression runs are made, the runs statistic can be evaluated rather than producing a new map after every regression run in which some model aspect has been modified. A runs statistic that becomes smaller in absolute value (closer to 0.0) indicates that the weighted residuals are becoming more randomly distributed.

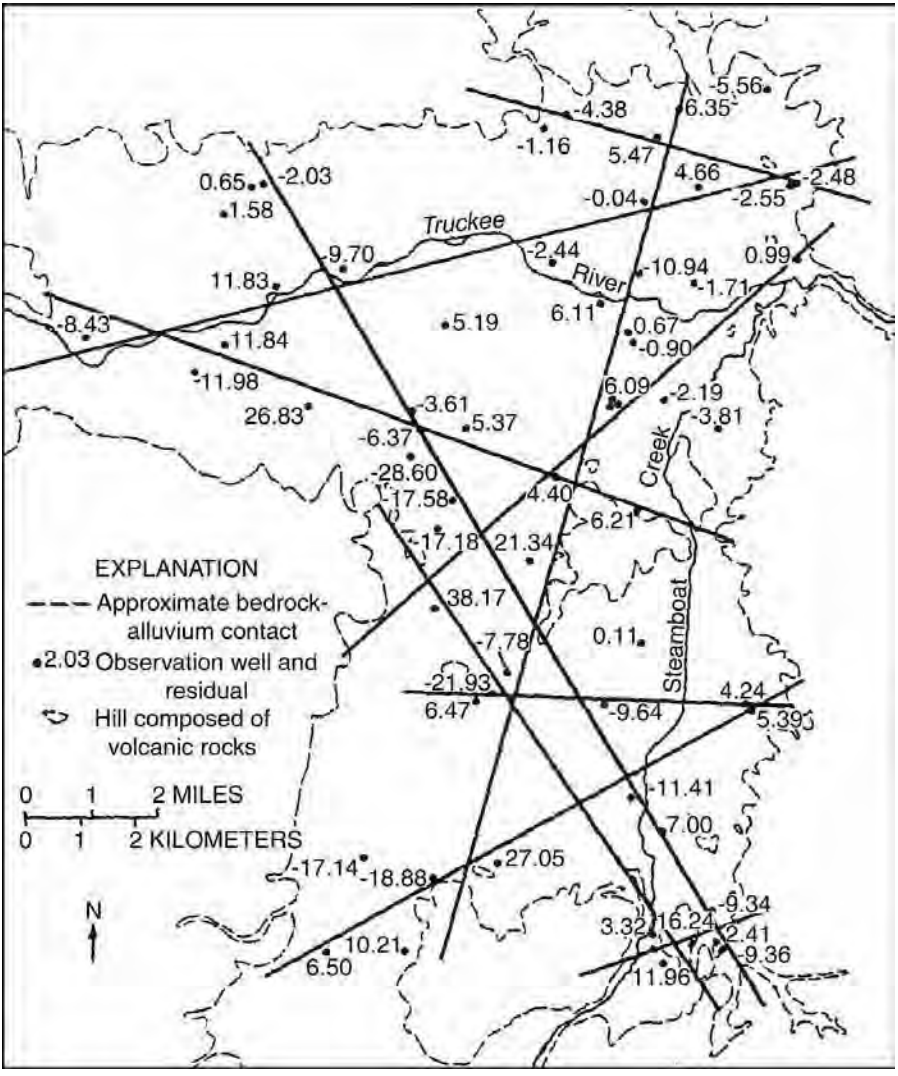


FIGURE 12.4 Hydraulic-head residuals from a model of the Truckee River Basin, Nevada, with lines used to conduct runs tests. The lines are located in the center of swaths for which the runs statistic is calculated. (From Cooley, 1979.)

The runs statistic also can be used to assess the spatial randomness of weighted residuals plotted on the model domain as illustrated in Figure 12.4. In this study, Cooley (1979) used runs tests to evaluate randomness for residuals distributed within a specified distance of selected transects. The results indicated that all the runs along each transect could have occurred by chance. MODFLOW-2000 and UCODE_2005 do not calculate runs statistics to evaluate the residuals in this manner, so this type of analysis requires the modeler to use a custom spreadsheet or code.

The fit of a calibrated model also can be tested using simulated equivalents for observations that either were not included in the model calibration process or are collected after model calibration. Such testing commonly is referred to as validation or a postaudit and is discussed in Guideline 13 in Chapter 14.

G9.2 Examine Fit for Existing Observations Important to the Purpose of the Model

It is important to closely examine the model fit for observations important to the purpose of the model. If the purpose is related to some aspect of model construction, the statistics listed in Table 10.2 that connect observations and parameters can be used to identify these observations. If the purpose is to predict unmeasured quantities, the *opr* statistic that connects observations and predictions can be used. The *opr* statistic is presented in Guideline 12 in Chapter 13 in the context of guiding additional field work. An example of using this statistic is presented in Chapter 15, Section 15.2.1.

G9.3 Diagnose the Cause of Poor Model Fit

Detailed evaluations of weighted residuals, such as those shown in Figures 12.2–12.4, can be used to diagnose the cause of poor model fit. Obvious locations of potential problems include areas in which the model fit is poor and/or biased. However, in models of natural systems, simulated conditions are generally sensitive to both local and distant aspects of model construction. Thus, discovering the cause of problems with model fit often requires considering problems located not only where the misfit occurs, but in a potentially large surrounding volume and, for transient models, at earlier simulated times. For example, discharge to springs in regional groundwater models can be influenced by hydrogeologic and hydrologic conditions at great distances upgradient and downgradient from the spring location. Water needs to supply the spring and some system characteristic or dynamic needs to make the water flow to the spring instead of to downstream locations. Similarly, recharge in high-elevation regions of a model can affect hydraulic heads and discharge at distances far downgradient.

In some cases, aspects of model construction make it impossible for the regression to match a given observation. Dimensionless scaled sensitivities (*dss*) (Chapter 4, Section 4.3.3) and leverage and influence statistics (Chapter 7, Section 7.3) can help reveal this problem. If the values of these statistics for an observation are near zero for all parameters, then the simulated equivalent is insensitive to changes in all parameters. This suggests that model construction precludes a good fit to the observation and can reveal problems with model construction. In groundwater modeling, an extreme example occurs when an observed head is located in a cell defined as constant head, and the value of the constant head is not being estimated by the regression. For a less extreme example of this problem, consider a geologic feature with very low hydraulic conductivity that has been interpreted as discontinuous, based on geologic data. However, differences in hydraulic head across the feature indicate that it is continuous and forms a substantial barrier to groundwater flow. If the model construction is not changed, the model fit to these head observations will be poor.

In many types of models, it can be difficult to address problems with model construction because of the inaccessibility of the true system and/or the expense of data collection. These limitations to investigating the true system may preclude modifying the model to alleviate all problems with poor model fit. In this case, the modeler needs to carefully evaluate the implications for the model predictions of the poor model fit.

An additional potential type of model error involves omission of processes that are important to simulating the observed values, or including processes that actually do not occur in the true system. This type of error can strongly affect the quality of the model fit to the observed values. Thus, when diagnosing the cause of poor fit, it is important to assess whether the model includes the relevant and important processes thought to occur in the true system. Determining the appropriate processes is especially important in transport models, where there are typically a large number of potential transport mechanisms that affect simulated concentrations, as discussed in Chapter 9, Section 9.2.

If the model fit is unsatisfactory, five aspects of the model or calibration effort can be investigated and possibly changed as described below. The magnitude of the changes can range from correcting data entry errors, to adding simulated processes, to completely reevaluating some or all facets of the conceptual model.

Parameter Definition Parameter definition can be modified, for example, by adding, omitting, dividing, or combining parameters. As always, the final parameterization needs to be consistent with all known information about the system; for example, in groundwater problems, hydrogeologic information needs to be respected. See the methods described in Chapters 4 and 7 and Guidelines 2 and 3 in Chapter 11.

Simulated Equivalents of the Observations Problems with the calculation of simulated equivalents to observations may become apparent as model calibration proceeds.

For example, consider a groundwater system with an observation from a well in which the screen spans several layers of the corresponding groundwater model. The simulated equivalent of the observed head is typically calculated as a weighted average of the simulated hydraulic heads in the model layers spanned by the screen. It is not always straightforward to define the contribution from each layer and the appropriate contribution may change as the model changes during calibration. If there is a poor fit to this type of observation, definition of the simulated equivalent may need to be modified. Alternatively, the methods included in, for example, the Multi-Node Well (MNW) Package (Halford and Hanson, 2002) of MODFLOW could be adapted to calculate the contributions from each model layer.

Problems with calculation of simulated equivalent also can occur when the defined elevations for head-dependent boundaries of a discretized model are determined from digital elevation maps (DEMs). Within the area of the model-grid cell the appropriate value might be the average elevation, the lowest elevation, or, depending on the resolution of the DEM, an elevation that is even somewhat lower than the lowest elevation. The latter circumstance can occur when there are narrowly incised rivers or springs ensuing from small depressions. Problems are generally indicated by too little simulated flow to the head-dependent boundaries, unexpected flow from the boundaries to the groundwater system, or too much flow from the boundaries into the groundwater system. Inspection of areal photographs and/or field work at selected representative sites often is needed to determine appropriate elevations to use in the model.

Other Aspects of Model Construction Model construction can be modified, for example, by correcting input data, changing the representation of boundary conditions and parameterization, and changing the processes simulated. In groundwater models, a surface-water body represented by a constant-head boundary might be changed to a head-dependent boundary, the pumping rates at wells might be updated based on new information, or temperature variations might be included explicitly or implicitly. Most of these changes are no different from modifications a modeler would consider as part of any model calibration effort.

Observations Affected by Processes that Are Not Simulated It is sometimes necessary to remove observations from the regression; however, this should be done only after careful consideration. For example, in groundwater systems, wells that intersect perched water do not directly reflect the dynamics of a regional flow system. Including measurements from such wells as observations in the calibration of a regional model is likely to produce fallacious results, and thus, these observations will typically be omitted from the regression.

Perched wells are one example of observations affected by systematic errors caused by omission from the model of a process important to the observation. Unlike random measurement error, systematic error cannot easily be accommodated by weighting and can be impossible to separate from the effects of simulated processes. An example is given by Pavelko (2004) for aquifer compaction and expansion data recorded by an extensometer in Las Vegas, Nevada. Extreme heating in the extensometer shed caused thermal effects on the extensometer, which were recorded as apparent diurnal fluctuations in aquifer deformation. When these data were employed as observations in regression runs used to calibrate a model of aquifer deformation, this resulted in poor model fit, unreasonable parameter estimates, and problems with regression convergence (M. Pavelko, U.S. Geological Survey, written communication, 2004). To correct this problem, the calibration observations were defined as aquifer deformation over time periods of 25 days or longer. This definition of the observations minimized the influence of the thermal effects.

Weighting Errors Errors in the weighting of the observations or prior information also are possible. However, use caution when considering changes to the weighting as an approach to resolving problems with model fit. It is easy to invest a great deal of time modifying weights and running regressions, with little consequent gain in model accuracy or in understanding the system dynamics. This does not mean that weighting never needs to be modified. Adherence to the principles described in Guideline 6 in Chapter 11 will help keep the effort spent determining and modifying the weight matrix consistent with its importance to the purpose of the model.

GUIDELINE 10: EVALUATE OPTIMIZED PARAMETER VALUES

Evaluating optimized parameter values involves five steps. (1) Quantify parameter-value uncertainty. (2) Detect model error by comparing the estimates and their linear and nonlinear confidence intervals to reasonable ranges determined from field data. (3) Diagnose the cause of unreasonable parameter values. (4) Identify observations important to the parameter estimates. (5) Determine whether fewer parameters are likely to produce as good a fit or if additional parameters can be supported by the available observations. These issues are discussed in the following five sections.

G10.1 Quantify Parameter-Value Uncertainty

Parameter-value uncertainty can be quantified using parameter confidence intervals, which are an integral part of the analyses discussed in Sections G10.2 to G10.5. Calculation of parameter confidence intervals is presented in Chapter 7.

The relative uncertainty of parameters can be important to the evaluations of Sections G10.4 and G10.5. Confidence intervals can be directly compared for parameters with the same units, such as in Figure 12.5. To compare the uncertainty of parameters with different units, such as hydraulic conductivity and recharge, confidence intervals can be expressed in terms of percent of estimated value, as shown in Figure 7.7, 7.8, and 9.19. Alternatively, parameter coefficients of variation (Eq. (7.4)) can be used.

G10.2 Use Parameter Estimates to Detect Model Error

The use of optimized parameter values to detect model bias was presented in Chapter 7, Section 7.6. This simple test can be an unexpectedly powerful indicator of model error, even given the wide ranges of reasonable values for many characteristics of natural systems. For example, in groundwater systems hydraulic

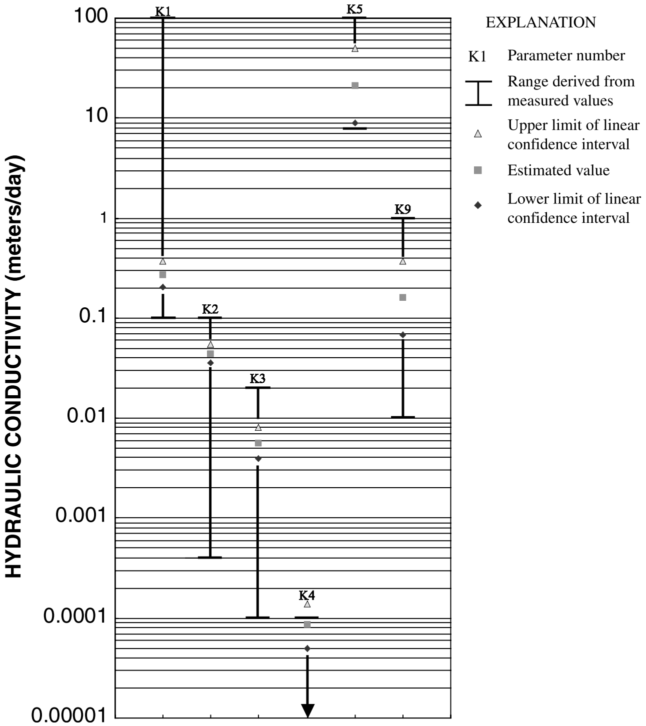


FIGURE 12.5 Optimized hydraulic-conductivity values, 95-percent linear confidence intervals, and the range of hydraulic-conductivity values derived from field and laboratory data. (From D'Agnese et al., 1997.)

conductivity can vary by many orders of magnitude in a single field site. Use of reasonable ranges to detect model error has been demonstrated using synthetic numerical test cases by Poeter and McKenna (1995), Anderman et al. (1996), Poeter and Hill (1996), Barlebo et al. (1998), and Hill et al. (1998). Field studies that have found this test to be useful include those by D'Agnese et al. (1997, 1999), Tiedeman et al. (1998b), McAda (1999), Faunt et al. (2004), and Gannett and Lite (2004). Relevant results from Barlebo et al. (1998) are presented in Chapter 15.

A graphical comparison of estimated hydraulic conductivities and ranges of expected values is presented in Figure 12.5 for the Death Valley regional flow system study of D'Agnese et al. (1997, 1999), which is discussed further in Chapter 15. Two features of Figure 12.5 deserve discussion: the large reasonable ranges and the small linear confidence intervals on the estimates.

The reasonable ranges in this example are large, but a number of conceptual models were rejected because optimized parameter values were outside these ranges. Thus, even in this circumstance with large ranges of expected values, requiring reasonable optimized parameter values produced an important constraint on model development.

Examination of the confidence intervals of Figure 12.5 could lead to the conclusion that the intervals are too small to realistically represent the uncertainty in the estimate. This judgment, however, needs to be made in the context of the meaning of the parameter estimates and confidence intervals. In this example, and in many situations, the defined parameters result from simplifying assumptions. The most relevant assumption in this example is that a few parameters and simple functions are used to represent the very complicated hydraulic-conductivity distribution that exists in the true flow system. In the Death Valley model, the simple functions are a zonation scheme in which the hydraulic conductivity is set to the same parameter value at all locations where rocks with certain characteristics occur. The simple functions also could involve using a few defined parameters to implement an interpolation scheme. Definition of a few parameter values to represent hydraulic conductivity throughout a model is very useful if broadly defined variations in hydraulic conductivity dominate system dynamics. The resulting estimated parameters represent effective or average values. The confidence intervals for these parameters represent the uncertainty in these effective or average values. In contrast, the reasonable ranges often represent the breadth of local values.

Confidence intervals on average (mean) values depend on the standard deviation of the original population, and on the sample size used to calculate the estimated average. Because the population statistics often are unknown, the sample standard deviation is commonly used. To demonstrate the importance of these dependencies, consider a simple example using a generated population of 300 normally distributed random numbers. Figure 12.6 shows the mean and range of the 300 numbers, as well as the mean and the confidence interval on the mean for different sample sizes drawn from the population. This simple example illustrates that even with very few samples, the confidence interval for the average is significantly smaller than the range of the population.

In Figure 12.5, the ranges of hydraulic conductivities are derived from measured field and laboratory values. Each of the six ranges is analogous to the population range in Figure 12.6. The six parameter estimates shown in Figure 12.5 for the Death Valley regional flow model are analogous to the three means of Figure 12.6, with one important difference. In Figure 12.5, the parameter estimates are derived through nonlinear regression. Thus, most of the data used to estimate the effective hydraulic-conductivity values are measurements of other quantities (hydraulic heads and spring flows). In contrast, the means of Figure 12.6 are calculated from samples taken from the population for which the range is plotted on the left side of the figure. Figure 12.6 reveals something important about Figure 12.5. That is, the wide ranges and much narrower confidence intervals such as those shown in Figure 12.5 are to be expected given that the confidence intervals are on the expected value.

Using independent information on the parameters to identify model error, as suggested here and in Chapter 7, Section 7.6, is an alternative to using the information on the parameters to define prior information or to impose limits on estimated parameter values, which are discussed in Chapter 5, Section 5.5 and in Guideline 5 in Chapter 11. As noted there, unreasonable optimized parameter

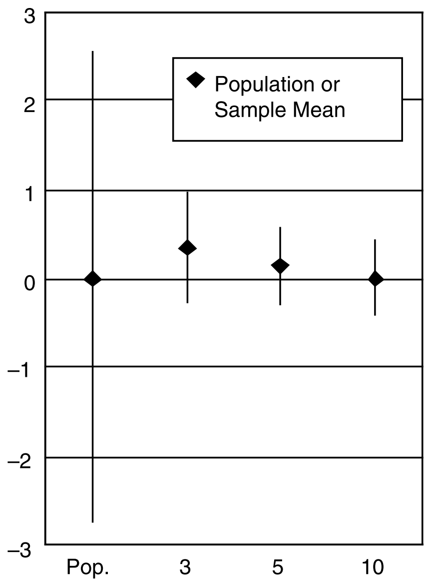


FIGURE 12.6 Population range and mean, and confidence intervals and means for different sample sizes. Means are calculated as the arithmetic average value (Table 7.1) The population range is noted by the bar labeled "Pop." The other bars are labeled with the sample size used (3, 5, and 10), and the lengths of the bars display the associated confidence interval on the mean, calculated as the mean $\pm 2s/n^{1/2}$, where s is the sample standard deviation (Table 7.1) and n is the sample size (Ott, 1993, pp. 201–202).

values can be disconcerting but can be important indicators of problems with model construction, the observations, or both.

G10.3 Diagnose the Cause of Unreasonable Optimal Parameter Estimates

If the analysis of parameter estimates and confidence intervals reveals imprecise and/or unreasonable parameter estimates, investigation of the issues discussed in Section G9.3 can help reveal the cause. Here, two strategies for diagnosing unreasonable estimates are discussed: influence statistics and inconsistencies between true and simulated processes. When attempting to diagnose why the regression is producing unreasonable parameter estimates, it is important to keep in mind that error in other model attributes (those not associated with the parameters with unreasonable estimates) also might be contributing to the problem.

Yager (1998) used *DFBETAS* influence statistics to help identify model error. In the model of regional groundwater flow through fractured dolomite depicted in Figure 11.2, an unreasonably large optimal value of horizontal anisotropy was estimated by nonlinear regression. The *DFBETAS* statistics were used to identify a set of influential head observations that were important to the anisotropy parameter and were located at the edge of a rural recharge zone that was adjacent to an urban recharge zone. The recharge rate in the rural zone was expected to be substantially lower than that in the urban zone. Evaluation of the calibrated model revealed that to optimize the overall model fit, the unrealistically large anisotropy value was estimated because it compensated for a recharge rate that was too low to provide a good fit to the influential heads. To resolve this problem, Yager (1998) modified the position of the boundary between the recharge zones, which was not clearly defined by field data, so that the influential observations were in the urban recharge zone. With this modification to model construction, the regression produced a realistic optimal estimate of horizontal anisotropy and of other model parameters and provided a good fit to the influential heads.

Investigating whether processes important to observed values are simulated in the model, as discussed in Guideline 9 with regard to diagnosing poor model fit, also can lead to identification of model error when diagnosing unrealistic optimized parameter values. For example, if observed solute concentrations in fractured rock are strongly controlled by advection, dispersion, and matrix diffusion, transport simulations using only advection and dispersion can produce unreasonable estimates of dispersion parameters. Matrix diffusion needs to be simulated to obtain reasonable estimates. In the example from Pavelko (2004) described in Guideline 9, unreasonable parameter estimates, as well as poor model fit, resulted when observations were defined in a way that emphasized diurnal signals in the data caused by heating of the extensometer.

G10.4 Identify Observations Important to the Parameter Estimates

The statistics presented in this book that can be used to identify observations important to parameters are listed in Table 10.2.

Statistics that can be used to identify observations that are important to individual parameter estimates include dimensionless scaled sensitivities (*dss*, Chapter 4, Section 4.3.3) and *DFBETAS* (Chapter 7, Section 7.3.2). The *dss* are fit-independent, but this attribute is not as important for Guideline 10 applied to a model that is substantially calibrated, as it is for Guideline 3 applied to a newly constructed model. *DFBETAS* has the advantage of representing the effects of both sensitivity and parameter correlation, so it is usually a better choice for the evaluations conducted as part of Guideline 10. Using *dss* to identify observations important to one parameter estimate is illustrated in Figure 8.1*c*. *DFBETAS* statistics can be presented similarly.

The statistics that can be used to identify observations that are important to a set of parameters include leverage (Chapter 4, Sections 4.3.6 and 4.4.3 and Chapter 7, Section 7.3.1) and Cook's *D* (Chapter 7, Section 7.3.2) Using Cook's *D* to identify observations important to all parameter values is illustrated in Chapter 15, Section 15.2.1. The statistics differ in that the leverage statistics are fit-independent, so that they do not account for model fit to observations. Cook's *D* is a measure of influence that accounts for model fit to observations. The choice of statistic, therefore, is likely to be based on whether the model is mature enough that inclusion of model fit is preferred.

G10.5 Reduce or Increase the Number of Parameters

If individual linear confidence intervals (Chapter 7, Section 7.5.1) for two or more parameters overlap, it may imply that the true parameter values are similar, even if the estimated values are different. An example is presented in Figure 11.8 and discussed in Section G8.4. In model B, the overlapping 95-percent linear individual confidence intervals and similar estimates suggest that the true hydraulic conductivities may be similar and it may be possible to assign the same hydraulic conductivity to model layers 3, 4, and 5 without a significant deterioration in model fit. Indeed, this was achieved using model A. If model fit significantly deteriorates, the parameters probably should not be combined. For nonlinear models, linear intervals are approximate. Nonlinear intervals (Chapter 7, Section 7.5.1) can be considered, but each limit of each interval requires as much execution time as a regression. It is often more effective to use linear intervals to identify likely parameter combinations that can then be tested using a single regression.

Analysis with the confidence intervals is analogous to performing a standard two-tailed, or two-sided, hypothesis test (Davis, 2002, pp. 61–64; Helsel and Hirsch, 2002, p. 104) in which the hypothesis for model B is that the hydraulic conductivity of the bedrock is uniform with depth. If the test results show that this hypothesis cannot be rejected, then it may be possible to define one hydraulic-conductivity parameter that applies to layers 3, 4, and 5 (model A).

At any stage of model calibration, composite scaled sensitivities can be analyzed as described in Guideline 3 (Chapter 11) to determine if the available data are likely to support additional detail in representing the system characteristics associated with the defined parameters. Parameters with composite scaled sensitivities that are significantly larger than 1.0 and large compared to *css* values for other parameters might be divided in ways that are consistent with other data, such as geologic and hydrogeologic data in groundwater problems. The new set of defined parameters could then be evaluated using the methods of Guideline 3, and regression pursued if warranted.

New parameters can also be added and estimated using, for example, the representer, super parameter, or constrained minimization method. See Chapter 1, Section 1.3.2 for references.

13

GUIDELINES 11 AND 12— POTENTIAL NEW DATA

In most natural systems, collecting meaningful data is expensive and time-consuming. Thus, it is important to collect data most beneficial to the modeling objectives. These objectives commonly include (1) better understanding of the processes and properties governing system dynamics and/or (2) simulating predictions of future conditions. Of course, (2) depends on (1), but identifying predictions that are of primary importance can be used to focus data collection efforts.

Models are powerful tools for guiding additional field data collection, as suggested in Chapter 8, Section 8.3. This effort is best achieved using the fit-independent statistics listed in Table 10.2. Fit-independence is important because the value of the potential new data is unknown. If fit-dependent statistics are used, they need to be evaluated for a reasonable range of potential observed values. The statistics can be used to identify observations important to parameters, parameters important to predictions, and observations important to predictions. Knowledge of the important parameters and observations can then be used to guide the data collection effort, as discussed in Guidelines 11 and 12.

To be useful for the task of identifying important potential new data, a model needs to represent the system with a reasonable level of accuracy. It can be difficult to determine when a model is sufficiently accurate, but at the very least, obvious errors in the system representation and in simulated equivalents to observations need to be resolved. Strategies to resolve these problems using analyses of model fit and optimal parameter estimates are presented in Guidelines 9 and 10 in Chapter 12.

Effective Groundwater Model Calibration: *With Analysis of Data, Sensitivities, Predictions, and Uncertainty.* By Mary C. Hill and Claire R. Tiedeman
Published 2007 by John Wiley & Sons, Inc.

In this chapter, Guideline 11 discusses identifying new data to improve the parameter estimates and distribution. Guideline 12 discusses identifying new data to improve model predictions. The analyses of model uncertainty discussed in Chapter 14 also often motivate and provide guidance for new data collection efforts. Modelers are encouraged to be creative in how they use the methods discussed in the guidelines.

For the approaches discussed here, results need to be considered carefully because they inherit all the simplifications and approximations in the model. To determine how to proceed with data collection, generally it is wise to use model results in combination with other information, such as existing observation data, existing knowledge of the system characteristics and observations, and information about past and future stresses, such as pumping in groundwater systems. That is, we do not suggest depending only on the model-generated results that are the primary focus of this discussion.

GUIDELINE 11: IDENTIFY NEW DATA TO IMPROVE SIMULATED PROCESSES, FEATURES, AND PROPERTIES

Sometimes models are constructed primarily to better understand the processes, features, and properties that govern system dynamics. New data can serve four roles in improving the representation of these entitites in models. Data can be used to support: (1) modifying system processes; (2) modifying the geometry of system features, including parameter structures such as zonation or interpolation; (3) defining system property values that relate directly to parameter values; and (4) new observations that provide indirect data about system information. Guideline 11 focuses on the fourth role and on methods for identifying useful new observations. Commonly, data related to observations are much easier and less expensive to collect than is system information. First, roles (1)–(3) are briefly discussed.

Collecting new data to support modification of processes or system features often is motivated by poor model fit or unreasonable parameter estimates. The first step typically is to evaluate the likely importance of the process or feature conceptually. Next, the process or feature is modified in the simulation model, and methods in Guidelines 8–10 can be used to test model improvement. If supported by these analyses, field data can be collected to further characterize the process or feature, and to improve its representation in the model, as discussed in Guideline 2.

Obtaining data that relate directly to parameter values can be difficult. System properties commonly are measured at scales that differ from those to which model parameters apply, as discussed in Chapter 9, Section 9.2.3 in relation to transport models. To the extent that the measurements do apply to parameter values, they can be used as reasonable ranges, prior information, or specified values, as discussed in Guidelines 2 and 5.

Data that support additional observations can be evaluated with the model using fit-independent statistics. We discuss methods that use sensitivities to evaluate potential new observation types and locations for the information they provide

TABLE 13.1 Dimensionless Scaled Sensitivities (*dss*) and Leverage for Two Potential Observations from Exercise 8.1c, and Composite Scaled Sensitivities (*css*) Calculated for the Existing Observations

	Dimensionless Scaled Sensitivities[a] (*dss*) for Parameter[b]:				
	HK_2	VK_CB	K_RB	RCH_2	Leverage
Potential head observation	-3.5	8.0×10^{-3}	-0.105	54.8	0.988
Potential flow observation	-3.2×10^{-5}	1.1×10^{-6}	-0.349×10^{-5}	-4.50	0.491
css for existing observations	3.1	0.22	0.20	25.3	

[a]For four of six parameters.
[b]*Parameter labels*: HK_2, hydraulic conductivity of model layer 2; VK_CB, vertical hydraulic conductivity of the confining unit; K_RB, vertical hydraulic conductivity of the riverbed; RCH_2, recharge rate away from the river.

about the model parameters. These methods include dimensionless and composite scaled sensitivities (*dss*, *css*), parameter correlation coefficients (*pcc*), and leverage statistics (Chapter 4, Sections 4.3.6 and 4.4.3, and Chapter 7, Section 7.5.2). For *dss*, *css*, and leverage statistics, the anticipated accuracy of the potential observations also can be considered because observation weights are included in the calculation. Weights for potential observations can be determined using the same strategies as for existing observations, discussed in Guideline 6.

Table 13.1 shows the *dss* calculated in Exercise 8.1c for two potential observations in the simple steady-state model with pumping, and the *css* calculated using only existing observations obtained before pumping began. In Exercise 8.1c, the potential observations were evaluated with respect to their contribution to reducing prediction uncertainty. Here they are evaluated with respect to their contribution to improving parameter estimates.

The *dss* in Table 13.1 are shown for three model parameters for which the existing observation data provide relatively little information (HK_2, VK_CB, and K_RB), as indicated by the *css*. The *dss* also are shown for parameter RCH_2, for which the existing observations provide ample information. The *dss* suggest that the potential head observation, which is located in the top model layer far upgradient from the river, is more important to all four model parameters than is the potential flow observation, which is the discharge along the entire length of the river.

In analyzing the *dss* in the context of the importance of potential observations to improving parameter estimates, it is important to assess them relative to the *css* calculated for the existing observations. To be helpful for improving a parameter estimate, the absolute value of the *dss* for a potential observation needs to be roughly of the same or greater magnitude than the *css* for the parameter. Comparison of the *dss* and *css* values in Table 13.1 suggests that the potential head observation is likely to improve the estimates of HK_2, K_RB, and RCH_2 but would contribute little toward estimating VK_CB. The potential flow observation is only likely to help improve the estimate of RCH_2. When evaluating the *dss* to determine the value of a potential observation, there is an additional consideration. As discussed in Chapter 4, Section 4.3.4, parameters with *css* less than 1.0 are more likely than those with larger *css* to be poorly estimated, and to cause regression convergence problems. Thus, potential observations that are likely to increase the *css* of a parameter to greater than 1.0 are of special interest. Potential observations that are likely to increase the *css* to a value less than 1.0 are not likely to improve the estimate of that parameter. By this analysis, the potential head observation is not likely to improve the estimate of K_RB.

Parameter correlation coefficients (*pcc*) also need to be considered when evaluating potential new observations. Potential observations that provide little information as indicated by the *dss* might be very important to improving the parameter estimates, if they help to reduce parameter correlations. This can be tested by comparing *pcc* calculated only with the existing observations to those calculated with the existing and potential observations. The latter calculation uses the parameter variance–covariance matrix with potential observations, discussed in Chapter 7, Sections 7.2.1 and 7.2.5. The results of this comparison are given in Exercise 8.1c for the example presented above and show that addition of the potential head observation reduces the absolute value of several correlations that are very large when only the existing observations are included. Addition of the flow observation as well further reduces the correlations, indicating that it is more important to improving the parameter estimates than is indicated by the *dss* alone, but how much more is not clear.

Leverage statistics also can be used to evaluate the potential effect of one or more observations on a set of parameter estimates. The actual effect is measured by influence statistics, which depend on the observed value, and so are not useful for evaluating potential observation data. In addition to the effects measured by *dss*, leverage statistics reflect the ability of the potential observation to reduce parameter correlations. The leverage statistics for the example are listed in Table 13.1. Leverage statistics can range from 0.0 to 1.0, so the potential head observation has extremely high leverage and the potential flow observation has moderate leverage. A disadvantage of leverage statistics is that they do not indicate the particular parameter(s) to which a potential observation is most important. In this example, the leverage statistic suggests that, overall, the head observation is likely to contribute more information than the flow observation, which is consistent with the analyses of the *dss* and *pcc*. Final decisions about data collection often also depend on which parameters are important to predictions, which is the topic of Guideline 12.

It can also be useful to plot the *dss* for potential observations in relation to independent variables such as time and location. The graph of *dss* versus time shown in Figure 13.1 indicates the relative importance of potential drawdown observations during pumpage. For parameters HK_1, HK_2, and Q_1&2, the sensitivity increases with time, indicating drawdown observations later in time provide the most information about these parameters. In contrast, drawdown at an intermediate time is most likely to improve the estimates of the storage coefficient parameters.

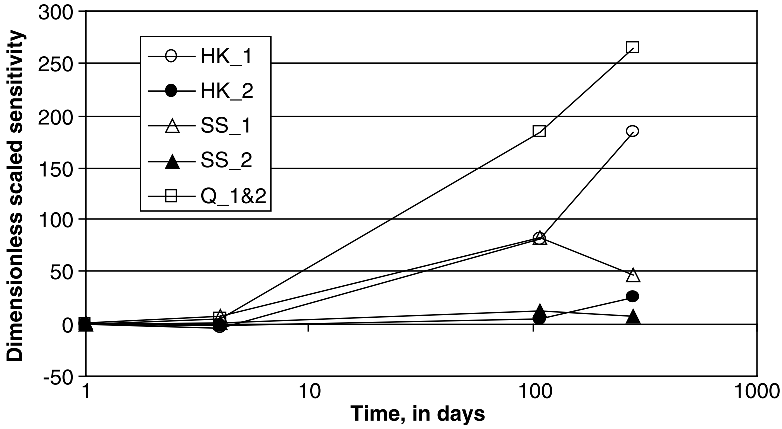


FIGURE 13.1 Dimensionless scaled sensitivities plotted in relation to time for an existing head observation (at time = 0 days, with no pumpage) and potential drawdown observations (at time >0 days, with constant pumpage) from well 2 of Exercise 9.6. Model parameter HK_1 represents the hydraulic conductivity in model layer 1, HK_2 is used to calculate the hydraulic conductivity of model layer 2, SS_1 and SS_2 are storage coefficients of the top and bottom layers, respectively, and Q_1&2 is the pumping rate in wells 1 and 2.

Additional uses of scaled sensitivities are discussed in Chapter 14 under Guideline 14 and in Chapter 4, Section 4.3.3. Using *dss* in this manner is similar to how sensitivity measures were used by Knopman and Voss (1988).

Maps of one-percent scaled sensitivities for hydraulic heads, such as those shown in Figure 4.4, are an additional tool for identifying areas and depths where hydraulic heads are important to one or more parameters but there are no existing observations. However, there are important limitations to the use of these maps, as discussed in Chapter 4, Section 4.3.7.

When evaluating potential new observations using *dss*, *css*, *pcc*, and leverage, model nonlinearity can produce misleading results. This is illustrated using the example from Anderman et al. (1996), discussed in Chapter 11, Section G3.1. Although in this example existing observations are considered, the results of analyzing the *css* and *pcc* would be identical if these observations were potential data. This example also provides an example of how nonlinearity can affect sensitivity analysis. Using initial parameter values, the advective-transport path entered a lake near the source instead of continuing a greater distance within the groundwater system. The longer path is more probable given the concentration data. The unrealistic short advective-travel path resulted in an underestimate of the importance of the advective-transport data when evaluated using the *css* and *pcc* calculated for the initial parameter values.

This situation demonstrates the importance of calculating statistics for multiple sets of parameter values, which also is discussed in Chapter 4, Section 4.4 and portrayed in Figure 4.2. If the statistics change considerably when calculated at a different, reasonable set of parameter values, then they may not be reliable indicators of the worth of the potential data to the model calibration. Reasonable parameter values are those that both respect the system information and produce a reasonable fit to observations. If the simulations produce statistics that support very different data acquisition efforts, the improved understanding of the system obtained from the analysis may still be helpful in making decisions about how to proceed with data acquisition and model development efforts.

GUIDELINE 12: IDENTIFY NEW DATA TO IMPROVE PREDICTIONS

Often models are developed primarily for predictive purposes. In this case, a high priority for field data collection is to improve predictions by increasing their accuracy or reducing their uncertainty. As noted in Guideline 11, new data can serve four roles in improving the representation of model processes, features, and properties governing system dynamics. Data can be used to (1) modify the processes included; (2) modify the geometry of system features, including the structure of parameterizations such as zonation or interpolation; (3) define system property values that relate directly to parameter values; (4) support additional observations. In the context of improving predictions, we expand the fourth role to include improving existing observations with poorly characterized attributes. The first role is discussed briefly below, (2) and (3) are considered in Section G12.1, and (4) is considered in Section G12.2.

Considering additional processes in the context of predictions follows the steps described for Guideline 11, except the effect on predictions also is considered. Once the process is included in the model, the methods used are identical to those described in Section G12.1.

G12.1 Potential New Data to Improve Features and Properties Governing System Dynamics

The most common method for identifying system features that are important to predicted values is to simulate the predictions using alternative conceptual models of the system in which selected features are added, removed, or modified. The process is similar to the sampling methods described in Chapter 14, Section G14.2, except that here the simulations are used to identify potential new data instead of evaluating uncertainty.

Methods presented in Chapter 8, Section 8.2 also can be used to guide collection of data important to the predictions. These include (1) combined use of composite and prediction scaled sensitivities (*css* and *pss*) and parameter correlation coefficients (*pcc*), as illustrated in Figure 8.2, and (2) the parameter–prediction (*ppr*) statistic. These methods focus on identifying parameters that are most important to the predictions. The results of these methods can be used to guide collection of data about the values of parameters associated with system features. Field activities to obtain this type of data in groundwater systems include, for example, hydraulic tests for estimating transmissivity and storativity values.

The results from the *css–pss–pcc* and *ppr* methods also can be used to guide collection of system information related to the representation of model features. By this approach, it is assumed that there is a link between model parameter importance and system feature importance. That is, it is assumed that information about system features is important to predictions if parameters related to the features are identified as important to predictions. The parameters identified as most important to the model predictions may not always correspond to the features of model construction that are most important to the model predictions, but it is expected that there will often be such a correspondence. In groundwater systems, such features might include the geometry and internal variability of a hydrogeologic unit associated with a hydraulic-conductivity parameter identified as important. Field activities might include geologic and geophysical investigation and interpretation of the extent and thickness of the hydrogeologic unit.

Tiedeman et al. (2003) discuss in more detail issues related to using the *pss* and *ppr* statistics to guide field data collection and provide an example of their application, which is summarized in Chapter 15, Section 15.2.1.

G12.2 Potential New Data to Support Observations

New data can be used to improve existing observations or to obtain new observations. It can be beneficial to improve existing observations if they are shown to be important to predictions and there is a resolvable deficiency in the observations. For example in a groundwater study, wells for which existing head observations are shown to be important to predictions might be the focus of downhole methods to better understand the condition of well screens where corrosion is suspected. In a surface-water study, high streamflow at a site may be important to predictions, but the flow might be derived from a stage measurement and a rating curve extrapolated beyond streamflow measurements. The new data might involve better delineating the local topography and vegetation and using the methods of Kean and Smith (2005) to improve the streamflow observation.

There are two primary tools for evaluating potential new observation data for improving the predictions, both of which are presented in Chapter 8, Section 8.3. The first involves using *dss*, *css*, *pss*, and *pcc* together, and the second is the observation–prediction (*opr*) statistic.

Using *dss–css–pss–pcc* involves first using *pss* to identify parameters that are important to a prediction, then using *css* to identify whether any of these parameters are not well supported by the existing observation data. Then, the methods discussed in Guideline 11 can be used to identify potential new observations likely to provide information about the identified parameters. Finally, *pcc* can be used to evaluate if the potential new observations help reduce parameter correlations that are problematic for predictions. This process has the advantage that each of the separate statistics is conceptually easy to understand and to convey to others. Disadvantages include that it can be cumbersome to display and evaluate the four different measures and associated graphs and it does not reflect the importance of parameter correlations to predictions.

The *opr* statistic of Chapter 8, Section 8.3.2 addresses the disadvantages of the *dss–css–pss–pcc* method by integrating the effects of both sensitivity and correlation. It can be used to evaluate an existing monitoring network to identify locations and types of data that are most advantageous to continue measuring under anticipated future scenarios. It also can be used to identify potential new observation types and locations that would be most beneficial to add to a monitoring network. The primary disadvantage is that *opr* may be more difficult to understand. Tiedeman et al. (2004) provide an example of applying the *opr* statistic to evaluate a hydraulic-head monitoring network associated with the Death Valley regional groundwater flow system. This application is summarized in Chapter 15, Section 15.2.1.

14

GUIDELINES 13 AND 14—PREDICTION UNCERTAINTY

An advantage of using optimization for model development and calibration is that optimization provides methods for evaluating and quantifying prediction uncertainty. Both deterministic and statistical methods can be used. Guideline 13 discusses using regression and postaudits, which we classify as deterministic methods. Guideline 14 discusses inferential statistics and Monte Carlo methods, which we classify as statistical methods.

GUIDELINE 13: EVALUATE PREDICTION UNCERTAINTY AND ACCURACY USING DETERMINISTIC METHODS

Deterministic methods are useful for evaluating and understanding prediction error. Here we consider two methods. The authors have discussed the first method with a number of people, including John Doherty (Watermark Consulting, Corinda, Australia, oral communication, 2002), but we are not aware that it has appeared in any previous publication.

G13.1 Use Regression to Determine Whether Predicted Values Are Contradicted by the Calibrated Model

In some circumstances the regression can be a useful tool for evaluating predictions and their uncertainty. For example, consider a model in which the simulated

Effective Groundwater Model Calibration: With Analysis of Data, Sensitivities, Predictions, and Uncertainty. By Mary C. Hill and Claire R. Tiedeman
Published 2007 by John Wiley & Sons, Inc.

concentration of a contaminant at a location is always below the drinking water standard, but resource managers question whether a small change in the parameter values could result in the simulated concentration exceeding the standard. This question can be addressed using linear and nonlinear confidence intervals, but the answer can sometimes be conveyed more clearly by revealing the parameter values or conditions that would be required to produce a specific simulated prediction or set of predictions. This can be accomplished using MODFLOW-2000, UCODE_2005, PEST, or other inverse models as follows.

1. Add the predicted value to the regression as an "observation" using a large weight (small statistic). In the example given above, this value would be a concentration that exceeds the drinking water standard.
2. Perform regression.

The conclusion is that the predicted value is contradicted by the observations and the calibrated model if (a) the predicted value cannot be matched by the regression, (b) it can be matched but the parameter values required produce a poor match to the calibration observations, or (c) the parameter values required to achieve the match are unreasonable. To the extent that the model represents the relevant aspects of the system, this suggests that the predicted value is unlikely to occur. This result also can be communicated using nonlinear confidence intervals on the predicted value, and possibly linear intervals.

The conclusion is that the predicted value is not contradicted by the observations and the calibrated model, and the concerns of the resource manager are substantiated, if the predicted value is matched without producing a poor match to the observations or unreasonable parameter values. This result can be communicated using the results of the regression and linear or nonlinear confidence intervals.

G13.2 Use Omitted Data and Postaudits

Model accuracy can be evaluated by comparing simulated predictions with existing data intentionally omitted from model calibration or new data. Here we concentrate on situations when the omitted or new data are related to predictions. Sometimes these tests are called model validation, but we agree with concerns expressed by, for example, Konikow and Bredehoeft (1992) and Bredehoeft and Konikow (1993), that this terminology is misleading. Different tests lead to different levels of confidence in the model, and saying each "validates" the model ignores that important distinction. Tests against new data are sometimes called postaudits.

These tests are meaningful when the new data represent stress conditions or aspects of the system that differ from those represented in the data used for model calibration. For example, consider a model calibrated using two cycles of tidally induced fluctuations. It is less meaningful to test the model using another cycle with the same amplitude and phase and measured at the same locations than to assess the ability of the model to reproduce a cycle with a different amplitude or system response to some other type of stress entirely, such as the imposition of pumpage. As another example, consider a groundwater model calibrated with hydraulic-head and flow data. A meaningful test might be to assess its ability to predict (1) heads and/or flows collected when pumpage had increased significantly or (2) another process such as transport.

Here we present a few published examples of using new data to test model predictive capabilities. The first two examples use new data collected under conditions similar to the calibration conditions.

Van Loon and Troch (2002) calibrated a suite of distributed hydrological models with varying temporal and spatial resolutions, using sets of soil moisture observations with different temporal and spatial densities. They then tested the ability of the calibrated models to predict a subset of soil moisture data collected later in time under similar hydrologic conditions. They concluded that prediction accuracy did not necessarily increase as model resolution increased.

Saiers et al. (2004) examined the dependence of prediction accuracy on the types of observations used to calibrate a groundwater flow and transport model. The observation sets consisted of heads; heads and flow; or heads, flows, and concentrations. The predictions were heads and flows measured at different times under similar conditions. The authors found that, for predicting heads, use of all three calibration observation sets performed equally well. For predicting flows, use of head observations alone did a poor job, and use of concentration observations did not produce increased prediction accuracy compared to use of only head and flow data. The latter conclusion resulted because the information about flow that the concentration observations provided was similar to that provided by the flow observations.

Most published postaudits of regional-scale groundwater flow and transport models have found that actual system responses differ from responses predicted by the model. For example, see the postaudits presented by Konikow and Person (1985), Alley and Emery (1986), Konikow (1986), Reichard and Meadows (1992), Hanson (1996), and Stewart and Langevin (1999), which involved regional-scale models with prediction times several years after the model calibration period. Results of these postaudits were used to gain considerable insight into the simulated groundwater systems, even though the predictions were incorrect to some degree. This insight was used to help detect model error and to identify data needs and changes to the conceptual model that could help reduce this model error. Andersen and Lu (2003) present a study in which remediation results are used for a postaudit analysis, which helped reveal error in the initial model. However, capture zones simulated with an updated model were similar to those with the initial model, indicating that the initial model was useful for designing remedial strategies despite the error.

GUIDELINE 14: QUANTIFY PREDICTION UNCERTAINTY USING STATISTICAL METHODS

Guideline 14 suggests two methods for quantifying prediction uncertainty: inferential statistics and random sampling (Monte Carlo) methods. For both these methods, the mechanism for communicating uncertainty is often some type of interval around the prediction.

The prediction uncertainty that can be quantified most readily by both inferential statistics and Monte Carlo methods is that produced by uncertainty in the defined parameters. Indeed, as noted in Chapter 8, Section 8.5.2, the two types of methods project parameter uncertainty onto predictions in ways that produce identical results in some circumstances. If the parameters do not represent all aspects of the model that may be incorrect, then the uncertainty represented by these methods tends to underestimate the actual uncertainty. If, however, defined parameters represent many aspects of the system, and other aspects of the model accurately represent system characteristics, then these methods can capture a substantial amount of the prediction uncertainty. This implies that one approach for better characterization of uncertainty is to represent more aspects of the system using defined parameters. This is a largely unexplored approach.

Predictions tend to be less accurate as they differ more from observations and as prediction conditions differ more from calibration conditions. The example by Saiers et al. (2004) presented in Section G13.1 showed that a groundwater model calibrated using heads produced poor predictions of flow. It is not clear how much measures of uncertainty can account for the differences between predictions and calibrations. Certainly if the predictions are affected by processes not represented in the model, the uncertainty calculated using any of the methods discussed here would be too small. There is no clear solution to this problem, but it is important to be aware of its possible existence in many types of models.

Inferential statistics, Monte Carlo methods, and other methods of uncertainty analysis, such as those presented by Sun (1994), are based on the assumption that the model accurately represents the real system. In truth, all models are simplifications of real systems, and the accuracy of the uncertainty analysis is in question. This accuracy is very difficult to evaluate definitively. Christensen and Cooley (1999) compared nonlinear prediction intervals with measured heads and flows and found good correspondence between the expected and realized significance level of the intervals. If model fit to data indicates model bias, theory suggests that the calculated intervals do not reflect all aspects of system uncertainty, and thus they might be best thought of as indicating the minimum amount of uncertainty. That is, actual uncertainty might be larger than indicated by the confidence intervals. If prediction intervals are dominated by the measurement error term, they are less likely to be prone to error. Unfortunately, in many circumstances the confidence intervals are of greater interest because they reflect model uncertainty most clearly. Cooley (1997, 2004) provides additional analysis of nonlinear confidence intervals.

Inferential statistics and Monte Carlo methods also can be used together. For example, Monte Carlo simulations based on alternative models could each calculate linear or nonlinear confidence intervals based on inferential statistics. Model uncertainty might then be represented by the range of predictions represented by the full set of confidence intervals. Such ideas are promising and are just beginning to be considered in the literature, as noted in Chapter 8, Section 8.6.

Clearly, prediction uncertainty is an area where there is much to be done and ongoing improvements in computer technology make advances more accessible than ever before. Here, we comment on using the methods presented in Chapter 8.

G14.1 Inferential Statistics

The most common and useful inferential statistics for quantifying prediction uncertainty are confidence and prediction intervals, which can be constructed using the methods described in Chapter 8, Section 8.4. Instead of reporting a single predicted value, a predicted value and a confidence or prediction interval are reported.

Given the different types of intervals discussed in Section 8.4—confidence and prediction, individual and simultaneous, and linear and nonlinear—confusion can arise as to when to use them. The following three points are provided for guidance.

1. Use *prediction intervals* to compare measured equivalents to predictions.
2. Use *simultaneous intervals* for multiple or vague predictions.
3. Suggested steps: calculate *linear intervals* and *test model linearity*. If the model is nonlinear, calculate a few *nonlinear intervals*. If needed, calculate more *nonlinear intervals*.

As noted in Chapter 8, Christensen and Cooley (1999) show that in nonlinear problems, nonlinear confidence intervals can be very different from linear intervals for some quantities, and can be very similar for others. It appears that linear confidence intervals are useful as a general indication of uncertainty in many circumstances, but, if at all possible given computer resources, some nonlinear intervals need to be calculated if the model is nonlinear. Brooks et al. (1994) calculated nonlinear confidence intervals for drawdowns. Keating et al. (2003) present nonlinear confidence intervals calculated on boundary fluxes predicted by a groundwater flow model. Besides quantifying the uncertainty, inferential statistics on predictions have been used to include risk assessment in design criteria by Tiedeman and Gorelick (1993).

Predictions and their confidence intervals need to be calculated for all reasonably accurate models to evaluate how different sets of observations and conceptual models are likely to affect both the simulated predictions and their likely uncertainty. Indeed, it can be useful to include at least linear confidence intervals when calculating predictions for each model calibration run.

Christensen et al. (1998) examined how nonlinear confidence intervals on predictions of streamflow gain varied with different observation sets used for calibrating a groundwater model. The observation sets included hydraulic heads and from zero to 18 streamflow gains. As expected, the confidence intervals were large for the model calibrated using only head data, but some intervals also were large even when the full set of streamflow gains was used for calibration.

G14.2 Monte Carlo Methods

Monte Carlo methods were described in Chapter 8, Section 8.5.

Computer technology and processor speed have greatly improved in recent years, making it much more feasible to conduct Monte Carlo analyses for models of natural systems. Parallel processing capabilities are advantageous to Monte Carlo studies in which the different runs are independent, because individual simulations easily can be distributed to different computer processors. These parallel processing capabilities can be achieved cost-effectively by using clusters of networked personal computers employing, for example, the parallel processing capabilities of the JUPITER API (Banta et al., 2006).

Monte Carlo methods in groundwater modeling have been used to assess the uncertainty of contributing areas to wells. For example, Evers and Lerner (1998) identified a zone of confidence defined as the area that is common to all contributing areas predicted by models that provide a reasonable fit to the calibration data. They also identified a zone of uncertainty, defined as the total area covered by all reasonable contributing areas. Starn et al. (2000) varied parameter values in a three-dimensional model using the variance–covariance matrix produced using regression, and simulated contributing areas using the generated parameter sets. Several Monte Carlo evaluations of capture zones that consider small-scale variations in hydraulic conductivity in two-dimensional systems have been published; for example, van Leeuwen et al. (2000), Feyen et al. (2001, 2003), and Stauffer et al. (2004). The latter was briefly described in Chapter 8, Section 8.5.2. Additional references are cited in the listed works.

Monte Carlo methods also have been integrated with regression to quantify model prediction uncertainty. Examples in groundwater modeling include Poeter and McKenna (1995) and McKenna and Poeter (1995). The Poeter and McKenna (1995) model was briefly described in Guideline 8 (Chapter 11) and provides an example of the six elements of a Monte Carlo analysis presented in Chapter 8, Section 8.5.1 for a groundwater problem. The work includes Monte Carlo runs conducted using three sets of information on the hydraulic-conductivity field, including (a) only hydrogeologic information (measurements of hydraulic conductivity), (b) hydrogeologic and geophysical information, and (c) hydrogeologic and geophysical information as well as hydraulic-head and streamflow gain and loss data integrated using nonlinear regression.

In all cases the goal was to quantify the uncertainty of concentration at a well. The six elements for the analyses were as follows:

1. The model input changed was the zonation used to represent the hydrogeology of the aquifer material.
2. The realizations were generated using indicator kriging.
3. Each Monte Carlo run for (a) and (b) consisted of a forward model simulation. For (c) each run consisted of an inverse model simulation to obtain the best-fit parameter values for the generated zonation. The observations were hydraulic heads and streamflow gains and losses. The concentration at a well was simulated for each Monte Carlo run. The system was simulated using MODFLOW, MODFLOWP, and MT3D.

4. Four hundred runs were conducted. The number of runs was determined largely by computational limitations.
5. For each Monte Carlo run, the following were saved: the zonation, estimated parameter values, information about parameter-estimation convergence, the standard error of the regression, and the predicted concentration.
6. Final results were analyzed by plotting histograms of the predicted concentrations. For (*a*) and (*b*), results for all 400 runs were plotted. For (*c*), results were omitted from the Monte Carlo analysis if one of the following conditions occurred: (i) the best-fit parameter values were unrealistic in that they were

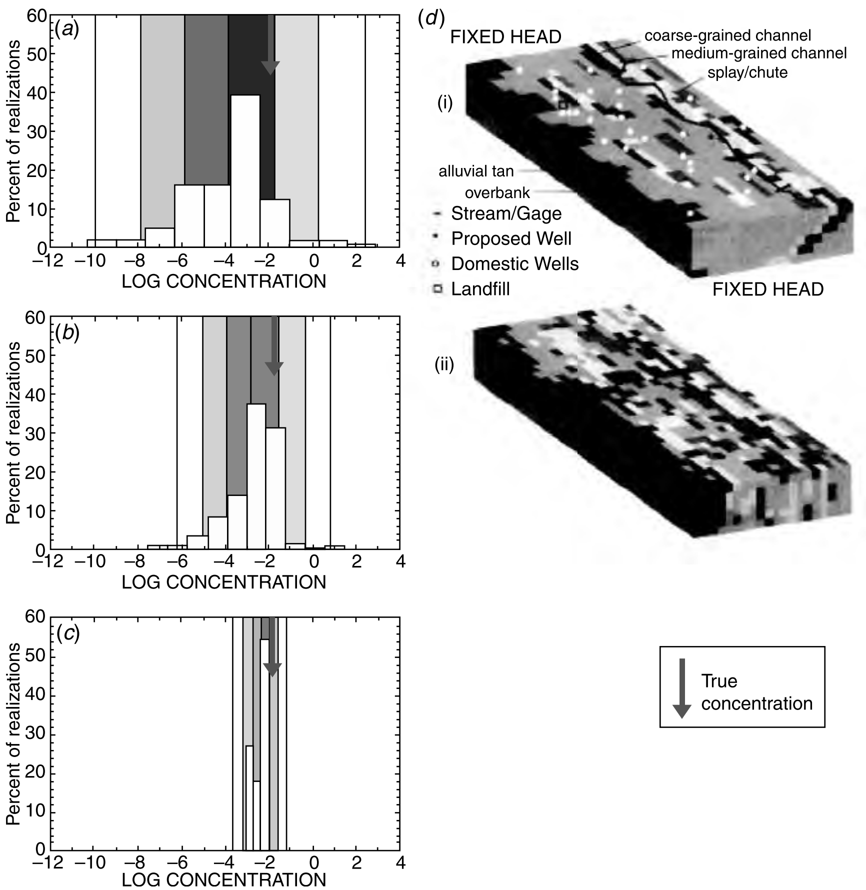


FIGURE 14.1 Histograms of simulated concentrations from models calibrated using three sets of data: (*a*) only hydrogeologic information (measurements of hydraulic conductivity), (*b*) hydrogeologic and geophysical information, and (*c*) hydrogeologic and geophysical information as well as hydraulic-head and streamflow gain and loss data integrated using nonlinear regression. (*d*) The true system and imposed boundary conditions, and a generated zonation. (From Poeter and McKenna, 1995.)

not in order from largest to smallest when such relations could be determined from system information, (ii) the best-fit parameter values were substantially different than expected, (iii) the model fit was significantly worse than for other models, or (iv) the regression did not converge. Ten realizations remained after these conditions were considered.

In this synthetic test case, the true solution was known so that performance of the different methods of characterizing the system could be definitively tested. Results are shown in Figure 14.1. Using nonlinear regression produced much more accurate predictions than were attained by (a) and (b). This is because nonlinear regression allowed conditioning to observations and comparison of estimated parameter values with realistic ranges and rankings based on system information. The dramatic improvement in the predictions produced by models screened using these criteria indicates that their application is likely to be useful for identifying more accurate models.

EXHIBIT 2

Designation: D 5490 – 93 (Reapproved 2002)

Standard Guide for
Comparing Ground-Water Flow Model Simulations to Site-Specific Information[1]

This standard is issued under the fixed designation D 5490; the number immediately following the designation indicates the year of original adoption or, in the case of revision, the year of last revision. A number in parentheses indicates the year of last reapproval. A superscript epsilon (ε) indicates an editorial change since the last revision or reapproval.

1. Scope

1.1 This guide covers techniques that should be used to compare the results of ground-water flow model simulations to measured field data as a part of the process of calibrating a ground-water model. This comparison produces quantitative and qualitative measures of the degree of correspondence between the simulation and site-specific information related to the physical hydrogeologic system.

1.2 During the process of calibration of a ground-water flow model, each simulation is compared to site-specific information such as measured water levels or flow rates. The degree of correspondence between the simulation and the physical hydrogeologic system can then be compared to that for previous simulations to ascertain the success of previous calibration efforts and to identify potentially beneficial directions for further calibration efforts.

1.3 By necessity, all knowledge of a site is derived from observations. This guide does not address the adequacy of any set of observations for characterizing a site.

1.4 This guide does not establish criteria for successful calibration, nor does it describe techniques for establishing such criteria, nor does it describe techniques for achieving successful calibration.

1.5 This guide is written for comparing the results of numerical ground-water flow models with observed site-specific information. However, these techniques could be applied to other types of ground-water related models, such as analytical models, multiphase flow models, noncontinuum (karst or fracture flow) models, or mass transport models.

1.6 This guide is one of a series of guides on ground-water modeling codes (software) and their applications. Other standards have been prepared on environmental modeling, such as Practice E 978.

1.7 The values stated in SI units are to be regarded as the standard.

1.8 *This standard does not purport to address all of the safety concerns, if any, associated with its use. It is the responsibility of the user of this standard to establish appropriate safety and health practices and determine the applicability of regulatory limitations prior to use.*

1.9 *This guide offers an organized collection of information or a series of options and does not recommend a specific course of action. This document cannot replace education or experience and should be used in conjunction with professional judgment. Not all aspects of this guide may be applicable in all circumstances. This ASTM standard is not intended to represent or replace the standard of care by which the adequacy of a given professional service must be judged, nor should this document be applied without consideration of a project's many unique aspects. The word "Standard" in the title of this document means only that the document has been approved through the ASTM consensus process.*

2. Referenced Documents

2.1 *ASTM Standards:*

D 653 Terminology Relating to Soil, Rock, and Contained Fluids[2]

E 978 Practice for Evaluating Mathematical Models for the Environmental Fate of Chemicals[3]

3. Terminology

3.1 *Definitions:*

3.1.1 *application verification*—using the set of parameter values and boundary conditions from a calibrated model to approximate acceptably a second set of field data measured under similar hydrologic conditions.

3.1.1.1 *Discussion*—Application verification is to be distinguished from code verification which refers to software testing, comparison with analytical solutions, and comparison with other similar codes to demonstrate that the code represents its mathematical foundation.

3.1.2 *calibration*—the process of refining the model representation of the hydrogeologic framework, hydraulic properties, and boundary conditions to achieve a desired degree of correspondence between the model simulations and observations of the ground-water flow system.

3.1.3 *censored data*—knowledge that the value of a variable in the physical hydrogeologic system is less than or greater

[1] This guide is under the jurisdiction of ASTM Committee D18 on Soil and Rock and is the direct responsibility of Subcommittee D18.21 on Ground Water and Vadose Zone Investigations.

Current edition approved Nov. 15, 1993. Published January 1994.

[2] *Annual Book of ASTM Standards*, Vol 04.08.

[3] *Annual Book of ASTM Standards*, Vol 11.04.

than a certain value, without knowing the exact value.

3.1.3.1 *Discussion*—For example, if a well is dry, then the potentiometric head at that place and time must be less than the elevation of the screened interval of the well although its specific value is unknown.

3.1.4 *conceptual model*—an interpretation or working description of the characteristics and dynamics of the physical system.

3.1.5 *ground-water flow model*—an application of a mathematical model to represent a ground-water flow system.

3.1.6 *hydrologic condition*—a set of ground-water inflows or outflows, boundary conditions, and hydraulic properties that cause potentiometric heads to adopt a distinct pattern.

3.1.7 *residual*—the difference between the computed and observed values of a variable at a specific time and location.

3.1.8 *simulation*—in ground-water flow modeling, one complete execution of a ground-water modeling computer program, including input and output.

3.1.8.1 *Discussion*—For the purposes of this guide, a simulation refers to an individual modeling run. However, simulation is sometimes also used broadly to refer to the process of modeling in general.

3.2 For definitions of other terms used in this guide, see Terminology D 653.

4. Summary of Guide

4.1 Quantitative and qualitative comparisons are both essential. Both should be used to evaluate the degree of correspondence between a ground-water flow model simulation and site-specific information.

4.2 Quantitative techniques for comparing a simulation with site-specific information include:

4.2.1 Calculation of residuals between simulated and measured potentiometric heads and calculation of statistics regarding the residuals. Censored data resulting from detection of dry or flowing observation wells, reflecting information that the head is less than or greater than a certain value without knowing the exact value, should also be used.

4.2.2 Detection of correlations among residuals. Spatial and temporal correlations among residuals should be investigated. Correlations between residuals and potentiometric heads can be detected using a scattergram.

4.2.3 Calculation of flow-related residuals. Model results should be compared to flow data, such as water budgets, surface water flow rates, flowing well discharges, vertical gradients, and contaminant plume trajectories.

4.3 Qualitative considerations for comparing a simulation with site-specific information include:

4.3.1 Comparison of general flow features. Simulations should reproduce qualitative features in the pattern of ground-water contours, including ground-water flow directions, mounds or depressions (closed contours), or indications of surface water discharge or recharge (cusps in the contours).

4.3.2 Assessment of the number of distinct hydrologic conditions to which the model has been successfully calibrated. It is usually better to calibrate to multiple scenarios, if the scenarios are truly distinct.

4.3.3 Assessment of the reasonableness or justifiability of the input aquifer hydrologic properties given the aquifer materials which are being modeled. Modeled aquifer hydrologic properties should fall within realistic ranges for the physical hydrogeologic system, as defined during conceptual model development.

5. Significance and Use

5.1 During the process of calibration of a ground-water flow model, each simulation is compared to site-specific information to ascertain the success of previous calibration efforts and to identify potentially beneficial directions for further calibration efforts. Procedures described herein provide guidance for making comparisons between ground-water flow model simulations and measured field data.

5.2 This guide is not meant to be an inflexible description of techniques comparing simulations with measured data; other techniques may be applied as appropriate and, after due consideration, some of the techniques herein may be omitted, altered, or enhanced.

6. Quantitative Techniques

6.1 Quantitative techniques for comparing simulations to site-specific information include calculating potentiometric head residuals, assessing correlation among head residuals, and calculating flow residuals.

6.1.1 *Potentiometric Head Residuals*—Calculate the residuals (differences) between the computed heads and the measured heads:

$$r_i = h_i - H_i \quad (1)$$

where:

r_i = the residual,
H_i = the measured head at point i,
h_i = the computed head at the approximate location where H_i was measured.

If the residual is positive, then the computed head was too high; if negative, the computed head was too low. Residuals cannot be calculated from censored data.

NOTE 1—For drawdown models, residuals can be calculated from computed and measured drawdowns rather than heads.

NOTE 2—Comparisons should be made between point potentiometric heads rather than ground-water contours, because contours are the result of interpretation of data points and are not considered basic data in and of themselves.[4] Instead, the ground-water contours are considered to reflect features of the conceptual model of the site. The ground-water flow model should be true to the essential features of the conceptual model and not to their representation.

NOTE 3—It is desirable to set up the model so that it calculates heads at the times and locations where they were measured, but this is not always possible or practical. In cases where the location of a monitoring well does not correspond exactly to one of the nodes where heads are computed in the simulation, the residual may be adjusted (for example, computed heads may be interpolated, extrapolated, scaled, or otherwise transformed) for use in calculating statistics. Adjustments may also be necessary when the times of measurements do not correspond exactly with the times when heads are calculated in transient simulations; when many observed heads are clustered near a single node; where the hydraulic gradient changes significantly from node to node; or when observed head data is affected by tidal fluctuations or proximity to a specified head boundary.

[4] Cooley, R. L., and Naff, R. L., "Regression Modeling of Ground-Water Flow," *USGS Techniques of Water Resources Investigations*, Book 3, Chapter B4, 1990.

6.1.2 *Residual Statistics*—Calculate the maximum and minimum residuals, a residual mean, and a second-order statistic, as described in the following sections.

6.1.2.1 *Maximum and Minimum Residuals*—The maximum residual is the residual that is closest to positive infinity. The minimum residual is the residual closest to negative infinity. Of two simulations, the one with the maximum and minimum residuals closest to zero has a better degree of correspondence, with regard to this criterion.

NOTE 4—When multiple hydrologic conditions are being modeled as separate steady-state simulations, the maximum and minimum residual can be calculated for the residuals in each, or for all residuals in all scenarios, as appropriate. This note also applies to the residual mean (see 6.1.2.2) and second-order statistics of the residuals (see 6.1.2.4).

6.1.2.2 *Residual Mean*—Calculate the residual mean as the arithmetic mean of the residuals computed from a given simulation:

$$R = \frac{\sum_{i=1}^{n} r_i}{n} \tag{2}$$

where:
R = the residual mean and
n = the number of residuals.

Of two simulations, the one with the residual mean closest to zero has a better degree of correspondence, with regard to this criterion (assuming there is no correlation among residuals).

6.1.2.3 If desired, the individual residuals can be weighted to account for differing degrees of confidence in the measured heads. In this case, the residual mean becomes the weighted residual mean:

$$R = \frac{\sum_{i=1}^{n} w_i r_i}{n \sum_{i=1}^{n} w_i} \tag{3}$$

where w_i is the weighting factor for the residual at point i. The weighting factors can be based on the modeler's judgment or statistical measures of the variability in the water level measurements. A higher weighting factor should be used for a measurement with a high degree of confidence than for one with a low degree of confidence.

NOTE 5—It is possible that large positive and negative residuals could cancel, resulting in a small residual mean. For this reason, the residual mean should never be considered alone, but rather always in conjunction with the other quantitative and qualitative comparisons.

6.1.2.4 *Second-Order Statistics*—Second-order statistics give measures of the amount of spread of the residuals about the residual mean. The most common second-order statistic is the standard deviation of residuals:

$$s = \left\{ \frac{\sum_{i=1}^{n} (r_i - R)^2}{(n-1)} \right\}^{\frac{1}{2}} \tag{4}$$

where s is the standard deviation of residuals. Smaller values of the standard deviation indicate better degrees of correspondence than larger values.

6.1.2.5 If weighting is used, calculate the weighted standard deviation:

$$s = \left\{ \frac{\sum_{i=1}^{n} w_i \, (r_i - R)^2}{(n-1) \sum_{i=1}^{n} w_i} \right\}^{\frac{1}{2}} \tag{5}$$

NOTE 6—Other norms of the residuals are less common but may be revealing in certain cases.[5,6] For example, the mean of the absolute values of the residuals can give information similar to that of the standard deviation of residuals.

NOTE 7—In calculating the standard deviation of residuals, advanced statistical techniques incorporating information from censored data could be used. However, the effort would usually not be justified because the standard deviation of residuals is only one of many indicators involved in comparing a simulation with measured data, and such a refinement in one indicator is unlikely to alter the overall assessment of the degree of correspondence.

6.1.3 *Correlation Among Residuals*—Spatial or temporal correlation among residuals can indicate systematic trends or bias in the model. Correlations among residuals can be identified through listings, scattergrams, and spatial or temporal plots. Of two simulations, the one with less correlation among residuals has a better degree of correspondence, with regard to this criterion.

6.1.3.1 *Listings*—List residuals by well or piezometer, including the measured and computed values to detect spatial or temporal trends. Figures X1.1 and X1.2 present example listings of residuals.

6.1.3.2 *Scattergram*—Use a scattergram of computed versus measured heads to detect trends in deviations. The scattergram is produced with measured heads on the abscissa (horizontal axis) and computed heads on the ordinate (vertical axis). One point is plotted on this graph for each pair. If the points line up along a line with zero intercept and 45° angle, then there has been a perfect match. Usually, there will be some scatter about this line, hence the name of the plot. A simulation with a small degree of scatter about this line has a better correspondence with the physical hydrogeologic system than a simulation with a large degree of scatter. In addition, plotted points in any area of the scattergram should not all be grouped above or below the line. Figures X1.3 and X1.4 show sample scattergrams.

6.1.3.3 *Spatial Correlation*—Plot residuals in plan or section to identify spatial trends in residuals. In this plot, the residuals, including their sign, are plotted on a site map or cross section. If possible or appropriate, the residuals can also be contoured. Apparent trends or spatial correlations in the residuals may indicate a need to refine aquifer parameters or boundary conditions, or even to reevaluate the conceptual model (for example, add spatial dimensions or physical processes). For example, if all of the residuals in the vicinity of a no-flow boundary are positive, then the recharge may need to be reduced or the hydraulic conductivity increased. Figure X1.5 presents an example of a contour plot of residuals in plan view. Figure X1.6 presents an example of a plot of residuals in cross section.

[5] Ghassemi, F., Jakeman, A. J., and Thomas, G. A., "Ground-Water Modeling for Salinity Management: An Australian Case Study," *Ground Water*, Vol 27, No. 3, 1989, pp. 384–392.

[6] Konikow, L. F., *Calibration of Ground-Water Models, Proceedings of the Specialty Conference on Verification of Mathematical and Physical Models in Hydraulic Engineering*, ASCE, College Park, MD, Aug. 9–11, 1978, pp. 87–93.

6.1.3.4 *Temporal Correlation*—For transient simulations, plot residuals at a single point versus time to identify temporal trends. Temporal correlations in residuals can indicate the need to refine input aquifer storage properties or initial conditions. Figure X1.7 presents a typical plot of residuals versus time.

6.1.4 *Flow-Related Residuals*—Often, information relating to ground-water velocities is available for a site. Examples include water budgets, surface water flow rates, flowing well discharges, vertical gradients, and contaminant plume trajectories (ground-water flow paths). All such quantities are dependent on the hydraulic gradient (the spatial derivative of the potentiometric head). Therefore, they relate to the overall structure of the pattern of potentiometric heads and provide information not available from point head measurements. For each such datum available, calculate the residual between its computed and measured values. If possible and appropriate, calculate statistics on these residuals and assess their correlations, in the manner described in 5.1 and 5.2 for potentiometric head residuals.

6.1.4.1 *Water Budgets and Mass Balance*—For elements of the water budget for a site which are calculated (as opposed to specified in the model input) (for example, base flow to a stream), compare the computed and the measured (or estimated) values. In addition, check the computed mass balance for the simulation by comparing the sum of all inflows to the sum of all outflows and changes in storage. Differences of more than a few percent in the mass balance indicate possible numerical problems and may invalidate simulation results.

6.1.4.2 *Vertical Gradients*—In some models, it may be more important to accurately represent the difference in heads above and below a confining layer, rather than to reproduce the heads themselves. In such a case, it may be acceptable to tolerate a correlation between the head residuals above and below the layer if the residual in the vertical gradient is minimized.

6.1.4.3 *Ground-Water Flow Paths*—In some models, it may be more important to reproduce the pattern of streamlines in the ground-water flow system rather than to reproduce the heads themselves (for example, when a flow model is to be used for input of velocities into a contaminant transport model). In this case, as with the case of vertical gradients in 6.1.4.2 it may be acceptable to tolerate some correlation in head residuals if the ground-water velocity (magnitude and direction) residuals are minimized.

7. Qualitative Considerations

7.1 *General Flow Features*—One criterion for evaluating the degree of correspondence between a ground-water flow model simulation and the physical hydrogeologic system is whether or not essential qualitative features of the potentiometric surface are reflected in the model. The overall pattern of flow directions and temporal variations in the model should correspond with those at the site. For example:

7.1.1 If there is a mound or depression in the potentiometric surface at the site, then the modeled contours should also indicate a mound or depression in approximately the same area.

7.1.2 If measured heads indicate or imply cusps in the ground-water contours at a stream, then these features should also appear in contours of modeled heads.

7.2 *Hydrologic Conditions*—Identify the different hydrologic conditions that are represented by the available data sets. Choose one data set from each hydrologic condition to use for calibration. Use the remaining sets for verification.

7.2.1 *Uniqueness (Distinct Hydrologic Conditions)*—The number of distinct hydrologic conditions that a given set of input aquifer hydrologic properties is capable of representing is an important qualitative measure of the performance of a model. It is usually better to calibrate to multiple conditions, if the conditions are truly distinct. Different hydrologic conditions include, but are not limited to, high and low recharge; conditions before and after pumping or installation of a cutoff wall or cap; and high and low tides, flood stages for adjoining surface waters, or installation of drains. By matching different hydrologic conditions, the uniqueness problem is addressed, because one set of heads can be matched with the proper ratio of ground-water flow rates to hydraulic conductivities; whereas, when the flow rates are changed, representing a different condition, the range of acceptable hydraulic conductivities becomes much more limited.

7.2.2 *Verification (Similar Hydrologic Conditions)*—When piezometric head data are available for two times of similar hydrologic conditions, only one of those conditions should be included in the calibration data sets because they are not distinct. However, the other data set can be used for model verification. In the verification process, the modeled piezometric heads representing the hydrologic condition in question are compared, not to the calibration data set, but to the verification data set. The resulting degree of correspondence can be taken as an indicator or heuristic measure of the ability of the model to represent new hydrologic conditions within the range of those to which the model was calibrated.

NOTE 8—When only one data set is available, it is inadvisable to artificially split it into separate "calibration" and "verification" data sets. It is usually more important to calibrate to piezometric head data spanning as much of the modeled domain as possible.

NOTE 9—Some researchers maintain that the word "verification" implies a higher degree of confidence than is warranted.[7] Used here, the verification process only provides a method for estimating confidence intervals on model predictions.

7.3 *Input Aquifer Hydraulic Properties*—A good correspondence between a ground-water flow model simulation and site-specific information, in terms of quantitative measures, may sometimes be achieved using unrealistic aquifer hydraulic properties. This is one reason why emphasis is placed on the ability to reproduce multiple distinct hydrologic stress scenarios. Thus, a qualitative check on the degree of correspondence between a simulation and the physical hydrogeologic system should include an assessment of the likely ranges of hydraulic properties for the physical hydrogeologic system at the scale of the model or model cells and whether the properties used in the model lie within those ranges.

[7] Konikow, L. F., and Bredehoeft, J. D., "Ground-Water Models Cannot Be Validated," *Adv. Wat. Res.* Vol 15, 1992, pp. 75–83.

8. Report

8.1 When a report for a ground-water flow model application is produced, it should include a description of the above comparison tests which were performed, the rationale for selecting or omitting comparison tests, and the results of those comparison tests.

9. Keywords

9.1 calibration; computer; ground water; modeling

APPENDIX

(Nonmandatory Information)

X1. EXAMPLES

X1.1 Fig. X1.1 and Fig. X1.2 present sample listings of residuals, as described in 6.1.3.1. These listings tabulate the residuals for simulations of two hydrologic conditions with the same model. Note that some of the wells do not have measurements for both simulations. Simulated heads for these wells are still reported as an aid to detecting temporal trends in the heads for different aquifer stresses. Some censored water level data were available for this site. For these data, the table merely indicates whether or not the simulation is consistent with the censored data.

Example Site
Stress scenario #1
Simulation #24-1

Residuals:
Number of residuals : 18
Maximum residual (m) : 2.62 at MW-31
Minimum residual (m) : -2.51 at MW-5
Residual mean (m) : 0.15
Standard deviation of residuals (m) : 1.49

Censored Data:
Number of inequalities met : 1
Number of inequalities not met : 1

WELL	MEASURED HEAD (M)	SIMULATED HEAD (M)	RESIDUAL (M)
MW-1	100.79	101.57	0.78
MW-2	104.52	103.14	-1.38
MW-3	103.07	101.26	-1.81
MW-4	<101.10	100.97	YES
MW-5	106.82	104.31	-2.51
MW-6	99.94	100.39	0.45
MW-7	101.43	102.84	1.41
MW-8	89.26	89.43	0.17
MW-9	89.34	87.53	-1.81
MW-10	<97.97	98.02	NO
MW-11		96.94	
MW-12		88.60	
MW-13		91.85	
MW-14		77.57	
MW-15		103.04	
MW-16		103.12	
MW-17	95.44	97.84	2.40
MW-18		104.80	
MW-19		95.32	
MW-20		103.14	
MW-21		94.31	
MW-22	101.02	99.54	-1.48
MW-23	70.79	71.69	0.90
MW-24		99.09	
MW-25		100.80	
MW-26	98.26	98.23	-0.03
MW-27	87.44	89.03	1.59
MW-28		98.79	
MW-29	83.30	83.14	-0.16
MW-30	82.99	85.03	2.04
MW-31	95.51	98.13	2.62
MW-32	97.63	97.80	0.17
MW-33	134.02	133.46	-0.56

FIG. X1.1 Example Listings of Residuals

Example Site
Stress scenario #2
Simulation #24-2

Residuals:
Number of residuals : 22
Maximum residual (m) : 2.30 at MW-24
Minimum residual (m) : -2.15 at MW-20
Residual mean (m) : 0.15
Standard deviation of residuals (m) : 1.22

Censored Data:
Number of inequalities met : 2
Number of inequalities not met : 0

WELL	MEASURED HEAD (m)	SIMULATED HEAD (m)	RESIDUAL (m)
MW-1	101.72	101.11	-0.61
MW-2	98.43	98.77	0.34
MW-3	100.04	100.80	0.76
MW-4	<101.10	100.57	YES
MW-5	102.95	104.45	1.50
MW-6	100.00	100.66	0.66
MW-7	101.56	102.80	1.24
MW-8	92.24	90.42	-1.82
MW-9	90.34	88.77	-1.57
MW-10	<97.97	96.88	YES
MW-11		97.69	
MW-12		90.01	
MW-13		93.43	
MW-14		80.27	
MW-15		103.58	
MW-16		103.32	
MW-17	96.33	98.62	2.29
MW-18		105.73	
MW-19		96.65	
MW-20	105.25	103.10	-2.15
MW-21	96.10	95.11	-0.99
MW-22		99.63	
MW-23	74.01	75.21	1.20
MW-24	96.66	98.96	2.30
MW-25	98.04	98.71	0.67
MW-26	97.39	98.21	0.82
MW-27	90.11	90.48	0.37
MW-28	100.23	98.76	-1.47
MW-29	84.92	84.98	0.06
MW-30	86.15	86.88	0.73
MW-31	97.87	97.38	-0.49
MW-32	97.31	97.17	-0.14
MW-33	134.43	133.96	-0.47

FIG. X1.2 Example Listings of Residuals

X1.2 Fig. X1.3 and Fig. X1.4 show sample scattergrams, as described in 6.1.3.2. The scattergram on Fig. X1.3 indicates a good match between modeled and measured potentiometric

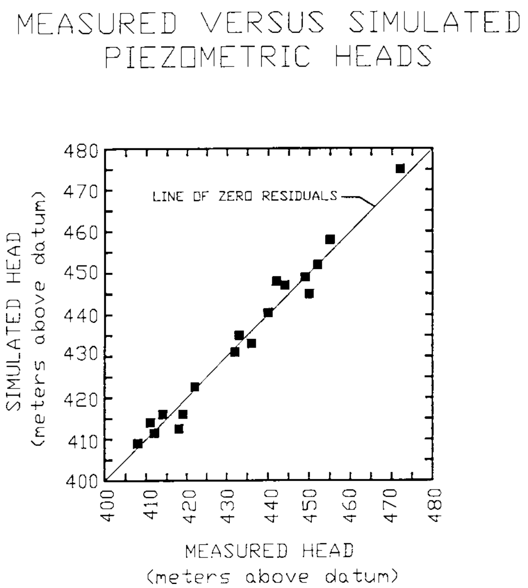


FIG. X1.3 Sample Scattergram

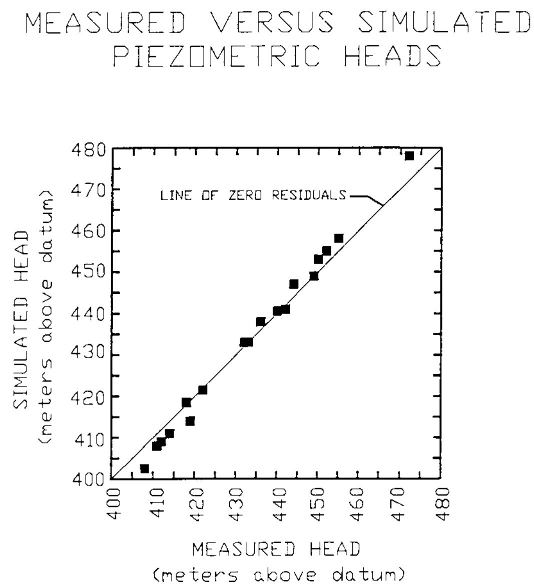


FIG. X1.4 Sample Scattergram

heads because there is little or no pattern between positive and negative residuals and because the magnitude of the residuals is small compared to the total change in potentiometric head across the site. The residuals shown on the scattergram on Fig. X1.4 have the same maximum, minimum, mean, and standard deviation as those shown on Fig. X1.3, but show a pattern of positiveresiduals upgradient and negative residuals downgradient. However, even though the statistical comparisons would indicate a good degree of correspondence, this model may overestimate seepage velocities because the simulated hydraulic gradient is higher than the measured hydraulic gradient. Therefore this model may need to be improved if the heads are to be input into a mass transport model.

X1.3 Fig. X1.5 and Fig. X1.6 show sample plots of residuals in plan and cross-section, as described in 6.1.3.3. In Fig. X1.5, there are sufficient data to contour the residuals. The contours indicate potentially significant correlations between residuals in the northwest and southwest corners of the model. Along the river, the residuals appear to be uncorrelated. In Fig. X1.6, residuals were not contoured due to their sparseness and apparent lack of correlation.

X1.4 Fig. X1.7 shows a sample plot of measured and simulated potentiometric heads and their residuals for one well in a transient simulation, as described in 6.1.3.4. The upper graph shows the measured potentiometric head at the well as measured using a pressure transducer connected to a data logger. In addition, simulated potentiometric heads for the same time period are also shown. The lower graph shows the residuals. This example shows how residuals can appear uncorrelated in a model that does not represent essential characteristics of the physical hydrogeologic system, in this case by not reproducing the correct number of maxima and minima.

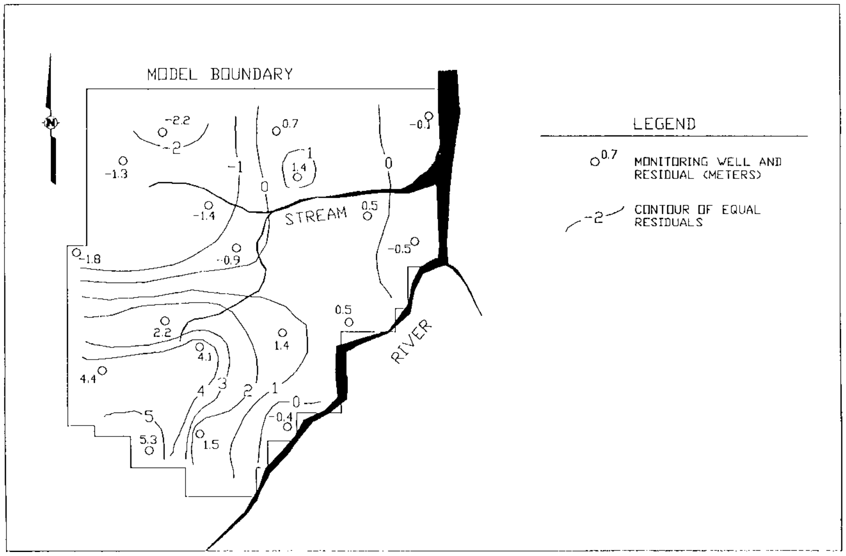


FIG. X1.5 Sample Contours of Residuals Plan View

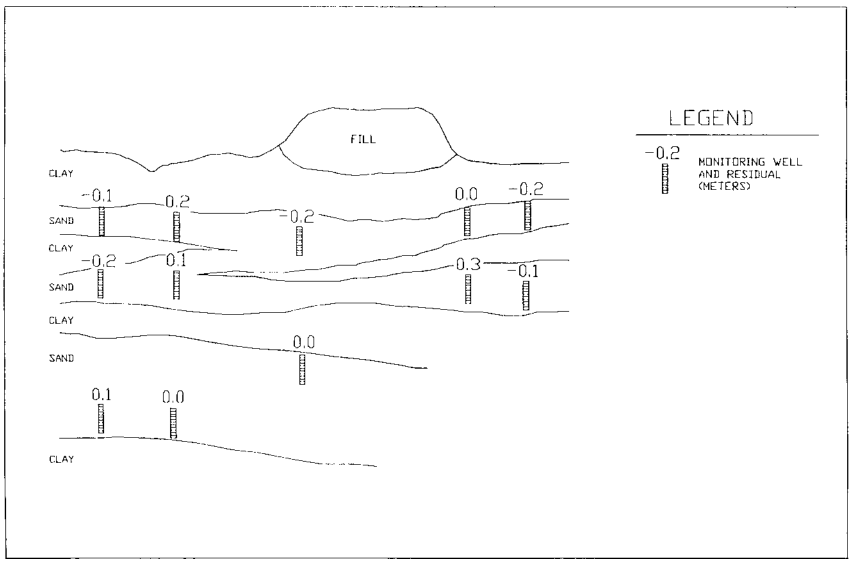


FIG. X1.6 Sample Plot of Residuals Section View

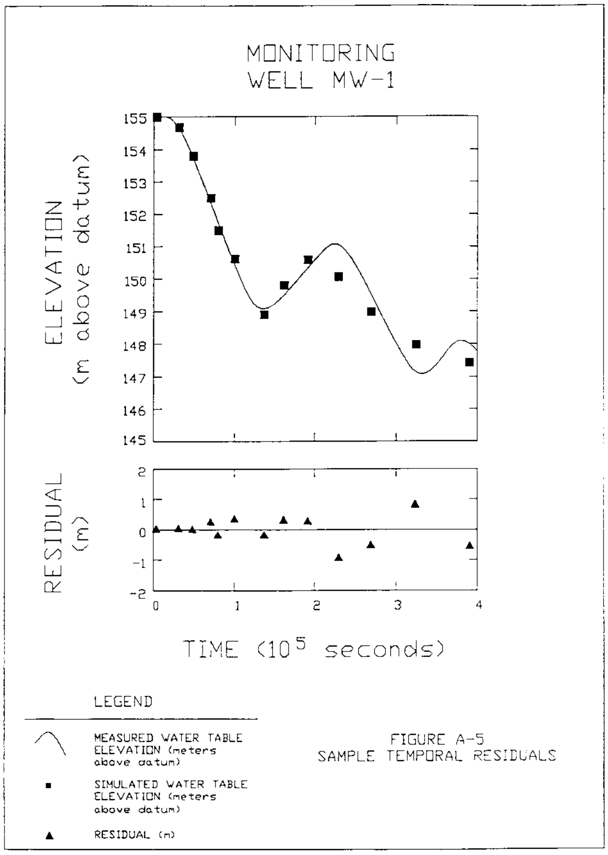


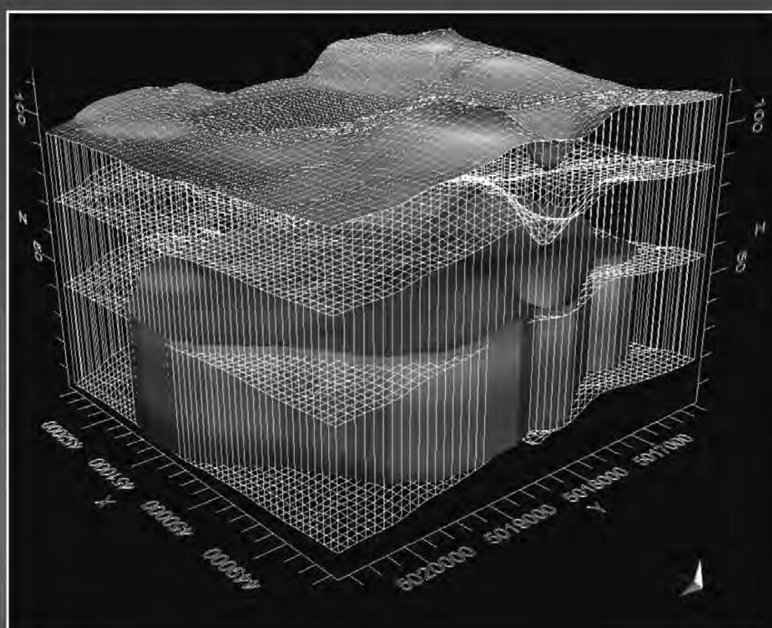
FIG. X1.7 Sample Temporal Residuals

EXHIBIT 3

Second Edition

Applied Groundwater Modeling

Simulation of Flow and Advective Transport



Mary P. Anderson
William W. Woessner
Randall J. Hunt

APPLIED GROUNDWATER MODELING

This page intentionally left blank

APPLIED GROUNDWATER MODELING

Simulation of Flow and Advective Transport

Second Edition

MARY P. ANDERSON

Department of Geoscience, University of Wisconsin-Madison, Madison, Wisconsin

WILLIAM W. WOESSNER

Department of Geosciences, University of Montana, Missoula, Montana

RANDALL J. HUNT

U.S. Geological Survey, Wisconsin Water Science Center, Cross Plains, Wisconsin

ELSEVIER

Amsterdam • Boston • Heidelberg • London
New York • Oxford • Paris • San Diego
San Francisco • Singapore • Sydney • Tokyo
Academic Press is an imprint of Elsevier

Academic Press is an imprint of Elsevier
125 London Wall, London EC2Y 5AS, UK
525 B Street, Suite 1800, San Diego, CA 92101-4495, USA
225 Wyman Street, Waltham, MA 02451, USA
The Boulevard, Langford Lane, Kidlington, Oxford OX5 1GB, UK

ISBN: 978-0-12-058103-0

British Library Cataloguing in Publication Data
A catalogue record for this book is available from the British Library

Library of Congress Cataloging-in-Publication Data
A catalog record for this book is available from the Library of Congress

For information on all Academic Press publications
visit our website at http://store.elsevier.com/

Acknowledgment

The front cover image is provided courtesy of Schlumberger Water Services. The image represents a uniform grid for a multi-layer finite-difference MODFLOW model and was produced using the software Visual MODFLOW Flex. Colors at the top of the image represent changes in land surface elevation; colors in the bottom layers represent geologic variability. The back cover graphic is a word cloud created using all text contained in Chapters 1—12. Word-cloud graphics included with the introductory sections of the book consist of text contained in each section. All word clouds were generated using Wordle, created by Jonathon Feinberg (www.wordle.net).

...to Charles, Jean, and Lori

This page intentionally left blank

CONTENTS

Boxes

Boxes

LIST OF FIGURES

LIST OF TABLES

This page intentionally left blank

PREFACE

Art and science have their meeting point in method.

Edward George Bulwer-Lytton

This second edition is motivated by the many significant developments in groundwater modeling since the first edition was published in 1992. The increased computational speed and capacity of present day multicore computers as well as the availability of sophisticated graphical user interfaces (GUIs) and geographical information systems have transformed groundwater modeling. But more importantly, new ways of calibrating models and analyzing uncertainty and new powerful codes that provide enhanced modeling tools are revolutionizing the science of groundwater modeling. In this second edition, we discuss many of the important advances in applied groundwater modeling introduced since 1992 and also update the treatment of fundamentals of groundwater flow modeling covered in the first edition. The chapters on model calibration and forecasting (Chapters 9 and 10 in the second edition) are entirely new and include discussion of new tools for parameter estimation and uncertainty analysis in forecast simulations. Similar to the first edition, our book is intended as an introduction to the applied science of modeling groundwater flow. We focus on groundwater modeling practice. For a more theoretical approach to groundwater modeling, the reader is referred to textbooks by Diersch (2014) and Bear and Cheng (2010).

Quantitative analysis of groundwater flow is essential to all hydrogeological problems, and groundwater models are the essential tools in such analyses. Groundwater flow models solve for what cannot be fully observed or measured—the distribution of head in space and time. Important associated information such as water budgets, flow rates, and flowpaths to and from surface water bodies and wells can be calculated from the head distribution. The focus of our book is mastering groundwater flow models, a critical first step for a groundwater modeler.

Although many groundwater problems can be solved by analyzing groundwater flow alone, some problems require analysis of the movement of solutes or contaminants in the subsurface. A transport model includes representation of advective transport, dispersion, and chemical reactions to solve for solute or contaminant concentrations. Transport modeling is beyond the scope of our textbook but is covered in detail by Zheng and Bennett (2002). However, the starting point for transport modeling is a good groundwater flow model because a transport code uses output from a groundwater flow model. Moreover, some transport problems can be addressed by considering only advective transport using a particle tracking code as a postprocessor to a groundwater flow model to calculate flowpaths and travel times. We discuss those types of problems in a chapter on particle tracking (Chapter 8 in the second edition) that was revised and updated from the first edition.

Mastery of groundwater modeling requires both art and science. The science of groundwater modeling includes basic modeling theory and numerical solution methods. There are many textbooks that provide advanced, intermediate, and elementary treatments of the science and underlying mathematics of numerical modeling of groundwater flow. Since 1992, applied groundwater science has expanded to include theory and methods for parameter estimation (inverse solutions) and uncertainty analysis, and there are books devoted exclusively to those topics (e.g., Doherty, 2015; Aster et al., 2013; Hill and Tiedeman, 2007). Although our text provides some of the background information for applying groundwater models to field problems, we assume that the reader knows the basic principles of hydrogeology and modeling as covered in standard textbooks such as Fitts (2013), Kresic (2007), Todd and Mays (2005), Schwartz and Zhang (2003), and Fetter (2001). A rudimentary knowledge of the theory of groundwater modeling including the basics of finite-difference and finite-element methods as contained in Wang and Anderson (1982) is also helpful.

Our book is meant to be accessible to those who want to apply groundwater models as tools. To use an analogy presented to us years ago by Professor John Wilson (New Mexico Tech), using a model is like driving a car. A good driver knows the rules of the road and has the skill to control the car under a wide variety of conditions and avoid accidents, but does not necessarily understand the intricacies of what goes on under the hood of the car. The goal of this book is to help the reader learn how to be a good driver and operate a model under a wide variety of conditions and avoid "accidents." To help in this, we have included a section at the end of each chapter in which we list common modeling errors—some we have encountered and many we have made ourselves. Eventually, after learning how to drive well, a modeler may want to explore the mechanics of a code (i.e., look under the hood of the car); familiarity with code mechanics helps the modeler understand the strengths and limitations of a specific code and will help the modeler modify the code if necessary.

The art of modeling is gained mainly through experience; by developing and applying groundwater models one develops "hydrosense" and modeling intuition (Hunt and Zheng, 2012). Our book provides guidance in the fundamental steps involved in the art of modeling: developing a conceptual model, translating the qualitative conceptual model to a quantitative (numerical) model, and assessing model input and output. Given that "art and science have their meeting point in method," our objective is to describe methods of applying groundwater flow models, and thereby provide a compact comprehensive reference to assist those wishing to develop proficiency in the art of modeling.

The book comprises four sections. Section 1, Modeling Fundamentals (Chapters 1, 2, and 3), lays out the motivation for modeling, describes the process of formulating a conceptual model, and provides the theoretical and numerical base. Section 2, Designing the

Numerical Model (Chapters 4 through 7), describes how to translate the conceptual model of groundwater flow into a numerical model, including grid/mesh design, selecting boundary and initial conditions, and setting parameter values. Section 3, Particle Tracking, Calibration, Forecasting, and Uncertainty Analysis (Chapters 8 through 10) discusses particle tracking and model performance. Section 4, The Modeling Report and Advanced Topics (Chapters 11, 12) discusses the modeling report and archive, model review, and briefly covers topics beyond basic groundwater flow modeling.

In the first edition, we made extensive reference to specific flow and particle tracking codes to illustrate examples of modeling mechanics. However, the number and capabilities of groundwater codes have increased dramatically since 1992. In the second edition, we illustrate how fundamental modeling concepts are implemented in two representative groundwater flow codes: MODFLOW (for finite-difference methods) and FEFLOW (for finite-element methods). We use MODFLOW (http://water.usgs.gov/ogw/modflow/MODFLOW.html) because it is freeware, open-source, well-documented, versatile, used worldwide and in the US is the standard code in regulatory and legal arenas. The proprietary code FEFLOW is widely used, versatile, well-supported, and well-documented both online (http://www.feflow.com/) and in a textbook (Diersch, 2014). We selected the PEST software suite (http://www.pesthomepage.org) to illustrate how concepts of parameter estimation can be implemented. The PEST suite of codes (Doherty 2014, 2015; Welter et al., 2012; Fienen et al., 2013) is freeware and open-source, includes widely used approaches for parameter estimation with many advanced options. A version of PEST (PEST++ by Welter et al., 2012) is supported by the U.S. Geological Survey (http://pubs.usgs.gov/tm/tm7c5/). In practice, the modeler will typically use these codes within a GUI. The details of how the codes work within a GUI are not covered in our book. The reader should expect to spend practice time with a GUI to be accomplished in using these or any other codes.

The many new developments and advances in groundwater modeling since the first edition are supported by an enormity of literature. Therefore, we developed some general guidelines for presentation of material in the second edition.

- We focus on "the norm" rather than "the exception" in order to guide the reader to the most likely productive approach for most problems.
- We use language and mathematics accessible to the beginning and intermediate level groundwater modeler and try to avoid jargon. Necessarily, the advanced modeler may find our presentation at times overly simple or lacking in rigor.
- For the most part, we reference widely available software; the vast majority of applied groundwater modeling is done with off-the-shelf software.
- We recognize that software, jargon, and methods will change in the future. Therefore, our text focuses on the basic principles of groundwater modeling that will endure. However, we use code-specific language and variable names when we believe that such specificity is beneficial.

- We mainly cite work published in the twenty-first century, as well as classic (benchmark) papers. References cited should be regarded as portals into the large body of pertinent literature on a specific topic. That is, the provided reference is cited not only for itself but also for all the work cited therein. In this way, the reader is given the opportunity to consult a broad body of literature and explore a research thread. Reports published by the U.S. Geological Survey are available for free download at http://www.usgs.gov or at the provided Universal Resource Locators (URLs).

With the maturing of the science, groundwater modeling has become more interdisciplinary and relevant publications are distributed across a wide variety of journals. No textbook can fully cover all the relevant literature. Therefore, we apologize in advance to those who may feel we have overlooked their contributions.

The second edition has an associated Web site that will contain background material, example problems, and links to other modeling resources (http://appliedgwmodeling.elsevier.com). We hope this material, together with the textbook, will be useful on two levels: (1) for teaching undergraduate and graduate level courses in applied groundwater modeling; (2) as a reference for environmental consultants and those in industry and governmental agencies. In its broadest intent, our book is meant for those who want to learn how to build, use, and assess groundwater flow models. We hope that reading this book will facilitate a life-long journey in groundwater modeling.

All things are ready, if our minds be so.

—Henry V, Act IV

Mary P. Anderson, Madison, Wisconsin
William W. Woessner, Missoula, Montana
Randall J. Hunt, Cross Plains, Wisconsin

REFERENCES

Aster, R.C., Borchers, B., Thurber, C.H., 2013. Parameter Estimation and Inverse Problems, second ed. Elsevier, 360 p.

Bear, J., Cheng, A.H.D., 2010. Modeling Groundwater Flow and Contaminant Transport. In: Theory and Applications of Transport in Porous Media, vol. 23. Springer, 834 p.

Diersch, H.-J.G., 2014. FEFLOW: Finite Element Modeling of Flow, Mass and Heat Transport in Porous and Fractured Media. Springer-Verlag, Berlin, Heidelberg, 996 p.

Doherty, J., 2014. PEST, Model-independent Parameter Estimation. User Manual (fifth ed., with slight additions). Watermark Numerical Computing, Brisbane, Australia.

Doherty, J., 2015. Calibration and Uncertainty Analysis for Complex Environmental Models. Watermark Numerical Computing, Brisbane, Australia, ISBN: 978-0-9943786-0-6, 227 p.

Fetter, C.W., 2001. Applied Hydrogeology, fourth ed. Pearson Education Limited, Prentice Hall, Upper Saddle River, N.J., 612 p.

Fienen, M.N., D'Oria, M., Doherty, J.E., Hunt, R.J., 2013. Approaches in Highly Parameterized Inversion: BgaPEST, a Bayesian Geostatistical Approach Implementation with PEST. U.S. Geological Survey Techniques and Methods Report 7(C9), 86 p. http://pubs.usgs.gov/tm/07/c09/.
Fitts, C.R., 2013. Groundwater Science, second ed. Academic Press, London, 672 p.
Hill, M.C., Tiedeman, C.R., 2007. Effective Groundwater Model Calibration. John Wiley & Sons, Hoboken, N.J., 455 p.
Hunt, R.J., Zheng, C., 2012. The current state of modeling. Groundwater 50 (3), 329–333.
Kresic, N., 2007. Hydrogeology and Groundwater Modeling, second ed. CRC Press, Boca Raton, FL, 807 p.
Schwartz, F.W., Zhang, H., 2003. Fundamentals of Ground Water. John Wiley & Sons, Hoboken, N.J., 583 p.
Todd, D.K., Mays, L.W., 2005. Groundwater Hydrology, third ed. John Wiley & Sons, Inc., Hoboken, N.J., 636 p.
Wang, H.F., Anderson, M.P., 1982. Introduction to Groundwater Modeling: Finite Difference and Finite Element Methods. Academic Press, San Diego, CA, 237 p.
Welter, D.E., Doherty, J.E., Hunt, R.J., Muffels, C.T., Tonkin, M.J., Schreüder, W.A., 2012. Approaches in Highly Parameterized Inversion—PEST++, a Parameter ESTimation Code Optimized for Large Environmental Models. U.S. Geological Survey Techniques and Methods 7(C5), 47 p. http://pubs.usgs.gov/tm/tm7c5/.
Zheng, C., Bennett, G.D., 2002. Applied Contaminant Transport Modeling, second ed. John Wiley & Sons, New York, 621 p.

This page intentionally left blank

DISCLAIMER

The material in this book is intended to guide those familiar with the basics of hydrogeology and groundwater flow modeling in developing numerical groundwater flow models of field problems. Although the information in this book is presented in the belief that it will help the reader to minimize errors, no responsibility is assumed by the authors, the U.S. Government and other institutions with which the authors are affiliated, or the publishers for any errors, mistakes, or misrepresentations that may occur from the use of this book, and no compensation will be given for any damages or losses whatever their cause.

Any use of trade, firm, or product names is for descriptive purposes only and does not imply endorsement by the U.S. Government.

This page intentionally left blank

ACKNOWLEDGMENTS

We are indebted to the many valuable comments by our reviewers who read the book in manuscript form. We especially thank Charles Andrews and Rodney Sheets who read the entire book and provided many helpful technical and editorial comments and Kevin Breen for his thorough and careful review of a near final version of the manuscript. Michael Cardiff, Michael Fienen, Andrew Leaf, and Jeremy White provided thoughtful and detailed comments on Chapters 9 and 10. Hans-Jörg Diersch, Henk Haitjema, and Kurt Zeiler gave us valuable comments on other chapters.

We also thank the many individuals who provided insights and help in conversations and via email over the years, including Daron Abby, Daniel Abrams, William Arnold, Jean Bahr, Mark Bakker, Paul Barlow, Brian Barnett, Okke Batelaan, Jordi Batlle-Aguilar, Steffen Birk, Kenneth Bradbury, John Bredehoeft, Philip Brunner, John Cherry, Steen Christensen, Brian Clark, K. William Clark, Thomas Clemo, Peter Cook, Le Dung Dang, Alyssa Dausman, Geoff Delin, Martin Dietzel, John Doherty, Matthew Ely, Daniel Feinstein, Charles Fitts, Devin Galloway, Joseph Guillaume, Keith Halford, Randall Hanson, Arlen Harbaugh, Glenn Harrington, David Hart, Mary Hill, Joseph Hughes, Steven Ingebritsen, Dylan Irvine, Anthony Jakeman, Scott James, Igor Jankovic, Paul Juckem, Elizabeth Keating, Victor Kelson, Stefan Kollet, Leonard Konikow, James Krohelski, Eve Kuniansky, Christian Langevin, Stanley Leake, Yu-Feng Lin, Fabien Magri, Marco Maneta, Steve Markstrom, Gregoire Mariethoz, Luis Marin, Ghislain de Marsily, Paul Martin, James McCallum, David McWhorter, Steffen Mehl, Allen Moench, Leanne Morgan, Eric Morway, Shlomo Neuman, Christopher Neuzil, Christopher Neville, Tracy Nishikawa, Richard Niswonger, Saskia Noorduijn, Gunnar Nützmann, Thomas Osborne, Sorab Panday, Berh Parker, Adam Perine, Eileen Poeter, Vincent Post, David Prudic, Larry Putnam, Todd Rayne, R. Steve Regan, James Rumbaugh, Willem Schreüder, Margaret Shanafield, Craig Simmons, Campbell Stringer, Otto Strack, Michael Sukop, Amelia Tallman, Michael Teubner, Lloyd Townley, Herbert Wang, Lieke Van Roosmalen, Chani Welch, David Welter, Adrian Werner, Stephen Westenbroek, Gerfried Winkler, Ray Wuolo, Yueqing Xie, Richard Yager, Chunmiao Zheng, Vitaly Zlotnik, and members of the 2011 and 2012 NCGRT Modeling and Research Groups at Flinders University, Australia. Marie Dvorzak provided library assistance at UW-Madison. Mary Devitt and her Crossroads Coffeehouse staff are kindly thanked for providing "office space" and "fuel" for a portion of the writing process.

Last but not least, we thank our families especially our spouses, and James and Johanna Hunt for their patience.

I can no other answer make but thanks,
And thanks, and ever thanks

—***Twelfth Night, Act III, Scene III***

This page intentionally left blank

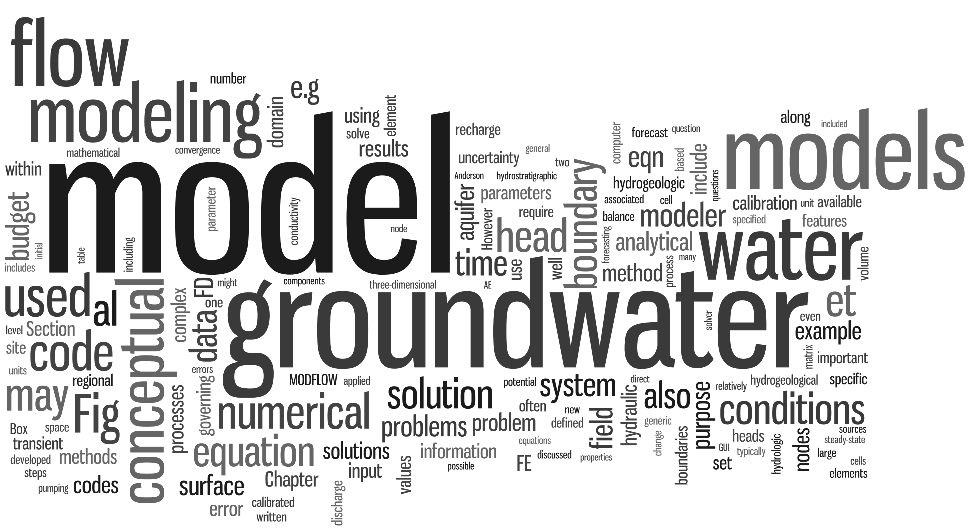
SECTION 1

Modeling Fundamentals

It is a capital mistake to theorise before one has data. Insensibly one begins to twist facts to suit theories, instead of theories to suit facts.

Sherlock Holmes in "Scandal in Bohemia" by Sir Arthur Conan Doyle.

In Chapters 1 and 2, we summarize the modeling process and discuss the modeling purpose and the conceptual model that forms the basis for the numerical model. Chapter 3 briefly reviews the differential equations and boundary conditions used in groundwater flow modeling and the methods for solving analytical, analytic element, and numerical (finite-difference, finite-element, and control volume finite-difference) models. We also discuss code selection and execution and the computed water budget.



This page intentionally left blank

CHAPTER 1

Introduction

Science, like art, is not a copy of nature but a re-creation of her.

Jacob Bronowski (1956, Science and Human Values Part 1)

Contents

Boxes

1.1 MOTIVATION FOR MODELING

Groundwater hydrologists are often asked questions about groundwater flow systems and management of groundwater resources. The following is a representative sampling of these types of questions.

Applied Groundwater Modeling
ISBN 978-0-12-058103-0, http://dx.doi.org/10.1016/B978-0-12-058103-0.00001-0

How will pumping affect groundwater levels in the North China Plain in the next 100 years?
How will proposed land use change affect groundwater discharge to wetlands and streams in Madison, Wisconsin, USA?
How will water management decisions related to water diversions affect groundwater levels in the Nubian Sandstone of Egypt and Libya in the next 50 years?
How will climate change affect groundwater levels and groundwater discharge to surface water bodies in temperate forests in northern Wisconsin, USA?
How long will it take for water levels in a lake created as a result of open pit mining in Guyana to reach equilibrium after dewatering operations cease?
What is the capture area of a well field that supplies municipal water to Graz, Austria?
Where and when should groundwater be sampled to identify potential leakage of a clay liner beneath a landfill in Mexico City?
How long will it take contaminants leaching into groundwater from an abandoned industrial site in Tokyo to reach the property boundary?

Providing answers to these seemingly straightforward questions requires considerable specific hydrogeologic information and analyses, as well as general hydrogeologic knowledge, insight, and professional judgment. Even relatively simple groundwater problems require values of aquifer parameters and hydrologic stresses such as pumping and recharge rates.

A groundwater model provides a quantitative framework for synthesizing field information and for conceptualizing hydrogeologic processes. The organization imposed by a model helps alert the modeler to errors in assumptions and to processes not previously considered. In other words: "…applying a model is an exercise in thinking about the way a system works" (Anderson, 1983). For this reason, mathematical modeling should be performed at the beginning of every hydrogeological study that addresses nontrivial questions (e.g., see Bredehoeft and Hall, 1995).

Tóth (1963) gave compelling justification for modeling, which is still valid today: "Whereas it is practically impossible to observe separately all phenomena connected with a regime of groundwater flow, a correct theory discloses every feature and draws attention to the most important properties of the flow." Or put another way, given that the subsurface is hidden from view and analysis is hampered by lack of field observations, a model is the most defensible description of a groundwater system for informed and quantitative analyses as well as forecasts about the consequences of proposed actions.

Therefore, although not all hydrogeological problems require a model, almost every groundwater problem will benefit from some type of model, if only as a way to organize field data and test the conceptual model. A corollary to the question "why model?" is the question "what else if not a model?" In the 1st edition of this book we included discussion of the debate over the worth of models then current in the literature. Today, groundwater models are accepted as essential tools for addressing groundwater problems.

1.2 WHAT IS A MODEL?

A *model* is a simplified representation of the complex natural world. For example, a road map is a kind of model (Wang and Anderson, 1982); it depicts a complex network of roads in a simplified manner for purposes of navigation. Similarly, a conceptual model of a groundwater system simplifies and summarizes what is known about the hydrogeology in the form of written text, flow charts, cross sections, block diagrams, and tables. A conceptual model is an expression of the past and current state of the system based on field information from the site, and knowledge available from similar sites (Section 2.2). A more powerful groundwater model is one that quantitatively represents heads in space and time in a simplified representation of the complex hydrogeologic conditions in the subsurface. Broadly speaking, groundwater models can be divided into physical (laboratory) models and mathematical models.

1.2.1 Physical Models

Physical models include laboratory tanks and columns packed with porous material (usually sand) in which groundwater heads and flows are measured directly. For example, in pioneering work Darcy (1856) measured head in sand-packed columns of various diameters and lengths to show that flow in porous media is linearly related to the head gradient. Physical models are mostly used at the laboratory scale (e.g., Mamer and Lowry, 2013; Illman et al., 2012; Sawyer et al., 2012; Fujinawa et al., 2009). Analog models are laboratory models that rely on the flow of electric current (electric analog models; e.g., Skibitzke, 1961) or viscous fluids (Hele-Shaw or parallel plate models; e.g., Collins and Gelhar, 1971) to represent groundwater flow. Analog models of groundwater flow, especially electric analog models, were important in the 1960s before digital computers were widely available (e.g., see Bredehoeft, 2012).

1.2.2 Mathematical Models

We consider two types of mathematical models: data-driven models and process-based models. *Data-driven or "black-box" models* (Box 1.1) use empirical or statistical equations derived from the available data to calculate an unknown variable (e.g., head at the water table) from information about another variable that can be measured easily (e.g., precipitation). *Process-based models* (sometimes called physically based models although that usage is discouraged by Beven and Young, 2013) use processes and principles of physics to represent groundwater flow within the problem domain. Process-based models are either stochastic or deterministic. A model is *stochastic* if any of its parameters have a probabilistic distribution; otherwise, the model is *deterministic*. The focus of our book is process-based deterministic models, although we briefly discuss stochastic models in Boxes 10.1 and 10.4 and Section 12.5.

A process-based mathematical groundwater flow model consists of a *governing equation* that describes the physical processes within the problem domain; *boundary conditions* that specify heads or flows along the boundaries of the problem domain; and for time-dependent problems, *initial conditions* that specify heads within the problem domain at the beginning of the simulation. Mathematical models can be solved analytically or numerically. Mathematical models for groundwater flow are solved for the distribution of head in space and also in time for transient problems.

Analytical models require a high level of simplification of the natural world in order to define a problem that can be solved mathematically to obtain a closed-form solution. The resulting analytical solution is an equation that solves for a dependent variable (e.g., head) in space and for transient problems also in time. Simple analytical solutions can be solved using a hand calculator but more complex solutions are often solved using a spreadsheet or a computer program (e.g., Barlow and Moench, 1998), or special software (e.g., MATLAB, http://www.mathworks.com/products/matlab/). Assumptions built into analytical solutions limit their application to relatively simple systems and hence they are inappropriate for most practical groundwater problems. For example, few analytical solutions allow for three-dimensional flow or hydrogeological settings with heterogeneity or boundaries with realistic geometries. Numerical models are even replacing the Theis (1935) analytical solution for aquifer test analysis (e.g., Li and Neuman, 2007; Yeh et al., 2014). Nevertheless, analytical solutions are still useful for some problems

Box 1.1 Data-Driven (Black-Box) Models

Data-driven models use equations that calculate system response (e.g., head) to input stresses (e.g., recharge from precipitation) without quantifying the processes and physical properties of the system. First, a site-specific equation is developed by fitting parameters either empirically or statistically to reproduce the historical record (time series) of fluctuations in water levels (or flows) in response to stresses. Then, the equation is used to calculate the response to future stresses. Data-driven models require a large number of observations of head that ideally encompass the range of all expected stresses to the system. They are used by themselves (e.g., Bakker et al., 2007) or with a process-based model (e.g., Gusyev et al., 2013; Demissie et al., 2009; Szidarovszky et al., 2007).

Early applications of data-driven models analyzed the response of karst aquifers (Dreiss, 1989) and applications to karst systems continue to be popular and successful (Fig. B1.1.1). Artificial neural network (ANN) models are data-driven models that have received much interest in the recent literature (e.g., Sepúlveda, 2009; Feng et al., 2008; Coppola et al., 2005). Data-driven models are also developed using Bayesian networks (e.g., Fienen et al., 2013).

Generally, process-based models are preferred over data-driven models because process-based models can make acceptable forecasts when large numbers of observations are not available and when future conditions lie outside the range of stresses in the historical record, such as response to climate change.

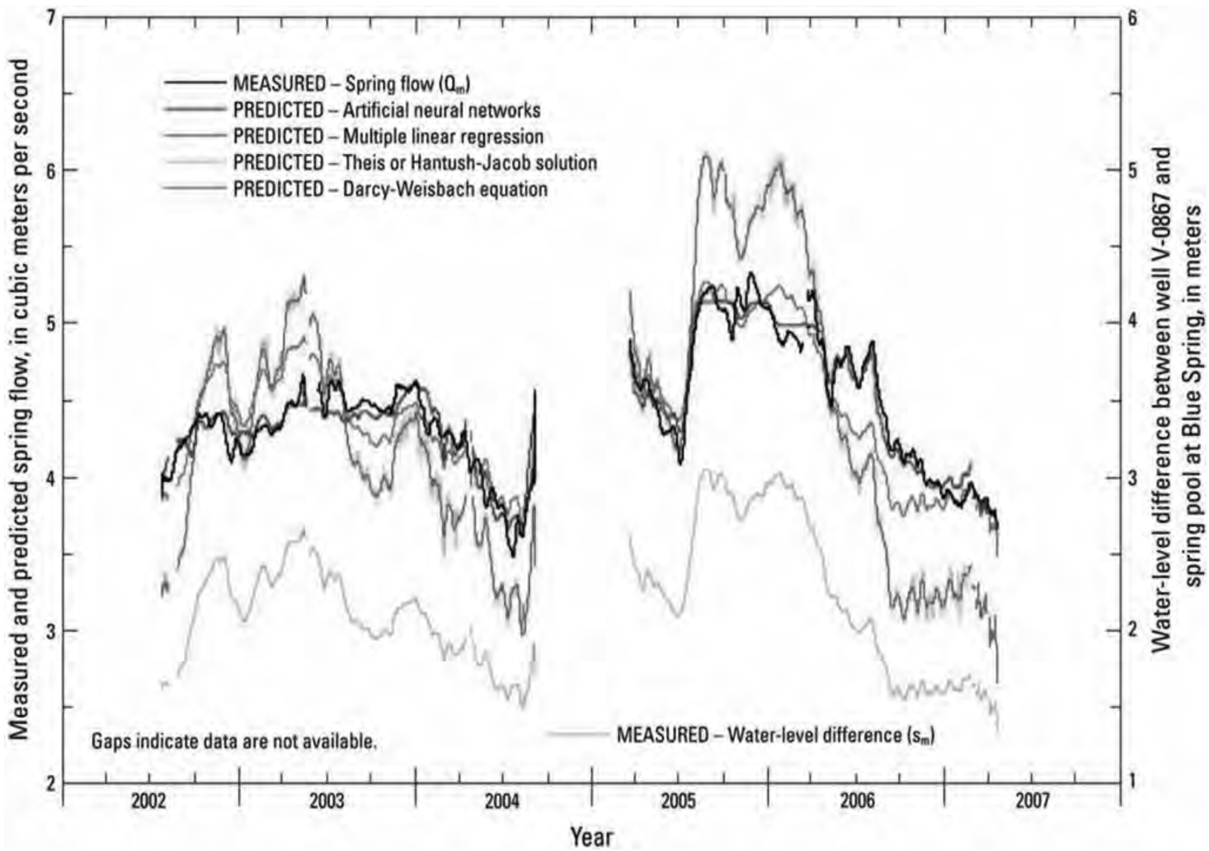


Figure B1.1.1 Springflow calculated using an ANN model and multiple linear regression compared with results from process-based models for continuous porous media (Theis or Hantush–Jacob solutions) and conduit flow (Darcy–Weisbach equation). Measured springflow is also shown *(Sepúlveda, 2009)*.

and also provide important insight into the behavior of groundwater systems (Box 3.2). Analytical models can be useful interpretive tools to guide construction of more complex numerical models (Haitjema, 2006). Analytical solutions are also used to verify that codes that solve numerical models are programmed correctly (Section 1.6).

The analytic element (AE) method (Haitjema, 1995; Strack, 1989) provides a way to extend analytical solutions to more complex problems. The AE method relies on a computer code to superpose certain types of analytical solutions, known as analytic elements, which are based on Green's functions and include solutions with point/line sources and sinks. AE models can incorporate complex boundary geometry and zones of heterogeneity, but currently have limited applicability for highly heterogeneous and transient problems (Hunt, 2006), although development of new AE solutions is an active area of research (e.g., Kuhlman and Neuman, 2009). Currently, AE models are most commonly applied to two-dimensional and steady-state groundwater flow problems (e.g., see Hunt, 2006; Haitjema, 1995). AE models are also useful for guiding assignment of regional boundary conditions for three-dimensional and transient modeling (Section 4.4).

Numerical models, typically based on either the finite-difference (FD) or the finite-element (FE) method, allow for both steady-state and transient groundwater flow in three dimensions in heterogeneous media with complex boundaries and a complex network of sources and sinks. Owing to their versatility, FD and FE models are most commonly used to solve groundwater problems and are the focus of our book.

Mathematical groundwater models are used to simulate both local and regional settings. Although some questions can, and should, be addressed with analytical models or simple numerical models, many problems require a more sophisticated representation of the groundwater system. Increased computing power and new codes and tools allow complex and large regional systems to be efficiently simulated. The sophistication, or complexity, of a numerical model is often measured by the number of processes included and the number of layers, cells/elements, and parameters it contains. Numerical methods assign parameter values to points (nodes) in the model domain and it is not uncommon for models to have millions of nodes. For example, Frind et al. (2002) described a three-dimensional, 30-layer FE model of the Waterloo Moraine aquifer system (Ontario, Canada) that used 1,335,790 nodes and 2,568,900 elements. A three-dimensional FD model of the Lake Michigan Basin (Feinstein et al., 2010) used over two million nodes. Kollet et al. (2010) discussed groundwater models that contained 8×10^9 FD cells. Although values of hydrogeologic parameters must be assigned to every node, cell, or element, in practice it is usual to delineate areas (zones) in the problem domain in which a constant value is assigned to all the nodes (Section 5.5). Hence, zonation effectively reduces the number of parameters. Other methods of parameterization and the issue of complexity in groundwater models are discussed in Chapter 9.

We use the term *groundwater model* or model to mean the mathematical representation and associated input data for a specific problem. A *code* is a computer program that processes the input data for a specific model and solves the process-based equations (Section 3.2) that describe groundwater processes. A code is written in one or more computer languages and consists of a set of equations that is solved by a computer. For example, PEST and the FD code MODFLOW are written in the computer language Fortran; PEST++ and the FE code FEFLOW are written in C/C++. A code that solves for groundwater flow calculates head in space and time, along with associated quantities such as flow. A *particle tracking code* takes output from a groundwater flow code and calculates groundwater flowpaths and associated travel times (Chapter 8). Codes are sometimes called groundwater models but we distinguish between a specific application of a code, which is a model, and the code itself, which is the tool for solving the model. A different groundwater model is designed for each application whereas the same code is used to solve many different problems.

1.3 PURPOSE OF MODELING

The starting point of every groundwater modeling application is to identify the purpose of the model (Fig. 1.1). The most common purpose is to forecast the effects of some future action or hydrologic condition, but models are also used to re-create past conditions (hindcasting) and also as interpretive tools. Reilly and Harbaugh (2004, p. 3) identify five broad categories of problems for groundwater modeling: basic understanding of groundwater systems; estimation of aquifer properties; understanding the present; understanding the past; and forecasting the future. We group the first three of these categories into interpretive models and the last two into forecasting/hindcasting models. We discuss forecasting/hindcasting models first.

1.3.1 Forecasting/Hindcasting Models

The objective of the vast majority of groundwater models is to forecast or predict results of a proposed action/inaction. Forecasting simulations are designed to address questions like those listed at the beginning of this chapter. We prefer the term forecast over prediction to emphasize that a forecast always contains some uncertainty. For example, a weather forecast is typically stated in terms of a probability (of rain, for example). Forecasting models (Chapter 10) are typically first tested by comparing model results to field measurements in a history matching exercise that is part of model calibration (Chapter 9). In history matching, parameters are adjusted within acceptable limits until model outputs, primarily heads and flows, give a satisfactory match to field-measured (observed) values. The calibrated model is then used as the base model for forecasting simulations.

Hindcasting (or back-casting) models are used to re-create past conditions. Hindcasting models may involve both a groundwater flow model and a contaminant transport model to simulate the movement of a contaminant plume. Examples of hindcasting models include those used in the well-known Woburn, Massachusetts Trial (Bair, 2001) and

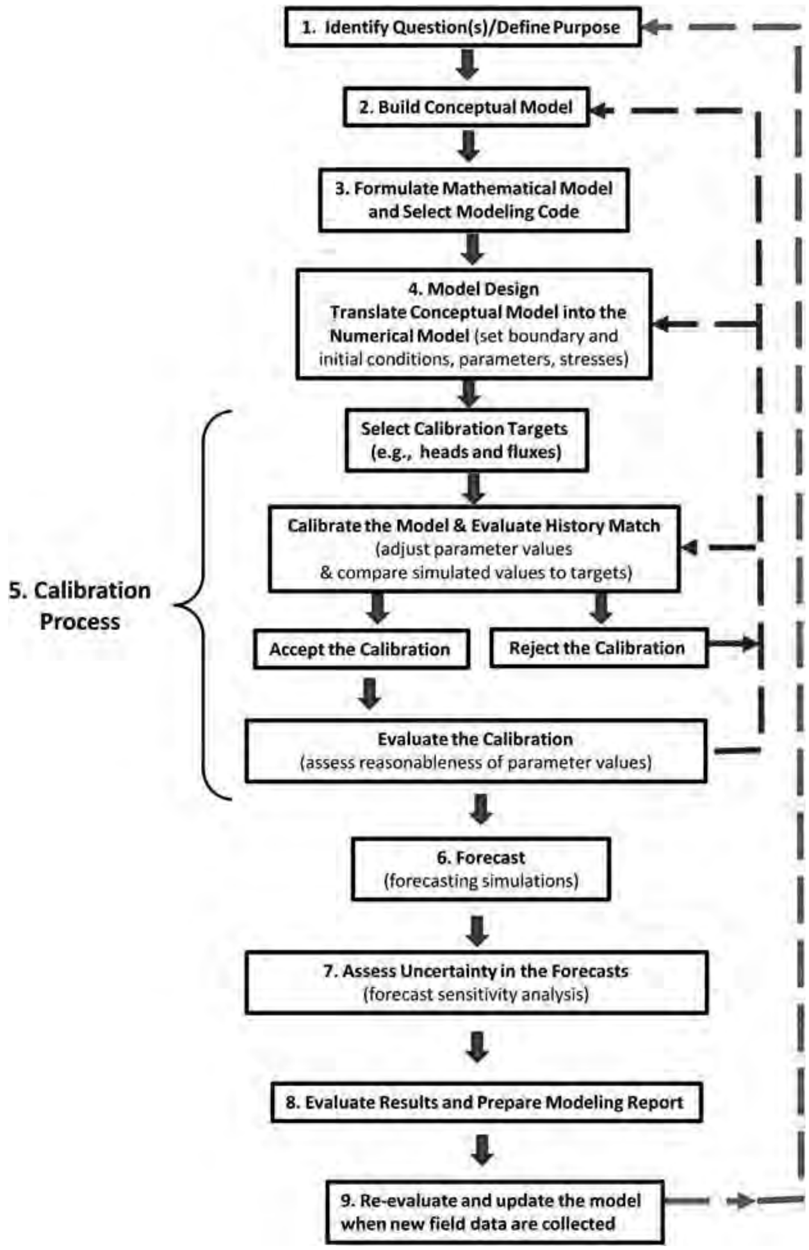


Figure 1.1 Workflow for groundwater modeling. As presented, the workflow assumes the objective of the model is a forecast but the workflow can be adapted for other modeling purposes, as described in the text. Although not shown in the figure, field data are critical for the workflow, especially conceptual model design and the calibration process.

at a military base in North Carolina (Clement, 2011). Hindcasting applications are "uniquely challenging" (Clement, 2011) because it is not possible to collect additional observations to augment the existing historical dataset, which is often meager.

1.3.2 Interpretative Models

Interpretive models include those used as: (1) *engineering calculators* that quickly give an answer to a specific engineering question; (2) *screening models* that help the modeler develop an initial understanding of a groundwater system and/or test hypotheses about the system; (3) *generic models* that explore processes in generic hydrogeologic settings. Models used as engineering calculators and generic models usually are not calibrated. Screening models may or may not be calibrated.

An example application of an interpretive model as an engineering calculator is the use of analytical and numerical models to calculate aquifer parameters from drawdown data obtained in an aquifer (pumping) test. Analytical models and sometimes numerical models are used as engineering calculators to verify new codes (Section 1.6).

A screening model vets a conceptual model or tests hypotheses about the flow system. A screening model might help in designing a more complex numerical model. For example, Hunt et al. (1998) developed a two-dimensional AE model as a screening model to develop boundary conditions for a three-dimensional FD model. Interpretive models also are used to conceptualize system dynamics and provide general insights into controlling parameters or processes at a field site. For example, during a major oil spill from a damaged well in the Gulf of Mexico, Hsieh (2011) quickly developed an interpretive MODFLOW model (adapted to simulate flow in a petroleum reservoir) to determine if measured shut-in pressure in the damaged well was indicative of a potential future catastrophic rupture of the capped well. The results were used to make the decision not to uncap the well to reduce reservoir pressure, which proved to be the correct course of action.

Generic models are interpretive models applied to idealized groundwater systems. Generic models were used in the early days of numerical modeling of groundwater flow and continue to be useful. For example, Freeze and Witherspoon (1967) and Zlotnik et al. (2011) used two-dimensional generic models to study the effects of heterogeneity on regional groundwater flow in cross section. Woessner (2000) and Sawyer et al. (2012) used generic models to study exchange between groundwater and streams at the aquifer/stream interface (the hyporheic zone). Sheets et al. (2005) used generic models to assess the effect of pumping near regional groundwater divides.

1.4 LIMITATIONS OF MODELS

Groundwater models are simplifications of reality and thus are limited by underlying simplifying approximations as well as by nonuniqueness and uncertainty (Chapters 9 and 10). Groundwater models never uniquely represent the complexity of the natural world. Therefore, groundwater models that represent the natural world have some level of uncertainty that must be evaluated and reported. In that respect, forecasting simulations for groundwater are similar to weather forecasts. Weather forecasts combine extensive datasets, representations of atmospheric physics, meteorology, and real-time satellite images within a highly sophisticated model, but the daily forecast is always given with probabilities. Similarly, results from groundwater models should be qualified by specifying the nature and magnitude of uncertainty associated with a forecast (Section 10.6).

1.4.1 Nonuniqueness

Nonuniqueness in groundwater models means that many different combinations of model inputs produce results that match field-measured data. Consequently, there will always be more than one possible reasonable model. Although early groundwater modeling applications typically reported only one calibrated model and presented only one possible forecast, this is unacceptable practice today. Either multiple calibrated models are carried forward in the analysis or the modeler choses a preferred calibrated model and constructs error bounds around forecasted outputs. In either case, it is acknowledged that a groundwater model cannot give a single true answer.

Although models are critical tools, professional judgment, guided by modeling intuition and hydrogeological principles, is always required during a modeling project. Recognition of model uncertainty and nonuniqueness motivates the following underlying philosophy of modeling: "…a model cannot promise the right answer. However, if properly constructed, a model can promise that the right answer lies within the uncertainty limits which are its responsibility to construct" (Doherty, 2011).

1.4.2 Uncertainty

Uncertainty in groundwater models (Sections 10.2, 10.3) arises from a number of factors related to representing groundwater processes. In selecting a particular code, the modeler indirectly makes assumptions about the set of hydrologic processes important to the modeling objective because the selection of a code in effect reduces all processes under consideration to only those included in the code. Furthermore, current and future hydrogeologic conditions represented in a model cannot be fully described or quantified. Hunt and Welter (2010) described one source of uncertainty as "unknown unknowns," which are "…things we do not know we don't know" (from Former US. Secretary of Defense Donald Rumsfeld, February 12, 2002 press briefing). In groundwater models, *unknown unknowns* include unexpected (and hence unmodeled) hydrogeologic features such as heterogeneities in subsurface properties, as well as unanticipated future stresses. Bredehoeft (2005) cautioned modelers to anticipate the model "surprise" that occurs when new data reveal system responses caused by unmodeled hydrologic processes. For example, in a forecasting model there is uncertainty over future hydrological conditions (e.g., recharge rates) as well as future pumping rates and locations of new wells, which depend on uncertain societal and economic drivers.

Although some types of forecasts are more uncertain than others (Section 10.3), uncertainty can only be reduced, never eliminated. Therefore, groundwater modelers need to develop an awareness of the uncertainties that influence modeling results and a healthy skepticism of modeling output. Modeling intuition (Haitjema, 2006) and "hydrosense" (Hunt and Zheng, 2012) help a modeler evaluate modeling output and identify flawed results. Modeling processes and results need to undergo rigorous "sensibility analyses" that are rooted in basic hydrogeologic principles.

1.5 MODELING ETHICS

Ethics refer to pursuing a course of action that leads to morally right outcomes. Ethics in groundwater modeling means that the groundwater modeler acts in a morally responsible manner when planning, designing, and executing models and presenting modeling results. Ethics also means that the modeler remains unbiased and objective and strives to model according to the best available science for the modeling purpose. The modeler must maintain scientific integrity even when the results are not what the client expects, and when models enter regulatory and legal arenas. Tensions can arise between the modeler and teams of interdisciplinary scientists, lawyers, regulators, and stakeholders including industrial clients and the public-at-large. The modeler must resist inappropriate pressure from those groups as well as the pressure of societal, environmental, and regulatory concerns and steadfastly perform ethical modeling.

Modeling may be driven by regulatory concerns or even mandated by regulations. For example, groundwater models are required by the European Water Framework Directive (Hulme et al., 2002) or regulations may be written in such a way that the best (perhaps even only) way to satisfy a regulatory obligation is by groundwater modeling. When models are discussed in the courtroom, the modeler must be especially vigilant to present objective, unbiased results based on sound science. The U.S. Federal Court trial regarding groundwater contamination in Woburn, Massachusetts, which was the subject of a popular book (Harr, 1995) and a movie (*A Civil Action*), was notable for the conflict and confusion that surrounded the interpretation of the hydrogeologic system (Bair, 2001; Bair and Metheny, 2011; also see *Science in the Courtroom: The Woburn Toxic Trial:* http://serc.carleton.edu/woburn/index.html). In that case, competing groundwater models (a one-dimensional steady-state model and a three-dimensional, transient model) and differences in opinion among three expert witnesses over the basic hydrogeology and appropriate parameter values led to difficulties in fact-finding needed to reach a verdict.

Ethical issues may arise over decisions about model design (especially as related to model complexity), model bias, presentation of results, and costs of modeling. Each of these is discussed below.

1.5.1 Model Design

In designing a model, the groundwater hydrologist, sometimes in concert with the client, regulators and stakeholders, proposes the analyses best suited to address the question(s) being posed. A numerical groundwater model may not be necessary if the questions can be answered more effectively using an analytical solution, an AE model, a data-driven model (Box 1.1), or analysis of field data without a model. For example, Kelson et al. (2002) showed that a simple AE model quickly provided the same insight into the effects of dewatering caused by a proposed mine as complex three-dimensional numerical models. However, for many complex problems a numerical model may be the best way to answer the questions. For the mine site considered by Kelson et al. (2002), questions about on-site disposal of mine tailings and the potential for contamination of groundwater and surface water were best addressed with a more comprehensive numerical model.

It may be clear before, during, or after a modeling effort that the available data are inadequate to constrain modeling results to a reasonable range suitable for decision-making. Clement (2011) discussed a highly complex state-of-the-art numerical hindcasting model where the historical data were judged insufficient to support the modeling effort. An independent panel of experts recommended that future hindcasting models for other parts of the site utilize simpler models including analytical models. The modelers disagreed with that assessment (Maslia et al., 2012), arguing that complex models are useful even when not fully supported by field data. The argument over simplicity *vs* complexity when designing groundwater models is a common topic in the literature (e.g., Simmons and Hunt, 2012; Hunt et al., 2007; Hill, 2006; Gómez-Hernández, 2006). Models should include processes and parameters essential to addressing the model's purpose, but exclude those that are not. Defining the optimal compromise between simplicity and complexity is part of the art of modeling and is one of the biggest challenges in modeling (Doherty, 2011). Simplifications come in many forms—for example, in the processes included or excluded from the model, and in the discretization of space and time, selection of boundary conditions, and parameter assignment. Each decision to simplify the complex natural world will influence the model's ability to simulate some facet of the actual hydrogeologic conditions.

1.5.2 Bias

Critics of modeling argue that models can be designed to produce whatever answer the modeler wants. Professionalism and ethics, however, require the modeler to design the model without introducing approximations that bias results. A simple example of deliberate bias is if a modeler consciously and inappropriately assigns a specified head boundary condition in order to minimize drawdown from pumping. (A specified head boundary allows an infinite amount of water to flow into the model and thereby mitigates the effect of pumping by maintaining heads at unnaturally high levels (Section 4.3).) Concerns over bias motivate a requirement for peer review of modeling reports (Section 11.4). In-house review by senior hydrogeologists or engineers and by outside experts, regulators, opposing parties, and even the interested public is common. Quality assurance review can be helpful to the modeler in identifying inadvertent modeling errors, but when performed by an independent party, especially one engaged by an opposing party, such errors can support concerns of deliberate bias. The perception of bias is reinforced if either the modeler or reviewers neglect to reveal any potential conflicts of interest and areas of personal bias.

Critics often question whether a modeler paid by a client can remain independent and avoid bias. It is essential that modelers maintain their independence and preserve their professional credibility. The modeler has the obligation to give honest scientific and engineering assessments in return for compensation for work performed. The payment for work performed is not itself at issue but there may be the perception that the resulting model is biased to produce results favorable to the client. Such concerns over perceived bias can be addressed by careful and deliberate presentation of results, as discussed below.

1.5.3 Presentation of Results

With today's sophisticated codes and graphics packages it is relatively easy to produce visually impressive figures and tables. But ethics require that assumptions and approximations built into the model are clearly identified in the modeling report and in oral presentations. Inadequacies in field data should be discussed and uncertainties in modeling results should be quantified and discussed. Directly addressing potential concerns about the model's trustworthiness helps safeguard the modeler against claims of bias. Preparation of the modeling report is discussed in Chapter 11.

1.5.4 Cost

The cost of designing and executing a numerical model is sometimes cited as a limitation of modeling, but we consider it an ethical concern. After an investment in hardware and software, the costs of modeling are primarily for the modeler's and modeling team's time. Obviously, a complicated model requires more time and money to construct than a simple model. Missteps in conceptualization, construction, execution, and interpretation of models cost time and money but are often an unavoidable part of the modeling process. Of course, models need field data, but field data are needed for any type of hydrogeologic analysis. Availability of funds may limit the type of model that can be constructed and the scope of the modeling effort; the modeler is ethically bound to provide the best possible model given the time and resources available. When cost is the dominant driver for the model presented, the report should clearly state how constraints on funding affected the design of the model and the output.

1.6 MODELING WORKFLOW

Steps in groundwater modeling (Fig. 1.1) follow the scientific method (Fig. 1.2). In the scientific method, a question is asked, a hypothesis is constructed and tested, then accepted or rejected. If rejected, the testing process is repeated with a revised hypothesis. Similarly, the workflow for groundwater modeling starts with a question. Modeling should never be an end in itself; a model is always designed to answer a specific question or set of questions. The question underpins all facets of the resulting groundwater model. A workflow for applying groundwater models in forecasting is presented in Fig. 1.1. The steps in the workflow build confidence in the model. Although not shown in the figure, field data and soft knowledge (i.e., any information that is not evaluated directly by model output) inform almost every step of the modeling process, especially the design of the conceptual model, parameterization, selection of calibration targets, and ending the calibration process.

The modeling process may start over when new field data become available and when there are new questions to answer. The cyclic nature of the workflow allows for the

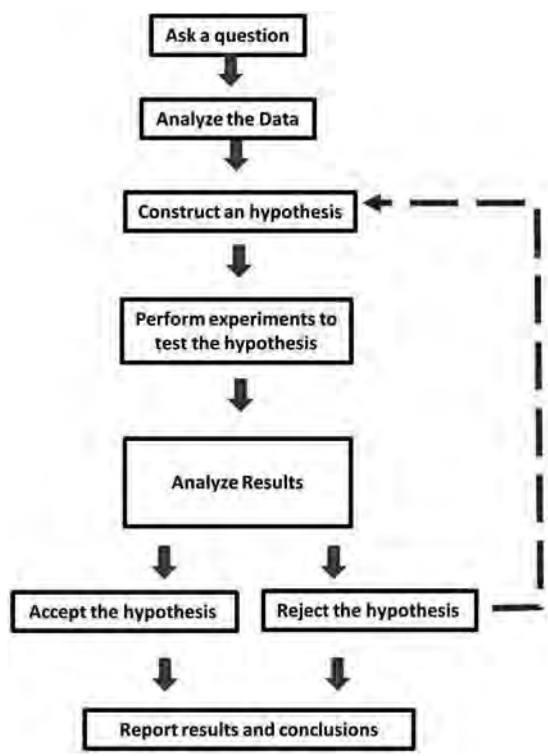


Figure 1.2 The scientific method *(modified from: http://www.sciencebuddies.org/science-fair-projects/project_scientific_method.shtml).*

potential to improve and update the model when a calibrated groundwater model is used routinely as a decision-making tool in water resources management. Modelers in the UK are working toward establishing a set of calibrated models for aquifer systems throughout the UK for water resources management (Shepley et al., 2012). The Netherlands has a countrywide AE groundwater model (De Lange, 2006) and multimodel system for water resources management (De Lange et al., 2014); large regional models designed for water resources management are also being developed in the US (Reeves, 2010). More often, however, a model is developed to answer a specific question and after the decision is made, the model is rarely used again.

1.6.1 Steps in the Workflow

Our book is structured to discuss each of the steps in Fig. 1.1 as summarized below.

1. The purpose of the model (Chapter 2) is to answer a specific question or set of questions. The purpose is the primary factor in deciding appropriate simplifications and assumptions and thereby determines the characteristics of the mathematical model and drives code selection and model design.
2. The conceptual model (Chapter 2) consists of a description of the groundwater flow system including associated surface water bodies, as well as hydrostratigraphic units and system boundaries. Field data are assembled and the hydrogeologic system is described; water budget components are estimated. Multiple conceptual models may be constructed in order to account for uncertainty in describing the field setting. If the modeler did not collect the field data, a visit to the field site is recommended. A field visit will help put the hydrogeologic setting in perspective, give context to the assignment of parameter values and guide decisions during the modeling process.
3. The modeling purpose and the conceptual model drive the choice of a mathematical model and associated code(s) (Chapter 3). The mathematical model consists of a governing equation, boundary conditions, and, for transient problems, initial conditions. Numerical methods programmed into the code approximate the mathematical model.
4. Model design (Chapters 4–7) involves translating the conceptual model into a numerical groundwater flow model by designing the grid/mesh, setting boundaries, assigning values of aquifer parameters, and hydrologic stresses, and, for transient models, setting initial conditions and selecting time steps. The model is run using an initial set of parameter values (Section 5.5) based on the conceptual model. A particle tracking code (Chapter 8) is used to check flow directions and interactions with boundary conditions, and calculate flowpaths and travel times.
5. Arguably calibration (Chapter 9) is the most important step in the modeling process because it helps establish the legitimacy of the conceptual and numerical models. Moreover, the calibrated model is the base model for forecasting simulations. During

the calibration process, the modeler selects calibration targets and calibration parameters, and performs history matching. History matching consists of adjusting the initial parameter assignments in sequential model runs until field observations are sufficiently matched by the model and final parameter values are reasonable. A parameter estimation code helps find the values of calibration parameters that give the best possible match to the field observations (calibration targets). Modelers often do not allow sufficient time for calibration; a guideline is to start calibration no later than halfway (defined by the timeline and budget) through the project and preferably earlier.

6. Forecasting simulations (Chapter 10) use the calibrated model or a set of acceptably calibrated models to forecast the response of the system to future events; or the calibrated model is used to reconstruct past conditions in a hindcasting simulation. In both forecasts and hindcasts, the model is run using calibrated values for aquifer parameters and stresses except for stresses that change under future (or past) conditions. Estimates of anticipated future hydrologic conditions (e.g., recharge rates and pumping rates) are needed to perform the forecast; past hydrologic conditions are needed in hindcasts.

7. Uncertainty (Chapter 10) in a forecast (or hindcast) arises from uncertainty in the calibrated model, including its parameters, as well as uncertainty in the magnitude and timing of future (or past) hydrologic conditions. A forecasting uncertainty analysis includes assessment of measurement error, errors in the design of the model, and uncertainty in future (or past) hydrologic conditions important to the forecast (or hindcast). A particle tracking code may be used to forecast flowpaths and travel times (Chapter 8).

8. The results are presented in the modeling report and stored in the modeling archive (Chapter 11). The modeling report chronicles the modeling process, presents model results and states conclusions and limitations. It includes introductory material, information on the hydrogeologic setting, explanation of the data and assumptions used to formulate the conceptual model, and a reference to the numerical methods and code selected. The report also describes how the model domain is discretized and how parameters were assigned, documents model calibration and presents calibration results, forecasts and associated uncertainty. Modeling reports are accompanied by an archive that contains datasets, codes, input and output files and other materials needed to re-create and execute the model in the future.

9. When the opportunity arises it is useful to evaluate model performance by performing a postaudit. A *postaudit* (Section 10.7) compares the forecast with the response that actually occurred in the field as a result of the action that was simulated by the model. The postaudit is performed long enough after the forecast to allow adequate time for significant changes to occur in the field system. New field data collected during a postaudit may be used to improve the model. In *adaptive management* the model is routinely updated as new data become available and used to guide management decisions.

A forecasting simulation proceeds through steps 1 through 8. Engineering calculators and generic models require steps 1 through 4 and then skip to step 6. The steps in the workflow for a screening model depend on the purpose; the workflow always includes the first four steps and might proceed through step 5 or even steps 6, 7, and 8. If multiple possible conceptual models are considered (e.g., Neuman and Wierenga, 2002), the workflow is executed multiple times.

1.6.2 Verification and Validation

The terms model verification, code verification, and model validation are not in the workflow because verification and validation, as historically used, are no longer critical elements in groundwater modeling. However, because these terms are still in use, we discuss them below and also in Box 9.5.

Model verification refers to a demonstration that the calibrated model matches a set of field data independent of the data used to calibrate the model. However, given the large number of parameters involved in calibrating most field-based groundwater models, it is advisable to use all available data in the calibration exercise itself (Doherty and Hunt, 2010, p. 15) rather than save some data for verification. Thus, groundwater model verification per se generally is not a useful exercise.

Code verification refers to a demonstration that a code can reproduce results from one or more analytical solutions or match a solution from a verified numerical code. Code verification is an important step in developing a code (ASTM, 2008) and information on code verification should be included in the user's manual. However, given that most applied modeling makes use of standard codes that have been verified by the code developer and well tested by the modeling community, additional code verification is not required for most modeling projects. Rather, it is reserved for cases when a new code is developed specifically for the modeling project or when an existing code is modified.

The term model validation has been much debated in the groundwater literature (e.g., Konikow and Bredehoeft, 1992; associated comments and reply; Bredehoeft and Konikow, 1993, 2012; Anderson and Bates, 2001; Hassan, 2004a,b; Moriasi et al., 2012). Validation has been equated with model calibration to suggest, incorrectly, that a calibrated model is a validated model. Furthermore, the term validation may incorrectly imply to nonmodelers that a model is capable of making absolutely accurate forecasts. This is fundamentally not supportable—truth cannot be demonstrated in any model of the natural world, or in any forecast using that model, because the truth is unknown (Oreskes et al., 1994). Therefore, models of the natural world cannot be validated in the same way as a computer code is verified or as a controlled laboratory experiment might be validated. Although such philosophical subtleties are not universally accepted, most groundwater modelers concur that a groundwater model cannot make absolutely accurate forecasts and therefore cannot be validated. We recommend the term "validation" not be used in reference to a groundwater model.

The modeling workflow described above provides a generic structure for best modeling practice. Modeling guidelines also provide strategies for modeling but are formulated as required or recommended steps tailored to application in a regulatory procedure (e.g., Barnett et al., 2012; Neuman and Wierenga, 2002). Technical guidance manuals (e.g., Ohio EPA, 2007; Reilly and Harbaugh, 2004) describe general modeling procedures usually intended for a specific audience of modelers. The ASTM International (http://www.astm.org/) has published a variety of technical guidance documents on groundwater modeling (e.g., ASTM, 2006, 2008).

1.7 COMMON MODELING ERRORS

At the end of each chapter, we present modeling errors that we have found to be common mistakes and misconceptions in groundwater modeling. Because no such list can be inclusive, the reader will undoubtedly make modeling errors and encounter errors in the work of other modelers that are not included in our lists.

- The modeler does not allow enough time for calibration. Certainly formulation of the conceptual model and design of the numerical model are critical steps in groundwater modeling. However, modelers often spend so much time on those initial steps that they run out of time and budget for robust model calibration; we suggest that half of the project's time and budget should be allocated for calibration.
- The modeler does not allow enough time for forecasting simulations. Modelers tend to think that the hard work of modeling is over when the model has been calibrated and assume that the forecasting simulations will be straightforward "production" runs. However, it is essential to perform an uncertainty analysis in conjunction with the forecast (Chapter 10) and uncertainty analysis may occupy more time than the modeler anticipates. Furthermore, sometimes surprises are encountered during the forecasting simulations that may require the modeler to revisit some of the earlier steps in the modeling workflow.
- The modeler does not allow enough time for report preparation. A readable and comprehensive modeling report is invaluable for reconstructing important modeling decisions and outcomes. A model is diminished without a good report to describe the model and its results.

1.8 USE OF THIS TEXT

Readers should be familiar with the basic principles of groundwater hydrology and basic concepts of groundwater modeling presented in standard hydrogeology textbooks such as Fitts (2013), Kresic (2007), Todd and Mays (2005), Schwartz and Zhang (2003), and

Fetter (2001). In Chapter 3, we review basic principles of FD and FE methods drawing on the elementary level text by Wang and Anderson (1982).

The problems following each chapter are intended to illustrate the main points of the chapter. Starting with Chapter 4, most of the problems require the use of an FD or FE code. Boxes amplify topics mentioned in the main text.

To supplement the material covered in the text, the reader is encouraged to consult the literature cited throughout the book as well as groundwater journals and modeling reports published by the US. Geological Survey and other governmental and regulatory groups. We have included links to many such resources on the companion Web site for this text (http://appliedgwmodeling.elsevier.com). The modeler can develop modeling intuition and hydrosense by studying the models described in journal papers and technical reports, starting with those cited in our book, and by the experience of developing and solving problems with models.

1.9 PROBLEMS

Problems for Chapter 1 are intended to introduce the modeling process and stimulate thinking about the level of modeling needed to address a stated modeling purpose.

P1.1 List the type of groundwater model (i.e., forecasting or interpretive (engineering calculator, screening, or generic)) that would most likely be used to solve each of the following problems. List the assumptions you made to reach your decision.

a. A regulatory agency wants to understand why the ages of water discharging from various springs that flow from an anisotropic and homogeneous sandstone aquifer are so variable. It is suggested that each spring is discharging water that is a mix of water coming from several different flowpaths, or that stratigraphic and structural controls affect groundwater residence times and thus determine the age of the spring discharge.

b. A lawyer wants a consultant to estimate seasonal fluctuations in the water table of an alluvial fan aquifer in Spain resulting from a change in the timing and distribution of groundwater recharge originating from flood irrigation practices. The change in recharge was brought about by recent litigation involving land ownership.

c. A consulting firm is tasked to determine the scales and magnitudes of aquifer heterogeneities that would cause a 25% reduction in the size of the capture zone of a well designed to pump contaminated water from what was thought to be a homogeneous unconfined outwash aquifer.

d. A stream ecologist wants to quantify the seasonal exchange of water between a stream and its contiguous floodplain aquifer.

e. An agency is planning a secure landfill for disposal of low-level nuclear waste in thick low permeability sedimentary deposits. The agency would like to assess the effect of changes in recharge on rates and directions of groundwater flow at the proposed site.

P1.2 Make a list of criteria you would use to determine if a model appropriately represented a particular hydrogeological system. Justify your selection and save the list for future reference.

P1.3 Read a recent report prepared by a consultant or governmental agency that describes the application of a groundwater flow model in your geographical area. Identify the purpose of the model and the modeling question(s). How was the conceptual model presented (e.g., in text, cross sections, tables)? Describe the mathematical model and identify the code used to solve the model. Describe the calibration process. If the model was used for forecasting, discuss how the modeler(s) evaluated forecast uncertainty. Create a flow chart of the modeling process used and compare and contrast it to Fig. 1.1.

REFERENCES

Anderson, M.G., Bates, P.D. (Eds.), 2001. Model Validation: Perspectives in Hydrological Science. John Wiley & Sons, Ltd, London, 500 p.

Anderson, M.P., 1983. Ground-water modeling—the emperor has no clothes. Groundwater 21 (6), 666–669. http://dx.doi.org/10.1111/j.1745-6584.1983.tb01937.x.

ASTM International, 2006. Standard guide for subsurface flow and transport modeling, D5880–06. American Society of Testing and Materials, Book of Standards 04 (09), 6 p.

ASTM International, 2008. Standard guide for developing and evaluating groundwater modeling codes, D6025–08. American Society of Testing and Materials, Book of Standards 04 (09), 17 p.

Bair, E.S., 2001. Models in the courtroom. In: Anderson, M.G., Bates, P.D. (Eds.), Model Validation: Perspectives in Hydrological Science. John Wiley & Sons Ltd, London, pp. 55–77.

Bair, E.S., Metheny, M.A., 2011. Lessons learned from the landmark "A Civil Action" trial. Groundwater 49 (5), 764–769. http://dx.doi.org/10.1111/j.1745-6584.2008.00506.x.

Bakker, M., Maas, K., Schaars, F., von Asmuth, J., 2007. Analytic modeling of groundwater dynamics with an approximate impulse response function for areal recharge. Advances in Water Resources 30 (3), 493–504. http://dx.doi.org/10.1016/j.advwatres.2006.04.008.

Barlow, P.M., Moench, A.F., 1998. Analytical Solutions and Computer Programs for Hydraulic Interaction of Stream-aquifer Systems. USGS Open-File Report: 98-415-A, 85 p. http://pubs.usgs.gov/of/1998/ofr98-415A/.

Barnett, B., Townley, L.R., Post, V., Evans, R.F., Hunt, R.J., Peeters, L., Richardson, S., Werner, A.D., Knapton, A., Boronkay, A., 2012. Australian Groundwater Modelling Guidelines. Waterlines Report. National Water Commission, Canberra, 191 p. http://nwc.gov.au/__data/assets/pdf_file/0016/22840/Waterlines-82-Australian-groundwater-modelling-guidelines.pdf.

Beven, K., Young, P., 2013. A guide to good practice in modeling semantics for authors and referees. Water Resources Research 49, 5092–5098. http://dx.doi.org/10.1002/wrcr.20393.

Bredehoeft, J., 2005. The conceptualization model problem—surprise. Hydrogeology Journal 13 (1), 37–46. http://dx.doi.org/10.1007/s10040-004-0430-5.

Bredehoeft, J., 2012. Modeling groundwater flow—the beginnings. Groundwater 50 (3), 324–329. http://dx.doi.org/10.1111/j.1745-6584.2012.00940.x.

Bredehoeft, J., Hall, P., 1995. Ground-water models. Groundwater 33 (4), 530–531. http://dx.doi.org/.

Bredehoeft, J.D., Konikow, L.F., 1993. Ground-water models: Validate or invalidate. Groundwater 31 (2), 178–179 (Reprinted in Groundwater 50 (4), pp. 493–494). http://dx.doi.org/10.1111/j.1745-6584.1993.tb01808.x.

Bredehoeft, J.D., Konikow, L.F., 2012. Reflections on our model validation editorial. Groundwater 50 (4), 495. http://dx.doi.org/10.1111/j.1745-6584.2012.00951.x.

Clement, T.P., 2011. Complexities in hindcasting models—When should we say enough is enough? Groundwater 49 (5), 620—629. http://dx.doi.org/10.1111/j.1745-6584.2010.00765.x.

Collins, M.A., Gelhar, L.W., 1971. Seawater intrusion in layered aquifers. Water Resources Research 7 (4), 971—979. http://dx.doi.org/10.1029/WR007i004p00971.

Coppola, E., Rana, A., Poulton, M., Szidarovszky, F., Uhl, V., 2005. A neural network model for predicting aquifer water level elevations. Groundwater 43 (2), 231—241. http://dx.doi.org/10.1111/j.1745-6584.2005.0003.x.

Darcy, H.P.G., 1856. Determination of the Laws of Water Flow through Sand, the Public Fountains of the City of Dijon, Appendix D — Filtration, Section 2 of Appendix D on Natural Filtration. Translated from the French by Patricia Bobeck. Kendall/Hunt Publishing Company, Iowa, 455—459.

De Lange, W.J., 2006. Development of an analytic element ground water model of the Netherlands. Groundwater 44 (1), 111—115. http://dx.doi.org/10.1111/j.1745-6584.2005.00142.x.

De Lange, W.J., Prinsen, G.F., Hoogewoud, J.C., Veldhuizen, A.A., Verkaik, J., Oude Essink, G.H.P., van Walsum, P.E.V., Delsman, J.R., Hunink, J.C., Massop, H.ThL., Kroon, T., 2014. An operational, multi-scale, multi-model system for consensus-based, integrated water management and policy analysis: The Netherlands Hydrological Instrument. Environmental Modelling & Software 59, 98—108. http://dx.doi.org/10.1016/j.envsoft.2014.05.009.

Demissie, Y., Valocchi, A.J., Minsker, B.S., Bailey, B., 2009. Integrating physically-based groundwater flow models with error-correcting data-driven models to improve predictions. Journal of Hydrology 364 (3—4), 257—271. http://dx.doi.org/10.1016/j.jhydrol.2008.11.007.

Doherty, J., 2011. Modeling: Picture perfect or abstract art? Groundwater 49 (4), 455. http://dx.doi.org/10.1111/j.1745-6584.2011.00812.x.

Doherty, J.E., Hunt, R.J., 2010. Approaches to Highly Parameterized Inversion: A Guide to Using PEST for Groundwater-Model Calibration. U.S. Geological Survey Scientific Investigations Report 2010—5169, 60 p. http://pubs.usgs.gov/sir/2010/5169/.

Dreiss, S.J., 1989. Regional scale transport in a karst aquifer: 2. Linear systems and time moment analysis. Water Resources Research 25 (1), 126—134. http://dx.doi.org/10.1029/WR025i001p00126.

Fienen, M.N., Masterson, J.P., Plant, N.G., Gutierrez, B.T., Thieler, E.R., 2013. Bridging groundwater models and decision support with a Bayesian network. Water Resources Research 49 (10), 6459—6473. http://dx.doi.org/10.1002/wrcr.20496.

Feinstein, D.T., Hunt, R.J., Reeves, H.W., 2010. Regional Groundwater-Flow Model of the Lake Michigan Basin in Support of Great Lakes Basin Water Availability and Use Studies. U.S. Geological Survey Scientific Investigations Report 2010—5109, 379 p. http://pubs.usgs.gov/sir/2010/5109/.

Feng, S., Kang, S., Huo, Z., Chen, S., Mao, X., 2008. Neural networks to simulate regional ground water levels affected by human activities. Groundwater 46 (1), 80—90. http://dx.doi.org/10.1111/j.1745-6584.2007.00366.x.

Fetter, C.W., 2001. Applied Hydrogeology, fourth ed. Prentice Hall. 598 p.

Fitts, C.R., 2013. Groundwater Science, second ed. Academic Press, London. 672 p.

Freeze, R.A., Witherspoon, P.A., 1967. Theoretical analysis of regional ground-water flow: 2. Effect of water table configuration and subsurface permeability variations. Water Resources Research 3 (2), 623—634. http://dx.doi.org/10.1029/WR003i002p00623.

Frind, E.O., Muhammad, D.S., Molson, J.W., 2002. Delineation of three-dimensional well capture zones for complex multi-aquifer systems. Groundwater 40 (6), 586—598. http://dx.doi.org/10.1111/j.1745-6584.2002.tb02545.x.

Fujinawa, K., Iba, T., Fujihara, Y., Watanabe, T., 2009. Modeling interaction of fluid and salt in an aquifer/lagoon system. Groundwater 47 (1), 35—48. http://dx.doi.org/10.1111/j.1745-6584.2008.00482.x.

Gómez-Hernández, J.J., 2006. Complexity. Groundwater 44 (6), 782—785. http://dx.doi.org/10.1111/j.1745-6584.2006.00222.x.

Gusyev, M.A., Haitjema, H.M., Carlson, C.P., Gonzalez, M.A., 2013. Use of nested flow models and interpolation techniques for science-based management of the Sheyenne National Grassland, North Dakota, USA. Groundwater 51 (3), 414—420. http://dx.doi.org/10.1111/j.1745-6584.2012.00989.x.

Haitjema, H.M., 1995. Analytic Element Modeling of Groundwater Flow. Academic Press, Inc., San Diego, CA, 394 p.

Haitjema, H., 2006. The role of hand calculations in ground water flow modeling. Groundwater 44 (6), 786–791. http://dx.doi.org/10.1111/j.1745-6584.2006.00189.x.

Harr, J., 1995. A Civil Action. Random House, New York, 512 p.

Hassan, A.E., 2004a. Validation of numerical ground water models used to guide decision making. Groundwater 42 (2), 277–290. http://dx.doi.org/10.1111/j.1745-6584.2004.tb02674.x.

Hassan, A.E., 2004b. A methodology for validating numerical ground water models. Groundwater 42 (3), 347–362. http://dx.doi.org/10.1111/j.1745-6584.2004.tb02683.x.

Hill, M.C., 2006. The practical use of simplicity in developing ground water models. Groundwater 44 (6), 775–781. http://dx.doi.org/10.1111/j.1745-6584.2006.00227.x.

Hsieh, P.A., 2011. Application of MODFLOW for oil reservoir simulation during the Deepwater Horizon crisis. Groundwater 49 (3), 319–323. http://dx.doi.org/10.1111/j.1745-6584.2011.00813.xs.

Hulme, P., Fletcher, S., Brown, L., 2002. Incorporation of groundwater modeling in the sustainable management of groundwater resources. In: Hiscock, K.M., Rivett, M.O., Davison, R.M. (Eds.), Sustainable Groundwater Development. Special Publication 193, Geological Society of London, pp. 83–90.

Hunt, R.J., 2006. Review paper: Ground water modeling applications using the analytic element method. Groundwater 44 (1), 5–15. http://dx.doi.org/10.1111/j.1745-6584.2005.00143.x.

Hunt, R.J., Anderson, M.P., Kelson, V.A., 1998. Improving a complex finite difference groundwater-flow model through the use of an analytic element screening model. Groundwater 36 (6), 1011–1017. http://dx.doi.org/10.1111/j.1745-6584.1998.tb02108.x.

Hunt, R.J., Doherty, J., Tonkin, M.J., 2007. Are models too simple? Arguments for increased parameterization. Groundwater 45 (3), 254–261. http://dx.doi.org/10.1111/j.1745-6584.2007.00316.x.

Hunt, R.J., Welter, D.E., 2010. Taking account of "unknown unknowns". Groundwater 48 (4), 477. http://dx.doi.org/10.1111/j.1745-6584.2010.00681.x.

Hunt, R.J., Zheng, C., 2012. The current state of modeling. Groundwater 50 (3), 329–333. http://dx.doi.org/10.1111/j.1745-6584.2012.00936.x.

Illman, W.A., Berg, S.J., Yeh, T.-C.J., 2012. Comparison of approaches for predicting solute transport: Sandbox experiments. Groundwater 50 (3), 421–431. http://dx.doi.org/10.1111/j.1745-6584.2011.00859.x.

Kelson, V.A., Hunt, R.J., Haitjema, H.M., 2002. Improving a regional model using reduced complexity and parameter estimation. Groundwater 40 (2), 132–143. http://dx.doi.org/10.1111/j.1745-6584.2002.tb02498.x.

Kollet, S.J., Maxwell, R.M., Woodward, C.S., Smith, S., Vanderborght, J., Vereecken, H., Simmer, C., 2010. Proof of concept of regional scale hydrologic simulations at hydrologic resolution utilizing massively parallel computer resources. Water Resources Research 46, W04201. http://dx.doi.org/10.1029/2009WR008730.

Konikow, L.F., Bredehoeft, J.D., 1992. Ground-water models cannot be validated. Advances in Water Resources 15, 75–83. http://dx.doi.org/10.1016/0309-1708(92)90033-X (Also see comment by Marsily, G. de, Combes, P., Goblet, P., 1993. Advances in Water Resources 15, pp. 367–369. Reply by Bredehoeft, J.D., Konikow, L.F., pp. 371–172.).

Kresic, N., 2007. Hydrogeology and Groundwater Modeling, second ed. CRC Press, Boca Raton, FL. 807 p.

Kuhlman, K.L., Neuman, S.P., 2009. Laplace-transform analytic-element method for transient, porous-media flow. Journal of Engineering Math 64, 113–130. http://dx.doi.org/10.1007/s10665-008-9251-1.

Li, Y., Neuman, S.P., 2007. Flow to a well in a five-layer system with application to the Oxnard Basin. Groundwater 45 (6), 672–682. http://dx.doi.org/10.1111/j.1745-6584.2007.00357.x.

Mamer, E.A., Lowry, C.S., 2013. Locating and quantifying spatially distributed groundwater/surface water interactions using temperature signals with paired fiber-optic cables. Water Resources Research 49, 1–11. http://dx.doi.org/10.1002/2013WR014235.

Maslia, M.L., Aral, M.M., Faye, R.E., Grayman, V.M., Suarez-Soto, R.J., Sautner, J.B., Anderson, B.A., Bove, J.F., Ruckart, P.Z., Moore, S.M., 2012. Comment on "complexities in hindcasting models—when should we say enough is enough". Groundwater 50 (1), 1–16. http://dx.doi.org/10.1111/j.1745-6584.2011.00884.x.

Moriasi, D.N., Wilson, B.N., Douglas-Mankin, K.R., Arnold, J.G., Gowda, P.H., 2012. Hydrologic and water quality models: Use, calibration and validation. Transactions American Society of Agricultural and Biological Engineers 55 (4), 1241–1247. http://dx.doi.org/10.13031/2013.42265.

Neuman, S.P., Wierenga, P.J., 2002. A Comprehensive Strategy of Hydrogeologic Modeling and Uncertainty Analysis for Nuclear Facilities and Sites. NUREG/CF-6805, 236 p. http://www.nrc.gov/reading-rm/doc-collections/nuregs/contract/cr6805/.

Ohio EPA (Environmental Protection Agency), 2007. Ground Water Flow and Fate and Transport Modeling, Technical Guidance Manual for Ground Water Investigations. Chapter 14, 32 p. http://www.epa.state.oh.us/ddagw/.

Oreskes, N., Shrader-Frechette, K., Belitz, K., 1994. Verification, validation, and confirmation of numerical models in the Earth Sciences. Science 263 (5147), 641–646. http://dx.doi.org/10.1126/science.263.5147.641.

Reeves, H.W., 2010. Water Availability and Use Pilot: A Multiscale Assessment in the U.S. Great Lakes Basin. U.S. Geological Survey Professional Paper 1778, 105 p. http://pubs.usgs.gov/pp/1778/.

Reilly, T.E., Harbaugh, A.W., 2004. Guidelines for Evaluating Ground-Water Flow Models. U.S. Geological Survey Scientific Investigation Report 2004-5038, 30 p. http://pubs.usgs.gov/sir/2004/5038/.

Sawyer, A.H., Cardenas, M.B., Buttles, J., 2012. Hyporheic temperature dynamics and heat exchange near channel-spanning logs. Water Resources Research 48. W01529. http://dx.doi.org/10.1029/2011WR011200.

Schwartz, F.W., Zhang, H., 2003. Fundamentals of Groundwater. John Wiley & Sons, 583 p.

Sepúlveda, N., 2009. Analysis of methods to estimate spring flows in a karst aquifer. Groundwater 47 (3), 337–349. http://dx.doi.org/10.1111/j.1745-6584.2008.00498.x.

Sheets, R.A., Dumouchelle, D.H., Feinstein, D.T., 2005. Ground-Water Modeling of Pumping Effects Near Regional Ground-water Divides and River/Aquifer Systems — Results and Implications of Numerical Experiments. U.S. Geological Survey Scientific Investigations Report 2005-5141, 31 p. http://pubs.usgs.gov/sir/2005/5141/.

Shepley, M.G., Whiteman, M.I., Hulme, P.J., Grout, M.W., 2012. Groundwater resources modelling: A case study from the UK, the Geological Society, London. Special Publication 364, 378 p.

Simmons, C.T., Hunt, R.J., 2012. Updating the debate on model complexity. GSA Today 22 (8), 28–29. http://dx.doi.org/10.1130/GSATG150GW.1.

Skibitzke, H.E., 1961. Electronic computers as an aid to the analysis of hydrologic problems. International Association of Scientific Hydrology, Publ. 52 347–358. Comm. Subterranean Waters, Gentbrugge, Belgium.

Strack, O.D.L., 1989. Groundwater Mechanics. Prentice Hall, Englewood Cliffs, New Jersey, 732 p.

Szidarovszky, F., Coppola, E.A., Long, J., Hall, A.D., Poulton, M.M., 2007. A hybrid artificial neural network-numerical model for ground water problems. Groundwater 45 (5), 590–600. http://dx.doi.org/10.1111/j.1745-6584.2007.00330.x.

Theis, C.V., 1935. The relation between lowering of the piezometric surface and rate and duration of discharge of a well using ground-water storage. Transactions of the American Geophysical Union 16, 519–524.

Todd, D.K., Mays, L.W., 2005. Groundwater Hydrology, third ed. John Wiley & Sons, Inc. 636 p.

Tóth, J., 1963. A theoretical analysis of groundwater flow in small drainage basins. Journal of Geophysical Research 68, 4795–4812. http://dx.doi.org/10.1029/JZ068i016p04795.

Wang, H.F., Anderson, M.P., 1982. Introduction to Groundwater Modeling: Finite Difference and Finite Element Methods. Academic Press, San Diego, CA, 237 p.

Woessner, W.W., 2000. Stream and fluvial plain ground water interactions: Rescaling hydrogeologic thought. Groundwater 38 (3), 423–429. http://dx.doi.org/10.1111/j.1745-6584.2000.tb00228.x.

Yeh, T.-C.J., Mao, D., Zha, Y., Hsu, K.-C., Lee, C.-H., Wen, J.C., Lu, W., Yang, J., 2014. Why hydraulic tomography works? Groundwater 52 (2), 168–172. http://dx.doi.org/10.1111/gwat.12129.

Zlotnik, V.A., Cardenas, M.B., Toundykov, D., 2011. Effects of multiscale anisotropy on basin and hyporheic groundwater flow. Groundwater 49 (4), 576–583. http://dx.doi.org/10.1111/j.1745-6584.2010.00775.x.

CHAPTER 9

Model Calibration: Assessing Performance

Clearly, many branches of science need an exquisite precision…and the infinitesimal decimals of calibration, so space launches, for example, are not scheduled for leap-second dates. But society as a whole neither needs that obsessive…measurement nor is well served by it.

Jay Griffith, A Sideways Look at Time

Contents

Boxes

Applied Groundwater Modeling
ISBN 978-0-12-058103-0, http://dx.doi.org/10.1016/B978-0-12-058103-0.00009-5

9.1 INTRODUCTION

Groundwater modeling would be straightforward if it were possible to characterize the natural world perfectly. Then boundary and parameter assignment would incorporate all relevant spatial and temporal information and the model would exactly simulate the real groundwater system. However, groundwater systems are never known exactly and, rather than reflecting the environmental system itself, we must map this system into a *model space* (Beven, 2009, p. 11). Model space is used here to define the range of feasible models and model inputs that are potentially appropriate for a field site. During the translation that occurs during this mapping, the already simplified view of the natural world represented by a conceptual model is further simplified so that a numerical model is computationally tractable. In order to judge how well this mapping of an environmental system to a model space was performed, model performance must be evaluated using field observations that can be compared with model output (*hard data*) as well as everything else we know about the system (*soft data*).

In the *forward problem*, parameters such as hydraulic conductivity, specific storage, storativity/specific yield, and recharge rate are specified, and heads and fluxes are calculated. However, in practice, field-measured values of heads and fluxes are usually known with a relatively higher degree of confidence and parameter values are less well known. In this context, the groundwater model is posed as an *inverse problem*, where head observations form the dependent variable in the governing equation and are used to solve for parameter values. Inverse problems are typically solved by *history matching*, a term that originated in the petroleum industry and refers to the matching model outputs to a historical time series of measured values by adjusting model inputs. For our purposes, history matching refers to matching field measurements (including at least heads and fluxes) in both steady-state and transient simulations (Chapter 7). The objective of history matching is to identify a set of parameters that produces a satisfactory match to the field observations. Parameters are adjusted within reasonable ranges in sequential forward runs of the model until the model produces an acceptable match. In its most general form (Fig. 9.1), history matching includes these steps:

1. select calibration targets from the set of field observations;
2. run the model using best estimates of input parameters (material property parameters and hydrologic parameters; Section 5.4);
3. compare simulated outputs to the targets;
4. adjust values of input parameters to obtain better fits of simulated values to targets;
5. select the model with the best fit possible given limitations on time and resources.

We distinguish between two phases of history matching: the first involving manual trial-and-error history matching shown in Fig. 9.1; and a subsequent phase where history matching is performed using software. History matching is important for evaluating a

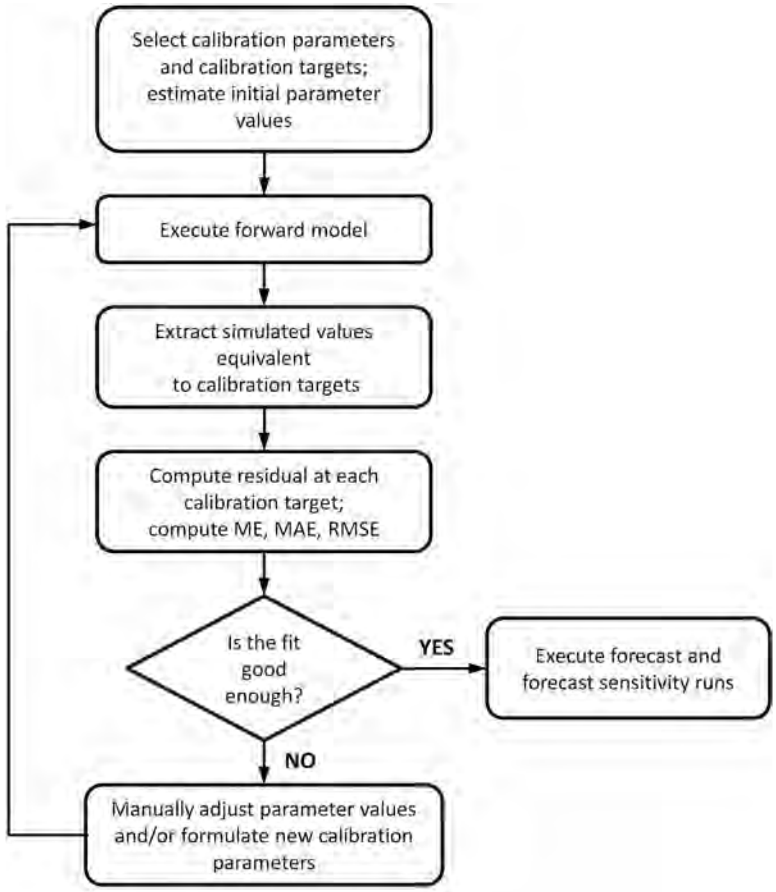


Figure 9.1 General workflow for manual trial and error, the first phase of history matching a model intended for forecasting (ME, mean error; MAE, mean absolute error; RMSE, root mean squared error).

model's fit for purpose: if a model cannot reproduce the measured heads and fluxes with sufficient accuracy, one can have little confidence that the calibrated model will adequately reproduce unmeasured heads and fluxes or forecast future conditions.

History matching can be considered a *hard knowledge* evaluation of model performance because field measurements can be directly compared with simulated values, sometimes also called *simulated equivalent values*. However, a good fit does not mean that the match is acceptable; the match is acceptable only if the parameters and assumptions used to obtain the fit are reasonable. Therefore, model performance evaluation also includes a *soft knowledge* evaluation of *hydrogeologic reasonableness*. Soft knowledge relies on expert knowledge about the system that is not directly comparable to quantitative model outputs, and draws on geological and hydrologic information of the site and basic hydrogeologic theory embodied in the conceptual model (Section 2.3). For example, if we know that the aquifer consists of gravel, a model calibrated with hydraulic conductivity values typical of silt and clay would be rejected even if the model satisfactorily reproduced field observations. Similarly, in most cases a model that produced a good fit but used recharge rates larger than precipitation rates would be rejected as hydrogeologically unreasonable. Effective soft knowledge assessment draws on the literature, knowledge of site conditions, hydrogeological principles, and professional experience. Guidelines for this type of assessment are not easily reduced to simple instructions or steps. Rather, soft knowledge assessments rely on "hydrosense" (Hunt and Zheng, 2012) that is developed with experience solving hydrogeological problems and designing and running models.

In practice, assessment of hydrogeological reasonableness using soft knowledge is done in concert with history matching. The combined evaluation of both hard and soft knowledge is *model calibration*, where a final *calibrated model* has an acceptable fit to observations and contains reasonable parameters and assumptions. If a model does not pass both assessments it cannot be considered calibrated. Typically, most effort and reporting focuses on the model's ability to fit observations (history matching), because assessments using hard knowledge can be easily communicated using summary statistics and visualization. Evaluation of a model's adherence to soft knowledge is not easily quantified and is often conveyed with words (e.g., "the calibrated parameter value is consistent with values reported for the site…"). In practice, model assessment using hard knowledge of model fit is sandwiched between two soft knowledge assessment activities: development of the conceptual model and evaluation of calibrated parameters for reasonableness. Although soft knowledge assessment of the calibrated parameter values is important, the focus of this chapter is on the five steps listed above that constitute history matching.

9.2 LIMITATIONS OF HISTORY MATCHING

Groundwater models simulate a portion of a complex natural world, much of which is unseen and uncharacterized (Freeze et al., 1990). Hence, the groundwater modeling problem is inherently tied to an *open system* (Oreskes et al., 1994) that, by definition, is impossible to characterize completely. As a result, a groundwater model is always a simplification of the true hydrogeologic system. Because the natural world is complex both in properties and processes, models almost always have more unknown parameter values than field measurements. As such, the inverse problem is said to be *underdetermined* by observations and therefore mathematically *ill-posed* (e.g., Freeze and Cherry, 1979; McLaughlin and Townley, 1996). A well-posed problem has a solution that depends continuously on the data, and is unique (Hadamard, 1902). In practice, what we know is typically not sufficient to constrain the problem to one unique solution. Rather, the modeler often must consider a "family" of possible reasonable models because groundwater models are fundamentally *nonunique*. In the broadest sense, a modeling problem might be considered an expression of multiple working hypotheses about how the system works, where model evaluation is a form of hypothesis testing rather than a matter of finding the optimal model (Beven, 2009, p. 18). In practice, however, decision-makers often require a single "best" model for the decision of interest. Therefore, the selected best calibrated model should ideally: (1) be based on the strongest conceptual model; (2) utilize all the information contained in the available observations; (3) avoid inappropriate simplification of natural world processes and structure important for the forecast(s) of interest; (4) be sufficiently discretized in space and time; and (5) have manageable run times given financial and time constraints of the project.

Fully understanding groundwater model nonuniqueness is critical for identifying an appropriate model, as well as forming the family of defensible models. We cannot objectively define a uniquely best model because all field-based groundwater modeling efforts necessarily use data sets that are incomplete and contain errors (e.g., Table 9.1). There will always be a number of possible defensible models that can reasonably simulate what we know about the real-world system that the model aims to represent. Hence, selection of a model that is considered the best representation of this reality will always be subjective (Doherty and Hunt, 2009a,b) even if unlimited resources and time were available.

This does not mean that all models are potentially acceptable nor is the selection of a "best" model based on whim. Rather, the corollary to a number of possible reasonable models is a much larger number of unreasonable ones. A skilled modeler discerns those dead-ends quickly and focuses on the reasonable subset. Therefore, although subjectivity operates within the realm of the family of reasonable models, those models outside this realm can be more objectively discarded. Models that fail calibration because they fail to achieve a satisfactory history match, use unreasonable parameter values, and/or do not conform to the conceptual model, may be discarded.

Table 9.1 Estimated accuracy of head data by measurement method (modified from Nielson, 1991). Measurement method is but one source of error for head targets

Measurement method	Accuracy, in feet	Major interference or disadvantage
Nonflowing wells		
Steel tape and chalk	0.01	Cascading water
Electric tape	0.02–0.1	Cable wear; hydrocarbons on water
Pressure transducers	0.01–0.1	Temperature change; electronic drift; blocked capillary
Acoustic probe	0.02	Cascading water; floating hydrocarbons on water
Ultrasonics	0.02–0.01	Temperature change; well materials
Floats	0.02–0.05	Float or cable drag; float size or lag
Poppers	0.1	Background noise in/around well; well depth
Air lines	0.25–1.0	Air line or fitting leaks; gage inaccuracies
Flowing wells		
Transducers	0.02	Temperature changes; electronic drift
Casing extensions	0.1	Limited range; awkward
Manometer/pressure gage	0.1–0.5	Gage inaccuracies; calibration required

Haitjema (2015) pointed out that the logical endpoint of calibration cannot be finding the *true model*, one that contains completely accurate properties of the field site. Nor is the logical endpoint even an *optimal model*, one that uses the most sophisticated methods to squeeze out every bit of information from every observation. Rather, in practice, the logical endpoint of modeling is an *appropriate model*—a model that balances sophistication and realistic representation with resources and time available. The concept of the appropriate model can be illustrated by the following example. If 80% of the project objective can be met with a model that used only 10% of the financial resources, can the decision the model was designed to address be made without expending additional resources on the remaining 20% of the objective? Can the uncertainty associated with the unknown 20% be handled in other ways, such as engineering safety factors? Or put another way, is it worth spending the remaining 90% of the resources to attempt to address the remaining 20% of the objective? The concept of the appropriate model recognizes that 80% of the answer may suffice for many problems that require modeling. However, at a minimum, an appropriate groundwater flow model must be a defensible representation of the groundwater system that, at a minimum, approximates large-scale observed groundwater flow directions and head trends.

9.3 CALIBRATION TARGETS

Commonly a modeler has a number of (imperfect) observations, typically heads and fluxes, which collectively give a partial snapshot of true field conditions at a site. Not all observations are equally certain; some may be relatively precise and accurate while others are decidedly approximate. The modeler selects all or some of these observations from similar conditions/time periods as *calibration targets*. Calibration targets are compared with simulated values during history matching to describe model fit, and contain the hard knowledge about the system. Hence, requiring that simulated values match the calibration targets forces the model to respond like the field system, at least for the conditions represented in the simulation. Information contained within the calibration targets, in turn, constrains model parameters that are adjusted during history matching.

Inclusion of several different types of calibration targets maximizes the amount of information that can be considered during calibration. At a minimum, both head and flux targets should routinely be used during history matching because one type of observation (e.g., heads) alone cannot mathematically constrain the inverse solution of the groundwater flow equation uniquely (Box 3.2, see also Haitjema, 2006). Ideally, the model should use as many types of available observations as can be compared to model outputs (Hunt et al., 2006). In addition to heads and fluxes, observations for history matching might include results from advective particle tracking (Chapter 8), as shown in Fig. 9.2, borehole flow measurements, indirect flux measurements based on isotope compositions, temperature, and solute concentrations, and observations from remote sensing (e.g., the

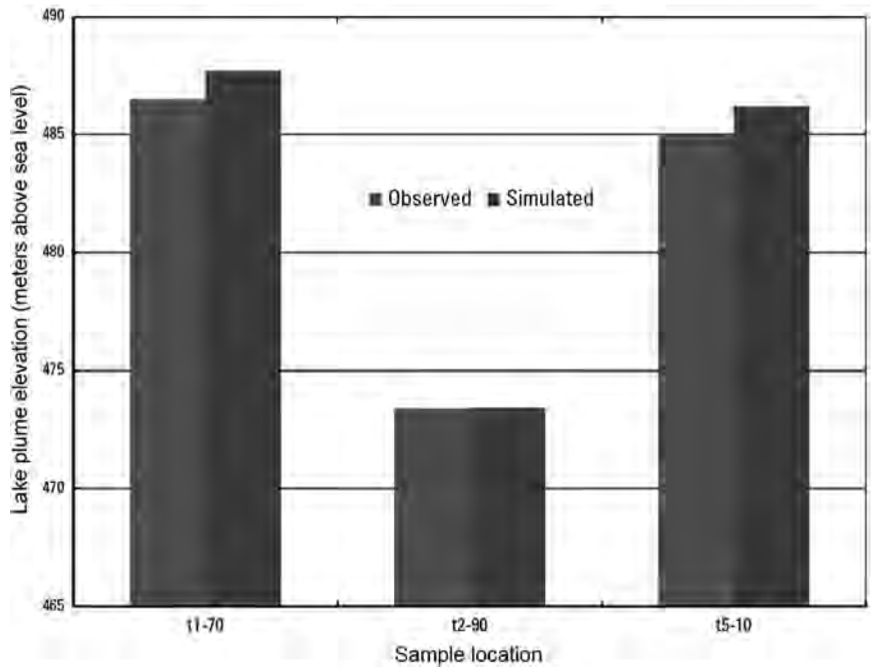


Figure 9.2 History matching to the depth of the interface between a plume of lake water and terrestrially recharged groundwater at three locations. The interface was located in the field by using measurements of stable isotopes of water (observed) and in the model by advective particle tracking (simulated) *(modified from Hunt et al., 2013).*

occurrence of saturated soils), and geophysics (e.g., extent of a contaminant plume). An objective of calibration is to extract the maximum information from all observations available while balancing the potentially contradictory information from different observations. Though many types of targets are desirable, our discussion will focus on the minimum recommended and most commonly used types, head and flux targets.

9.3.1 Head Targets

Head is the only type of target that is a direct output of the groundwater flow equation, and at least some measurements of head are available in most groundwater investigations. Ideally, head values provide the modeler with a relatively large number of observations distributed in space and time (Fig. 7.11). Even with large numbers of head measurements, it is important to note that head data have associated uncertainty. *Measurement errors* include uncertainty associated with the accuracy of the water level measuring device (Table 9.1), potential operator error, and errors that result from inaccurate surveying of the elevation of a well's measuring point. *Interpolation errors* occur when the field head target is not located on a node in the grid or mesh. Comparison of simulated and observed heads can be improved by the use of postprocessing algorithms (included in some graphical user interfaces (GUIs)) that interpolate simulated heads in order to make a target location-specific comparison. Heads may be measured in wells with screens that partially penetrate a model layer or penetrate more than one model layer (Section 6.2). Heads measured in wells with long screens may be appropriate for history matching vertically averaged head output from a two-dimensional areal model. However, vertically distinct head measurements at a given location are better suited for 3-D modeling. Such data are obtained from nested and multilevel piezometers, where multiple discrete measuring points are open to different elevations (e.g., Meyer et al., 2014). The difference in head between vertically separated observation points can also be processed for use as *head difference targets*. Head difference targets increase the signal-to-noise ratio of the head data and are especially useful for calibration of vertical hydraulic conductivity (Doherty and Hunt, 2010, p. 13) but are typically used together with unprocessed head targets. *Transient errors* are introduced when a single value of head is used as a target when multiple measurements over a period of time show temporal changes in head (Fig. 7.1). Steady-state models may be calibrated using temporally averaged head targets where the measurements span time periods meaningful for the modeling objective (Figs 7.2 and 7.3). However, in some locations heads can fluctuate 10s of meters over a selected time period, and a steady-state model is inappropriate (Section 7.2). In transient models, *temporal head difference targets* can be calculated from a time series (Fig. 7.11) as the difference between observed heads measured at two different times and are often superior to absolute head targets in transient models (Doherty and Hunt, 2010, p. 13).

Head target uncertainty is usually expressed as a *standard deviation* (the square root of the average of squared differences of the values from their average value) or *variance* (the square of the standard deviation) around the observed head value. Head target uncertainty can also be expressed as the 95% confidence interval (approximately ± two standard deviations) around the reported value. Clearly, information on the magnitude of the types of errors described above helps quantify the uncertainty associated with a head target. Surveying error should be recorded when a well's measurement point is surveyed; instrument and operator errors should be estimated and recorded when the well is monitored for head. Details of well construction are needed to assess scaling error, and time series of head measurements are required to assess temporal error. Total combined errors of head targets are never perfectly known; thus a modeler commonly states an assessment of head target certainty without detailed breakdown of all components of uncertainty present.

9.3.2 Flux Targets

Flux observations include a variety of types of flows such as baseflow, springflow, infiltration from a losing stream, groundwater inflow to a lake, and evapotranspiration across the water table, and all may be used as calibration targets. Spatially integrated values of groundwater fluxes to and from streams are often estimated from stream gage data or miscellaneous stream discharge measurements. Point estimates of fluxes can be upscaled from direct field measurements or computed using field data and Darcy's law. Fluxes can also be estimated indirectly using tracers (e.g., McCallum et al., 2012; Gardner et al., 2011; Cook et al., 2008; Hunt et al., 1996; Krabbenhoft et al., 1994). Typically, the modeler has many fewer flux observations than head measurements. Nevertheless, flux observations at different locations in the problem domain are extremely helpful during calibration because they give insight into processes in different areas represented in the model. Not all locations of flux targets are equally valuable for calibration: for example, a baseflow measurement at the most downstream location of a model domain commonly has high importance because it integrates the most model area, while locations upstream represent the distribution of groundwater flow within smaller areas of the model domain (Hunt et al., 2006).

For transient models, flux targets are most useful when averaged over time periods suited to the modeling objective (e.g., mean monthly baseflow; defined using flow duration/cumulative probability curves). Time periods used for averaging should correspond to the time period for temporal averaging of head targets when possible. *Spatial flux difference targets* (differences between fluxes at different locations measured during a similar time period) and *temporal flux difference targets* (difference between fluxes at the same location at different times) help maximize the extraction of information contained within raw observed flow data. Difference targets should be used together with standard flux targets whenever possible.

Similar to head targets, flux targets have associated measurement error, and in practice their measurement error is commonly larger than for heads because it is more difficult to measure fluxes accurately in the field. Transient errors in streamflow targets are usually relatively large because surface water flows tend to be more temporally variable than groundwater fluxes. Indirect estimation of flux involves a number of assumptions, which introduce additional error to the flux target. In practice, therefore, each flux target will have its own associated measurement error.

Flux target uncertainty is commonly expressed as *coefficient of variation* (standard deviation divided by the expected, or average, value) relative to the observed value (e.g., ±20%). This type of reporting normalizes the uncertainty to the magnitude of the flux, which is useful for reporting uncertainty of flux targets of different magnitudes. For steady-state models, a coefficient of variation is often assigned to a single flux target to express the uncertainty based on the range of flux measurements in the time series. Similar to head targets, flux target uncertainty can also be expressed as the 95% confidence interval (approximately plus or minus two standard deviations) around the reported value. For example, uncertainty in steady-state flux targets is shown by error bars in Fig. 9.7(a). When possible field data are used to quantify the magnitude of uncertainty (for example, time series data from a stream gage), but in many cases uncertainty is assigned using professional judgment and based on the importance of the target to the modeling objective.

9.3.3 Ranking Targets

Not all targets are equally certain or important to the modeling purpose (e.g., Townley, 2012), and no model can match all calibration targets equally well. Therefore, it is necessary to decide which targets are most important. This is done by *ranking* the targets, where the rank expresses the modeler's judgment of the importance of simulating a specific target during history matching. The modeler tries to find a good match to the higher ranked targets and may accept a model that poorly matches lower ranked targets. The set of ranked targets is the single most important expression of what the modeler holds to be important for calibration, and by extension, the modeling objective. The ranked targets affect both the identification of an appropriate model and the forecasts (Chapter 10) made using the final calibrated model.

From the perspective of statistical theory, ranking targets according to their measurement error is a primary consideration (e.g., Hill and Tiedeman, 2007), and target measurement error is a recommended first approximation for specifying target importance. However, this first ranking typically is adjusted to reflect practical considerations related to the type and location of the target (Doherty and Hunt, 2010, p. 12). For example, there may be hundreds of one type of target (commonly heads) and only one or a few of another (commonly fluxes and/or head difference targets). If measurement error were used as the only ranking criterion, model fit would be overwhelmingly dominated by a large number of head values, which would imply that matching all head targets is more important than matching the fewer flux targets. Likewise, head and flux measurements from the area of primary modeling interest (the *near-field*) are likely most relevant to the modeling purpose and forecast. Targets distributed in the model domain outside the area of interest (the *far-field*) typically have relatively less importance due simply to their location. Therefore, even though near-field and far-field targets might have the same measurement error, they would not be considered equally valuable for finding the best appropriate model. As a result, far-field targets are assigned a lower rank. The ranking might also include consideration of target type; if the modeling purpose required forecasts of future fluxes at a near-field flux target location, for example, a modeler would likely be willing to trade worse fit in heads simulated at far-field targets in order to get a better simulation of the flux target of interest.

Ultimately, the best appropriate model is the one that provides the best forecasts of interest for the system. As such, the ranking of targets should anticipate the needs of the forecasting simulation (Chapter 10). Consequently, because each model is uniquely characterized by its purpose, there is no universally appropriate way to rank targets; rather, it is recognized that this ranking will always include subjective elements that rely on professional experience and the modeling objective (Doherty and Hunt, 2010, p. 12). In the first phase of history matching (manual trial-and-error calibration; Section 9.4), subjectivity is obvious because targets are ranked qualitatively in order of importance. In the second phase of history matching (automated trial-and-error calibration; Section 9.5), targets are quantitatively ranked using numerical weights (e.g., Table 7.1) but still rely on the subjective judgment of the modeler.

9.4 MANUAL HISTORY MATCHING

Once calibration targets are selected and ranked, the groundwater flow model is executed using a set of initial parameter values based on the conceptual model. For some screening models and heuristic modeling exercises where observations do not exist (e.g., Beven, 2009, p. 49), the first forward run might produce results sufficient for the modeling objective. In that case, all subsequent work focuses on forecasting and estimating uncertainty in the forecasts (Chapter 10). Typically, however, multiple runs are necessary to obtain an acceptable history match. The first step in the history matching process involves measuring and improving model fit with *manual trial-and-error* history matching where the modeler manually changes parameter values and evaluates output after each forward run. The second step uses computer codes that automate trial-and-error history matching (Sections 9.5 and 9.6). In both phases, an assessment of the fit is made using both qualitative and quantitative methods. Given the importance to all aspects of history matching, we start by discussing methods for assessing model fit.

9.4.1 Comparing Model Output to Observations

Visual comparisons of simulated values and targets together with calculation of summary statistics are efficient ways to assess model fit. These methods are used to report results obtained via both manual and automated trial and error history matching. Most straightforward is a plot of the observed and simulated water table (e.g., Fig. 9.3) and/or potentiometric surface(s) in each layer of the model. However, observed surfaces are not equivalent to the hard data represented by the point measurements themselves because subjective decisions were needed for their creation. For transient models, observed and simulated hydrographs (Fig. 7.11) depict the model's ability to capture the dynamics of the groundwater system (Fig. 9.4). *Scatter plots* (Fig. 9.5(a)) show calibration targets versus simulated values and allow for a quick assessment of model fit; *categorized scatter plots* (Fig. 9.5(b)) are useful for distinguishing between data with different sources. In addition to fit, scatter plots also visualize *bias* in the calibration. Bias is absent when points in the scatter plot are more or less equally distributed around the central line shown on the plot, which indicates one-to-one correspondence between simulated and observed values (i.e., this line is not a regression line fitted to the data set). If simulated heads in a scatter plot are biased high, for example, it could mean that recharge rates are too high and/or hydraulic conductivities are too low.

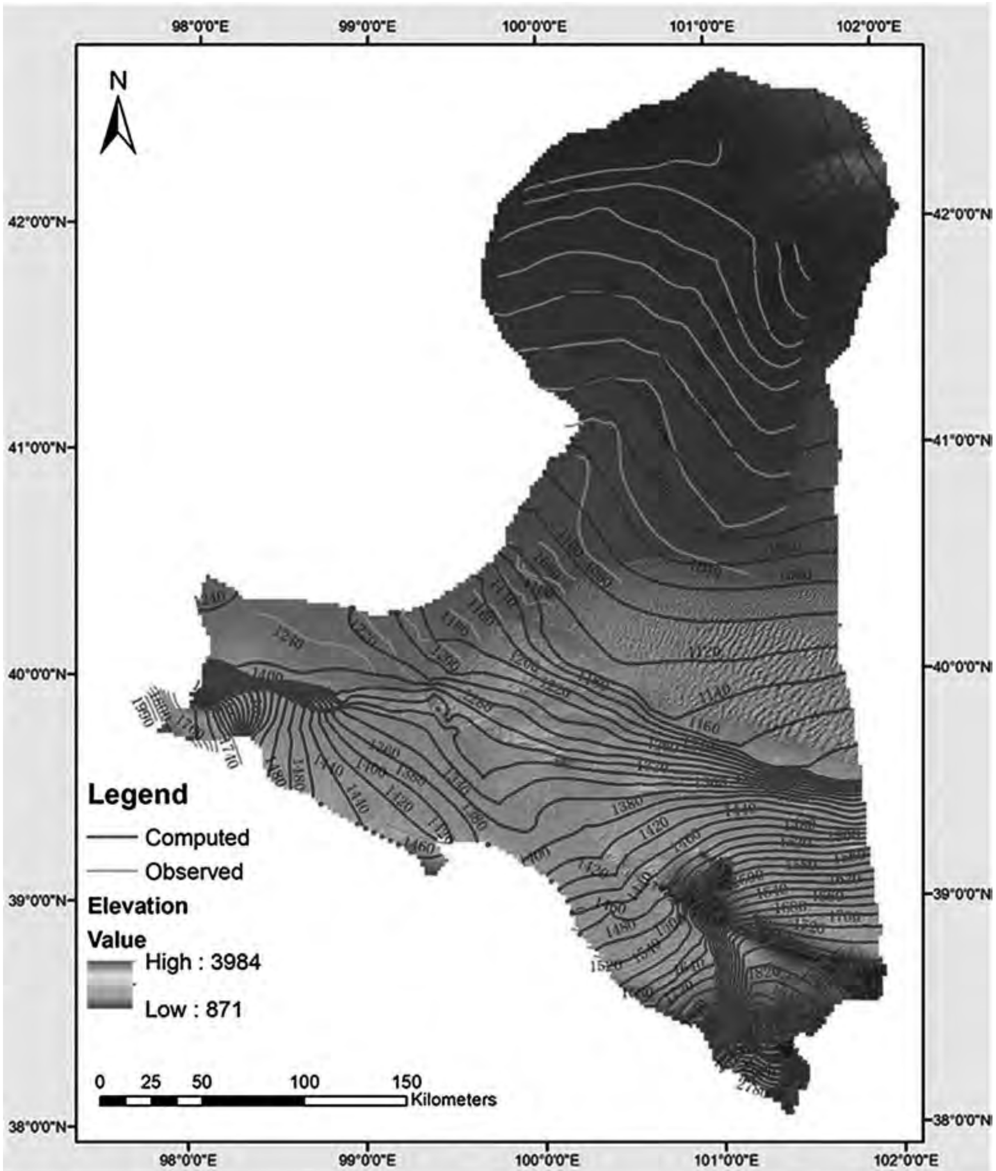


Figure 9.3 Map view of observed (green) and simulated (red) water table (shown by contours) in an arid inland river basin in China. Topographic elevations are shown by color shading *(Yao et al., 2014)*.

Plots of *residual errors* (or *residuals*) are also useful for visualizing calibration results. Residual error is the difference between the target's observed value and its simulated value; for example, the residual in head is ($h_m - h_s$), where h_m is the measured (observed) head and h_s is the simulated head. Residual errors can be plotted spatially in map view

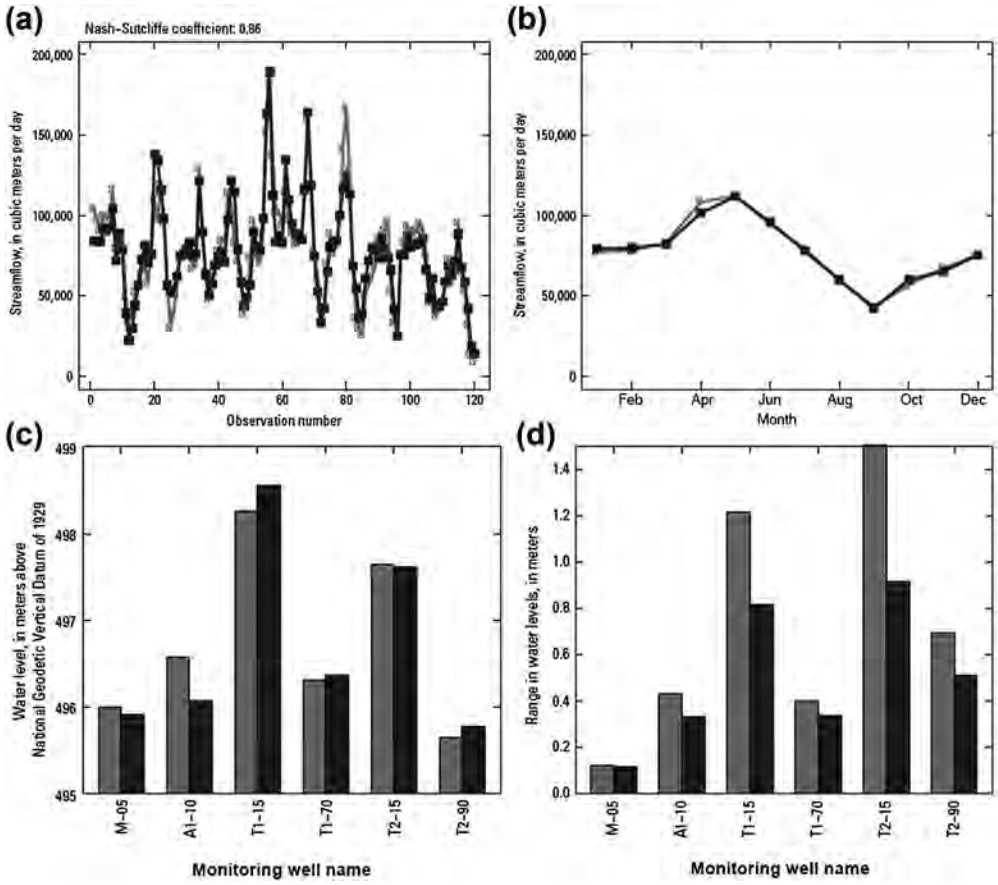


Figure 9.4 Four ways to visualize the comparison of history matching observed (blue) to simulated (reddish-brown) targets in a transient model. (a) Hydrograph of observed and simulated streamflow with Nash–Sutcliffe coefficient (Eqn (9.4)) reported; Fig. 7.11 shows an example of this type of plot using observed and simulated heads. (b) Monthly plot of mean observed and simulated streamflow over the same months in different years using data shown in panel (a). (c) Comparison of mean observed and simulated heads. (d) Comparison of the observed and measured range of values for mean head values shown in panel c *(modified from* Hunt et al., 2013*)*.

(e.g., heads: Fig. 9.6(a); fluxes: Fig. 9.6(b)) or in a cross section to illustrate the magnitude and spatial distribution of residuals. Residuals can also be shown by using graphs (Fig. 9.7). For transient simulations, residuals can be shown on a hydrograph (Fig. 7.11) of each target or a summary plot for groups of targets, such as by hydrogeologic unit (Fig. 7.1).

Although valuable, visual representations of results are necessarily subjective. Therefore, quantitative *summary statistics* are also calculated to measure the goodness of fit. The search for the best appropriate model focuses on finding a model that minimizes those statistics.

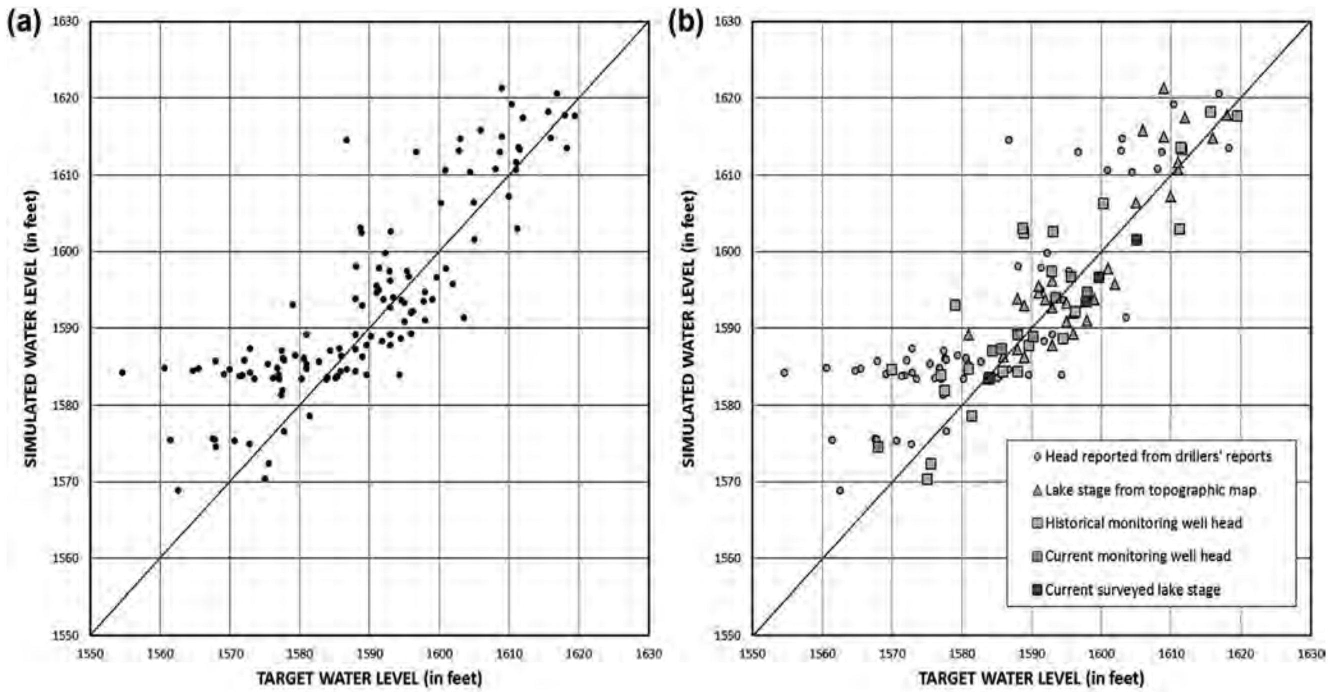


Figure 9.5 Scatter plot (a) and categorized scatter plot (b) of simulated to observed fit of water levels. The categories in (b) can convey the modeler's assessment of target quality, here ranging between observations roughly estimated (small, gray dots) and more accurate observations (larger, colored symbols). The 1:1 perfect fit line is also shown for reference to visualize bias *(modified from* Juckem et al., 2014*).*

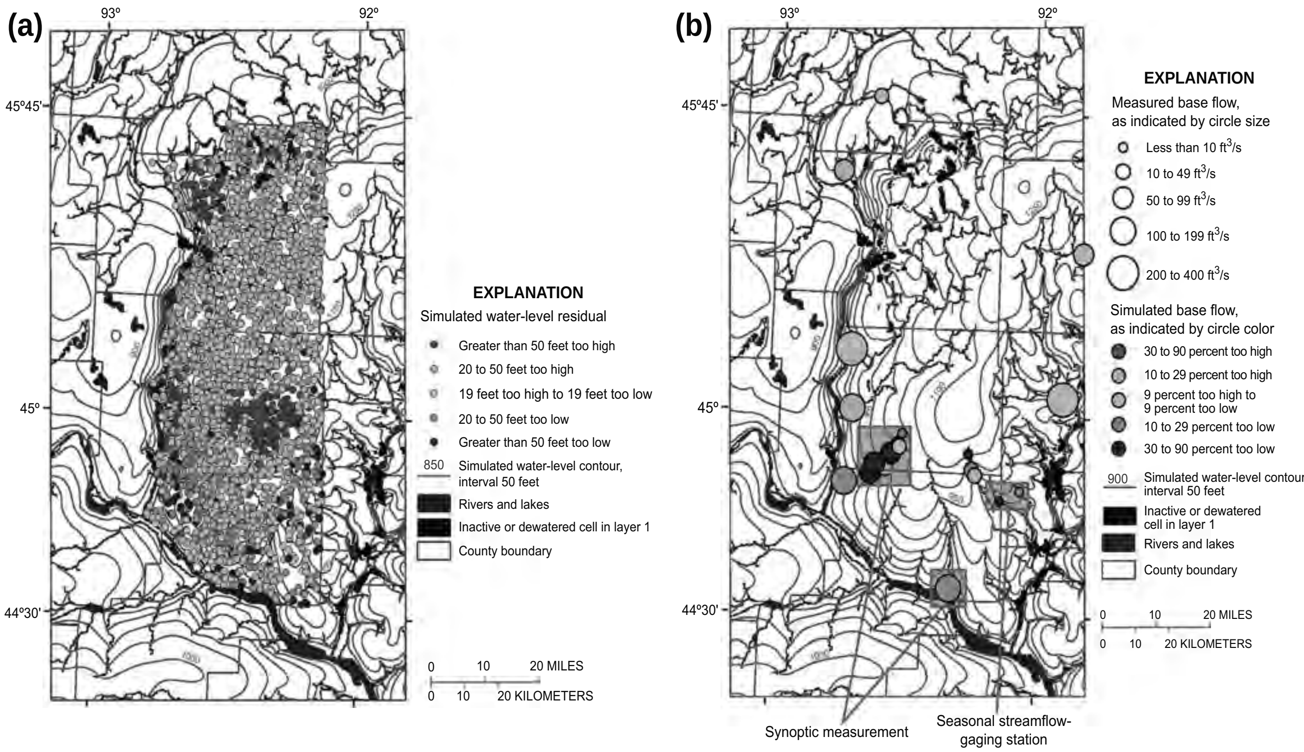


Figure 9.6 Two examples of representing residual errors. (a) Similar size symbols with different colors can be effective when many data are shown, as is the case for head data from the large-scale groundwater model shown in the figure. With such a representation the spatial bias of simulated heads is effectively conveyed. (b) Different sizes and colors can be used when data are few, such as with flux targets in the same model domain as shown in (a). Color relates to degree of fit and symbol size relates to magnitude of the measured flux target—information important when judging the fit of a regional model. Small data sets of lesser quality from synoptic measurements and seasonal stream gages are highlighted to distinguish them from higher quality long-term streamflow measurements *(modified from Juckem, 2009)*.

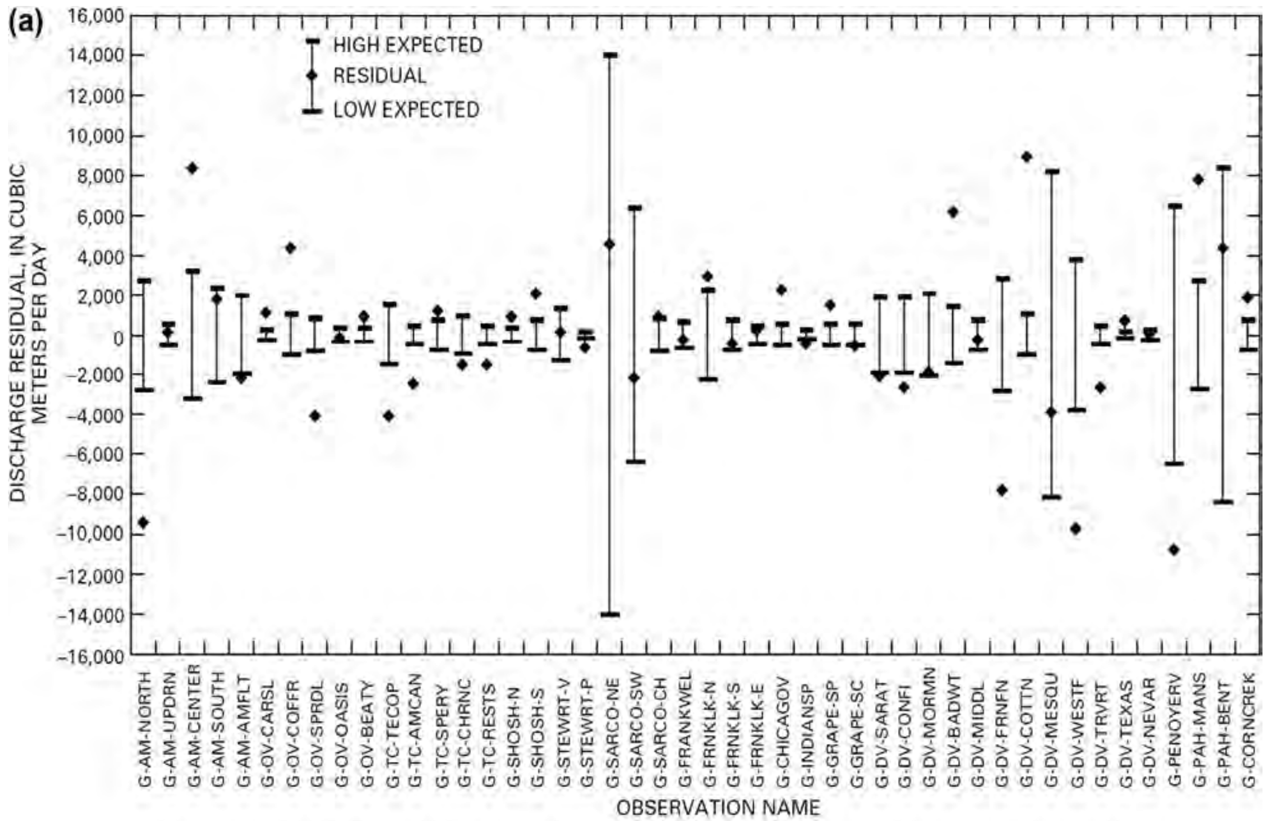


Figure 9.7 History match of flux targets: (a) flux targets with residual error related to uncertainty in measured values *(D'Agnese et al., 2002)*;

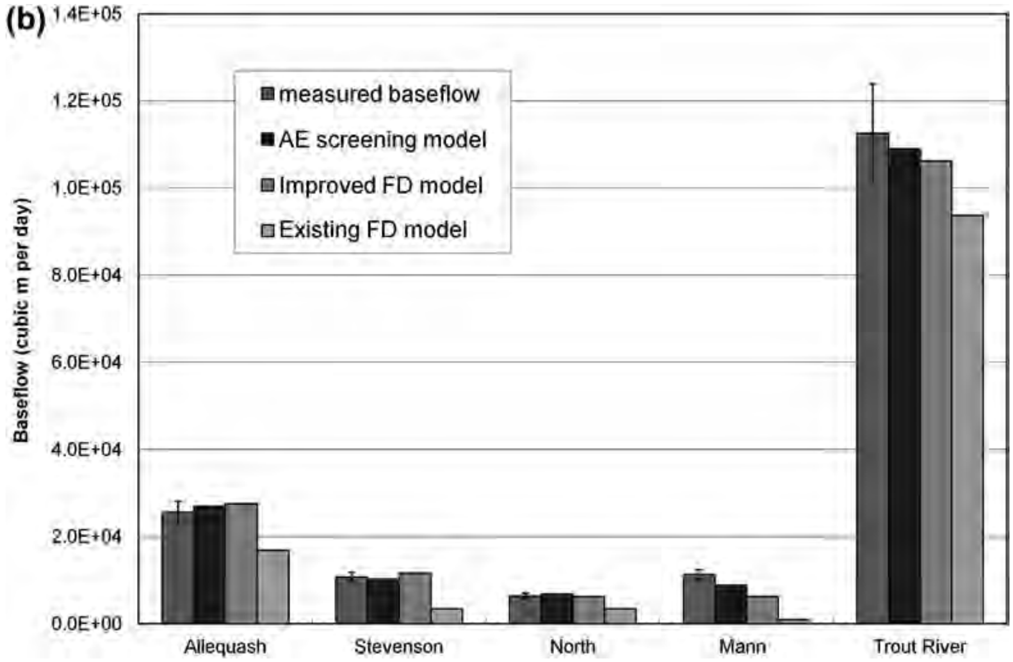


Figure 9.7 Cont'd (b) spatial flux difference targets of baseflow in five streams for three different models showing uncertainty in measured values *(modified from* Hunt et al., 1998*).*

Examples of summary statistics, commonly reported together, are given below; the examples use head data as example observations, but the statistics can be calculated for any type of observation.

1. The *mean error* (*ME*) is the mean difference of the residual errors (measured heads h_m minus simulated heads h_s):

$$ME = \frac{1}{n}\sum_{i=1}^{n}(h_m - h_s)_i \tag{9.1}$$

where n is the number of targets. The *ME* is simple to calculate but is not an ideal statistic. It provides a general description of model bias but because both negative and positive differences are included in the mean, the errors may cancel each other, thus reducing the overall error reported. A small *ME* suggests that the overall model fit is not biased (the simulated values are on average not too high or too low), but this by itself is a weak indicator of goodness of model fit.

2. The *mean absolute error* (*MAE*) is the mean of the absolute value of the residual. Using head as the example:

$$MAE = \frac{1}{n}\sum_{i=1}^{n}|(h_m - h_s)|_i \tag{9.2}$$

Taking the absolute value of the residuals ensures that positive and negative residuals do not cancel. As a result, the *MAE* is usually larger than the *ME*, and is generally a better indicator of model fit than the *ME*.

3. The *root mean squared error* (*RMSE*) is the average of the squared residuals.

$$RMSE = \left[\frac{1}{n}\sum_{i=1}^{n}(h_m - h_s)_i^2\right]^{0.5} \tag{9.3}$$

RMSE is less robust to the effects of outlier residuals; thus, the *RMSE* is typically larger than the *MAE*.

For transient models, other summary statistics can be used to compare individual simulated to observed hydrographs, such as the Nash–Sutcliffe coefficient of efficiency (NS):

$$NS = 1 - \frac{\sum_{i=1}^{n} |(h_m - h_s)|_i^2}{\sum_{i=1}^{n} \left|\left(h_m - \overline{h}_m\right)\right|_i^2} \tag{9.4}$$

where $\overline{h}_{\mathrm{m}}$ is the mean of observed head. *NS* ranges from $-\infty$ to 1; values close to 1 indicate a good fit. For a value of 0, the mean of the data is as good a predictor as the transient series of simulated values. For a value less than 0, the mean of the data would be a better predictor. In practice, lower values such as 0.5 might be deemed acceptable depending on the difficulty of the problem, and many times it is the improvement in *NS* results after a new history match that is of primary focus rather than the value itself.

Even with quantitative summary statistics, deciding that a model's history match is good enough for the modeling purpose is not straightforward because "good enough" remains subjective. Some guidelines use summary statistics as goodness of fit criteria (e.g., Murray–Darling Basin Commission, 2001; ASTM, 2008). For example, a model might be considered sufficiently calibrated if the *RMSE* is less than some set percentage of the calibration target range of values. That is, if head targets range from 50 to 150 m, an acceptable *RMSE* is on the order of 10 m using 10% as a criterion. However, no reasoning supports an assertion that simply meeting such a criterion defines an appropriately calibrated model. Nor are there established industry guidelines regarding the acceptable magnitude of the *ME*, *MAE*, or *RMSE*, other than it is desirable to minimize these values. Although the utility of standard criteria is recognized, uniform calibration standards have not been adopted by the modeling community. In part, this reflects the awareness that all modeling requires subjective judgment (e.g., Silver, 2012; Fienen, 2013). Moreover, it is unlikely that a universally appropriate methodology could be formulated because the acceptability of a calibration is directly dependent on the modeling objective, and there are many possible modeling objectives.

9.4.2 Choosing the Parameters to Adjust

As discussed above, the first forward model run using best estimates for model parameter values is unlikely to obtain a model fit sufficient for the modeling purpose. Therefore, parameter values must be adjusted from the modeler's initial estimate to obtain a better fit. The translation of real-world properties to the model requires assigning parameter values to every node in the grid/mesh (Section 5.5). For purposes of calibration, the modeler reduces the set of all possible parameters (Section 5.4) to a set of *calibration parameters* that are allowed to vary during history matching. Calibration parameters may include any model input: vertical and horizontal hydraulic conductivities, boundary conditions, recharge rates, as well as other sources and sinks of water. Calibration parameters will not be equally valuable for improving model fit; during manual trial-and-error, the modeler identifies *insensitive parameters* that minimally affect the model output of simulated targets, and *sensitive parameters* that have a larger effect. Because the goal of adjusting parameter values is to find a sufficiently good history match, the modeler focuses on adjusting sensitive parameters. The final set of *optimal calibration parameter* values reflects the solution to the inverse problem supported by hard knowledge (Fig. 9.1). However, even then, this set should be recognized as *conditionally optimal* because it is dependent on the calibration data (and their errors), and criteria for judging what is optimal, selected by the modeler (Beven, 2009, p. 106).

One might ask why not make all parameters calibration parameters? When the number of calibration parameters (the unknowns) is greater than the number of observations (the knowns), the inverse problem is considered mathematically ill-posed and underdetermined (Section 9.2). One general approach to obtain an *overdetermined*, and therefore hopefully mathematically tractable, problem is to reduce the number of calibration parameters to a number fewer than the number of calibration targets. This approach for obtaining a tractable inverse problem has been extensively developed (e.g., see Hill and Tiedeman, 2007).

The advantage to simplifying the model by reducing the number of calibration parameters a priori is that at some point excluding enough calibration parameters will always result in a tractable inverse problem. Excluding parameters from the history matching process is also conceptually straightforward. However, when simplifications introduced during parameterization are done poorly, model outputs are adversely affected in ways not obvious to the modeler or easily corrected (Doherty and Welter, 2010). This is because the degree of simplification is a subjective choice of the modeler and, once set, further analysis of model error is difficult. As a result, it becomes difficult to assess whether large residuals are caused by poor choices of parameter values or if caused by defects in the model resulting from "incorrect hypotheses, unmodeled processes, or unknown correlations between processes" (Gaganis and Smith, 2001); this latter source of model misfit is called *structural error* (sometimes called "model error"). Although structural error appears self-evident, in practice complexities that are left out while defining the model are often "quietly forgotten" (Beven, 2009, p. 6).

A straightforward method of reducing the number of calibration parameters involves *zonation* (Section 5.5), whereby areas of the model domain are assigned the same parameter value; adjusting the calibration parameter for the zone adjusts the parameter at all nodes in the zone simultaneously. Hence, zonation creates areas of *piecewise constant* parameters so that when the parameter is changed it affects model input for all nodes within the zone. The piecewise constant structure inherent to zonation is a modeling artifact—a simplification that helps models handle a complex natural world. When present, zones exist only approximately in the field. One concern is that the structural error imparted by zonation on model results can be large (e.g., Moore and Doherty, 2005). Yet zones are commonly used to reduce the number of calibration parameters, and thus zonation helps obtain a well-posed inverse problem.

Although impossible to quantify completely, it is clear that structural error associated with a model is not random. Its magnitude is a direct function of the type and degree of simplification imposed by the modeler (e.g., Beven, 2005). For example, a model with only one zone has relatively large structural error and will be less successful in fitting targets than a model with more zones. Recognizing the relation of the total number of parameters to structural error, and its effect on model calibration and forecasting, is important because structural error is usually the largest component of model error in sparsely parameterized groundwater models (Sun et al., 1998; Gaganis and Smith, 2001; Moore and Doherty, 2005). When the level of simplification imposed by the modeler unacceptably degrades a model's performance, the model is considered *oversimplified*. The issue of oversimplification is not new to groundwater modeling—the development of numerical models was driven by attempts to overcome oversimplification inherent in the limiting assumptions typical of analytical solutions (e.g., Freeze and Witherspoon, 1966). This selection and grouping of calibration parameters for history matching is called *parameterization*; we revisit the topic of parameterization and its effect on model performance in Section 9.6.

9.4.3 Manual Trial-and-Error History Matching

Similar to the initial forward run of the model, a second run of the forward model using different calibration parameters is unlikely to provide a satisfactory history match. The process of trying additional parameter sets becomes an iterative *manual trial-and-error* matching procedure whereby the modeler manually adjusts parameter values and compares model output to targets using successive forward runs of the model. By manually adjusting parameters, the modeler explores how changes to the number, magnitude, and location of calibration parameters influence the fit between simulated values and targets. In this way, manual trial-and-error history matching not only improves the fit but also provides important insight into how the simulated groundwater system behaves.

Some parameters and boundary conditions may be known with a high degree of certainty and, therefore, should be modified only slightly from initial values, if at all, during this phase of history matching. The modeler identifies insensitive parameters by observing that changes (made within a predetermined reasonable range) produce little change in model outputs. Therefore, during subsequent trial runs insensitive parameters are set as invariant, or *fixed*, values that are based on field data, literature values, professional judgment, and/or other soft knowledge. A parameter that is insensitive during history matching may be sensitive in forecasting simulations, however. Therefore, a parameter that is fixed during history matching may need to be freed during the forecasting phase of modeling (Chapter 10).

When changing multiple parameters in the same forward run of the model, the modeler may also identify parameters that are *correlated*. Two or more parameters are correlated when the effects of changes in one parameter can be offset by changes to others such that model outputs are not appreciably changed. For example, examination of the groundwater flow equation (e.g., Eqns (3.12) and (3.13(a,b))) (and hydrogeologic intuition) indicates that decreases in hydraulic conductivity and increases in recharge both increase heads. Therefore, both are sensitive parameters when considered independently. However, a decrease in hydraulic conductivity can be offset with a commensurate decrease in recharge rate resulting in no net effect on simulated heads. This is an important insight for model calibration because it means that history matching to head data only is fundamentally nonunique. Head data alone can only constrain the ratio of recharge and hydraulic conductivity (Box 3.2; Haitjema, 2006); unique individual values for both recharge and hydraulic conductivity cannot be obtained. However, if a flux target (e.g., observed baseflow) is considered along with head data, parameter correlation is reduced and unique estimates of both hydraulic conductivity and recharge can be obtained. In cases where additional observations are not available to break parameter correlation, the modeler attempts to determine best estimates for correlated parameters manually. Such manual intervention can be difficult in practice because parameter correlation is harder to identify than insensitivity, especially if many parameters and processes are simulated.

9.4.4 Limitations of a Manual Approach

Manual trial-and-error calibration remains a fundamental first step for history matching because it gives the modeler much insight about the site modeled and how parameter changes affect different areas of the model and types of observations. In this way, manual trial-and-error helps develop a modeler's "hydrosense." Manual trial-and-error is also an efficient first test of the conceptual model because it can quickly demonstrate that a specific conceptual model is ill-suited to match field observations and thus does not belong in the family of reasonable models. These positive aspects notwithstanding, manual trial-and-error history matching is an imperfect process because even though some insight is gained, feedbacks between sources and sinks and other correlated parameters and processes in most groundwater systems are complex. As a result, it is impossible to track effects of all changes in calibration parameters to system-wide effects on all observations. The inherent subjectivity and deficiencies of manual trial-and-error calibration were summarized by Carrera and Neuman (1986):

> *The method of calibration used most often in real-world situations is manual trial and error. However, the method is recognized to be labor intensive (therefore expensive), frustrating (therefore often left incomplete), and subjective (therefore biased and leading to results the quality of which is difficult to evaluate).*

The last point is critically important: the very ad hoc nature of manual trial and error makes comprehensive testing and identification of all insensitive and correlated parameters difficult. As a result, using manual trial-and-error calibration alone is problematic. It cannot guarantee that the modeler has found the quantifiable best fit for a given conceptual model. At the end of even the most rigorous manual trial-and-error procedure it is likely that untested sets of parameters might yield a better model. For some modeling purposes, this lack of a guarantee of best fit is undesirable but not problematic. In other cases, failure to present a defensible best model can have serious repercussions, especially when groundwater models are used in regulatory and legal arenas (e.g., Bair, 2001; Bair and Metheny, 2011). In recognition of this fact, mathematically rigorous automated trial-and-error methodologies (Box 9.1; Sections 9.5 and 9.6) were developed. Yet, even with these methods, it should be recognized that advanced methods can never fully replace insight and hydrosense gained from the manual trial-and-error process. Instead, advanced methods are best applied after a model is at least roughly calibrated using a manual trial-and-error approach.

9.5 PARAMETER ESTIMATION: AUTOMATED TRIAL-AND-ERROR HISTORY MATCHING

Parameter estimation is an indirect solution of the inverse problem (Box 9.1) that is effectively automated trial-and-error calibration because computer algorithms perform the same general steps as described in Section 9.4 and shown in Fig. 9.1. Parameter estimation starts with an initial set of reasonable parameters derived from a manual history match and perfects the ad hoc and subjective manual results using a computer program (inverse code) and statistical methods. Parameter estimation codes also formalize the history matching process in that the modeler must explicitly address elements loosely handled in a manual trial-and-error process. These include:

1. the computer code(s) for the forward runs;
2. the calibration parameters;
3. calibration targets and their weights;
4. criteria for when to stop looking for a better fit.

Box 9.1 Historical Context for Parameter Estimation

The inverse problem is called "inverse" because what we know (heads) must be inverted to find what we do not know (e.g., aquifer material properties). In other words, in solving the inverse problem for groundwater flow, we can find values for the parameters because we assume heads are known. Pioneering papers by Stallman (1956a,b) proposed a direct solution to this inverse problem. The direct approach was explored by Nelson (1960, 1961, 1962), among others (e.g., Emsellem and de Marsily, 1971; Neuman, 1973). In the direct method, the partial differential equation for groundwater flow is written with hydraulic conductivity as the dependent variable; heads must be specified completely in space and time. However, heads are never completely known, which necessitates interpolation of field-measured heads. Interpolation introduces small errors into the head distribution that can cause large errors when solving the inverse problem for hydraulic conductivity. Therefore, even though the direct approach is appealing owing to its mathematical elegance and computational efficiency, it was found to be unstable for most realistic problems.

The inverse problem, however, can also be solved indirectly. The indirect method essentially automates the manual trial-and-error process where properties are estimated iteratively using statistical regression and computer algorithms. Yeh and Tauxe (1971), Cooley and Sinclair (1976), and Cooley (1977, 1979) advocated an indirect approach to solve for groundwater parameters, now called *parameter estimation*. Richard Cooley (Cooley, 1977, 1979; Cooley and Naff, 1990) developed a pioneering inverse code using nonlinear regression, an approach later extended to the parameter estimation code MODINV (Doherty, 1990), MODFLOWP (Hill, 1992), and UCODE (Poeter et al., 2005). PEST (*P*arameter *EST*imation; Doherty 2014a,b) replaced MODINV in 1994, and currently the PEST software suite is widely used for applied groundwater modeling. Late in the twentieth century, groundwater modelers began routinely applying inverse codes to sparsely parameterized problems and a wider use of parameter estimation was advocated (e.g., Yeh, 1986; Carrera, 1988; Poeter and Hill, 1997). Researchers in other fields such as geophysics were also addressing inverse problems at this time by applying advanced statistical theory and mathematics (e.g., Aster et al., 2013) to solve highly parameterized problems. Many of these advanced methods (e.g., singular value decomposition, Tikhonov regularization) are now available to groundwater modelers through the PEST software suite (www.pesthomepage.org).

It is clear that indirect methods for solving the inverse problem are valuable and essential tools for groundwater modeling. There is a textbook focusing primarily on calibration of sparsely parameterized models (Hill and Tiedeman, 2007), and guidelines for highly parameterized groundwater modeling are available (Doherty and Hunt, 2010). Large increases in computer power and access to parallel processing have expanded parameter estimation to complex models with 1000s of calibration parameters (e.g., BeoPEST: Schreüder, 2009; GENIE: Muffels et al., 2012; PEST++: Welter et al., 2012), and cloud computing (e.g., Hunt et al., 2010). Inverse codes include modern programming techniques, provide simplified access to advanced methods (e.g., PEST++, Welter et al., 2012), and have been updated to incorporate the Bayesian geostatistical approach (bgaPEST—Fienen et al., 2013) and the null-space Monte Carlo method (Tonkin and Doherty, 2009; Doherty et al., 2010b). Inverse methods are still evolving and finding better ways to solve the inverse problem continues to be an active area of research (e.g., Zhou et al., 2014).

For example, parameter estimation requires the modeler to translate an observation's subjective importance (i.e., its rank; Section 9.3) into a numerical weight (Table 7.1). Parameter estimation also requires the modeler to quantify the reasonable ranges for the calibration parameters. Perhaps most importantly, parameter estimation quantitatively determines when a fit is sufficiently good. Thus, parameter estimation utilizes the power of modern computing methods to alleviate the labor intensive aspects of manual trial-and-error calibration (e.g., Figs 9.8 and 9.9). For example, a typical parameter estimation algorithm automates: (1) adjustment of calibration parameters; (2) evaluation of output; (3) tracking the effect of changes in all calibration parameters on all calibration targets; and (4) estimating better values for calibration parameters. Because the calibration steps in Fig. 9.9 are formalized in the input for the parameter estimation code, the quantitative description of the calibration can be expressed in a way that is transparent and easily documented.

Although the general steps in parameter estimation (Fig. 9.9) are formalized in the code, the automated process cannot be considered automatic calibration because the modeler is fully involved in all aspects of defining the calibration. If the fit is unacceptable, the modeler modifies the target types, weights, and calibration parameters, after which the parameter estimation process is repeated. The modeler will also perform a soft knowledge assessment of the calibration by deciding whether the calibrated parameter values are hydrogeologically reasonable and conform to the conceptual model. If the best fit model is still unacceptable, a new conceptual model and a new numerical model must be formulated and the calibration process, starting with manual trial-and-error history matching, is repeated.

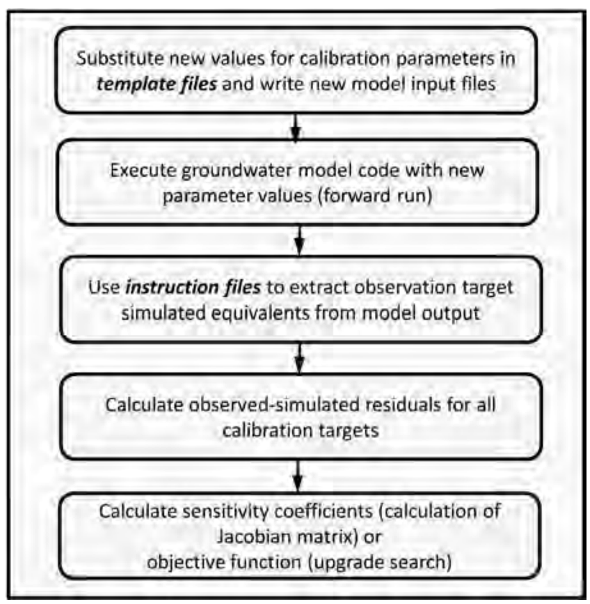


Figure 9.8 A schematic workflow diagram of the mechanics of each forward run automated by a universal nonlinear regression parameter estimation code. The shaded background in the figure indicates that the steps are performed internally by the code without user intervention. Two types of ASCII (American Standard Code for Information Interchange) files are required before the parameter estimation code can be run: (1) a template file that specifies where to place new values of calibration parameters in the model input file; and (2) an instruction file that extracts relevant model outputs for comparison to observed calibration targets. Both required files are typically created by a graphical user interface (GUI).

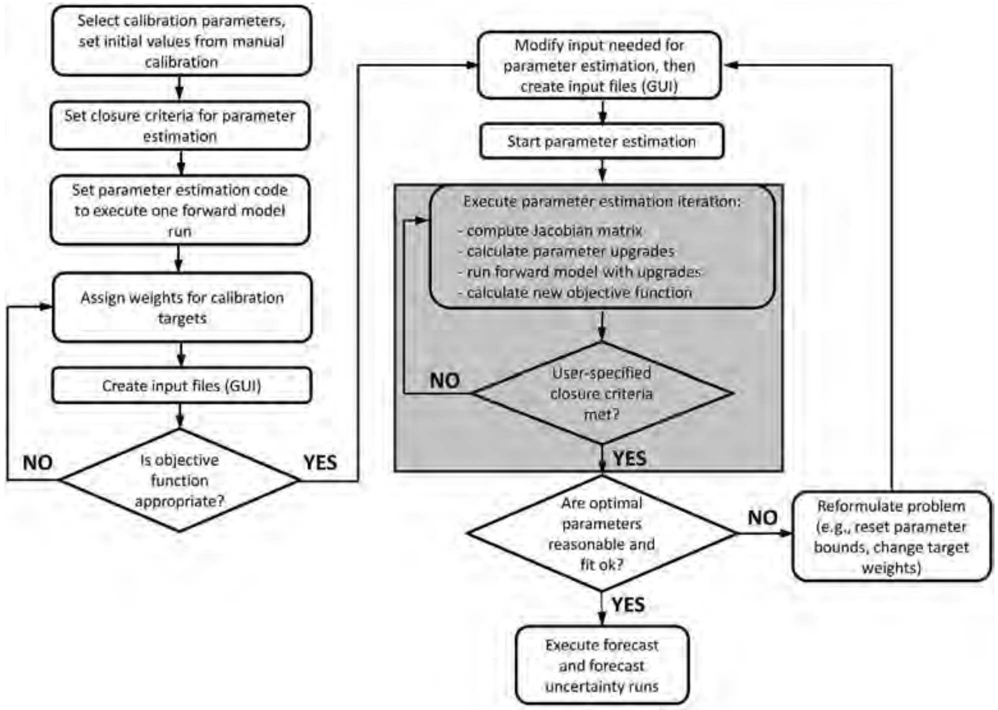


Figure 9.9 A schematic diagram of a general workflow for parameter estimation, the second phase of history matching for a model designed for forecasting. Shaded box contains steps automated by the parameter estimation code; steps in the unshaded areas require modeler action. An objective function is appropriate when all targets are included but targets important to the modeling objective are more prominently weighted (GUI, graphical user interface).

As outlined above, parameter estimation appears to be straightforward, and general guidelines are well developed (Box 9.2). However, automating the inverse problem is difficult and many approaches have been developed. Zhou et al. (2014) broadly group inverse methods into deterministic and stochastic approaches. Deterministic inverse methods seek a single representation of parameters that produces a best fit to the calibration targets. Stochastic inverse methods generate multiple realizations of parameter distributions, all of which give acceptable fits to the calibration parameters; the ensemble of realizations is carried forward to make forecasts (Chapter 10) and convey parameter uncertainty. We focus here primarily on deterministic inverse methods that are programmed into "universal" parameter estimation codes. Universal parameter estimation codes are widely used for applied modeling because they can interface with any computer code that can: (1) run in batch mode (reach completion and write model output without user intervention) and (2) read input and write output files. The input/output file format required is most commonly American Standard Code for Information Interchange

(ASCII) files, which is the computer file type recognized by simple text editors. Most GUIs for groundwater flow codes build input and can execute a universal parameter estimation code. The essential elements of formalizing the calibration problem for universal parameter estimation codes are considered in more detail below and in Section 9.6. Tips for running the code are given in Box 9.2.

Parameter estimation theory uses advanced mathematical and statistical methods, and can be quite sophisticated. Fortunately, advanced parameter estimation techniques are accessible to the applied modeler through widely available software, and their appropriate use does not require detailed knowledge of underlying theory. In this section, we discuss some general concepts relevant to all deterministic inverse methods, but in Section 9.6 we emphasize specific approaches embodied in the PEST (*P*arameter *EST*imation) suite of codes (Doherty, 2014a,b; Welter et al., 2012; Fienen et al., 2013). Similar to our use of MODFLOW and FEFLOW to illustrate concepts of groundwater modeling, PEST is used to illustrate concepts of calibration. The PEST software suite is currently widely used for parameter estimation of applied groundwater models, and includes many advanced capabilities (some of which are discussed in Section 9.6). Although not a stochastic inverse code in the sense discussed by Zhou et al. (2014), PEST has an option that allows generation of multiple realizations of parameters in a Monte Carlo framework (Section 10.5).

Those who wish to delve further into the details of parameter estimation theory should consult references provided at the end of this chapter, and associated literature cited therein. Zhou et al. (2014) provides a review of inverse modeling applied to groundwater systems and many references. User manuals or guidance documents provided with specific codes (e.g., Doherty, 2014a,b; Doherty and Hunt, 2010; for PEST) typically include the theoretical background, as well as instructions and examples for creating input and running the code itself.

9.5.1 Weighting the Targets

In Section 9.3, we ranked targets qualitatively considering errors, uncertainty, and the importance of the target for addressing the modeling purpose. This same approach is used to rank targets for parameter estimation except that targets are now numerically weighted (Table 7.1). In an ideal statistical world, assigned individual target weights directly express the associated measurement error of the observation. However, as discussed in Section 9.3, the ideal rarely holds when models are applied in practice; thus, initial measurement-based weights are often adjusted to reflect other modeling considerations such as the need to balance the numbers of each type of target, the spatial distribution (e.g., declustering—Bourgault, 1997), and the importance of the target to the modeling purpose, such as location in the near-field or far-field.

Mathematically, weights are used to increase or decrease the contribution of individual residuals to the total sum of model error called the *objective function* (often represented by $\mathbf{\Phi}$). Most universal parameter estimation codes calculate the objective function as the sum of squared weighted residuals. That is, the residual calculated for each target is multiplied by its weight, squared (making all residuals positive), and then summed. A quantitative best fit model has the minimum value of the objective function. If the targets include only head observations, the objective function, $\mathbf{\Phi}$, is:

$$\mathbf{\Phi} = \sum_{i=1}^{n} \left[w_{hi} (h_m - h_s)_i \right]^2 \tag{9.5}$$

where w_{hi} is the weight for the ith head observation; h_m is the measured (observed) head target; h_s is the simulated head. For better posed history matching, both head and flux observations are used as targets and the objective function is written:

$$\mathbf{\Phi} = \left\{ \sum_{i=1}^{n} \left[w_{hi} (h_m - h_s)_i \right]^2 + \sum_{i=1}^{n} \left[w_{fi} (f_m - f_s) \right]^2 \right\} \tag{9.6}$$

where w_{hi} is the weight for the ith head observation; h_m is the measured (observed) head target; h_s is the simulated equivalent head; w_{fi} is the weight for the ith flux observation; f_m is the measured (observed) flux target; f_s is the simulated equivalent flux.

From Eqns (9.5) and (9.6), it is evident that the objective function can be expanded to include any type of observation that has a simulated equivalent quantity. Indeed, including as many observation types in the objective function as possible helps constrain the parameter estimation process and ensure better correspondence between the simulated and real-world systems (Hunt et al., 2006). Moreover, raw observations as in Fig. 9.4(a) can be processed (e.g., Fig. 9.4(b)−(d)) and also included in the objective function to emphasize aspects of the system deemed important. Equations (9.5) and (9.6) show that assigned weights directly influence the objective function − a higher weight increases the importance of the residual by giving it a larger contribution to the objective function.

The best fit model has the minimum value of the objective function, which is directly dependent on the weights assigned to each target. It follows that targets with relatively small measurement errors and that are important for the forecast should be assigned relatively larger weights. Weighting also quantifies a modeler's judgment regarding the importance of target type relative to other types (e.g., heads versus fluxes, far-field heads versus near-field heads, baseflow targets versus miscellaneous streamflow measurements). The goal of target weighting is to achieve a balanced initial objective function (Fig. B9.2.1 in Box 9.2) where all targets have a presence. However, the objective function does not need to be perfectly balanced; rather, it should reflect the modeling purpose, where targets important to the modeling objective are more prominent. Because expression of what the modeler holds important for the modeling purpose is part of the art of modeling, there is no one set of definitive rules for weighting. Different views of weighting are explored by Doherty and Hunt (2010) and Hill and Tiedeman (2007).

9.5.2 Finding a Best Fit

The objective function provides a single numerical value that encapsulates the model's fit to all targets and the importance assigned to each target by the modeler. Because a best fit corresponds to the minimum of the objective function, finding the best fit becomes a search for a minimum on a multidimensional *objective function surface* (Fig. 9.10). For a

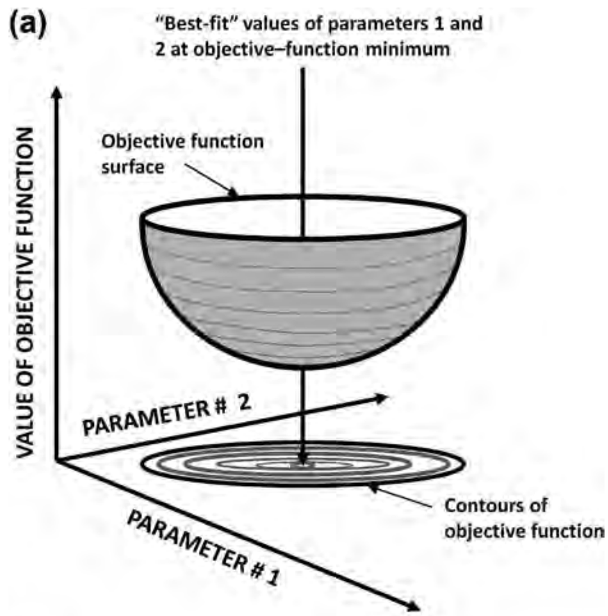
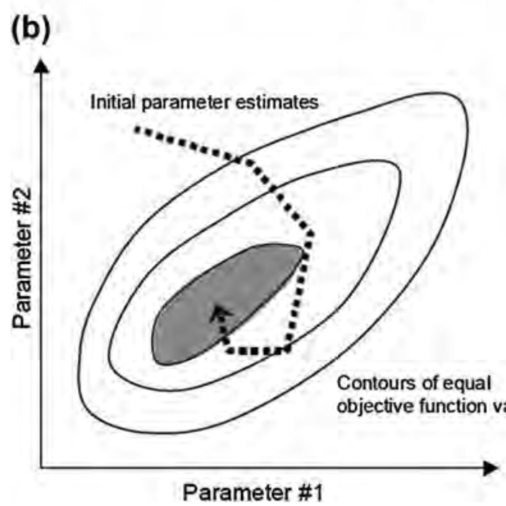


Figure 9.10 (a) Idealized objective function surface for a two-parameter problem *(modified from Himmelblau, D.M., 1972,* Applied Nonlinear Programming, *McGraw-Hill, New York, reproduced with permission of McGraw-Hill Education).*



(b) improvement in the solution via parameter upgrade in successive parameter estimation iterations (shown by the dashed line) leading to the objective function minimum *(from Doherty, 2014a).*

simple two-parameter model as shown in Fig. 9.10, the objective function surface is easily visualized as contours of the objective function. Most history matching occurs with more than two parameters, however, which results in a multidimensional surface difficult to visualize. Nevertheless, concepts discussed below for the simple case of a two-parameter model are similar for a multidimensional surface. To find the objective function minima, the parameter estimation code performs a series of forward model runs, each with a different set of values for calibration parameters. The algorithm then calculates the objective function using an equation like Eqn (9.6). The search for optimal parameters typically is not random; *derivative-based nonlinear* search techniques used for most applied modeling evaluate the slopes of the objective function surface and adjust parameters to force the forward model to progress toward the global minimum of the objective function. The search technique must accommodate nonlinearity because the responses of heads and flows to changes in parameters are usually nonlinear (e.g., Eqn (3.12)).

One widely used method to search the objective function surface for the minimum is based on the *Gauss–Marquardt–Levenberg (GML) method*, also known as the *damped least squared method* (Levenberg, 1944; Marquardt, 1963; Hill and Tiedeman, 2007; Doherty, 2014a). *Derivative-based methods* such as GML assume that simulated values of targets vary as a continuous function in response to changes in calibration parameters. That is, the GML method assumes that model inputs (parameters) and outputs (simulated values of targets) are continuously differentiable. In general, the groundwater flow equation conforms to this assumption. As discussed previously, however, nonuniqueness inherent to groundwater models means that multiple combinations of parameters can provide similar fits to the targets. In the two-parameter case, nonuniqueness can be visualized as a set of optimal values lying in the "trough" of the objective function surface (Fig. 9.11(a)). However, even when the inverse problem is well posed (e.g., giving the unique best fit in Fig. 9.11(b)), a multidimensional objective function surface can have multiple local minima in addition to the global minimum (Fig. 9.12) that represents the best model fit. For some models, guaranteeing that an objective function minimum is the global minimum can be difficult, especially when the derivatives are noisy (i.e., not perfectly continuously differentiable due to machine or code precision issues or solver closure selected—compare Figs. 9.13(a) and (b)). *Global methods* do not rely on derivatives to explore the objective function surface; however, they are much more computationally expensive than gradient-based methods, and thus typically consider a relatively small number of calibration parameters (usually <100). As a result, derivative-based methods are more commonly used than global methods for most applied modeling problems.

Universal parameter estimation codes can manipulate model input files and process model output files from any groundwater flow code. Therefore, they can calculate the objective function slope required by derivative-based methods using almost any code, not just the subset that internally include such capabilities. Observation-to-parameter

Figure 9.11 Objective function surfaces from a two-parameter model of a field site where contour lines with warmer colors represent lower objective function value: (a) example of a solution that did not converge; that is, the objective function surface has no unique minimum (shaded pink trough). Nonconvergence was caused by using only head data as calibration targets;

(b) the objective function surface for a solution that converged. The solution included both heads and groundwater temperature as observation targets. Dashed lines represent the approach to the surface minimum and reddish circles represent parameter upgrades *(modified from* Bravo et al., 2002*).*

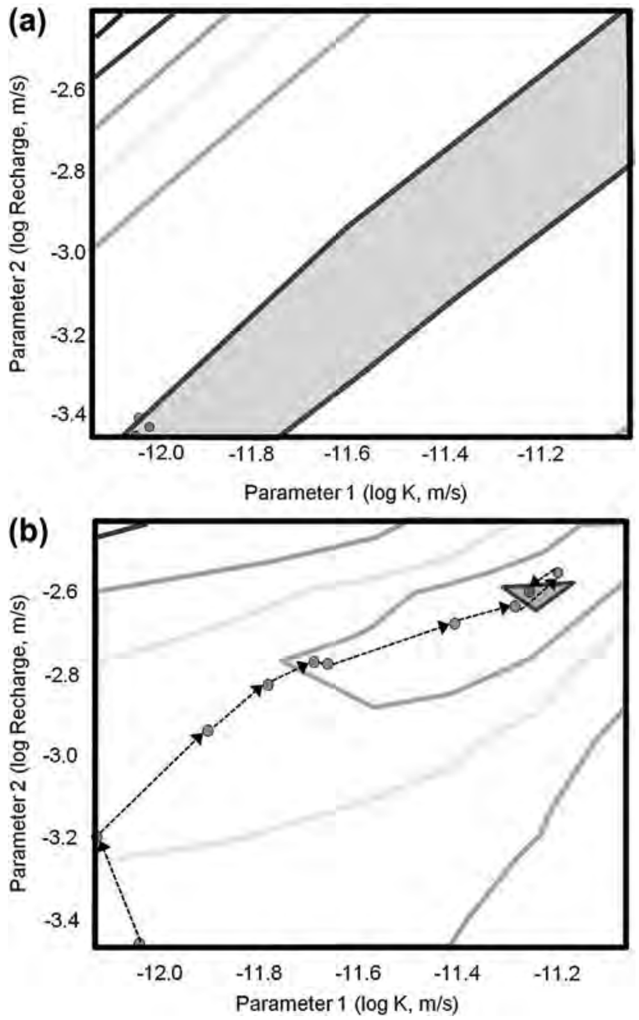
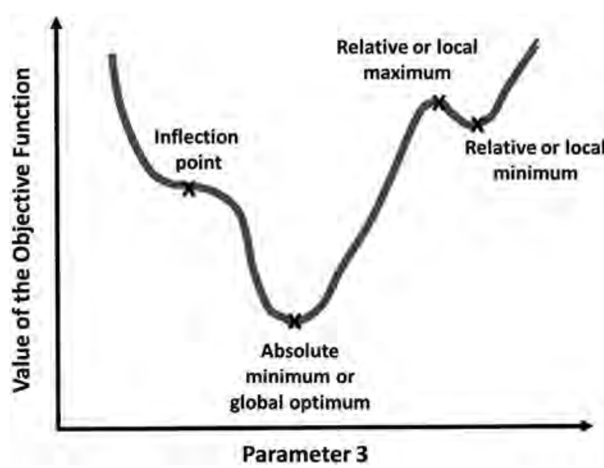


Figure 9.12 Cross section of an objective function surface showing local and global minima *(modified from* Zheng and Bennett, 2002*).*



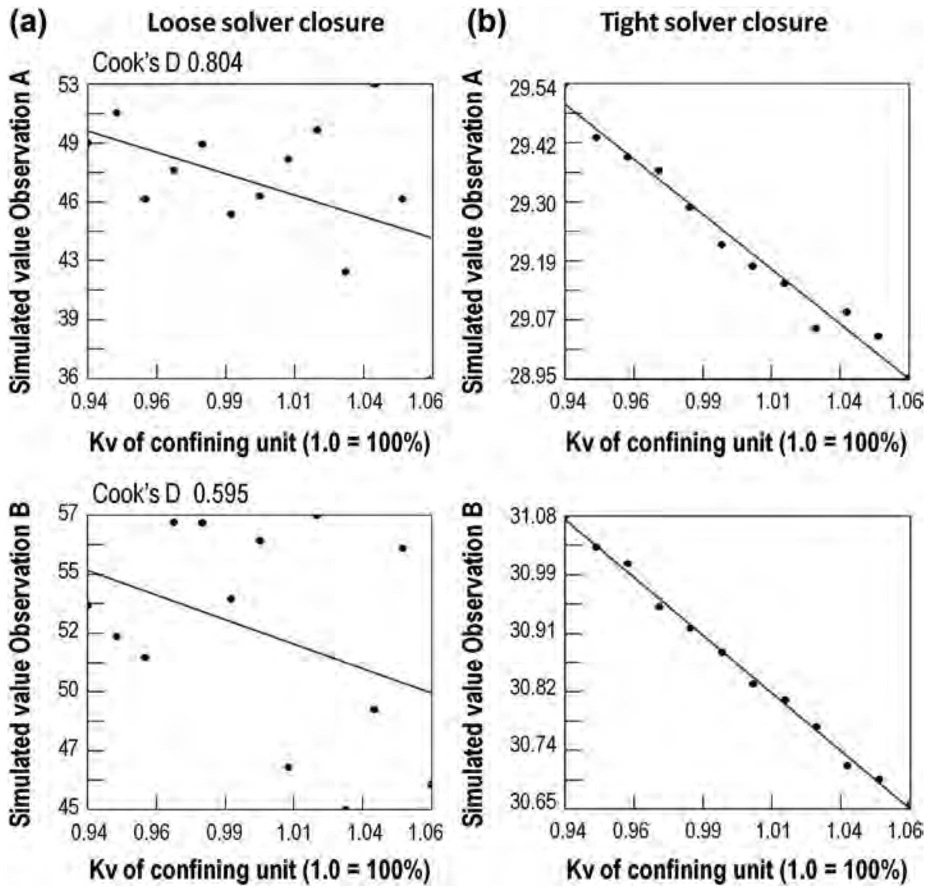


Figure 9.13 Plot of change in model outputs (y-axes) to small increments of change in one model parameter (x-axes) for two different observations. Each dot represents one model run; the straight line is the best fit through the dots. Because the true parameter sensitivity derivative is approximated using a 1% parameter perturbation sequential 1% perturbations should provide a coherent change (e.g., the monotonically changing line shown in (b)). Poor derivatives calculated by perturbation (a) can confound derivative-based parameter estimation methods; tighter solver closure as shown in (b) provides more coherent derivatives. An influence statistic (Cook's D, Box 9.6) for the two observations is also listed, where higher values represent more influence on the regression *(modified from Feinstein et al., 2008)*.

derivatives relate the change in the simulated value of the target (Δ*observation*) to a change in the value of the calibration parameter (Δ*parameter*), and are known as *sensitivity coefficients* (also called *parameter sensitivity*):

$$\textit{sensitivity coefficient}_{ij} = \frac{\Delta\ \textit{observation}_i}{\Delta\ \textit{parameter}_j} \tag{9.7}$$

where $\Delta observation_i$ is the change in simulated value of the *i*th target and $\Delta parameter_j$ is the change in value of the *j*th calibration parameter. The set of sensitivity coefficients forms a two-dimensional array of values of *i* rows and *j* columns commonly known as the *Jacobian matrix* or *sensitivity matrix* (Fig. 9.14). The heads computed by using initial parameter values at the start of the parameter estimation process form the basis for comparison; changes in output are calculated by changing parameter values from their initial values. After the initial forward run, a series of forward runs is performed where each individual calibration parameter is changed by a small amount (usually 1%) and the model is run while all other parameters are held constant at their initial values.

Changes in the simulated values for each target ($\Delta observation_i$) are calculated by subtracting the model output from the run with the perturbed parameter from the output of the initial model run that used unperturbed parameters. The sensitivity for the parameter that was perturbed is calculated from Eqn (9.7) and entered into the Jacobian matrix. The minimum number of forward runs needed to calculate a Jacobian matrix is equal to the number of calibration parameters plus one (i.e., the initial unperturbed run). Perturbation-based sensitivity information stored in the Jacobian matrix only approximate the actual derivatives of the observations to changes in each parameter, but has been found to be sufficiently accurate for applied models (Yager, 2004).

Once the Jacobian matrix is calculated, the slope of the objective function surface as represented by the derivative information is used to identify changes in calibration parameters that move toward the objective function minimum. From these slopes: revised estimates of the calibration parameters are selected; a new forward run is performed, and a new objective function is calculated. In practice, the complex objective function surface and deviations from linearity preclude a simple determination of a single best new set of calibration parameters; therefore, a small number (usually <10) of candidate parameter sets are calculated and run in the forward model. An objective function is then calculated from each candidate parameter set, and the one with the lowest value is used to update the calibration parameters. A first update to initial parameter values does not complete the parameter estimation process because the groundwater inverse problem is nonlinear and sensitivities contained in the initial Jacobian matrix cannot accurately represent the sensitivities of the solution using the new parameter values. Therefore, a new Jacobian matrix is calculated using the parameters that gave the lowest objective function, which becomes the new unperturbed base case, and the slopes are used to develop a new set of candidate calibration parameters. The set of runs that starts with the calculation of a new Jacobian matrix and includes the set of forward runs for the corresponding new parameter estimates is called a *parameter estimation iteration*. Replacing a parameter set with a new parameter set that lowers the objective function constitutes a *parameter upgrade*—indicating that parameters are not merely updated but improved.

Parameters (columns)

Observations (rows)

	k_unconsol	k_bedrock	recharge	c_drainagelakes	c_seepagelakes	c_stream
Head_11_poor	-1.15129	0.00000	0.308674	-6.864546E-06	3.222347E-04	-7.712651E-07
Head_12_poor	-2.87823	-5.756463E-02	1.80995	-0.172709	-5.642061E-02	2.47528
Head_13_fair	-12.9520	-0.402952	8.10971	-4.250797E-04	2.104297E-02	11.8007
Head_16_fair	7.59851	-0.230259	2.94640	5.831008E-02	2.083643E-02	10.5920
Head_18_fair	-33.3875	2.300745E-14	8.67094	-5.791823E-02	1.759003E-02	0.518045
Head_23_fair	-8.00148	-1.533830E-14	2.20281	0.172619	3.733688E-03	0.575639
Head_36_fair	0.633211	0.00000	-0.182398	6.825390E-06	-3.094240E-04	-0.115128
Head_39_fair	-21.0687	-5.756463E-02	11.6735	-0.114699	3.664815E-02	11.3978
Head_46_fair	1.26643	-1.533830E-14	2.14669	-5.775567E-02	9.476421E-03	5.06567
Head_50_fair	-1.72694	-5.756463E-02	4.86862	-0.172693	3.120432E-04	9.95868
Head_52_fair	-39.6620	-5.756463E-02	15.6582	-0.115823	3.457457E-02	10.0162
Head_55_best	-52.9019	-5.756463E-02	20.1199	-0.171774	1.216745E-02	20.7809
Head_56_best	-80.7632	0.00000	24.6799	5.718392E-02	1.862524E-02	16.5210
Head_57_poor	-44.6701	7.669149E-15	12.0242	-1.301467E-04	6.561156E-03	2.01475

Figure 9.14 An example of a Jacobian matrix with 6 columns of parameters and 14 rows of observations. Each entry in the matrix is a parameter sensitivity (sensitivity coefficient) calculated from Eqn (9.7). The numbers in the left-hand column are the labels for head targets where best, fair, and poor indicate the quality of the target.

The search for parameter upgrades continues until one of three modeler-designated parameter estimation *closure criteria* is met: (1) the model fit cannot be further improved; (2) changes to the upgraded parameters are sufficiently small that one is not substantively different from another; or (3) the maximum number of parameter estimation iterations specified by the modeler has been reached. Because initial parameter values specified by the modeler may or may not be near final optimal values, there is no general guideline for how much the initial objective function should be reduced. Rather, in practice an acceptable value of the final objective function is the decision of the modeler. Thus, even though the trial-and-error process is automated, deciding when to end the parameter estimation is not automatic but depends on choices made by the modeler.

Box 9.2 Tips for Running a Parameter Estimation Code

Calibration guidelines presented in this chapter and by others (e.g., Hill and Tiedeman, 2007 for sparsely parameterized models) primarily pertain to conceptual aspects of modeling. Successful parameter estimation also involves more mechanistic aspects because input to a parameter estimation code can be lengthy and involve complex statistical concepts. Fortunately, most codes use default settings that are appropriate for many applied groundwater modeling problems, and utility software and graphical user interfaces simplify access to a code. Nevertheless, proper application of a parameter estimation code still requires attention to user manuals and guidelines included with the code itself. Running example problems or tutorials included with the code will give the user familiarity with its operation and troubleshooting options. Regardless of the code chosen, the following practices can facilitate efficient execution of the parameter estimation process.

- Run all input checking utilities (e.g., PESTCHEK.exe for PEST) before starting the parameter estimation run. Such utilities are tuned to identify and describe common errors that will cause parameter estimation to fail.
- When extracting values from the model output to align with the observation targets, carry the maximum numerical precision possible even if numerical precision is higher than reasonable for the associated field-measured observation. This will ensure a more accurate derivative calculation during construction of the Jacobian matrix, which in turn facilitates a better parameter upgrade by the derivative method.
- Use the parameter estimation code's option to log transform all calibration parameters that do not go negative (e.g., hydraulic conductivity). This dampens changes in extremely sensitive parameters and enhances parameter estimation performance.
- Recognize that tighter closure criteria in the solver of the groundwater code for the forward problem may appreciably speed and improve the parameter estimation process even if the forward run time increases. Gradient-based methods like Gauss–Marquardt–Levenberg rely on coherent/linear derivatives, but loose closure criteria can affect derivative quality (Fig. 9.13) even if the overall computed water budget is acceptable.
- Perform an initial check run that makes one pass through the parameter estimation steps including model input file creation, forward model run, extraction of model output, and

Box 9.2 Tips for Running a Parameter Estimation Code—cont'd

Figure B9.2.1 Pie charts of an initial objective function that is: (a) unbalanced because the number of head targets is much larger than other targets and (b) more balanced because no one target type dominates or is dominated by other groups. The more balanced objective function was obtained by simply normalizing the observation weights by the number of targets in each group.

calculation of residuals in order to verify that the steps are performed correctly. Moreover, this initial pass-through will give a value for the starting objective function, which should be evaluated for balance among target types (Fig. B9.2.1), and to make sure the initial objective function reflects the modeler's view of the importance of different observation target types.

- After the first Jacobian matrix is calculated, parameter sensitivities reported as zero, if any, should be evaluated. An unexpected zero sensitivity indicates a possible error in the handling of the parameter estimation file where a model input file is being created but is not being called by the associated model run file.
- If the chain of programs run for a forward model run contains intermediate utility codes that preprocess input for the groundwater model, it is good practice to have the output of the utility code be deleted at the top of that batch file/script used to call the forward model run. This ensures that the parameter estimation process is not using an old version of utility output, which may not be discovered until the completion of the parameter estimation run and poor results are obtained.
- Set the initial range of possible parameter values defined by their upper and lower bounds larger than what is realistic to assess potential issues with the conceptual model and effects of processes omitted from the model. Near the conclusion of parameter estimation, set the upper and lower bounds to the expected realistic range (e.g., 95% confidence interval) to ensure realistic parameters and to provide first estimates of parameter uncertainty for evaluating forecast uncertainty (Chapter 10).
- Recognize that at the end of the parameter estimation process the results are not necessarily better than a manual trial-and-error calibration, and may even be worse. For example, the parameter estimation process may find that unreasonable parameter values gave the best model fit whereas unreasonable parameter values would have been excluded at the beginning of a manual trial-and-error calibration. The modeler should never allow the parameter estimation to dictate what parameter set is best if a modeler's hydrosense indicates otherwise. Parameter estimation simply reflects the history matching problem as defined by information provided by the modeler. Often this information can be improved after initial parameter estimation results are obtained and reviewed.

9.5.3 Statistical Analysis

Prior to the widespread availability of parameter estimation methods, groundwater models were calibrated exclusively by manual trial and error. Then, parameter sensitivity was evaluated by a manual *sensitivity analysis*. The sensitivity of a given parameter was determined by fixing all calibration parameters at their calibrated values except for the selected parameter, which was varied in sequential forward runs of the model by incrementally increasing and decreasing its value by some percent from its calibrated value (e.g., ±25%). This type of sensitivity analysis showed how much the model moved out of calibration by changes in selected calibration parameters—a subset of all possible calibration parameters subjectively selected by the modeler. This approach was limited, not only to the subset of parameters manually adjusted, but also by reporting the change using a summary of all calibration target residuals, regardless of importance to the modeling objective. Hill and Tiedeman (2007, p. 184–185) discussed other limitations of this traditional type of sensitivity analysis. Modern parameter estimation codes make such sensitivity analysis unnecessary because parameter sensitivity coefficients are automatically calculated for all calibration targets and included in the Jacobian matrix. Hence, parameter sensitivities can be more thoroughly evaluated.

Parameter sensitivity analysis uses the Jacobian matrix to develop quantitative statistical insights about the model. *Insensitive parameters* (Section 9.4) are now defined as those having sensitivity coefficients less than a modeler-specified threshold. For practical purposes, an insensitive parameter is defined as those having a sensitivity coefficient more than two orders of magnitude lower than the sensitivity of the most sensitive parameter (Hill and Tiedeman, 2007, p. 50). In addition, information contained in the Jacobian matrix allows calculation of *parameter correlation coefficients* between calibration parameters. In a simple parameter sensitivity analysis, the modeler ranks calibration parameters by sensitivity and identifies both insensitive parameters and correlated parameters (e.g., correlation coefficient >0.95). *Parameter identifiability* (Doherty and Hunt, 2009a; Fig. 10.10) combines parameter insensitivity and correlation information, and reflects the "ease with which particular parameter values in a model might be calibrated" (Beven, 2009, p. 273). An identifiable parameter is both sensitive and relatively uncorrelated and thus is more likely to be estimated (identified) than an insensitive and/or correlated parameter. Parameter sensitivity analysis can also include evaluating the *statistical influence*, which quantitatively relates the importance of observations to calibration parameters and the determination of best fit (e.g., Yager, 1998; Hunt et al., 2006; Hill and Tiedeman, 2007).

Parameter estimation has greatly reduced the effort needed to perform sensitivity analyses, and introduced new quantitative measures such as identifiability and influence. General guidelines for performing parameter sensitivity analysis (e.g., Hill and Tiedeman, 2007) and sophisticated software tools are available. However, there is debate among modelers over how much effort should be expended on parameter sensitivity analyses because they only identify underlying calibration issues; they cannot overcome them. Model calibration still requires intervention by the modeler to overcome problems of parameter insensitivity and correlation. As we will see in Section 9.6, advanced parameter estimation methods can automatically overcome parameter insensitivity and correlation without modeler intervention. Just as calculating the Jacobian matrix is an interim step toward identifying upgraded parameters, parameter sensitivity analysis is an interim step in finding a best model for forecasts. Therefore, in many cases modeling resources may be better spent on other methods of parameter estimation that allow the modeler to overcome problems only identified in parameter sensitivity analysis. This should, in turn, allow additional resources to be spent on uncertainty analyses of the forecast (Chapter 10).

9.6 HIGHLY PARAMETERIZED MODEL CALIBRATION WITH REGULARIZED INVERSION

As the conceptual model is formulated, the numerical model is designed, and parameters are assigned to the nodal network, the modeler must make decisions on how to simplify the natural world for the purposes of the model. So far in this chapter, we have described the traditional approach for making the inverse problem tractable: the modeler reduces the complexity of the natural world to a small number of calibration parameters and thereby simplifies the problem to a sparsely parameterized model (e.g., as advocated by Hill (2006)). Once history matching of the sparsely parameterized model is complete, the modeler must assess the suitability of the simplification by evaluating parameter sensitivity, correlation, and the distribution of residuals that result from the conceptualization. If the fit of simulated values to targets is judged inadequate, more calibration parameters may be added. If the number of calibration parameters is too large to identify a best fit, insensitive and correlated parameters are set to fixed values to reduce the number of calibration parameters. The sparsely parameterized approach requires the modeler to spend time and effort initially deciding how best to simplify the model. If the first attempt at simplification fails to produce an acceptable calibration, more time and effort must be spent reformulating the calibration parameters for additional attempts at history matching. Moreover, if the conceptual model itself is found wanting after failed attempts to calibrate successively simpler (or more complex) models, the entire process must start over with the development of a new conceptual model.

Recognition of the disadvantages of sparsely parameterized methods in other fields of science led to the development of alternatives. One branch of these methods is *regularized inversion* (Engl et al., 1996), which is attractive because it addresses many of the issues of arbitrarily simplified groundwater models (Hunt et al., 2007). “Inversion” refers to solving the inverse problem. "Regularization" describes any general process that makes a mathematical function (like the objective function surface in Fig. 9.11(b)) more stable or smooth. Regularization can be broadly interpreted as any method that helps provide an approximate and meaningful answer to an ill-posed problem. With this definition, it follows that the traditional approach of specifying a relatively few number of parameters acts as a regularization strategy, albeit an informal and subjective one. In the form most commonly used for applied groundwater modeling, regularized inversion consists of:

1. assigning a large number of parameters to the model domain—many more than are used in the traditional sparsely parameterized approach; the model is said to be *highly parameterized* and all parameters are selected as calibration parameters;
2. constraining the larger parameter set with mathematical regularization, which allows the parameter estimation problem to be solved.

When properly performed, regularized inversion provides a systematic and quantitative framework for achieving parameter simplification whereby the mathematical rationale for the simplification is formally documented, transparent, and readily conveyed to others. Moreover, regularized inversion produces a single best fit appropriate model, which is required for many models used in decision-making. It also is attractive because it achieves parameter parsimony in more rigorous ways than zonation and other ad hoc simplification approaches.

It is important to note that regularized inversion was not simply overlooked by previous generations of modelers, but was recognized to be computational challenging due to the high number of parameters considered. Major advances in computing power, numerical solution techniques, and advanced techniques for formulating the parameter estimation problem made regularized inversion possible. Doherty and Hunt (2010) discuss detailed methodology for application of regularized inversion to groundwater flow models; many GUIs have regularized inversion capabilities. The main tenets and approaches are discussed below.

9.6.1 Increasing the Number of Calibration Parameters

The inherent subjectivity of traditional ad hoc parameter simplification introduces unquantifiable degrees of structural error (Section 9.4). Zonation, for example, defines the geometry of a set number of piecewise constant zones, thereby creating boundaries where properties change abruptly. The abrupt change across boundaries is usually not geologically realistic, and geographical delineations of zone boundaries are usually not well supported by field data. As a result, there is always uncertainty whether the zones are optimally constructed. Specifying too few zones decreases the ability of the observations to inform the parameter estimation process because the coarse model structure does not have receptacles to use the information and may bias the forecasts made using the calibrated model. Sparsely parameterized models may produce an acceptable history match, but in effect their parameters are *surrogates* for the true complexity in the natural world. Although surrogate parameters may be given names intended to reflect their physical significance, the values of those parameters needed to get good model performance will depend on the model structure used (Beven, 2009, p. 9). Such surrogacy may produce acceptable forecasts when, for example, observations used for history matching are the same type and time period as the forecast. When this is not the case, however, artifacts from the simplification process can degrade the forecast to an unknown degree because effects of simplification cannot be completely characterized (Doherty and Welter, 2010). *Highly parameterized approaches* were developed in an effort to avoid the problems of difficult to measure parameter oversimplification on model performance. Rather than reducing the number of model parameters a priori, the modeler retains all parameters that are of potential use for calibration and forecasting as calibration parameters. Therefore, the emphasis is on retaining model *flexibility* afforded by using many parameters. The concept of flexibility allows for more avenues to pursue model fit. Furthermore, more information contained within the observations can be extracted because observations are less likely to be competing with other observations to constrain the same calibration parameter. In addition, flexibility also facilitates more encompassing analysis of forecast uncertainty (Chapter 10).

Highly parameterized approaches have sometimes been characterized as the pursuit of model *complexity* (e.g., Hill, 2006). The definition of model complexity, however, is not straightforward (Gómez-Hernández, 2006) and involves more than the number of parameters in a model. For example, highly parameterized models provide more flexibility, but that does not equate to each parameter having a unique value, or that the resulting hydraulic conductivity field is highly heterogeneous. In a model described by Fienen et al. (2009a), each node was assigned a calibration parameter yet the high parameterization collapsed to a relatively simply three zone conceptualization after calibration. An advantage of the highly parameterized approach over traditional zonation is that the simple conceptualization is not specified beforehand, but is identified after information in the observations is considered during calibration. Application of the highly parameterized approach requires a large number of model runs, however, to assess the effect of each parameter on model output. Therefore, the goal is to find a middle ground where the calibration parameters provide sufficient flexibility so that the maximum amount of information is extracted from the calibration targets and structural error is reduced, but the parameters are not so numerous as to confound or preclude calibration. Finding this middle ground is part of the art of modeling and continues to be actively discussed (e.g., Hunt and Zheng, 1999; Hill, 2006; Gómez-Hernández, 2006;

Hunt et al., 2007; Voss, 2011; Doherty and Christensen, 2011; Doherty, 2011; Simmons and Hunt, 2012; Doherty and Simmons, 2013).

A highly parameterized model includes as much detail as necessary to address the modeling purpose. For example, parameterization could include heterogeneity in hydraulic properties at a level of detail important for a forecast, such as representing high hydraulic conductivity preferential flowpaths, which are important in transport simulations. In some cases, properties in every model cell/element in an area of interest are specified as calibration parameters (e.g., Fienen et al., 2009a). In practice, there are still practical limits to how many calibration parameters can be included in the inverse problem. Therefore, the computational burden is commonly reduced by the use of *pilot points* (Marsily et al., 1984; Certes and Marsily, 1991; Ramarao et al., 1995; McLaughlin and Townley, 1996; Doherty, 2003; Alcolea et al., 2006; Doherty et al., 2010a). In this approach, parameter values are estimated at discrete locations (pilot points) distributed throughout the model domain. Once the pilot point locations and parameter values are assigned, spatial interpolation (Section 5.5) such as kriging is used to assign parameter values to all remaining nodes or elements. The number and locations of pilot points are selected to balance parameter flexibility while reducing the computational burden and addressing the modeling objective (Fig. 9.15; Box 9.3). Pilot points can be assigned to zones so that known geologic boundaries can be represented. A pilot point approach is a compromise between extremely large numbers (hundreds of thousands) of possible parameters and the traditional sparsely parameterized approach using an arbitrarily small number of parameters (usually fewer than 100).

9.6.2 Stabilizing Parameter Estimation

Regularization, in the broadest sense, includes any mechanism that stabilizes the ill-posed inverse problem. For example, reducing the number of calibration parameters by using pilot points is a form of regularization because fewer parameters make the parameter estimation process more tractable. Two main types of regularization are commonly used in applied groundwater modeling: adding soft knowledge and reducing problem dimensionality. These methods can be used by themselves but are most commonly used in combination.

9.6.2.1 Adding Soft Knowledge: Tikhonov Regularization

In Section 9.1 we emphasized that model calibration consists of both a hard knowledge and a soft knowledge assessment. In manual trial-and-error calibration and simple parameter estimation (Section 9.5), soft knowledge assessment is done independently of the hard knowledge assessment. That is, the model is first calibrated using hard knowledge via history matching and then the calibrated parameters are assessed for hydrogeological reasonableness using soft knowledge. Or put another way: a calibrated model is one that

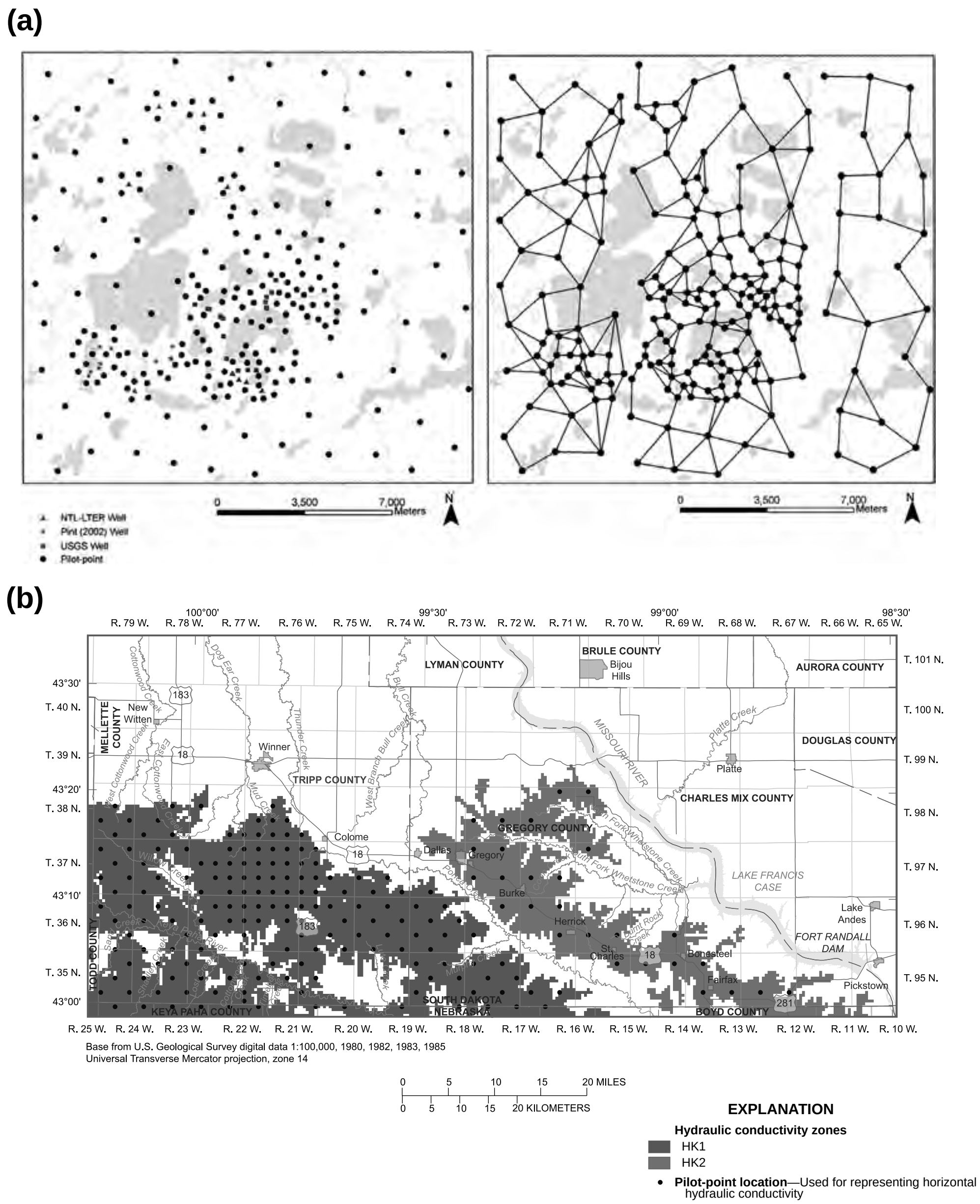


Figure 9.15 Pilot Points. (a) Network of pilot points in a watershed-scale groundwater flow model (left); linkages between pilot points (right) used to calculate Tikhonov regularization constraints for preferred homogeneity *(modified from* Muffels, 2008*)*. (b) Network of pilot points used to represent two hydraulic conductivity zones where Tikhonov regularization is applied to pilot points within the same zone *(modified from* Davis and Putnam, 2013*)*.

Box 9.3 Tips for Effective Pilot Point Parameterization

There is no universal set of rules for the placement of pilot points used for parameterization. However, Doherty et al. (2010a) provided the following suggestions based on a mathematical analysis of pilot point parameterization schemes:

1. Generally place pilot points in a uniform pattern to ensure some minimal level of coverage over the entire model domain. Then place additional pilot points in areas of interest. Avoid large gaps between pilot points so that single pilot points are not representing large areas of the domain. The separation between pilot points should be equal to or greater than the characteristic length of any heterogeneities in hydraulic properties in the model domain.
2. Pilot points that are used to estimate horizontal hydraulic conductivity should be placed between observation targets along the direction of the groundwater gradient.
3. Place pilot points at wells where aquifer test data are available so that hydraulic property estimates derived from aquifer test results can serve as initial and/or preferred parameter values.
4. Place pilot points that are used to estimate storage parameters at locations where fluctuations in head have been measured.
5. Place pilot points that are used to estimate hydraulic conductivity parameters between outflow boundaries and upgradient observation wells.
6. Increase pilot point density where calibration target data density is high. But do not place pilot points at locations containing head observations to minimize "bulls eyes" in the hydraulic conductivity.
7. If the number of pilot points is limited by computing resources (e.g., long-forward run times and few resources to run the problem), consider using fewer pilot points to represent vertical hydraulic conductivity in confining or semiconfining units and more pilot points to represent horizontal hydraulic conductivity.

Pilot points can be placed in zones (Section 5.5); some zones may have many pilot points and others just one. When a single pilot point is assigned to a zone, the parameter estimation process assigns one value to each node in that zone; thus the pilot point parameter acts as a piecewise constant zone, which is insensitive to the location of the pilot point. When more than one pilot point is located in a zone, spatial interpolation from pilot points to the nodal points, and associated regularization (Section 9.6), do not take place across zonal boundaries.

has the best fit to hard data but also whose parameters have the smallest deviation from soft knowledge available for a modeled area. This informal representation of a soft knowledge penalty, however, can be mathematically included along with the expression of goodness of fit from Eqn (9.6):

$$\Phi_{total} = \Phi_{hard\ data\ misfit} + \Phi_{soft\ knowledge\ deviation} \tag{9.8}$$

which can also be expressed as:

$$\Phi_{total} = \sum_{i=1}^{n} (w_i r_i)^2 + \sum_{j=1}^{q} \left(f_j(p)\right) \tag{9.9}$$

The first term to the right of the equals sign is the measurement objective function from Eqn (9.6), which is calculated as the sum of squared weighted residuals, where n residuals, r_i, are calculated from hard knowledge and w_i are their respective weights. The second term quantifies the penalty resulting from deviations from soft knowledge as the sum of q deviations from j soft knowledge conditions f_j, where f_j is a function of model parameters p. A calibrated model, therefore, is found by minimizing both the measurement objective function (hard data) and the soft knowledge penalty.

The Russian mathematician Andrey Tikhonov developed an approach for mathematically including soft knowledge at the beginning of the calibration process (Tikhonov 1963a,b; Tikhonov and Arsenin, 1977), now known as *Tikhonov regularization*. With Tikhonov regularization, the modeler's soft knowledge can be used along with hard knowledge during parameter estimation. Soft knowledge includes intuitive knowledge, professional judgment, regional literature values, and geological expertise—information that is often qualitative or marginally relevant to the site being modeled. Yet, this approach is widely used because even such qualitative information can help stabilize an ill-posed parameter estimation problem, particularly when the type of information conveyed by the soft knowledge is not contained in the targets.

Tikhonov regularization formally incorporates soft knowledge into the calibration process by augmenting the objective function, here called the *measurement objective function* (described by Eqn (9.6)), with a second *regularization objective function* that expresses the soft knowledge penalty (i.e., the two additive components of Eqn (9.9), respectively). The regularization objective function captures the parameters' deviation from the modeler's understanding of the system as expressed by *preferred conditions* for parameters (e.g., Doherty, 2003, pp. 171−173); thus, minimizing the regularization objective function reduces the soft knowledge penalty. Preferred conditions are usually expressed as a preferred parameter value (e.g., "this area is thought to have a hydraulic conductivity of 4 m/d") and/or a preferred difference, most often a difference of zero indicating a preferred homogeneity condition (e.g., "these two areas are thought to have the same properties"). The more the parameter estimation process deviates from the preferred conditions, the larger the value of the regularization objective function. The model is calibrated by minimizing both the measurement and regularization objective functions (Φ_{total}, Eqn (9.9)); when both minima are obtained a unique solution to the inverse solution is obtained (see De Groot-Hedlin and Constable, 1990).

Note that obtaining a unique solution is directly dependent on the modeler's formulation of the problem—if the modeler changes observation weights or regularization preferred conditions, minimization of both the measurement and regularization measurement functions must be performed again. Mathematically, the regularization objective function is tracked separately from the targets and related measurement objective function. Thus, parameter estimation using Tikhonov regularization is a "dual constrained minimization" process. Functionally, the modeler-specified preferred conditions constitute a suite of fallback values for parameters (or for relations between parameters) that are applied when information contained in the observations is insufficient for unique estimation of a parameter (e.g., insensitive parameters). When the hard knowledge from observations informs the parameter value, deviation from these fallback preferred values is allowed. Such deviations, however, penalize the combined objective function by increasing the value of the regularization objective function. Therefore, deviations from soft knowledge are only allowed if they provide sufficiently large reduction in the measurement objective function (better fit to the targets) to offset the increase in the combined objective function.

Tikhonov regularization also allows the modeler to specify how strongly to enforce the soft knowledge constraints. This is done through the *target measurement objective function*. This additional input provided by the modeler (e.g., in PEST via the variable PHIMLIM) limits the level of fit the calibration process is allowed to achieve (Doherty, 2003; Fienen et al., 2009b). When the target measurement objective function is unrealistically below the lowest possible measurement objective function (Fig. 9.16(a)), soft knowledge is weakly enforced. This can lead to unreasonably extreme values for parameters. Higher values of the target measurement objective function cause the soft knowledge to be more strongly enforced and the resulting parameter field is smoother (Fig. 9.16(b)). In practice, a very low value for the target measurement objective function is typically specified in an initial run to minimize soft knowledge and obtain a best fit to hard data (e.g., Fig. 9.16(a)). The best fit value of the measurement objective function is then used to estimate a target measurement objective function that is somewhat higher than the best fit (e.g., around 10% higher, Fig. 9.16(b)).

As expected given the issues described in Section 9.1, there are many possible models that could be considered calibrated depending on the modeler's expression of the strength of soft knowledge. The trade-off between soft knowledge and hard knowledge can be shown graphically by a *Pareto front* diagram (Fig. 9.17). A Pareto front is commonly used in economics to describe the trade-off between two objectives when it is not possible for both to be attained simultaneously. In Fig. 9.17, the calibration that favors the soft knowledge preferred condition (smallest value on y-axis scale) gives the worst model fit (i.e., the largest value on the x-axis scale); the calibration that favors the hard knowledge and gives the best history match (smallest value on x-axis scale) deviates the most from the soft knowledge. The best calibrated model selected from the Pareto front is an expression of the modeler's subjective judgment as to the optimal trade-off between hard and soft knowledge, which is the essence of the art of modeling. For

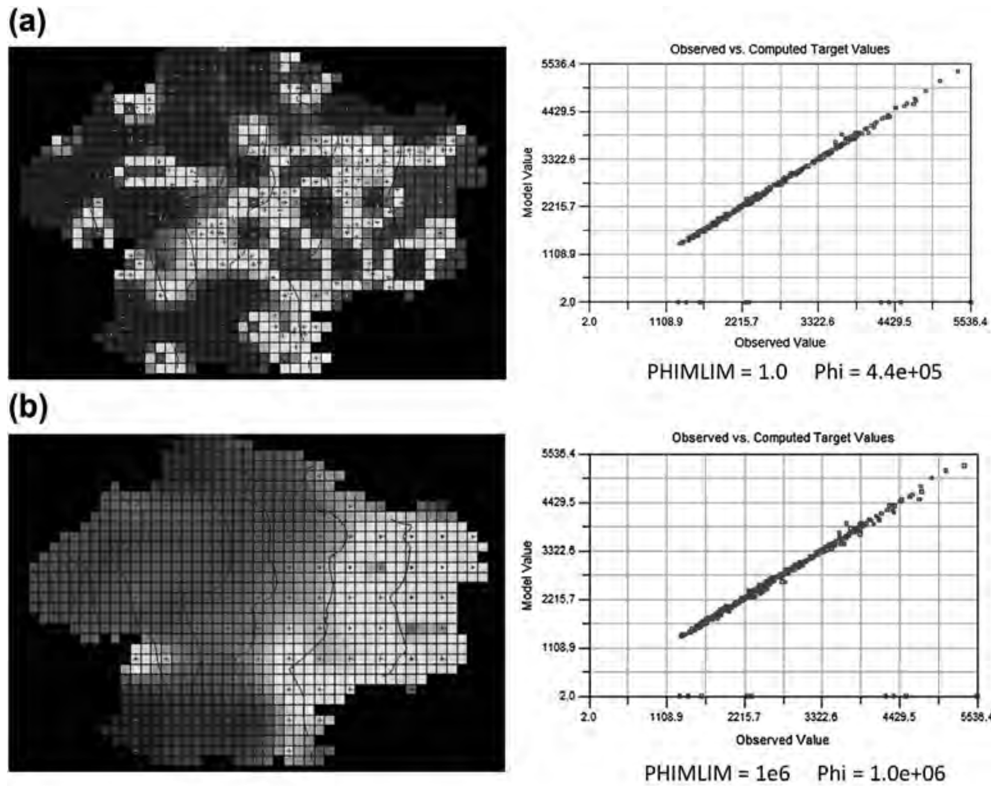


Figure 9.16 Visualization of parameter estimation using alternative Tikhonov regularization, where the same parameter estimation problem is solved using two different values of the target objective function (PHIMLIM variable in PEST). (a) When the target objective function is set unrealistically low (PHIMLIM = 1), user soft knowledge is disregarded and optimality of the inverse solution is defined solely by the model's fit to calibration targets (i.e., minimization of the measurement objective function, Phi). The resulting field has extreme contrasts and parameter "bulls eyes" that reflect the code's unchecked pursuit of the best fit. (b) When the target objective function is set to a value around 10% higher than the best Phi obtained (PHIMLIM = 1e6), the resulting fit is slightly worse (as shown by a slightly larger spread around the 1:1 line in the scatter plot of heads), but heterogeneity in the optimal parameter field is reduced. Whether the heterogeneity expressed is reasonable is the decision of the modeler; thus both models might be considered part of the Pareto front shown in Fig. 9.17 *(modified from USGS unpublished data).*

most groundwater models, we can assume that neither extreme of the Pareto front is optimal. That is, a history match that is too good reflects noise associated with the field measurements and/or inadequacies of the model rather than the properties of the natural system, and the model is said to be *overfit*. At the other extreme of the Pareto front, hard knowledge from the targets is unacceptably diminished and the model is dominated by a modeler's preconceived notions of the system; such a model is said to be *underfit*. When

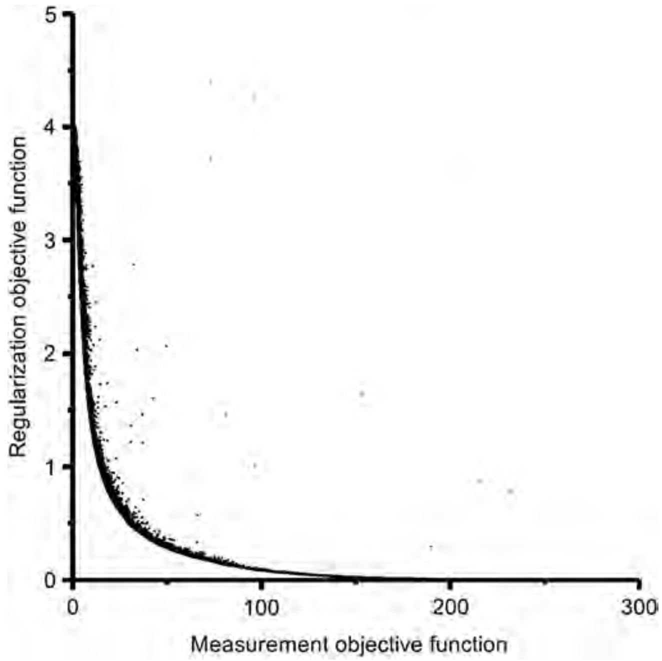


Figure 9.17 A Pareto front diagram. Multiple calibrations by Tikhonov regularized inversion of the same model are shown by dots, which coalesce into a thick black line along a "front"; the only difference among calibrations is the strength of the soft knowledge constraint expressed during parameter estimation. The Pareto front illustrates the inherent trade-off between a perfect model fit (zero on x-axis) and perfect adherence to the modeler's soft knowledge (zero on y-axis). The "best" model is the modeler's subjective pick of one calibration from the many calibration results along the Pareto front *(modified from Moore et al., 2010).*

properly balanced, the soft knowledge constraint defines an *optimal parameter field* where heterogeneity is included at locations and in ways that are supported by the calibration targets. Therefore, changes to the target measurement objective function allow the modeler to evaluate whether departures from initial values of the parameters based on soft knowledge used to construct the conceptual model are supported by observations and are hydrogeologically realistic (e.g., Fienen et al., 2009b). Put another way, although the complexity of the natural world can never be known, Tikhonov regularization gives the modeler a mathematically defensible way to include as much parameter complexity as their observations support.

9.6.2.2 Collapsing Problem Dimensionality: Subspace Regularization

In contrast to Tikhonov regularization, which adds information to the calibration process in order to achieve numerical stability, subspace methods achieve numerical stability by reducing the dimensionality of the Jacobian matrix through subtraction of parameters and/or by combining parameters (Aster et al., 2013). Only those parameters and linear combinations of parameters that are sufficiently constrained by the targets are estimated. The determination of which parameters to estimate is automated using *singular value decomposition* (SVD—Box 9.4) of the Jacobian matrix (e.g., Moore and Doherty, 2005; Tonkin and Doherty, 2005).

Although understanding the theoretical underpinnings is not critical for using SVD for model calibration, a brief discussion is included here to familiarize the reader with terminology associated with SVD. SVD uses linear algebra for matrix decomposition; it conveys the maximum signal energy (information from the observations) into as few coefficients (calibration parameters) as possible, and thus is widely used in applications in engineering, signal processing, and statistics. Recall from Section 9.5 that the Jacobian matrix consists of sensitivity coefficients (Eqn (9.7)) that relate all parameters (i.e., *base parameters*) to all observations. SVD operates on the Jacobian matrix to divide parameter space into a set of linearly independent combinations of parameters. Each of

Box 9.4 A "Singularly Valuable Decomposition"[1]—Benefits for Groundwater Modeling

When large numbers of parameters are added to a model, some will be insensitive and others highly correlated with other parameters. As a result, even though a parameter is important to the modeling objective, it does not mean that it is *identifiable* (capable of being estimated given the available calibration targets). Doherty and Hunt (2010) point out that what is needed is an intelligent calibration tool—one that detects what can and cannot be inferred from the calibration targets. This tool should estimate what it can leave out and what it cannot—all automatically, without user intervention. Singular value decomposition (SVD) is such a tool, fondly referred to as a "singularly valuable decomposition" by Kalman (1996).

SVD is a way of processing matrices into a smaller set of independent linear approximations that represent the underlying structure of the matrix; thus, it is called a *subspace method*. It is used widely for such tasks as image processing, for example, as commonly experienced in the sequentially updated resolution of images displayed by an Internet browser (similar to Fig. B9.4.1). In this way, SVD gives the user progressively more useful information, even from a blurry image, earlier rather than waiting for the entire image to download.

In the context of groundwater model calibration, rather than solving for all details of an inverse problem (represented by all calibration parameters), SVD utilizes a reduced representation of the problem. It recognizes that certain combinations of observations are uniquely informative and also creates linear combinations of the parameters. Similar to the image processing example, this subspace represents a blurry view of the subsurface, but a view that defines where combinations of informative observations (the *solution space*) run out, thereby defining the combinations of parameters that cannot be estimated (the *null space*). SVD-based parameter estimation fixes initial values of insensitive parameters and does not

(Continued)

Box 9.4 A "Singularly Valuable Decomposition"[1]—Benefits for Groundwater Modeling—cont'd

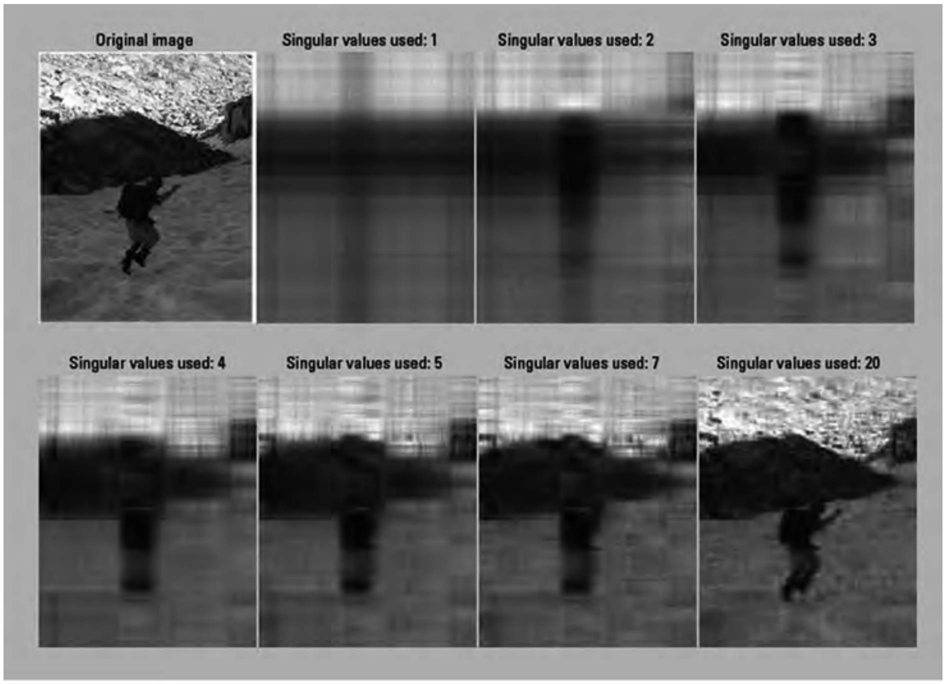


Figure B9.4.1 Singular value decomposition of a photographic image. When the matrix is perfectly known (defined by 240 pixels/singular values in the image), it reflects the highest resolution and thus the highest number of singular values can be shown visually. For reference, the image with 20 singular values represents less than 10% of the information contained in the original image in the upper left, yet it contains enough information that the subject matter can be easily identified. A similar concept applies to groundwater problems—if too few singular values are selected, a needlessly coarse and blurry representation of the groundwater system results. When the information content of the calibration data set is increased, a larger number of data-supported singular values can be included, resulting in a sharper "picture" of the groundwater system. In practice, most field observations only support a relatively blurry depiction of subsurface properties *(from Doherty and Hunt, 2010; image and SVD processing by Michael N. Fienen, USGS).*

use them in the parameter estimation process. Therefore, parameter combinations in the solution space become the heart of the calibration process. Because only parameter combinations that can be estimated are used in the parameter estimation process, solution of the inverse problem is unique and unconditionally stable. By using parameter combinations, known as superparameters, such as in SVD-Assist (Section 9.6), the size of the Jacobian matrix is reduced, as is processing time.

[1] *Kalman, D., 1996. A singularly valuable decomposition—The SVD of a matrix. College Mathematics Journal 27(1), 2–23.*

these combinations is multiplied by a factor known as a *singular value*, and summed to reproduce the full parameter field. In this way, singular values constitute a reduced set of linear combinations of the full suite of calibration parameters (here called *base parameters*).

Singular values are usually listed in decreasing order (i.e., singular value of index 1 is more constrained by information contained in observations than singular value 2). In practice, those parameters associated with singular values of lower index tend to represent spatially averaged parameters; those associated with higher index tend to represent local system detail. After SVD, *singular value truncation* is performed where parameter combinations associated with singular values that are greater than a user-specified threshold (i.e., have lower index number) are considered supported by the observation data and assigned to the *solution space*; parameters and parameter combinations that cannot be estimated from the targets (e.g., insensitive parameters) are not included in the solution space and are assigned to the *null space* (Fig. 9.18). A parameter or combination of parameters residing in the null space is considered uninformed by the observations and retains the

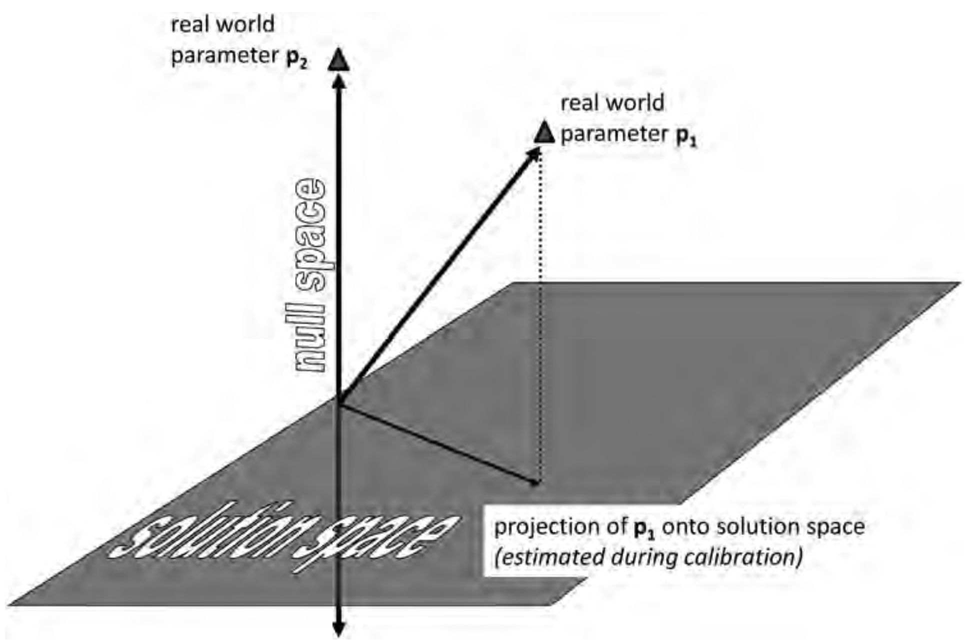


Figure 9.18 A schematic depiction of the relation of two parameters (p_1 and p_2) to the solution space and null space defined by a set of calibration targets. Because neither parameter lies on the plane of the solution space, the parameters are not perfectly constrained by the observations. Parameter p_1 is partially informed by the observations; thus it has a projection into the solution space and can be estimated during parameter estimation. Parameter p_2, however, cannot be projected onto the solution space and cannot be estimated given the calibration targets *(modified from Doherty et al., 2010b).*

initial values specified by the modeler during calibration. Therefore, it is important when using SVD that initial parameter values are hydrogeologically reasonable. By using linear combinations of parameters rather than individual parameters, correlated parameters that cannot be estimated individually can be estimated in combination with associated correlated parameters. In this way, SVD automatically accounts for the insensitive and correlated parameters that a modeler must otherwise address manually using the methods discussed in Sections 9.4 and 9.5.

If too many combinations of parameters are estimated (too many singular values), the problem will still be ill-posed and numerically unstable. If too few parameters are estimated, the model fit may be unnecessarily poor, and forecasting errors may be larger than for an optimally parameterized model. Even when the problem includes an appropriate number of singular values, SVD can still be ruthless in its search for a best fit (Doherty and Hunt, 2010). Therefore, when used alone, SVD can result in overfitting, producing calibrated parameter fields that lack geologically realistic characteristics. As a result, SVD is often used in conjunction with Tikhonov regularization, which produces geologically realistic parameter distributions owing to soft knowledge constraints. When the two approaches are combined, the degree of fitting is controlled by the soft knowledge input under Tikhonov regularization, but the fitting is performed on an inverse problem that is unconditionally stable (Box 9.4).

9.6.3 Speeding the Parameter Estimation Process

Although SVD can provide an unconditionally stable and unique model calibration, it does not alleviate the high computational burden of a highly parameterized approach because the full Jacobian matrix is computed for each parameter estimation iteration. Recall from Section 9.5 that the minimum number of model runs required for calculation of the full Jacobian matrix is equal to the number of calibration parameters plus one. Fortunately, parameter estimation is an "embarrassingly parallel" problem (Foster, 1995). That is, to construct the Jacobian matrix each parameter is perturbed independently from all others, and thus one run does not require information from other runs to start or complete. Large speedups in total run time can be achieved by distributing the runs across multiple processors and calculating the Jacobian matrix and parameter upgrade searches simultaneously (e.g., Schreüder, 2009; Doherty, 2014a). Advances in run management and computational networking allow the runs to be distributed over multiple processor cores on a single personal computer or, for larger problems, over the Internet (e.g., Muffels et al., 2012) and in the cloud computing environment (Hunt et al., 2010).

In addition to the brute force approach of simply adding more computer units to perform parameter estimation, the SVD process itself can be sped up using *SVD-Assist* (SVDA) (Tonkin and Doherty, 2005), whereby the solution and null subspaces are defined just once by using the Jacobian matrix calculated from initial parameter values. Before the parameter estimation process starts, a set of *superparameters* is defined from sensitivities calculated from the full set of calibration (base) parameter values using SVD, thereby reducing the full parameter space to a subset of the solution space that relates to the full set of base parameters. Being derived from SVD, superparameters are comprised of linear combinations of parameters informed by the observation targets. Significant speedups in the parameter estimation process are obtained because, once defined by SVD, the number of superparameters is less than the set of base parameters but can be estimated as if they were ordinary base parameters. Derivatives in the Jacobian matrix are calculated using the smaller number of superparameters rather than the full set of base parameters. However, it is possible that a Jacobian matrix calculated from final optimized parameters would be appreciably different from that calculated from the initial values because of nonlinearity. If sufficiently different, the underlying assumption of SVDA is violated because superparameters defined using initial values would not approximate those calculated from optimal values. In that case, following the initial SVDA run, the Jacobian matrix is recalculated from calibrated parameter values, superparameters are redefined, and another SVDA parameter estimation run is performed with the newly defined superparameters. A parameter estimation code (PEST++—Welter et al., 2012) automates these relinearization and singular value redefinition steps, thereby freeing the modeler from performing this check.

The number of superparameters may be sufficiently small for their values to be estimated using traditional calibration methods for well-posed inverse problems (Section 9.5). In most cases, however, Tikhonov regularization (with default conditions applied to the base calibration parameters) should be included in a *hybrid SVDA/Tikhonov* (Fig. 9.19) parameter estimation process. Doherty and Hunt (2010) suggest this as the preferred method for applied modeling because: (1) large reductions in run times are achieved because the number of runs needed for most parameter estimation iterations is related to the number of superparameters; (2) simultaneous application of Tikhonov regularization constraints allows the user to interject soft knowledge into the parameter estimation process and thus rein in the pursuit of a best fit to calibration targets. SVD and SVDA have been incorporated into some GUIs and codes (PEST++—Welter et al., 2012), and utility software is also available (e.g., SVDAPREP—Doherty, 2014a). Because of the complementary increase in speed and likelihood of obtaining geologically realistic parameter fields, the hybrid SVDA/Tikhonov approach is currently the most efficient and numerically stable means of attaining a hydrogeologically reasonable, highly parameterized groundwater model. However, the decision as to what constitutes hydrogeologically reasonable is subjective (e.g., Fig. 9.17) and the modeler may perform several iterations through the loop shown in Fig. 9.19, where alternate Tikhonov regularization schemes are tested to refine the trade-off of soft and hard knowledge (e.g., Fig. 9.16).

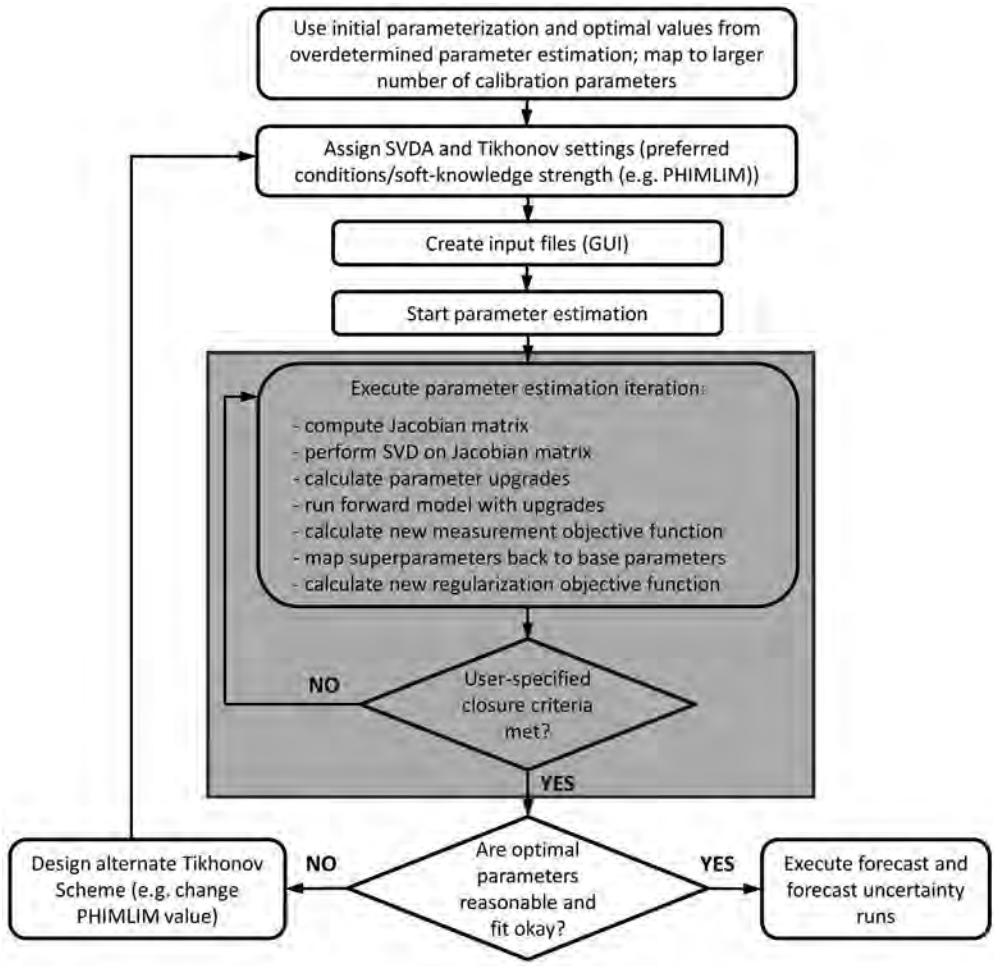


Figure 9.19 A schematic diagram of a general workflow for parameter estimation using a hybrid SVD-Assist (SVDA)/Tikhonov regularization approach. Shaded box contains the steps performed internally by the parameter estimation code without user intervention; unshaded steps require modeler action. The trade-off between soft knowledge and the model's fit to hard knowledge is adjusted by changing the target objective function for Tikhonov regularization (the PHIMLIM parameter in PEST); (GUI, graphical user interface; SVD, singular value decomposition).

9.7 A WORKFLOW FOR CALIBRATION AND MODEL PERFORMANCE EVALUATION

Model calibration, which includes history matching and an assessment of parameter reasonableness, is in essence an exercise in evaluating model performance. Most groundwater modelers accept that a groundwater model can never be validated (Box 9.5).

Box 9.5 Code/Model Verification and Model Validation

When discussing model calibration, the terms verification and validation (Section 1.5) are often used. Given the state of modeling in the twenty-first century and the availability of new approaches for calibration (Sections 9.5 and 9.6), these concepts have become largely unnecessary. Nevertheless, the terms continue to be used (e.g., Moriasi et al., 2012; Anderson and Bates, 2001; Beven and Young, 2013) and are discussed here to provide the reader with a context for their use in applied groundwater modeling.

Code verification refers to establishing that a computer program (code) is correctly written so that it accurately solves the relevant partial differential equation. Most codes for groundwater modeling that are in use today have been verified by the developer of the code and thus code verification by the user is unnecessary. Code verification is usually documented in the user's manual.

An interest in *model verification* (as opposed to code verification) arose from the practice among streamflow modelers to divide field observations into groups using a split sample method. One portion of the sample of observations was used to calibrate the model to a specific time period and the other portion of the sample was used to test the calibrated model. It is sometimes recommended that groundwater models be calibrated against one time period and "verified" against another, or for different time periods that represent different hydraulic conditions (e.g., average annual heads versus heads from a short-term aquifer test); or that a groundwater flow model be "verified" by demonstrating that calibrated heads and fluxes can reasonably reproduce observations of another dependent variable such as concentrations (using a solute transport model) or temperatures (using a heat transport model). Doherty and Hunt (2010), however, point out that while these exercises demonstrate that a calibrated model is able to reproduce certain aspects of system response under field conditions, the data used in a verification exercise are more valuable when incorporated into the calibration. In most cases, any additional confidence gained by withholding data will be overwhelmed by the uncertainty that remains. Nonuniqueness and uncertainty can be reduced by including more and varied calibration targets in the calibration. Different time periods and data types contain information pertinent to different aspects of the modeled system. Therefore, history matching exercises (and the final calibrated model) are poorer by the omission of data. Using concepts discussed in Section 9.6, including data withheld for the purpose of verification could add dimensions to the parameter solution space, and thereby decrease the dimensionality of the null space. Where data are scarce, uncertainty margins will be wide—an inescapable consequence of not having data. Therefore, for most groundwater modeling projects, verification will not lead to increased confidence in the model's performance. Rather, time and resources are better spent in parameter estimation using the full set of observations followed by forecast uncertainty analysis (Chapter 10).

The term *model validation* implies that the model is in some sense "correct" and therefore capable of making accurate (valid) forecasts. In the twentieth century, attempts were made to establish validation protocols, especially for siting geologic repositories for high-level nuclear waste. However, concerns over nonuniqueness and model uncertainty led to the current

(Continued)

Box 9.5 Code/Model Verification and Model Validation—cont'd

view that a model cannot be validated; it can only be invalidated (e.g., Konikow and Bredehoeft, 1992). Furthermore, it can only be invalidated at a certain level of confidence (Oreskes et al., 1994; Oreskes and Belitz, 2001). In short, validation has been replaced with other types of model performance evaluation such as parameter estimation and forecast uncertainty analysis. These activities can build confidence in the model while recognizing that it is impossible to guarantee that the model is 100% correct. Rather, the goal is to assess a model's fit for purpose, which evaluates whether it is conditionally suitable for use in a stated type of application (Beven and Young, 2013). The situation is well summarized by Doherty (2011): "When it makes a prediction, a model cannot promise the right answer. However, if properly constructed, a model can promise that the right answer lies within the uncertainty limits which are its responsibility to construct."

Therefore, calibration is the primary way to assess model performance. Calibration of groundwater models should start with manual trial-and-error history matching (Fig. 9.1), followed by automated trial-and-error history matching (parameter estimation, Fig. 9.9). A general workflow for calibration would typically calibrate the steady-state model first, focusing on hydraulic conductivity, recharge, and leakance/resistance parameters. If transient modeling is required, the transient model is typically calibrated separately after the steady-state calibration, where history matching is attempted by adjusting only storage parameters. Temporal difference targets (Section 9.3) are best suited for the primary focus for transient history matching. The quality of the match can be judged by the representation of system dynamics (Fig. 7.11; Fig. 9.4(a) and (d)), and history matching is not confounded by the need to overcome systematic misfit in absolute model outputs inherited from the steady-state calibration. A separate calibration of steady-state and transient models prevents the steady-state best fit from being degraded during transient calibration when adjustment of storage parameters alone can obtain a good fit to the transient observation targets. Moreover, the number of calibration parameters estimated with the transient model is limited to storage parameters; a small number of transient calibration parameters is desirable because transient models typically have appreciably longer forward run times than steady-state models. In some cases, the separate calibration approach may not yield a satisfactory transient history match; in these cases the steady-state and transient models are run together, and model outputs are evaluated using a combined objective function that includes both steady-state and transient observations.

If simple methods alone are used for parameter estimation (Section 9.5), final calibrated parameter values must be assessed for reasonableness using a manual soft knowledge assessment. For most applied modeling, the preferred approach is to use PEST with Tikhonov regularization to include soft knowledge formally in the parameter estimation solution. SVD helps stabilize the solution (Section 9.6) and SVDA speeds up the calibration process. Moreover, modern desktop computers have multiple processors that allow for parallel processing (running multiple workers) on a single machine. Because most parameter estimation codes have parallel processing capabilities, the user can take advantage of the pleasingly parallel aspects of parameter estimation. If multiple networked computers are used for parallel processing of proprietary software, the modeler must ensure that each additional machine has appropriate software licenses. Open source software typically can be copied to multiple machines without such licensing concerns.

The results of the calibration should be documented by reporting summary statistics (*ME*, *MAE*, *RMSE* for steady-state models: Eqns (9.1)—(9.3); NS for transient models: Eqn (9.4), Fig. 9.4(a)), a plot of observed versus simulated values (Fig. 9.5; Fig. 7.11), a map and spatial plot showing locations and magnitudes of residuals (Fig. 9.6), and an evaluation of the simulated water budget (Fig. 7.5(b)). Summary statistics and residual plots are typically represented using unweighted residuals because they represent the true departure from observed values and are not obscured by weights, which are subjectively chosen by the modeler. The modeler should report and discuss both the rank (weight—e.g., Table 7.1) of the observation targets and the choice of calibration parameters, and discuss how soft knowledge was included in the calibration. If Tikhonov regularization was used, a Pareto front diagram (Fig. 9.17) is helpful.

Evaluation of model performance must also identify data gaps and uncertainties in the conceptual model and limitations of the numerical model. The modeler evaluates recalcitrant misfit of targets and the spatial and temporal distribution of residuals by examining scatter plots of observed versus simulate values (Fig. 9.5) and spatial maps of residuals (Fig. 9.6). Additional statistical tools are also available that can evaluate how the selected conceptual model performed (Box 9.6). If such examination leads to the conclusion that the best fit model is inadequate, it is likely that the underlying assumptions and/or conceptual model are inadequate, or that the calibration targets poorly represent the hydrogeological site conditions. The usefulness of any forecast based on an inadequate calibrated model is questionable. If potentially significant flaws in the conceptual model are suspected, the modeler may decide to examine *alternative conceptual models* (Section 1.6). Alternative conceptual models allow the modeler to expand the evaluation to other plausible representations of the system, within constraints of the available data and what is known about the system. One or more new conceptual models would form the basis of new or refined numerical models. With each new model, the model assessment processes begin again, including calibration. The advantage of parameter estimation is that the quantitative best fit for a given conceptual model is identified efficiently and in a mathematically rigorous way, and shortcomings in the conceptual model are transparent. Therefore, parameter estimation facilitates testing more than one conceptual model. An alternative conceptual model may supplant the original conceptual model and become the preferred basis for forecasting simulations. Or as we will see in Chapter 10, several conceptual models may be carried forward to help represent uncertainty in the forecasts. Uncertainty estimates have become an important part of applied modeling.

Box 9.6 Additional Parameter Estimation Tools

The quantitative framework inherent in parameter estimation allows for evaluating a model beyond approaches discussed in Sections 9.4–9.6. Two additional statistical metrics are briefly discussed in this box: (1) parameter and observation influence; (2) global sensitivity. Both of these metrics are included in currently available software, but are not as widely used as other methods covered in this chapter. Parameter estimation is an active area of research and we expect that these and many more tools will eventually be incorporated into the standard applied modeling software toolkit.

An objective of parameter estimation is to maintain the same importance (ranking) of observations as in manual trial-and-error calibration (Section 9.5). Before calibration begins, the leverage an observation exerts on the parameters can be calculated (e.g., Hill and Tiedeman, 2007, p. 134; INFSTAT utility in PEST—Doherty, 2014b). With this information the modeler can identify observations that have the potential to dominate the parameter estimation process, and thus can assess whether its influence is consistent with the modeling purpose. When an observation has too much leverage, its weight (Section 9.5) can be reduced to lessen its effect. After calibration is performed, the modeler may question results if the parameter values fall outside the range of values considered representative for the site. Information regarding which observation(s) are better fit by using parameter values outside the range of reasonable values may be helpful in evaluating the calibration. Yager (1998) describes the use of the influence statistic DFBETAS (Belsley et al., 1980), which statistically measures an observation's effect on a single parameter. With this information, observations can be ranked in order of influence on an estimated parameter (e.g., Hunt et al., 2006). The *SSSTAT* (using subspace methods discussed in Section 9.6) tool in the PEST software suite (Doherty, 2014b) is designed to trace observation influence to parameters in underdetermined inverse problems.

The sensitivity coefficient (Eqn (9.7)) measures local sensitivity because it is based on small perturbations around a given parameter value. Local sensitivity, while computationally efficient, also assumes linearity, which means that sensitivity coefficients calculated for one set of parameters apply for the entire range of possible input and output, which may not be a good assumption. Global sensitivity analyses (e.g., Saltelli et al., 2008) address nonlinear sensitivity for a wide range of parameter values. According to Mishra et al. (2009) global sensitivity analyses are well suited for determining parameters that have the greatest impact on overall uncertainty and factors that cause extreme forecasts.

Mishra et al. (2009) compared results from global sensitivity to local sensitivity analyses and the Method of Morris (Morris, 1991), which provides a "bridge" between local and global methods. Global methods are more computationally intensive, and the number of runs required is unknown a priori because it depends on problem-specific factors such as degree of nonlinearity and number of parameters. A practical alternative is to "simplify the model via reduction in spatial dimensions, simplification of processes, screening for key parameters based on expert judgment…", to help guide subsequent work. Another such bridge is the Distributed Evaluation of Local Sensitivity Analysis statistic (Rakovec et al., 2014). The insight such methods provide can facilitate more efficient direct sampling-based uncertainty analyses such as Monte Carlo.

Whereas reporting results from a single calibrated model was standard practice in the past, it is now widely recognized that modeling must include some expression of uncertainty in the conceptual model, calibrated numerical model, and forecast conditions. Uncertainty analyses are explored in Chapter 10.

9.8 COMMON MODELING ERRORS

- Too much time and effort are spent on model design and construction; calibration is started too late and the project is nearly out of time and money. Consequently, the final model does not have an acceptable history match and/or has unreasonable parameters.
- Calibration is deemed complete simply because a summary statistic (e.g., a limit on the MAE) is met. Alternatively, an appropriate model is discarded because a summary statistic is not met.
- Calibration is deemed complete after a history matching exercise but optimized calibration parameters include unreasonable values.
- History matching only includes manual trial-and-error when the modeling objective requires a quantitative best fit. Model calibration should include parameter estimation.
- Weights assigned to calibration targets for parameter estimation do not reflect the same importance the modeler used for manual trial-and-error history matching. Consequently, the results of parameter estimation do not reflect the modeler's judgment of observation importance.
- The modeler accepts a history match produced by an oversimplified model that does not fully leverage information contained in the observations and degrades the model's forecasting ability.
- The initial model used for parameter estimation is overly complex and has not been tested via manual trial-and-error calibration. Models should illuminate system complexity, not create it (Saltelli and Funtowicz, 2014).
- Parameter results are accepted without evaluation simply because they are produced by a computer algorithm. The modeler should examine parameter estimation results for hydrogeological reasonableness.
- Too much time and effort are given to performing parameter estimation statistical analyses leaving little or no time for the primary modeling objectives of forecasting and related uncertainty analyses.
- SVD is not used on an ill-posed problem and the parameter estimation cannot find a best fit.
- SVD is used without some form of additional regularization (e.g., Tikhonov regularization). The process reports best fit calibrated parameters that are outside the range of reasonable values when a model with values within the range produces a fit that is only negligibly worse.

9.9 PROBLEMS

Chapter 9 problems are designed to provide experience in using trail-and-error and automated history matching to calibrate models. The best calibrated model from these problems will be used in the problems in Chapter 10 for forecasting and forecast uncertainty analysis.

P9.1 Design a 2-D areal model of an unconfined sand and gravel aquifer; the dimensions of the problem domain are 1500 m by 1500 m (Fig. P9.1). Use a uniform nodal spacing of 100 m. The modeling objective is to forecast the effects on heads and river flows from proposed pumping of well M (Fig. P9.1). It is desirable to minimize the effects of pumping on river flows because farms downstream rely on river water for irrigation.

The north, east, and west boundaries of the problem domain are no flow boundaries representing impermeable bedrock. The south boundary is represented by a 100 m wide gravel-bottomed eastward sloping ditch that carries water out of the basin. The ditch leaks large quantities of water continuously. Leakage also enters the problem domain from many other such ditch systems south of the modeled area (see Fig. P9.1). The eastward flowing river just south of the northern boundary of the model is 100 m wide. The average stage (m above sea level) is given in Fig. P9.1 at the points indicated. The river has an average depth of 2 m and a bottom composed of 2 m of sand and fine gravel with a vertical hydraulic conductivity of 30 m/d. The river flows adjacent to an outcrop of impermeable bedrock in the area labeled "area not contributing groundwater" (Fig. P9.1). The entire area receives an average daily recharge of 0.0001 m/d.

The driller's logs for wells shown in Fig. P9.1 generally listed river sand and gravel with isolated lenses of silt and clay from land surface to the aquifer base. The geologic logs for wells N and E (Fig. P9.1) show over 50% silt and clay, which are interpreted as overbank and oxbow sediments. Aquifer tests of wells finished in sand and gravel yielded hydraulic conductivities ranging from 30 to 120 m/d with an average of 75 m/d $\pm$ 40%. The steady-state groundwater discharge to the river was 45,550 $m^3/d \pm 10\%$. Inflow from the river to the aquifer was 350 $m^3/d \pm 10\%$. All head measurements (Table P9.1) used as calibration targets contain a measurement error of about $\pm$0.002 m and a survey error of $\pm$0.02 m.

a. Use information in the geologic logs (described above) to delineate zones of hydraulic conductivity. Then calibrate a 2-D areal model to the steady-state heads in Table P9.1 and river fluxes given above using manual trail-and-error history matching. The number and assigned hydraulic conductivity values of the zones can be varied. Justify your values. Keep a simulation log (Section 3.7, Table 3.1) in which you record each trial calibration run and the effect

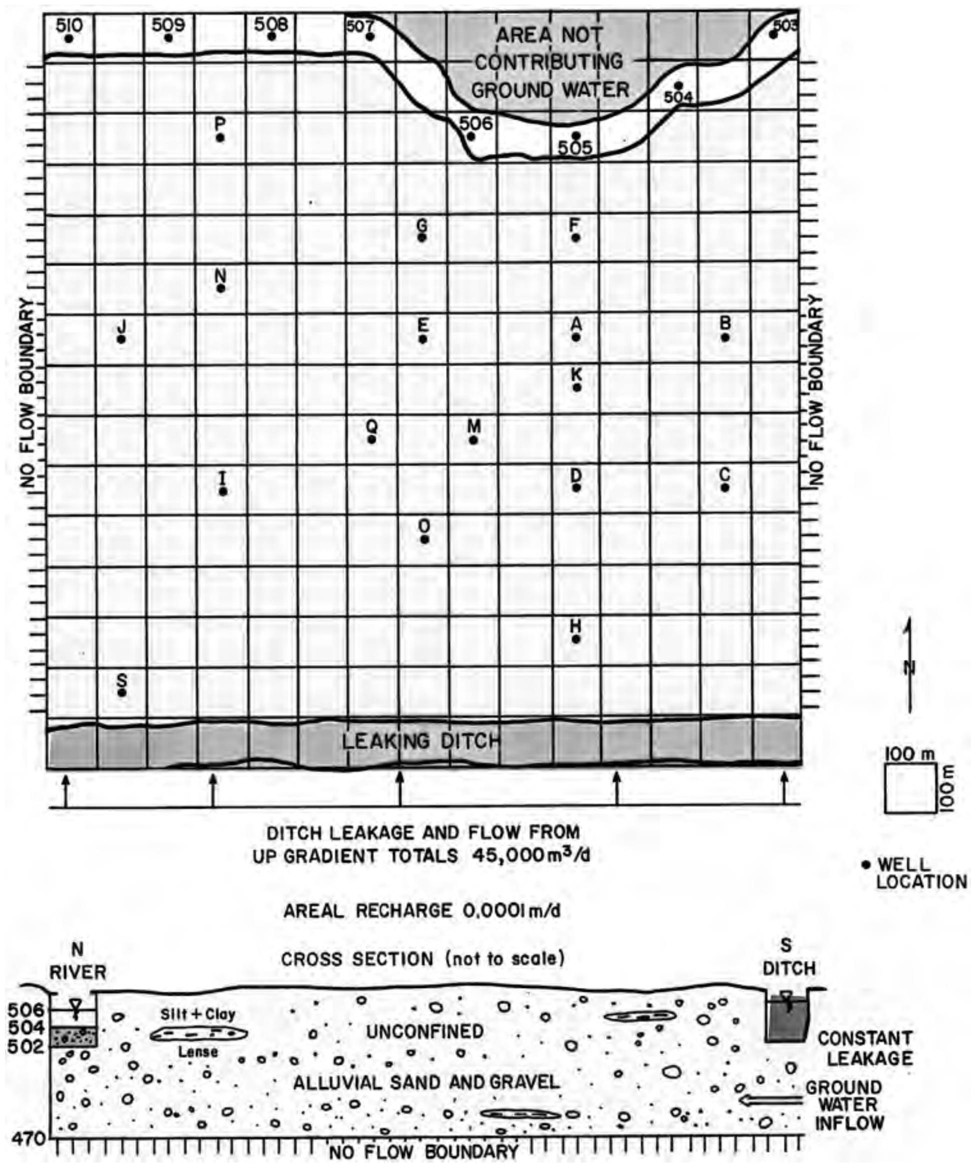


Figure P9.1 Map view and cross section of an unconfined sand and gravel aquifer. The areal dimensions of the problem domain are 1500 m by 1500 m and the nodal spacing is uniformly 100 m. Impermeable bedrock along the northern boundary of the problem domain and north of the river does not contribute water to the river. Numbers refer to river stage in meters above sea level. Letters refer to pumping and observation wells (Table P9.1). The cross section is oriented N—S along column 9. Elevations are given in meters above sea level.

Table P9.1 Head targets for the aquifer shown in Fig. P9.1

Well	Row	Column	Head (m) I[a]	Head (m) II[b]
P	3	4	509.12	509.11
G	5	8	508.19	507.99
F	5	11	508.17	507.79
N	6	4	512.83	512.83
J	7	2	515.71	515.71
E	7	8	513.17	513.04
A	7	11	512.22	508.8
B	7	14	511.95	511.29
K	8	11	513.88	512.21
Q	9	7	518.32	518.18
M	9	9	517.12	516.68
I	10	4	519.28	518.86
D	10	11	516.71	516.17
C	10	14	516.03	515.66
O	11	8	519.02	518.86
H	13	11	519.70	519.55
S	14	2	521.96	521.95

[a]I, Steady-state heads.
[b]II heads after 3 days of pumping well A; all heads are averages for a 100 m by 100 m area centered on the well.

of changing parameter values on the resulting history match. Calibration will mostly require adjusting values of hydraulic conductivity. Calculate summary statistics (Eqns (9.1)—(9.3)) to judge your calibration. Also show simulated and measured values on a scatter plot and residuals on a map. Use the heads from the best calibrated model to generate a water table contour map, showing both field and simulated equipotential lines. List the values of the parameters for the best calibrated model. Discuss the calibration results; are your parameter values hydrogeologically reasonable? Justify your selection of the best calibrated model.

b. Repeat the process using parameter estimation (i.e., automated trail and error) with the zone configuration from the manual trial-and-error calibration. Describe how you formulated the objective function and justify the weights used. Compare and contrast the RMSE of heads and the river discharge from manual trial-and-error calibration in part (a) with the results from parameter estimation. Also compare and contrast the final calibrated hydraulic conductivity values and comment on differences and similarities.

P9.2 History matching sometimes includes calibration to transient conditions. Transient data form a second set of calibration data.

The specific yield of the sand and gravel aquifer was estimated to be about 0.10. Design a transient model to simulate results of a three-day aquifer test whereby well A (Fig. P9.1) is pumped continuously at a constant rate of 20,000 m^3/d. The cumulative three-day groundwater discharge to the river during the test was about 125,700 $m^3 \pm 10\%$ and cumulative river inflow to the aquifer was 1030 $m^3 \pm 10\%$.

a. Use the parameter values and zones from the steady-state calibration of Problem P9.1(b) and final heads as initial conditions. Run the transient model and examine the heads and the cumulative flux to and from the river after 3 days of simulated pumping. Attempt to calibrate to the observations using only the specific yield and river fluxes. Do the simulated heads match the transient calibration head targets (Table P9.1) and the flows to and from the river measured during the aquifer test?

b. If your head and flux matches were unacceptable in part (a) recalibrate the steady-state model by altering the zonation as needed using automated trail-and-error methods. Then attempt transient calibration using zones and hydraulic conductivities from the new steady-state model and adjust values of specific yield. Justify your objective function design, and the final aquifer parameter values.

c. Comment on your methods and the calibration results. How confident are you that the model is calibrated so that it could appropriately forecast the response of the aquifer to pumping a new well at location M?

P9.3 The previous calibration methods used zones of hydraulic conductivity. In this problem, we will use pilot points with parameter estimation. Use initial parameter values from your best calibrated steady-state model from Problem P9.2 (a) and (b).

a. Remove all the zones and use a regular grid of pilot points; calibrate the steady-state model again. Derive initial hydraulic conductivities for the pilot points from your results (Problem P9.2(b)). Compare and contrast your results with those of Problems P9.1(a), P9.1(b)).

b. Use the calibrated parameter values from Problem P9.3(a) and the heads as the initial conditions and place a pumping well at A to simulate the three-day aquifer test. Calibrate the transient model to river fluxes using specific yield. Compare and contrast your results with results from Problem P9.2(b).

c. Pick a best model (base model) and support your selection. This model will be used in Chapter 10 for forecasting and uncertainty analysis.

P9.4 Read the report by Doherty and Hunt (2010) (given in the reference list), which advocates highly parameterized models. Construct a flow chart of the process they advocate for parameter estimation.

REFERENCES

Alcolea, A., Carrera, J., Medina, A., 2006. Pilot points method incorporating prior information for solving the groundwater flow inverse problem. Advances in Water Resources 29 (11), 1678–1689. http://dx.doi.org/10.1016/j.advwatres.2005.12.009.

Anderson, M.G., Bates, P.D. (Eds.), 2001. Model Validation: Perspectives in Hydrological Science. John Wiley & Sons Ltd., London, UK, 512 pp.

Aster, R.C., Borchers, B., Thurber, C.H., 2013. Parameter Estimation and Inverse Problems, second ed. Elsevier Academic Press. 301 p.

ASTM (International), 2008. Standard guide for calibrating a groundwater flow model application D5981 – 96(2008). American Society of Testing and Materials, ASTM International, 6 p.

Bair, E.S., 2001. Models in the courtroom. In: Anderson, M.G., Bates, P.D. (Eds.), Model Validation: Perspectives in Hydrological Science. John Wiley & Sons Ltd., London, pp. 55–77.

Bair, E.S., Metheny, M.A., 2011. Lessons learned from the landmark "A Civil Action" trial. Groundwater 49 (5), 764–769. http://dx.doi.org/10.1111/j.1745-6584.2008.00506.x.

Belsley, D.A., Kuh, E., Welsch, R.E., 1980. Regression Diagnostics: Identifying Influential Data and Source of Collinearity. John Wiley, New York, 292 p.

Beven, K.J., 2005. On the concept of model structural error. Water Science & Technology 52 (6), 167–175. http://www.iwaponline.com/wst/05206/wst052060167.htm.

Beven, K.J., 2009. Environmental Modelling: An Uncertain Future? An Introduction to Techniques for Uncertainty Estimation in Environmental Prediction. Routledge, 310 p.

Beven, K., Young, P., 2013. A guide to good practice in modeling semantics for authors and referees. Water Resources Research 49 (8), 5092–5098. http://dx.doi.org/10.1002/wrcr.20393.

Bourgault, G., 1997. Spatial declustering weights. Mathematical Geology 29 (2), 277–290. http://dx.doi.org/10.1007/BF02769633.

Bravo, H.R., Jiang, F., Hunt, R.J., 2002. Using groundwater temperature data to constrain parameter estimation in a groundwater flow model of a wetland system. Water Resources Research 38 (8), 28-1–28-14. http://dx.doi.org/10.1029/2000WR000172.

Carrera, J., 1988. State of the art of the inverse problem applied to flow and solute transport equations. In: Custodio, E., et al. (Eds.), Groundwater Flow and Quality Modelling. D. Reidel Publication Company, pp. 549–583.

Carrera, J., Neuman, S.P., 1986. Estimation of aquifer parameters under transient and steady state conditions: 1. Maximum likelihood method incorporating prior information. Water Resources Research 22 (2), 199–210. http://dx.doi.org/10.1029/WR022i002p00199.

Certes, C., Marsily, G. de, 1991. Application of the pilot points method to the identification of aquifer transmissivities. Advances in Water Resources 14 (5), 284–300. http://dx.doi.org/10.1016/0309-1708(91)90040-U.

Cook, P.G., Wood, C., White, T., Simmons, C.T., Fass, T., Brunner, P.A., 2008. Groundwater inflow to a shallow, poorly-mixed wetland estimated from a mass balance of radon. Journal of Hydrology 354 (1–4), 213–226. http://dx.doi.org/10.1016/j.jhydrol.2008.03.016.

Cooley, R.L., 1977. A method of estimating parameters and assessing reliability for models of steady state groundwater flow, 1. Theory and numerical properties. Water Resources Research 13 (2), 318–324. http://dx.doi.org/10.1029/WR013i002p00318.

Cooley, R.L., 1979. A method of estimating parameters and assessing reliability for models of steady state groundwater flow, 2. Application of statistical analysis. Water Resources Research 15 (3), 603–617. http://dx.doi.org/10.1029/WR015i003p00603.

Cooley, R.L., Sinclair, P.J., 1976. Uniqueness of a model of steady-state groundwater flow. Journal of Hydrology 31 (3–4), 245–269. http://dx.doi.org/10.1016/0022-1694(76)90127-X.

Cooley, R.L., Naff, R.L., 1990. Regression Modeling of Ground-water Flow. U.S. Geological Survey Techniques of Water-Resources Investigations, 03–B4, 232 p. http://pubs.usgs.gov/twri/twri3-b4/.

D'Agnese, F.A., O'Brien, G.M., Faunt, C.C., Belcher, W.R., San Juan, C., 2002. A Three-dimensional Numerical Model of Predevelopment Conditions in the Death Valley Regional Ground-water Flow

System, Nevada and California. U.S. Geological Survey Water-Resources Investigations Report, 02-4102, 114 p. http://pubs.usgs.gov/wri/wri024102/.
Davis, K.W., Putnam, L.D., 2013. Conceptual and Numerical Models of Groundwater Flow in the Ogallala Aquifer in Gregory and Tripp Counties, South Dakota, Water Years 1985–2009. U.S. Geological Survey Scientific Investigations Report 2013-5069, 82 p. http://pubs.usgs.gov/sir/2013/5069/.
De Groot-Hedlin, C., Constable, S., 1990. Occam's inversion to generate smooth, two-dimensional models from magnetotelluric data. Geophysics 55 (12), 1613–1624. http://dx.doi.org/10.1190/1.1442813.
Doherty, J., 1990. MODINV – Suite of Software for MODFLOW Preprocessing, Postprocessing, and Parameter Optimization. User's Manual: Australian Centre for Tropical Freshwater Research (various pagings).
Doherty, J., 2003. Ground water model calibration using pilot points and regularization. Groundwater 41 (2), 170–177. http://dx.doi.org/10.1111/j.1745-6584.2003.tb02580.x.
Doherty, J., 2011. Modeling: Picture perfect or abstract art? Groundwater 49 (4), 455. http://dx.doi.org/10.1111/j.1745-6584.2011.00812.x.
Doherty, J., 2014a. PEST, Model-independent Parameter Estimation—User Manual (fifth ed., with slight additions). Watermark Numerical Computing, Brisbane, Australia.
Doherty, J., 2014b. Addendum to the PEST Manual. Watermark Numerical Computing, Brisbane, Australia.
Doherty, J., Christensen, S., 2011. Use of paired simple and complex models to reduce predictive bias and quantify uncertainty. Water Resources Research 47 (12), W12534(21). http://dx.doi.org/10.1029/2011WR010763.
Doherty, J., Hunt, R.J., 2009a. Two statistics for evaluating parameter identifiability and error reduction. Journal of Hydrology 366 (1–4), 119–127. http://dx.doi.org/10.1016/j.jhydrol.2008.12.018.
Doherty, J., Hunt, R.J., 2009b. Response to comment on: Two statistics for evaluating parameter identifiability and error reduction. Journal of Hydrology 380 (3–4), 489–496. http://dx.doi.org/10.1016/j.jhydrol.2009.10.012.
Doherty, J., Hunt, R.J., 2010. Approaches to Highly Parameterized Inversion: A Guide to Using PEST for Groundwater-model Calibration. U.S. Geological Survey Scientific Investigations Report 2010-5169, 60 p. http://pubs.usgs.gov/sir/2010/5169/.
Doherty, J., Simmons, C.T., 2013. Groundwater modeling in decision support: Reflections on a unified conceptual framework. Hydrogeology Journal 21 (7), 1531–1537. http://dx.doi.org/10.1007/s10040-013-1027-7.
Doherty, J., Welter, D.E., 2010. A short exploration of structural noise. Water Resources Research 46 (5), W05525. http://dx.doi.org/10.1029/2009WR008377.
Doherty, J.E., Fienen, M.N., Hunt, R.J., 2010a. Approaches to Highly Parameterized Inversion: Pilot-point Theory, Guidelines, and Research Directions. U.S. Geological Survey Scientific Investigations Report 2010-5168, 36 p. http://pubs.usgs.gov/sir/2010/5168/.
Doherty, J.E., Hunt, R.J., Tonkin, M.J., 2010b. Approaches to Highly Parameterized Inversion: A Guide to Using PEST for Model-parameter and Predictive-uncertainty Analysis. U.S. Geological Survey Scientific Investigations Report 2010–5211, 71 p. http://pubs.usgs.gov/sir/2010/5211/.
Emsellem, Y., Marsily, G. de, 1971. An automatic solution for the inverse problem. Water Resources Research 7 (5), 1264–1283. http://dx.doi.org/10.1029/WR007i005p01264.
Engl, H.W., Hanke, M., Neubauer, A., 1996. Regularization of Inverse Problems. Kluwer Academic, Dordrecht, The Netherlands, 321 p. ISBN 978-0-7923-4157-4.
Feinstein, D.T., Hunt, R.J., Reeves, H.W., 2008. Calibrating a big model: Strategies and limitations. In: MODFLOW and More 2008: Ground Water and Public Policy, Proceedings of the 9th International Conference of the International Ground Water Modeling Center. Colorado School of Mines, Golden, CO, pp. 430–434.
Fienen, M.N., 2013. We speak for the data. Groundwater 51 (2), 157. http://dx.doi.org/10.1111/gwat.12018.
Fienen, M., Hunt, R., Krabbenhoft, D., Clemo, T., 2009a. Obtaining parsimonious hydraulic conductivity fields using head and transport observations—A Bayesian geostatistical parameter estimation approach. Water Resources Research 45 (8), W08405(23). http://dx.doi.org/10.1029/2008WR007431.

Fienen, M.N., Muffels, C.T., Hunt, R.J., 2009b. On constraining pilot point calibration with regularization in PEST. Groundwater 47 (6), 835–844. http://dx.doi.org/10.1111/j.1745-6584.2009.00579.x.

Fienen, M.N., D'Oria, M., Doherty, J.E., Hunt, R.J., 2013. Approaches in Highly Parameterized Inversion: bgaPEST, A Bayesian Geostatistical Approach Implementation with PEST. U.S. Geological Survey Techniques and Methods. Book 7, Section C, (Chapter 9), 86 p. http://pubs.usgs.gov/tm/07/c09/.

Foster, I., 1995. Designing and Building Parallel Programs. Addison-Wesley Pearson Education, Upper Saddle River, New Jersey, 430 p. ISBN 9780201575941.

Freeze, R.A., Cherry, J.A., 1979. Groundwater. Prentice-Hall, 604 p.

Freeze, R.A., Witherspoon, P.A., 1966. Theoretical analysis of regional groundwater flow, 1. Analytical and numerical solutions to the mathematical model. Water Resources Research 2 (4), 641–656. http://dx.doi.org/10.1029/WR002i004p00641.

Freeze, R.A., Massmann, J., Smith, L., Sperling, T., James, B., 1990. Hydrogeological decision analysis: 1. A framework. Groundwater 28 (5), 738–766. http://dx.doi.org/10.1111/j.1745-6584.1990.tb01989.x.

Gaganis, P., Smith, L., 2001. A Bayesian approach to the quantification of the effect of model error on the predictions of groundwater models. Water Resources Research 37 (9), 2309–2322. http://dx.doi.org/10.1029/2000WR000001.

Gardner, W.P., Harrington, G., Solomon, D.K., Cook, P., 2011. Using terrigenic ^{4}He to identify and quantify regional groundwater discharge to streams. Water Resources Research 47 (6), W06523(13). http://dx.doi.org/10.1029/2010WR010276.

Gómez-Hernández, J.J., 2006. Complexity. Groundwater 44 (6), 782–785. http://dx.doi.org/10.1111/j.1745-6584.2006.00222.x.

Hadamard, J., 1902. Sur les problèmes aux dérivées partielles et leur signification physique. Princeton University Bulletin, 49–52.

Haitjema, H., 2006. The role of hand calculations in ground water flow modeling. Groundwater 44 (6), 786–791. http://dx.doi.org/10.1111/j.1745-6584.2006.00189.x.

Haitjema, H.M., 2015. The cost of modeling. Groundwater 53 (2), 179. http://dx.doi.org/10.1111/gwat.12321.

Hill, M.C., 1992. A Computer Program (MODFLOWP) for Estimating Parameters of a Transient, Three-dimensional, Ground-water Flow Model Using Nonlinear Regression. U.S. Geological Survey Open-File Report 91-484, 358 p. http://pubs.er.usgs.gov/publication/ofr91484.

Hill, M.C., 2006. The practical use of simplicity in developing ground water models. Groundwater 44 (6), 775–781. http://dx.doi.org/10.1111/j.1745-6584.2006.00227.x.

Hill, M.C., Tiedeman, C.R., 2007. Effective Groundwater Model Calibration—with Analysis of Data, Sensitivities, Predictions, and Uncertainty. Wiley-Interscience, Hoboken, NJ, 455 p.

Himmelblau, D.M., 1972. Applied Nonlinear Programming. McGraw-Hill, New York, 477 p.

Hunt, R.J., Anderson, M.P., Kelson, V.A., 1998. Improving a complex finite difference ground water flow model through the use of an analytic element screening model. Groundwater 36 (6), 1011–1017. http://dx.doi.org/10.1111/j.1745-6584.1998.tb02108.x.

Hunt, R.J., Zheng, C., 1999. Debating complexity in modeling. Eos (Transactions, American Geophysical Union) 80 (3), 29. http://dx.doi.org/10.1029/99EO00025.

Hunt, R.J., Krabbenhoft, D.P., Anderson, M.P., 1996. Groundwater inflow measurements in wetland systems. Water Resources Research 32 (3), 495–507. http://dx.doi.org/10.1029/95WR03724.

Hunt, R.J., Feinstein, D.T., Pint, C.D., Anderson, M.P., 2006. The importance of diverse data types to calibrate a watershed model of the Trout Lake Basin, northern Wisconsin, USA. Journal of Hydrology 321 (1–4), 286–296. http://dx.doi.org/10.1016/j.jhydrol.2005.08.005.

Hunt, R.J., Doherty, J., Tonkin, M.J., 2007. Are models too simple? Arguments for increased parameterization. Groundwater 45 (3), 254–261. http://dx.doi.org/10.1111/j.1745-6584.2007.00316.x.

Hunt, R.J., Luchette, J., Schreüder, W.A., Rumbaugh, J.O., Doherty, J., Tonkin, M.J., Rumbaugh, D.B., 2010. Using a cloud to replenish parched groundwater modeling efforts. Rapid Communication for Groundwater 48 (3), 360–365. http://dx.doi.org/10.1111/j.1745-6584.2010.00699.x.

Hunt, R.J., Zheng, C., 2012. The current state of modeling. Groundwater 50 (3), 329–333. http://dx.doi.org/10.1111/j.1745-6584.2012.00936.x.

Hunt, R.J., Walker, J.F., Selbig, W.R., Westenbroek, S.M., Regan, R.S., 2013. Simulation of Climate-change Effects on Streamflow, Lake Water Budgets, and Stream Temperature Using GSFLOW and SNTEMP, Trout Lake Watershed, Wisconsin. U.S. Geological Survey Scientific Investigations Report 2013-5159, 118 p. http://pubs.usgs.gov/sir/2013/5159/.

Juckem, P.F., 2009. Simulation of the Groundwater-flow System in Pierce, Polk, and St. Croix Counties, Wisconsin. U.S. Geological Survey Scientific Investigations Report 2009-5056, 53 p. http://pubs.usgs.gov/sir/2009/5056/.

Juckem, P.F., Fienen, M.N., Hunt, R.J., 2014. Simulation of Groundwater Flow and Interaction of Groundwater and Surface Water on the Lac du Flambeau Reservation, Wisconsin. U.S. Geological Survey Scientific Investigations Report 2014-5020, 34 p. http://dx.doi.org/10.3133/sir20145020.

Kalman, D., 1996. A singularly valuable decomposition: The SVD of a matrix. College Mathematics Journal 27 (1), 2—23. http://dx.doi.org/10.2307/2687269.

Konikow, L.F., Bredehoeft, J.D., 1992. Ground-water models cannot be validated. Advances in Water Resources 15 (1), 75—83. http://dx.doi.org/10.1016/0309-1708(92)90033-X.

Krabbenhoft, D.P., Bowser, C.J., Kendall, C., Gat, J.R., 1994. Use of oxygen-18 to assess the hydrology of groundwater-lake systems. In: Baker, L.A. (Ed.), Environmental Chemistry of Lakes and Reservoirs, American Chemical Society Advances in Chemistry Series, vol. 237, pp. 67—90.

Levenberg, K., 1944. A method for the solution of certain non-linear problems in least squares. Quarterly of Applied Mathematics 2, 164—168.

Marquardt, D., 1963. An algorithm for least-squares estimation of nonlinear parameters, SIAM. Journal on Applied Mathematics 11 (2), 431—441. http://dx.doi.org/10.1137/0111030.

Marsily, G. de, Lavendan, C., Boucher, M., Fasanino, G., 1984. Interpretation of interference tests in a well field using geostatistical techniques to fit the permeability distribution in a reservoir model. In: Verly, G., David, M., Journel, A.G., Marechal, A. (Eds.), Geostatistics for Natural Resources Characterization. NATO, C 182, Boston, Massachusetts, pp. 831—849.

McCallum, J., Cook, P., Berhane, D., Rumpf, C., McMahon, G., 2012. Quantifying groundwater flows to streams using differential flow gaugings and water chemistry. Journal of Hydrology 416—417, 118—132. http://dx.doi.org/10.1016/j.jhydrol.2011.11.040.

McLaughlin, D., Townley, L.R., 1996. A reassessment of the groundwater inverse problem. Water Resources Research 32 (5), 1131—1161. http://dx.doi.org/10.1029/96WR00160.

Meyer, J.R., Parker, B.L., Cherry, J.A., 2014. Characteristics of high resolution hydraulic head profiles and vertical gradients in fractured sedimentary rocks. Journal of Hydrology 517, 493—507. http://dx.doi.org/10.1016/j.jhydrol.2014.05.050.

Mishra, S., Deeds, N., Ruskauff, G., 2009. Global sensitivity analysis techniques for probabilistic ground water modeling. Groundwater 47 (5), 727—744. http://dx.doi.org/10.1111/j.1745-6584.2009.00604.x.

Moore, C., Doherty, J., 2005. Role of the calibration process in reducing model predictive error. Water Resources Research 41 (5), 1—14. http://dx.doi.org/10.1029/2004WR003501.

Moore, C., Wöhling, T., Doherty, J., 2010. Efficient regularization and uncertainty analysis using a global optimization methodology. Water Resources Research 46 (8), W08527. http://dx.doi.org/10.1029/2009WR008627.

Moriasi, D.N., Wilson, B.N., Douglas-Mankin, K.R., Arnold, J.G., Gowda, P.H., 2012. Hydrologic and water quality models: Use, calibration and validation. Transactions American Society of Agricultural and Biological Engineers 55 (4), 1241—1247. http://dx.doi.org/10.13031/2013.42265.

Morris, M.D., 1991. Factorial sampling plans for preliminary computational experiments. Technometrics 33 (2), 161—174. http://www.jstor.org/stable/1269043.

Muffels, C.T., 2008. Application of the LSQR Algorithm to the Calibration of a Regional Groundwater Flow Model—Trout Lake Basin, Vilas County, Wisconsin (M.S thesis). University of Wisconsin-Madison, 106 p.

Muffels, C.T., Schreüder, W.A., Doherty, J.E., Karanovic, M., Tonkin, M.J., Hunt, R.J., Welter, D.E., 2012. Approaches in Highly Parameterized Inversion—GENIE, A General Model-independent TCP/IP Run Manager. U.S. Geological Survey Techniques and Methods. Book 7, Chapter C6, 26 p. http://pubs.usgs.gov/tm/tm7c6/.

Murray–Darling Basin Commission (MDBC), January 2001. Groundwater Flow Modelling Guideline. Report prepared by Aquaterra.
Nelson, R.W., 1960. In place measurement of permeability in heterogeneous media, 1. Theory of a proposed method. Journal of Geophysical Research 65 (6), 1753–1760. http://dx.doi.org/10.1029/JZ065i006p01753.
Nelson, R.W., 1961. In place measurement of permeability in heterogeneous media, 2. Experimental and computational considerations. Journal of Geophysical Research 66 (6), 2469–2478. http://dx.doi.org/10.1029/JZ066i008p02469.
Nelson, R.W., 1962. Conditions for determining areal permeability distributions by calculation. Society of Petroleum Engineers Journal 2 (3), 223–224. http://dx.doi.org/10.2118/371-PA.
Neuman, S.P., 1973. Calibration of distributed parameter groundwater flow models viewed as a multiple-objective decision process under uncertainty. Water Resources Research 9 (4), 1006–1021. http://dx.doi.org/10.1029/WR009i004p01006.
Nielson, D.M., 1991. Practical Handbook of Ground-Water Monitoring. Lewis, Chelsea, MI, 717 p.
Oreskes, N., Belitz, K., 2001. Philosophical issues in model assessment. In: Anderson, M.G., Bates, P.D. (Eds.), Model Validation: Perspectives in Hydrological Science. John Wiley & Sons Ltd., London, UK, pp. 24–41.
Oreskes, N., Shrader-Frechette, K., Belitz, K., 1994. Verification, validation, and confirmation of numerical models in the earth sciences. Science 263 (5147), 641–646. http://dx.doi.org/10.1126/science.263.5147.641.
Poeter, E.P., Hill, M.C., 1997. Inverse models—a necessary next step in ground-water modeling. Groundwater 35 (2), 250–260. http://dx.doi.org/10.1111/j.1745-6584.1997.tb00082.x.
Poeter, E.P., Hill, M.C., Banta, E.R., Mehl, S., Christensen, S., 2005. UCODE_2005 and Six Other Computer Codes for Universal Sensitivity Analysis, Calibration, and Uncertainty Evaluation. U.S. Geological Survey Techniques and Methods, 6 A11, 47 p. 283 p. http://pubs.usgs.gov/tm/2006/tm6a11/.
Rakovec, O., Hill, M.C., Clark, M.P., Weerts, A.H., Teuling, A.J., Uijlehoet, R., 2014. Distributed Evaluation of Local Sensitivity Analysis (DELSA), with application to hydrologic models. Water Resources Research 50 (1), 409–426. http://dx.doi.org/10.1002/2013WR014063.
Ramarao, B.S., Lavenue, A.M., Marsily, G. de, Marietta, M.G., 1995. Pilot point methodology for automated calibration of an ensemble of conditionally simulated transmissivity fields, 1. Theory and computational experiments. Water Resources Research 31 (3), 475–493. http://dx.doi.org/10.1029/94WR02258.
Saltelli, A., Ratto, M., Andres, T., Campolongo, F., Cariboin, J., Gatelli, D., Saisana, M., Tarantola, S., 2008. Global Sensitivity Analysis: The Primer. Wiley-Interscience, Hoboken NJ, 302 p.
Saltelli, A., Funtowicz, S., 2014. When all models are wrong. Issues in Science and Technology 79–85. Winter 30. http://www.issues.org/30.2/.
Schreüder, W.A., 2009. Running BeoPEST. In: Conference Proceedings from the 1st PEST Conference, November 1–3, 2009, Potomac, MD. Lulu Press, Inc., Raleigh, NC, USA, 7 p.
Silver, N., 2012. The Signal and the Noise: Why Most Predictions Fail but Some Don't. Penguin Press, New York, NY, 534 p.
Simmons, C.T., Hunt, R.J., 2012. Updating the debate on model complexity. GSA Today 22 (8), 28–29. http://dx.doi.org/10.1130/GSATG150GW.1.
Stallman, R.W., 1956a. Numerical analysis of regional water levels to define aquifer hydrology. Eos, Transactions American Geophysical Union 37 (4), 451–460. http://dx.doi.org/10.1029/TR037i004p00451.
Stallman, R.W., 1956b. Use of Numerical Methods for Analyzing Data on Ground-water Levels. International Association of Scientific Hydrology Pub. 41, Tome II, pp. 227–331. (Reproduced in Freeze, R. A. and Back, W., editors, 1983: Physical Hydrogeology, Benchmark Papers in Geology, v. 72, Hutchinson Ross Publishing Company, Stroudsburg, Pennsylvania, pp. 193–197).
Sun, N.Z., Yang, S.L., Yeh, W.W-G., 1998. A proposed stepwise regression method for model structure identification. Water Resources Research 34 (10), 2561–2572. http://dx.doi.org/10.1029/98WR01860.
Tikhonov, A.N., 1963a. Solution of incorrectly formulated problems and the regularization method. Soviet Mathematics Doklady 4, 1035–1038.

Tikhonov, A.N., 1963b. Regularization of incorrectly posed problems. Soviet Mathematics Doklady 4, 1624−1637.

Tikhonov, A.N., Arsenin, V.Y., 1977. Solutions of Ill-Posed Problems. Halstead Press-Wiley, New York, 258 p.

Tonkin, M.J., Doherty, J., 2005. A hybrid regularized inversion methodology for highly parameterized models. Water Resources Research 41 (10), W10412. http://dx.doi.org/10.1029/2005WR003995.

Tonkin, M.J., Doherty, J., 2009. Calibration-constrained Monte-Carlo analysis of highly parameterised models using subspace techniques. Water Resources Research 45 (12), W00B10. http://dx.doi.org/10.1029/2007WR006678.

Townley, L.R., 2012. Calibration and sensitivity analysis. In: Barnett, B., Townley, L.R., Post, V., Evans, R.E., Hunt, R.J., Peeters, L., Richardson, S., Werner, A.D., Knapton, A., Boronkay, A. (Eds.), Australian Groundwater Modelling Guidelines, Waterlines Report 82. National Water Commission, Canberra, pp. 57−78, 191 p. ISBN 978-1-921853-91-3.

Voss, C.I., 2011. Editor's message: Groundwater modeling fantasies—Part 1, adrift in the details. Hydrogeology Journal 19 (7), 1281−1284. http://dx.doi.org/10.1007/s10040-011-0789-z.

Welter, D.E., Doherty, J.E., Hunt, R.J., Muffels, C.T., Tonkin, M.J., Schreüder, W.A., 2012. Approaches in Highly Parameterized Inversion: PEST++, A Parameter ESTimation Code Optimized for Large Environmental Models. U.S. Geological Survey Techniques and Methods, 7(C5), 47 p. http://pubs.usgs.gov/tm/tm7c5/.

Yager, R.M., 1998. Detecting influential observations in nonlinear regression modeling of groundwater flow. Water Resources Research 34 (7), 1623−1633. http://dx.doi.org/10.1029/98WR01010.

Yager, R.M., 2004. Effects of model sensitivity and nonlinearity on nonlinear regression of ground water flow. Groundwater 42 (2), 390−400. http://dx.doi.org/10.1111/j.1745-6584.2004.tb02687.x.

Yeh, W., 1986. Review of parameter identification procedures in groundwater hydrology: The inverse problem. Water Resources Research 22 (2), 95−108. http://dx.doi.org/10.1029/WR022i002p00095.

Yeh, W.W-G., Tauxe, G.W., 1971. Optimal identification of aquifer diffusivity using quasilinearization. Water Resources Research 7 (4), 955−962. http://dx.doi.org/10.1029/WR007i004p00955.

Yao, Y., Zheng, C., Liu, J., Cao, G., Xiao, H., Li, H., Li, W., 2014. Conceptual and numerical models for groundwater flow in an arid inland river basin. Hydrological Processes 29 (6), 1480−1492. http://dx.doi.org/10.1002/hyp.10276.

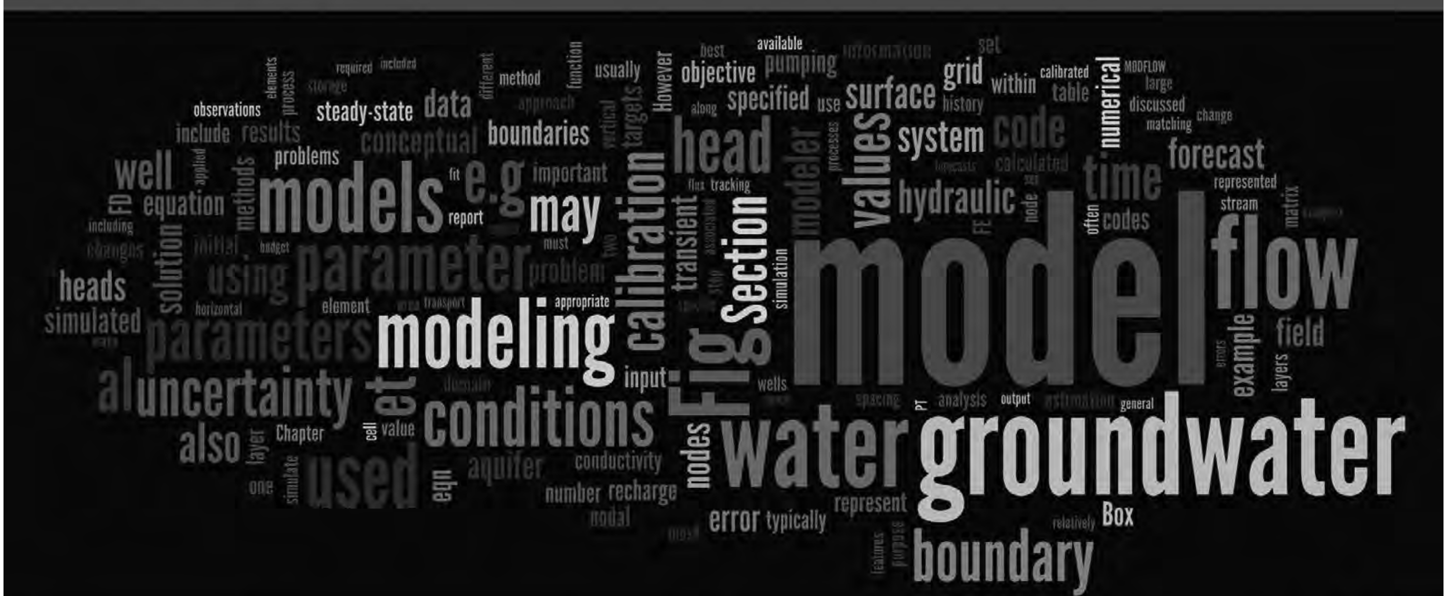
Zheng, C., Bennett, G.D., 2002. Applied Contaminant Transport Modeling, second ed. John Wiley & Sons, New York, 621 p.

Zhou, H., Gómez-Hernández, J.J., Liangping, L., 2014. Inverse methods in hydrogeology: Evolution and recent trends. Advances in Water Resources 63, 22−37. http://dx.doi.org/10.1016/j.advwatres.2013.10.014.

This second edition is extensively revised throughout with expanded discussion of modeling fundamentals and coverage of advances in model calibration and uncertainty analysis that are revolutionizing the science of groundwater modeling. The text is intended for undergraduate- and graduate-level courses in applied groundwater modeling and as a comprehensive reference for environmental consultants and scientists/engineers in industry and governmental agencies.

Key features:

- Explains how to formulate a conceptual model of a groundwater system and translate it into a numerical model
- Demonstrates how modeling concepts, including boundary conditions, are implemented in two groundwater flow codes—MODFLOW (for finite differences) and FEFLOW (for finite elements)
- Discusses particle tracking methods and codes for flowpath analysis and advective transport of contaminants
- Summarizes parameter estimation and uncertainty analysis approaches using the code PEST to illustrate how concepts are implemented
- Discusses modeling ethics and preparation of the modeling report
- Includes boxes that amplify and supplement topics covered in the text
- Each chapter presents lists of common modeling errors and problem sets that illustrate concepts



elsevier.com

ISBN 978-0-12-058103-0

EXHIBIT 4

Advances in Water Resources **15** (1992) 167–173

The role of the postaudit in model validation

Mary P. Anderson

Department of Geology and Geophysics, University of Wisconsin-Madison, Madison, Wisconsin 53706, USA

&

William W. Woessner

Department of Geology, University of Montana, Missoula, Montana 59812, USA

Most researchers agree that validation is a demonstration that a model is capable of making accurate predictions at a site-specific field setting. A successful demonstration of validation requires completion of a series of steps that form a modeling protocol. These steps include model design and calibration, and verification of the governing equation, the computer code, and the model itself. The strictest form of validation is to demonstrate that the model can accurately predict the future. This type of validation test has been called a postaudit. Results of five postaudits suggest that it will be difficult and probably impossible to validate groundwater models by means of a postaudit because it is impossible to characterize the field setting in sufficient detail. Attention should instead be focused on good modeling protocol including providing a complete description of model design, a thorough assessment of model calibration, and an uncertainty analysis.

Key words: model validation, postaudit, modeling protocol, uncertainty analysis.

INTRODUCTION

A groundwater model is generally recognized to be the preferred tool for synthesizing the many factors involved in analyzing complex groundwater problems. But at the same time, results of groundwater models are often viewed with skepticism. In the last 5 years or so an 'enormous amount of skepticism appears to have developed, with a resulting attitude of 'Prove it!' having replaced the more passive and accepting faith of earlier years'.[1] Skepticism arises from an increasing concern over the validity of using models to make long-term predictions about the configuration of a flow system or concentrations of contaminants in groundwater. The absence of proof that models can make accurate long-term predictions has led to demands for what is usually termed model validation, where validation is usually understood to be a demonstration of accuracy.

A model consists of a governing equation and a set of boundary and initial conditions specific to a given field problem. The model is also understood to have associated ranges of site-specific parameter values. The code is a generic computer program that contains an algorithm capable of solving the mathematical model numerically. The modeling process consists of using the code to solve a site-specific field problem. Model validation takes place during the final steps in the modeling process when the accuracy of the model is tested. As such, the success of model validation depends on satisfactory completion of all the other steps in the modeling process. This sequence of steps forms a protocol for modeling. There have been numerous applications of groundwater models to field problems, but as yet there is no standard protocol to provide guidance during modeling or when reporting modeling results. Efforts to develop such a protocol are currently underway.[2,3] The modeling protocol advocated by Anderson and Woessner[26] is shown in Figure 1.

The concept of validation is sometimes confused with verification. Verification, like validation, refers to establishing accuracy. It can be used in reference to the governing equation, the code, or the model. All three types of verification are part of a modeling protocol. Verification of the governing equation consists of demonstrating that the equation used in the model accurately describes the processes of flow and/or transport in porous media, i.e. that the governing

Advances in Water Resources 0309-1708/92/$05.00

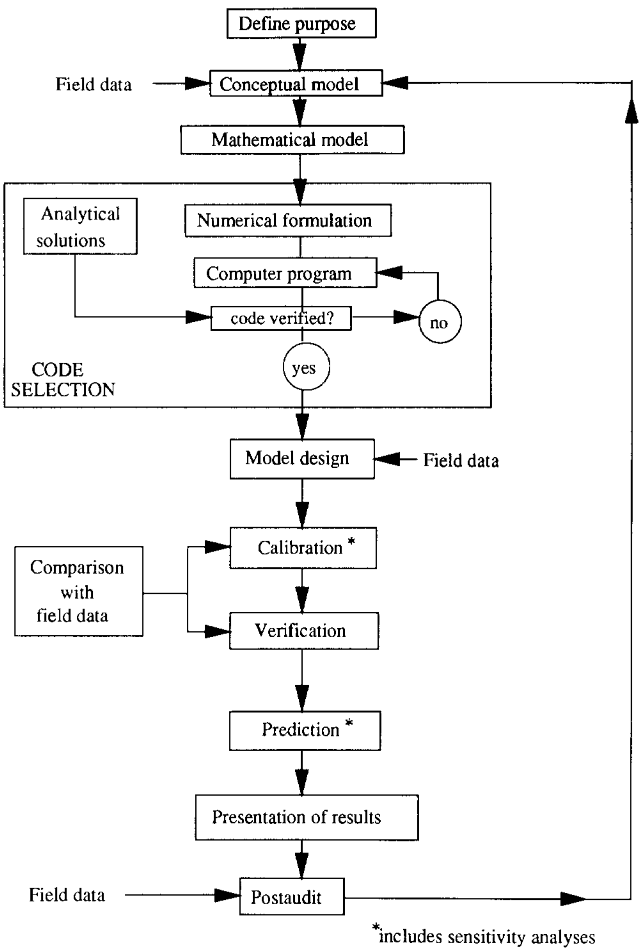


Fig. 1. A modeling protocol.[26]

equation is appropriate for the processes of interest. Verification of a governing equation may consist of a demonstration that a model based on the equation can reproduce and predict short-term results from laboratory and field experiments. Groundwater flow models are accepted as verified in this sense; it is commonly believed that Darcy's law and conservation of mass accurately describe groundwater flow at a macroscopic scale and that average or 'effective' parameters may be defined to characterize the porous medium at the scale of a representative elementary volume. Mass transport models, on the other hand, have not passed this type of generic verification test. Laboratory studies and calibration of models to field data demonstrate that the advection–dispersion equation, currently used in most solute transport models, does not always reproduce system behavior. Consequently, there is much debate over the appropriate way to quantify terms for dispersion and certain chemical reactions. If the governing equation used in a model has not passed a verification test, it must be recognized that modeling results may be incorrect.

Code verification involves comparison of the numerical solution generated by the model with one or more analytical solutions or with other numerical solutions. Verification of the code ensures that the computer program accurately solves the equations that constitute the mathematical model.

Model verification has been used synonymously with model validation, but we prefer to distinguish between these two concepts. We also treat model calibration separately from verification and validation, although all three are tests of model accuracy. During calibration a set of values for aquifer parameters and stresses is found that approximately reproduces field-measured heads and flows and/or concentrations. Calibration is done by trial-and-error adjustment of parameters or by using an automated parameter estimation code. The purpose of model verification is to establish greater confidence in the model by using the set of calibrated parameter values and stresses to reproduce a second set of field data. According to Konikow,[4] a model is verified 'if its accuracy and predictive capability have been proven to lie within acceptable limits or error by tests independent of the calibration data.' This step is also sometimes called historical data validation.[5] In a typical verification exercise, values of parameters and hydrologic stresses determined during calibration are used to simulate a transient response that has been measured in the field. Unfortunately it is often impossible to verify a model because only one set of field data is available. That data set, of course, is needed for calibration. If this is the case, the model cannot be verified. A calibrated but unverified model can still be used to make predictions as long as careful sensitivity analyses of both the calibrated model and the predictive model are performed and evaluated. Predictions resulting from calibrated but unverified models generally will be more uncertain than predictions derived from verified models.

Whereas model calibration and verification demonstrate that the model can mimic past behavior, model validation, as defined here, tests whether the model can predict the future. This type of validation test has been called a predictive validation[5] or a postaudit. In a postaudit, new field data are collected several years after the modeling study was completed to determine whether the prediction came true. If the model's prediction was accurate the model may be considered valid for that particular site for the conditions simulated. Several authors[1,6–10] stressed that claims of validation require qualifiers as to the conditions for which the model has been validated and those for which it should not be used. For example, Tsang[8] observed that it may not be reasonable to require the current generation of transport models to predict concentrations at a point in space at a given moment in time. However, it may be reasonable to expect the model to simulate average transport behavior within the problem domain. Hence, it is necessary to state the performance measures used as one of the qualifiers of the validation.

In this paper the role of the postaudit as a form of validation is considered. The postaudit should occur long enough after the prediction was made to ensure that there has been adequate time for significant changes to occur. A postaudit performed too soon after the initial calibration may lead to the conclusion that the prediction came close to estimating the observed values, when in fact not enough time elapsed to allow the system to move sufficiently far from the calibrated solution. In the literature, validation has been used mainly in reference to models for assessing the potential of contaminant movement from high level radioactive waste repositories.[11] This type of modeling requires prediction on the order of 10 000 or 100 000 years, whereas in most other engineering applications of groundwater models the time frame is of the order of tens of years. Because of the long-term nature of predictions required to assess the potential for contaminant movement from high level radioactive waste repositories, model validation by means of a postaudit will have limited utility in this context.

Postaudits have not been considered a routine part of the modeling process and in fact they may not be necessary if the purpose of the model is to analyze current steady-state behavior or to make short-term predictions. However, when the model is used to make predictions on the order of tens or hundreds of years, a postaudit is an important step in building the case that a model produces meaningful results.

The modeling process, including analysis of the postaudit, requires subjective judgements about the magnitude of acceptable error.[12] Errors include measurement error in the field data and modeling error represented by the differences between field and simulated values. While the magnitude and distribution of errors can be analyzed quantitatively, a subjective judgement is always required in deciding whether the errors are tolerable. Such judgements must be tied to the purpose of the modeling effort and based on hydrogeologic expertise and evidence.

LESSONS FROM POSTAUDITS

To date, five postaudits of modeling studies have been reported in the literature.[13–17] Three of these include postaudits of solute transport models. In all five cases the models did not accurately predict the future. Two conclusions emerge:

(1) Inaccurate predictions were partly caused by errors in the conceptual model of the hydrogeological system.
(2) Inaccurate predictions resulted from a failure to use appropriate values for assumed future stresses such as recharge, pumping and contaminant loading rates.

The more serious problem from the perspective of using a postaudit as a proof of validation is the first of these. It is unfortunate but true that there will always be errors in the conceptual model. Even a detailed site characterization can never eliminate uncertainties about parameter values, processes, and conditions at a site. While it is true that uncertainties involved in estimating future stresses are often large, these are less serious because the model could be rerun using accurate values for the stresses once they become known. Then if the conceptual model and the calibrated parameter values accurately represent system behavior, the validation would be successful.

Uncertainty about future stresses should be built into predictive simulations by means of a sensitivity analysis of the prediction (Fig. 1) in which several different scenarios are simulated using different assumed trends in the applied stresses in order to define a range in the predicted values. In the modeling work analyzed in the postaudits described below, and for most modeling done in the 1960s and 1970s, this step was not performed.

Summaries of postaudits

Postaudit results are reviewed by Anderson and Woessner[26] and are briefly summarized below.

(1) Konikow[13] performed a postaudit of a two-dimensional electric analog model of the Salt River and Lower Santa Cruz River Basins, Arizona, that was calibrated against 40 years of record (1923–64) and then used to predict water-level changes during the following 10 years (1965–74). During the postaudit, analysis of observed water-level changes in 77 wells during 1965–74 showed that the model consistently predicted lower water levels than actually occurred.

The errors in the prediction can be accounted for, in part, by the failure to use accurate future pumping stresses in the simulation. The modeler assumed that future pumping would continue at the 1964 rate when in fact pumping declined after 1965. During the postaudit, examination of the distribution of pumping and the predicted errors in water levels suggested that incorrect assumed pumping rates were partly responsible for the erroneous prediction but that other sources of error were also present. Because the analog model has been disassembled, it was not possible to run the model again to isolate the sources of error. However, it is likely that improvements in the conceptual model, e.g. including land subsidence and a three-dimensional representation of the system, would improve the model's predictive ability by better representing changes in aquifer storage and transmissivity.

(2) Alley and Emery[14] examined predictions of 1982 water-level declines and streamflow depletions for the Blue River Basin, Nebraska, made in 1965 with an electric analog model. Declines in water levels and streamflow were predicted to occur as a result of increases in pumpage for irrigation. The postaudit showed that the model overestimated the decline in

groundwater levels and underestimated the amount of streamflow depletion.

Net groundwater withdrawals in agricultural areas are difficult to estimate because it is usually necessary to infer net withdrawals from estimates of irrigated acreage, groundwater recharge, and consumptive use of irrigation water (irrigation efficiency). Analyses performed by Alley and Emery[14] suggested that net groundwater withdrawals used in the analog simulation were too low. The model overestimated groundwater level declines because it assumed that all of the net groundwater withdrawals would come from storage in the aquifer, when in fact some water comes from induced recharge from the stream. Furthermore, Alley and Emery[14] speculated that storage coefficients used in the model were too low. They concluded that: 'Considerable uncertainty about the basic conceptualization of the hydrology of the Blue River basin greatly limits the reliability of groundwater models developed for the basin.'

(3) Konikow and Bredehoeft[18] used an early version of the USGS Method of Characteristics model[19] to predict concentrations of dissolved solids in the aquifer adjacent to a portion of the Arkansas River in southeastern Colorado. Salinity is a problem in this area, owing to recycling of irrigation water. Konikow and Bredehoeft[18] calibrated the flow model to a transient flow field determined from data collected during the 1971–72 study. The solute transport model was also calibrated to data obtained during 1971–72. The model predicted that dissolved solids concentrations would increase steadily through 1982. Statistical evaluation of the historical data set including data collected in 1982, showed that dissolved solids had not increased in the aquifer above 1971–72 levels. This suggested that the aquifer is in dynamic equilibrium with respect to salinity.[15] If true, this would mean that current irrigation practices could be continued indefinitely without causing further groundwater salinity degradation.

Konikow and Person[15] showed that the error in the original prediction was due to calibration during a period of decreasing river discharge. During the 1971–72 calibration period, river discharge was declining after a record high in 1966. Concentration of dissolved solids in the river is inversely proportional to discharge; during 1971–72, river water recharging the aquifer was increasing in salinity. The model propagated this trend into the future. Statistical tests showed that this short-term trend, although statistically significant, was not representative of the long-term salinity trend. The postaudit showed that the flow portion of the model was adequately calibrated.

Person and Konikow[20] recalibrated the model using an improved regression equation to relate salinity to measured specific conductance. Data from 1971, 1972, and 1982, were used in calculating the new regression equation. Calibration of the model is sensitive to this relationship because about half of the irrigation water is diverted from the river. They also improved the conceptual model of the system by incorporating a lag time for solutes to travel through the unsaturated zone. The recalibrated model successfully simulated the observed long-term trend in salinity from 1971 to 1982. Finally, they used the recalibrated model to demonstrate that the system is in dynamic equilibrium with current irrigation practices.

Although the recalibrated model could accurately simulate the observed long-term trend in salinity, it should be noted that the recalibration used field data collected in 1982 in order to simulate 1982 conditions. Only 3 years of detailed data, including 1982, were available for the 1971–82 simulation. It is therefore relevant to ask whether the model could have predicted the long-term trend in the absence of the 1982 data. Through statistical analysis of temporal salinity trends using a 32-year record of estimated stream salinities, Person and Konikow[20] demonstrated that a 4-year sampling period was needed to calibrate the solute transport model to within 10% of the observed mean salinity, while 1 year's worth of data was sufficient to calibrate the flow model. The implication is that the long-term trend could have been predicted without the 1982 data, as long as a 4-year record of salinity trends was available for calibration. This finding suggests that evaluation of a conceptual model should include not only the spatial properties of the system, but also the hydrologic response time and temporal trends that characterize the system.

(4) Robertson[21] used a two-dimensional groundwater flow model to simulate flow in a basalt aquifer beneath the Idaho National Engineering Laboratory (INEL). Robertson[21] calibrated the model to an assumed steady-state flow field. He coupled the flow model to a solute transport model calibrated to the observed concentrations of chloride in groundwater in 1958 and 1969. Simulation of tritium and strontium-90 plumes were also simulated and compared with field data.

Robertson[21] then used the calibrated model to predict chloride and tritium concentrations in 1980. Lewis and Goldstein[16] performed a postaudit of those predictions and concluded that the contaminant plumes predicted by the simulation extended farther downgradient than the actual plumes because of conservative worst-case assumptions in the model input and inaccurate approximations of subsequent waste discharge and aquifer recharge conditions. The model assumed that waste disposal through a disposal well south of the river would continue at 1973 rates when disposal rates actually increased. The model also assumed that the Big Lost River would recharge the aquifer in odd-numbered years, when in fact there were high flows from 1974 to 1976, followed by 4 years of low flows when no recharge occurred.

Lewis and Goldstein[16] also pointed out that the conceptual model used by Robertson[21] was highly simplified. It was not unusual in the 1970s to use simplistic conceptual models in contaminant transport modeling, assuming two-dimensional, steady-state flow and a homogeneous and isotropic aquifer. We now know that these assumptions are usually inappropriate for simulations of complex contaminant plumes such as those at the INEL. However, recent modeling of this system by Goode and Konikow[22] demonstrated that the inclusion of transient effects in the model does not explain the anomalies in the Robertson simulation. Another possibility would be to use a fracture flow model to simulate the basalt aquifer. The conceptual model used by Robertson[21] viewed the aquifer as a continuous porous medium. It is likely that flow in this aquifer would be better approximated using a dual porosity model that included flow through the fractures as well as matrix diffusion.

(5) Flavelle *et al.*[17] simulated the release of hydrogen ions (H^+) from a tailings pile situated in glaciofluvial deposits in Ontario, Canada. The flow model was calibrated to heads observed in 1989 in the inner part of the plume where pH was less than 4·8. The solute transport model was calibrated by varying the distribution coefficient so that the velocity of contaminants in the inner part of the plume matched the observed positions of the plume in 1983 and 1984. The calibrated model was then used to predict the plume configuration in 1989.

Field measurements collected in 1989 showed that the model predicted pH in the inner portion of the plume reasonably well but not at the outer edges of the plume because the simulated velocities were too low. The values of distribution coefficient calibrated to the inner portion of the plume poorly represented conditions at the outer edge of the plume. It is not surprising that a single value for the distribution coefficient did not simulate the complex geochemistry occurring within the plume. The investigators concluded that even though their site is one of the most thoroughly studied uranium tailings sites in Canada, the data were not complete enough for a successful model validation.

Discussion

All of the postaudits indicate that errors in the predictions can be attributed at least partly to errors in the conceptual model. Model validation, therefore, requires a good conceptual model. Herein lies a major difficulty because a good conceptual model requires accurate and complete field characterization. Field characterization is always incomplete, thereby introducing uncertainty into the conceptual model. Continual improvement of the conceptual model requires periodic collection of field data and a trial and error process of model improvement over many years. It is rare to find such a large commitment of time and money to a modeling effort.

It is likely that there have been hundreds of predictive modeling studies performed since the 1960s. The fact that only five postaudits are reported in the literature suggests that at least in the USA, models are often used in a crisis mode rather than a management mode. In other words, a model is constructed to answer some pressing question so that a management decision can be made. After the model has served this purpose, it is 'shelved' and forgotten or discarded. Most models constructed in the USA are not used for management of the groundwater system on a day-to-day, month-to-month, or even year-to-year basis.

Ideally, models should be archived so that the model can be revived years later when a new modeling objective is defined or new field data become available. For example, Jorgensen[23] described a succession of three increasingly more sophisticated models used to predict drawdowns in the aquifer system underlying Houston, Texas, and the surrounding area. The first model was an electric analog model constructed in the early 1960s. The model accurately simulated observed water-level declines in and adjacent to the City of Houston, but did not reliably simulate drawdowns in outlying areas. The failure of the model was attributed to the lack of sufficient field data to formulate an adequate conceptual model of the system. Between 1965 and 1975, the conceptual model of the system was improved following the acquisition of new field data. A second analog model was constructed in 1975 using a four-layer representation of the system and including the effects of vertical leakage across clay units and the release of water from storage owing to compaction of clays. The simulated clay compaction was used to assess the ability of the model to predict land subsidence. Although the model accurately simulated drawdown, except near the boundaries, it did not accurately simulate the distribution of observed land subsidence. In the late 1970s, as part of a Regional Aquifer System Assessment (RASA) study, a five-layer finite difference model was used to simulate the Houston area once again. This model simulated a larger area than the 1975 analog model and thereby eliminated boundary effects that had been a problem with the analog simulation. The finite difference model used essentially the same conceptual model as the 1975 analog model but incorporated a revised distribution of clay layers and time-dependent storage coefficients for the clays. This model accurately simulated both drawdowns and land subsidence.

The example described by Jorgensen[23] is not a postaudit because a long-term prediction of the model was not evaluated. Rather, successive improvements in the conceptual model were made in an effort to achieve a better calibration to observed conditions. Jorgensen's example also illustrates the iterative way in which a model may be improved as new information is obtained.

Ideally, this is the way all models should develop. Improvements in the conceptual model will result in improved predictions.

SUMMARY AND DISCUSSION

Model validation carries the implication that site-specific models can make accurate predictions. If we require that a model accurately reproduce existing conditions and make accurate short-term predictions, it may be sufficient to follow the steps in the modeling protocol shown in Fig. 1 up to the postaudit.

If we require that a model make accurate long-term predictions in order to be considered valid, a postaudit is recommended. However, it is necessary to wait several years after a prediction is made before a postaudit can be performed. In applications to high level radioactive waste disposal, for example, it may not be practical to wait the length of time necessary before the prediction can be tested under the conditions for which validation is required.

Another difficulty is that a successful postaudit requires an accurate conceptual model of the site and accurate estimates of the magnitude and timing of future stresses. Defining an accurate conceptual model is an iterative process of continually up-dating and improving the field data base. Even with a large commitment of time and money, it is likely that the complete 'truth' about a site will never be known. Estimation of future stresses requires that the modeler foresee the future. Such forecasting necessarily introduces another large source of uncertainty into the model, as the results of the postaudits reviewed above demonstrate. For this reason, it is important to perform a series of predictive simulations to establish a range of probable outcomes. (Each of the postaudits reviewed above assessed the accuracy of only one predictive simulation.) Alternatively, the calibrated model could be rerun after the postaudit when the future stresses are known. If the calibrated model formulated prior to the postaudit accurately predicts field measurements when accurate stresses are input, the model can be considered validated for the conditions simulated.

The issue of validation is mainly a regulatory one, not a scientific one.[6] Tsang[5] pointed out that validation is not possible without a thorough understanding of the relevant physical and chemical processes and the system structure. Because our understanding of a system will always be incomplete a model can never be proven valid from a scientific standpoint. Hence, regulators must be content with some degree of partial validation, which requires detailed qualification of the conditions of validation. Such limited validation may be less than satisfying.

Given the difficulties of carrying out a successful validation and the low probability of success, it seems wise to seek an alternative to validation as a regulatory objective. Model validation is not a fruitful exercise because uncertainties in the conceptual model will always exist. Hence, uncertainty analysis should be built into the modeling strategy from the onset. For example, a modeling strategy involving uncertainty analysis coupled with probability and risk assessment was described by Freeze *et al.*[24] According to NRC[1] (p. 232): 'Such information is ultimately both more useful and more realistic than a certification that a model is or is not validated.' The regulatory focus should shift from demands for validation to demands for good modeling protocol, including providing a complete description of model design, a thorough assessment of model calibration, and an uncertainty analysis. Existing protocols for validation, e.g. the protocol proposed by the US Department of Energy (Voss[25]), should be replaced by protocols for performing and documenting the entire modeling process.

REFERENCES

1. NRC (National Research Council), *Ground Water Models: Scientific and Regulatory Applications*. National Academy Press, Washington, DC, 1990.
2. GRMR (Ground Water Monitoring Review), An update on ASTM Subcommittee D-18.21 on ground water and vadose zone investigations, *Ground Water Monitoring Review*, **X** (1990) 74–7.
3. State of California, Department of Health Services, Scientific and Technical Standards of Hazardous Waste Sites (Draft), Vol. 2: Exposure Assessment, 1990.
4. Konikow, L.F., Calibration of ground-water models. In *Verification of Mathematical and Physical Models in Hydraulic Engineering*, American Society of Civil Engineers, New York, 1978, pp. 87–93.
5. Tsang, C.-F., The modeling process and model validation. *Ground Water*, **29** (1991) 825–31.
6. Davis, P.A. & Goodrich, M.T., A proposed strategy for the validation of ground-water flow and solute transport models. In *GEOVAL-1990: Symposium on Validation of Geosphere Flow and Transport Models*. Organisation for Economic Co-Operation and Development (OECD), Nuclear Energy Agency, Paris, France, 1991, pp. 580–88.
7. Tsang, C.-F., Comments on model validation. *Transport in Porous Media*, **2** (1987) 623–9.
8. Tsang, C.-F., Tracer travel time and model validation. *Radioactive Waste Management and the Nuclear Fuel Cycle*, **13** (1989) 311–323.
9. Heijde, P.K.M. van der, El-Kadi, A.I. & Williams, S.A., Groundwater Modeling: An Overview and Status Report, EPA/600/2-89/028, US EPA, 1988.
10. Heijde, P.K.M. van der, Quality assurance in the development and application of groundwater models. In *Calibration and Reliability in Groundwater Modeling*, ed. K. Kovar, IAHS Publication No. 195, 1990, pp. 271–8.
11. *GEOVAL-1990: Symposium on Validation of Geosphere Flow and Transport Models*. Organisation for Economic Co-Operation and Development (OECD) Nuclear Energy Agency, Paris, France, 1991.
12. Woessner, W.W. & Anderson, M.P., Selecting calibration values and formulating calibration targets for ground

water flow simulations. In *Proceedings of: Solving Ground Water Problems with Models*. Association of Ground Water Scientists and Engineers, National Ground Water Association, Dallas, TX, 1992, pp. 199–212.
13. Konikow, L.F., Predictive accuracy of a ground-water model — lessons from a postaudit. *Ground Water*, **24** (1986) 173–84.
14. Alley, W.M. & Emery, P.A., Groundwater model of the Blue River Basin, Nebraska — twenty years later. *Journal of Hydrology*, **85** (1986) 225–50.
15. Konikow, L.F. & Person, M. Assessment of long-term salinity changes in an irrigated stream-aquifer system. *Water Resources Research*, **21** (1985) 1611–24.
16. Lewis, B.D. & Goldstein, F.S., Evaluation of a predictive ground-water solute-transport model at the Idaho National Engineering Laboratory, Idaho. Water Resources Investigations Report 82–85, US Geological Survey, 1982.
17. Flavelle, P., Nguyen, S. & Napier, W., Lessons learned from model validation — a regulatory perspective. In *GEOVAL-1990: Symposium on Validation of Geosphere Flow and Transport Models*. Organisation for Economic Co-Operation and Development (OECD), Nuclear Energy Agency, Paris, France, 1991, pp. 441–8.
18. Konikow, L.F. & Bredehoeft, J.D., Modeling flow and chemical quality changes in an irrigated stream-aquifer system. *Water Resources Research*, **10** (1974) 546–562.
19. Konikow, L.F. & Bredehoeft, J.D., Computer model of two-dimensional solute transport and dispersion in ground water. In *Techniques of Water-Resources Investigation*, Book 7, Chapter C2, US Geological Survey, 1978.
20. Person, M. & Konikow, L.F., Recalibration and predictive reliability of a solute transport model of an irrigated stream-aquifer system. *Journal of Hydrology*, **87** (1986) 145–65.
21. Robertson, J.B., Digital modeling of radioactive and chemical waste transport in the Snake River Plain aquifer at the National Reactor Testing Station, Idaho. Open File Report IDO-22054, US Geological Survey, 1974.
22. Goode, D.J. & Konikow, L.F., Reevaluation of large-scale dispersivities for a waste chloride plume: effects of transient flow. In *Calibration and Reliability in Groundwater Modeling*, ed. K. Kovar. IAHS Publ. 195, D. Reidel, Dorchrecht, 1990, pp. 417–26.
23. Jorgensen, D.G., Geohydrologic models of the Houston District, Texas. *Ground Water*, **19** (1981) 418–28.
24. Freeze, R.A., Massmann, J., Smith, L., Sperling, T. & James, B., Hydrogeological decision analysis: 1. A framework. *Ground Water*, **28** (1990) 738–66.
25. Voss, C.I., A proposed methodology for validating performance assessment models for the DOE Office of Civilian Radioactive Waste Management Program. In *High Level Radioactive Waste Management*, Vol. 1. American Society of Civil Engineers, New York, 1990, pp. 359-63.
26. Anderson, M.P. & Woessner, W.W., *Applied Groundwater Modeling: Simulation of Flow and Advective Transport*. Academic Press, New York, 1992.

EXHIBIT 5

Designation: D5447 − 17

Standard Guide for Application of a Numerical Groundwater Flow Model to a Site-Specific Problem[1]

This standard is issued under the fixed designation D5447; the number immediately following the designation indicates the year of original adoption or, in the case of revision, the year of last revision. A number in parentheses indicates the year of last reapproval. A superscript epsilon (ε) indicates an editorial change since the last revision or reapproval.

1. Scope*

1.1 This guide covers the application and subsequent documentation of a groundwater flow model to a particular site or problem. In this context, "groundwater flow model" refers to the application of a mathematical model to the solution of a site-specific groundwater flow problem.

1.2 This guide illustrates the major steps to take in developing a groundwater flow model that reproduces or simulates an aquifer system that has been studied in the field. This guide does not identify particular computer codes, software, or algorithms used in the modeling investigation.

1.3 This guide is specifically written for saturated, isothermal, groundwater flow models. The concepts are applicable to a wide range of models designed to simulate subsurface processes, such as variably saturated flow, flow in fractured media, density-dependent flow, solute transport, and multiphase transport phenomena; however, the details of these other processes are not described in this guide.

1.4 This guide is not intended to be all inclusive. Each groundwater model is unique and may require additional procedures in its development and application. All such additional analyses should be documented, however, in the model report.

1.5 This guide is one of a series of standards on groundwater model applications. Other standards include D5981, D5490, D5609, D5610, D5611, and D6033.

1.6 *This standard does not purport to address all of the safety concerns, if any, associated with its use. It is the responsibility of the user of this standard to establish appropriate safety, health, and environmental practices and determine the applicability of regulatory limitations prior to use.*

1.7 *This guide offers an organized collection of information or a series of options and does not recommend a specific course of action. This document cannot replace education or experience and should be used in conjunction with professional judgment. Not all aspects of this guide may be applicable in all circumstances. This ASTM standard is not intended to represent or replace the standard of care by which the adequacy of a given professional service must be judged, nor should this document be applied without consideration of a project's many unique aspects. The word "Standard" in the title of this document means only that the document has been approved through the ASTM consensus process.*

1.8 *This international standard was developed in accordance with internationally recognized principles on standardization established in the Decision on Principles for the Development of International Standards, Guides and Recommendations issued by the World Trade Organization Technical Barriers to Trade (TBT) Committee.*

2. Referenced Documents

2.1 *ASTM Standards:*[2]

D653 Terminology Relating to Soil, Rock, and Contained Fluids

D5490 Guide for Comparing Groundwater Flow Model Simulations to Site-Specific Information

D5609 Guide for Defining Boundary Conditions in Groundwater Flow Modeling

D5610 Guide for Defining Initial Conditions in Groundwater Flow Modeling

D5611 Guide for Conducting a Sensitivity Analysis for a Groundwater Flow Model Application

D5981 Guide for Calibrating a Groundwater Flow Model Application (Withdrawn 2017)[3]

D6033 Guide for Describing the Functionality of a Groundwater Modeling Code

3. Terminology

3.1 *Definitions:*

[1] This guide is under the jurisdiction of ASTM Committee D18 on Soil and Rock and is the direct responsibility of Subcommittee D18.21 on Groundwater and Vadose Zone Investigations.

Current edition approved Dec. 15, 2017. Published January 2018. Originally approved in 1993. Last previous edition approved in 2010 as D5447–04(2010). DOI: 10.1520/D5447-17.

[2] For referenced ASTM standards, visit the ASTM website, www.astm.org, or contact ASTM Customer Service at service@astm.org. For *Annual Book of ASTM Standards* volume information, refer to the standard's Document Summary page on the ASTM website.

[3] The last approved version of this historical standard is referenced on www.astm.org.

***A Summary of Changes section appears at the end of this standard**

3.1.1 For common definitions of technical terms used in this standard, refer to Terminology D653.

3.2 *Definitions of Terms Specific to This Standard:*

3.2.1 *boundary condition, n—in hydrogeologic properties*, a mathematical expression that constrains the equations of the mathematical model to account for the addition or removal of fluid or solutes to or from the mathematical model.

3.2.2 *calibration (model application), n—in hydrogeologic properties*, the process of refining the model representation of the hydrogeologic framework, hydraulic properties, and boundary conditions to achieve a desired degree of correspondence between the model simulation and observations of the groundwater flow system.

3.2.3 *groundwater flow model, n—in hydrogeologic properties*, application of a mathematical model to represent a site-specific groundwater flow system.

3.2.4 *model, n—in hydrogeologic properties*, an assembly of concepts in the form of mathematical equations that portray understanding of a natural phenomenon.

3.2.5 *sensitivity (model application), n—in hydrogeologic properties*, the degree to which the model result is affected by changes in a selected model input representing hydrogeologic framework, hydraulic properties, and boundary conditions.

3.3 The following terms are contained in Terminology D653, but are included here for the convenience of the user:

3.3.1 *conceptual model, n—in hydrogeologic properties*, an interpretation or working description of the characteristics and dynamics of the physical system.

4. Summary of Guide

4.1 The application of a groundwater flow model ideally would follow several basic steps to achieve an acceptable representation of the physical hydrogeologic system and to document the results of the model study to the end-user, decision-maker, or regulator. These primary steps include the following:

4.1.1 Define study objectives,

4.1.2 Develop a conceptual model,

4.1.3 Select a computer code,

4.1.4 Construct a groundwater flow model,

4.1.5 Calibrate model and perform sensitivity analysis,

4.1.6 Make predictive simulations,

4.1.7 Document modeling study, and

4.1.8 Perform postaudit.

4.2 These steps are designed to ascertain and document an understanding of a system, the transition from conceptual model to mathematical model, and the degree of uncertainty in the model predictions. The steps presented in this guide should generally be followed in the order they appear in the guide; however, there is often significant iteration between steps. All of the steps outlined in this guide are required for a model that simulates measured field conditions. In cases where the model is only used to understand a problem conceptually, some steps are unnecessary. For example, if no site-specific data are available, the calibration step would be omitted.

5. Significance and Use

5.1 Model applications **(1)**,[4] are useful tools to:

5.1.1 Assist in problem evaluation,

5.1.2 Design remedial measures,

5.1.3 Conceptualize and study groundwater flow processes,

5.1.4 Provide additional information for decision making, and

5.1.5 Recognize limitations in data and guide collection of new data.

5.2 Groundwater models are routinely employed in making environmental resource management decisions. The model supporting these decisions should be scientifically defensible and decision-makers informed of the degree of uncertainty in the model predictions. This has prompted some state agencies to develop standards for groundwater modeling **(2)**. This guide provides a consistent framework within which to develop, apply, and document a groundwater flow model.

5.3 This guide presents steps ideally followed whenever a groundwater flow model is applied. The groundwater flow model will be based upon a mathematical model that may use numerical, analytical, or other appropriate technique.

5.4 This guide should be used by practicing groundwater modelers and by those wishing to provide consistency in modeling efforts performed under their direction.

5.5 Use of this guide to develop and document a groundwater flow model does not guarantee that the model is valid. This guide simply outlines the necessary steps to follow in the modeling process. For example, development of an equivalent porous media model in karst terrain may not be valid if significant groundwater flow takes place in fractures and solution channels. In this case, the modeler could follow the steps in this guide and not end up with a defensible model.

6. Procedure

6.1 The procedure for applying a groundwater model includes the following steps: define study objectives, develop a conceptual model, select a computer code or algorithm, construct a groundwater flow model, calibrate the model and perform sensitivity analysis, make predictive simulations, document the modeling process, and perform a post-audit. These steps are generally followed in order, however, there is substantial overlap between steps, and previous steps are often revisited as new concepts are explored or as new data are obtained. The iterative modeling approach may also require the reconceptualization of the problem. An example of these feedback loops is shown in Fig. 1. These basic modeling steps are discussed below.

6.2 Definition of the study objectives is an important step in applying a groundwater flow model. The objectives aid in determining the level of detail and accuracy needed in the model simulation. Complete and detailed objectives would ideally be specified prior to modeling activities.

[4] The boldface numbers in parentheses refer to the list of references at the end of this standard.

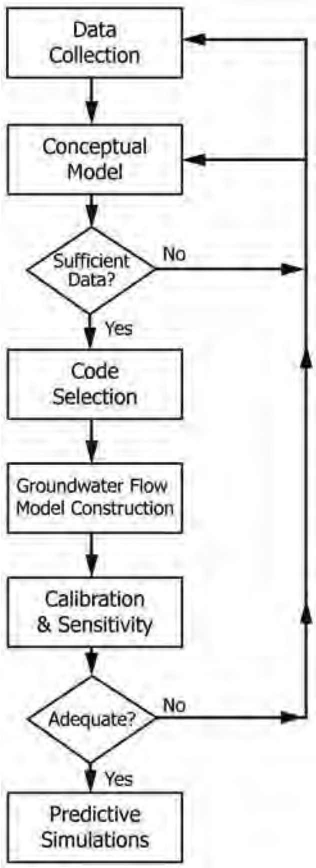


FIG. 1 Flow Chart of the Modeling Process

6.3 A conceptual model of a groundwater flow and hydrologic system is an interpretation or working description of the characteristics and dynamics of the physical hydrogeologic system. The purpose of the conceptual model is to consolidate site and regional hydrogeologic and hydrologic data into a set of assumptions and concepts that can be evaluated quantitatively. Development of the conceptual model requires the collection and analysis of hydrogeologic and hydrologic data pertinent to the aquifer system under investigation. Standard guides and practices exist that describe methods for obtaining hydrogeologic and hydrologic data.

6.3.1 The conceptual model identifies and describes important aspects of the physical hydrogeologic system, including: geologic and hydrologic framework, media type (for example, fractured or porous), physical and chemical processes, hydraulic properties, and sources and sinks (water budget). These components of the conceptual model may be described either in a separate document or as a chapter within the model report. Include illustrations, where appropriate, to support the narrative, for example, contour maps, cross sections, or block diagrams, or combination thereof. Each aspect of the conceptual model is described as follows:

6.3.1.1 Geologic framework is the distribution and configuration of aquifer and confining units. Of primary interest are the thickness, continuity, lithology, and geologic structure of those units that are relevant to the purpose of the study. The aquifer system domain, that may be composed of interconnected aquifers and confining units, often extends beyond the domain of interest. In this case, describe the aquifer system in detail within the domain of interest and at least in general elsewhere. Analysis of the geologic framework results in listings, tabulations, or maps, or combination thereof, of the thickness, extent, and properties of each relevant aquifer and confining unit.

6.3.1.2 Hydrologic framework in the conceptual model includes the physical extents of the aquifer system, hydrologic features that impact or control the groundwater flow system, analysis of groundwater flow directions, and media type. The conceptual model should address the degree to which the aquifer system behaves as a porous media. If the aquifer system is significantly fractured or solutioned, the conceptual model should address these issues. Hydrologic framework also includes flow system boundaries that may not be physical and can change with time, such as groundwater divides. Fluid potential (head) measurements allow assessment of the rate and direction of groundwater flow. In addition, the mathematical model is typically calibrated against these values (see 6.5). Water level measurements within the groundwater system are tabulated, both spatially and temporally. This analysis of the flow system includes the assessment of vertical and horizontal gradients, delineation of groundwater divides, and mapping of flow lines.

6.3.1.3 Hydraulic properties include the transmissive and storage characteristics of the aquifer system. Specific examples of hydraulic properties include transmissivity, hydraulic conductivity, storativity, and specific yield. Hydraulic properties may be homogeneous or heterogeneous throughout the model domain. Certain properties, such as hydraulic conductivity, may also have directionality, that is, the property may be anisotropic. It is important to document field and laboratory measurements of these properties in the conceptual model to set bounds or acceptable ranges for guiding the model calibration.

6.3.1.4 Sources and sinks of water to the aquifer system impact the pattern of groundwater flow. The most common examples of sources and sinks include pumping or injection wells, infiltration, evapotranspiration, drains, leakage across confining layers and flow to or from surface water bodies. Identify and describe sources and sinks within the aquifer system in the conceptual model. The description includes the rates and the temporal variability of the sources and sinks. A water budget should be developed as part of the conceptual model.

6.3.2 Provide an analysis of data deficiencies and potential sources of error with the conceptual model. The conceptual model usually contains areas of uncertainty due to the lack of field data. Identify these areas and their significance to the conceptual model evaluated with respect to project objectives. In cases where the system may be conceptualized in more than one way, these alternative conceptual models should be described and evaluated.

6.4 Computer code selection is the process of choosing the appropriate software algorithm, or other analysis technique, capable of simulating the characteristics of the physical hydrogeologic system, as identified in the conceptual model. The computer code should also be tested for the intended use and be well documented **(2-4)**.

6.4.1 Other factors may also be considered in the decision-making process, such as model analyst's experience and those described below for model construction. Important aspects of the model construction process, such as dimensionality, will determine the capabilities of the computer code needed for the model. Provide a narrative in the modeling report justifying the computer code selected for the model study.

6.5 Groundwater flow model construction is the process of transforming the conceptual model into a mathematical form. The groundwater flow model typically consists of two parts, the data set and the computer code. The model construction process includes building the data set utilized by the computer code. Fundamental components of the groundwater flow model include: dimensionality, discretization, boundary and initial conditions, and hydraulic properties.

6.5.1 Spatial dimensionality is determined both by the objectives of the investigation and by the nature of the groundwater flow system. For example, conceptual modeling studies may use simple one-dimensional solutions in order to test alternate conceptualizations. Two-dimensional modeling may be warranted if vertical gradients are negligible. If vertical gradients are significant or if there are several aquifers in the flow system, a two-dimensional cross section or (quasi-)three-dimensional model may be appropriate. A quasi-three-dimensional approach is one in which aquitards are not explicitly discretized but are approximated using a leakage term **(5)**.

6.5.2 Temporal dimensionality is the choice between steady-state or transient flow conditions. Steady-state simulations produce average or long-term results and require that a true equilibrium case is physically possible. Transient analyses are typically performed when boundary conditions are varied through time or when study objectives require answers at more than one point in time.

6.5.3 In numerical models, spatial discretization is an important step in the model construction process **(5)**. In general, finer discretization produces a more accurate solution to the governing equations. There are practical limits to the number of nodes, however. In order to achieve acceptable results with the minimum number of nodes, the model grid may require finer discretization in areas of interest or where there are large spatial changes in aquifer parameters or hydraulic gradient. In designing a numerical model, it is advisable to locate nodes as close as possible to pumping wells, to locate model edges and hydrologic boundaries accurately, and to avoid large contrasts in adjacent nodal spacings **(6)**.

6.5.4 Temporal discretization is the selection of the number and size of time steps for the period of transient numerical model simulations. Choose time steps or intervals to minimize errors caused by abrupt changes in boundary conditions. Generally, small time steps are used in the vicinity of such changes to improve accuracy **(7)**. Some numerical time-stepping schemes place additional constraints on the maximum time-step size due to numerical stability.

6.5.5 Specifying the boundary conditions of the groundwater flow model means assigning a boundary type to every point along the three-dimensional boundary surface of the aquifer system and to internal sources and sinks **(8)**. Boundary conditions fall into one of five categories: specified head or Dirichlet, specified flux or Neumann, and mixed or Cauchy boundary conditions, free surface boundary, and seepage face. It is desirable to include only natural hydrologic boundaries as boundary conditions in the model. Most numerical models, however, employ a grid that has to end somewhere. Thus, it is often unavoidable to specify artificial boundaries at the edges of the model. When these grid boundaries are sufficiently remote from the area of interest, the artificial conditions on the grid boundary do not significantly impact the predictive capabilities of the model. However, the impact of artificial boundaries should always be tested and thoroughly documented in the model report.

6.5.6 Initial conditions provide a starting point for transient model calculations. In numerical groundwater flow models, initial conditions consist of hydraulic heads specified for each model node at the beginning of the simulation. Initial conditions may represent a steady-state solution obtained from the same model. Accurately specify initial conditions for transient models. Steady-state models do not require initial conditions.

NOTE 1—Steady-state models do not require initial conditions, specifying initial conditions, such as head values, can speed convergence or avoid destabilizing behavior that may prevent convergence.

6.5.7 In numerical modeling, each node or element is assigned a value for each hydraulic property required by the groundwater flow model. Other types of models, such as many analytical models, specify homogeneous property values. The most common hydraulic properties are horizontal and vertical hydraulic conductivity (or transmissivity) and storage coefficients. Hydraulic property values are assigned in the model based upon geologic and aquifer testing data. Generally, hydraulic property values are assigned in broad zones having similar geologic characteristics **(9)**. Geostatistical techniques, such as kriging, are also commonly used to assign property values at model nodes when sufficient data are available.

6.6 Calibration of the groundwater flow model is the process of adjusting hydraulic parameters, boundary conditions, and initial conditions within reasonable ranges to obtain a match between observed and simulated potentials, flow rates, or other calibration targets. The range over which model parameters and boundary conditions may be varied is determined by data presented in the conceptual model. In the case where parameters are well characterized by field measurements, the range over which that parameter is varied in the model should be consistent with the range observed in the field. The degree of fit between model simulations and field measurements can be quantified using statistical techniques **(D5981)**.

6.6.1 In practice, model calibration is frequently accomplished through trial-and-error adjustment of the model's input data to match field observations **(9)**. Automatic inverse techniques are another type of calibration procedure **(10-12)**. The calibration process continues until the degree of correspondence between the simulation and the physical hydrogeologic system is consistent with the objectives of the project.

6.6.2 The calibration is evaluated through analysis of residuals. A residual is the difference between the observed and simulated variable. Calibration may be viewed as a regression analysis designed to bring the mean of the residuals close to zero and to minimize the standard deviation of the residuals **(9)**. Statistical tests and illustrations showing the distribution of residuals are presented to document the calibration. Ideally, criteria for an acceptable calibration should be established prior to starting the calibration.

6.6.3 Calibration often necessitates reconstruction of portions of the model, resulting in changes or refinements in the conceptual model. Both possibilities introduce iteration into the modeling process whereby the modeler revisits previous steps to achieve a better representation of the physical system.

6.6.4 In both trial-and-error and inverse techniques, sensitivity analysis plays a key role in the calibration process by identifying those parameters that are most important to model reliability. Sensitivity analysis is used extensively in inverse techniques to make adjustments in model parameter values.

6.6.5 Calibration of a groundwater flow model to a single set of field measurements does not guarantee a unique solution. In order to reduce the problem of nonuniqueness, the model calculations may be compared to another set of field observations that represent a different set of boundary conditions or stresses. This process is referred to in the groundwater modeling literature as either validation **(1)** or verification **(13, 14)**. The term verification is adopted in this guide. In model verification, the calibrated model is used to simulate a different set of aquifer stresses for which field measurements have been made. The model results are then compared to the field measurements to assess the degree of correspondence. If the comparison is not favorable, additional calibration or data collection is needed. Successful verification of the groundwater flow model results in a higher degree of confidence in model predictions. A calibrated but unverified model may still be used to perform predictive simulations when coupled with a careful sensitivity analysis **(14)**.

6.7 Sensitivity analysis is a quantitative method of determining the effect of parameter variation on model results. The purpose of a sensitivity analysis is to quantify the uncertainty in the calibrated model caused by uncertainty in the estimates of aquifer parameters, stresses, and boundary conditions **(5)**. It is a means to identify the model inputs that have the most influence on model calibration and predictions **(1)**. Perform sensitivity analysis to provide users with an understanding of the level of confidence in model results and to identify data deficiencies **(15)(D5611)**.

6.7.1 Sensitivity analysis is performed during model calibration and during predictive analyses. Model sensitivity provides a means of determining the key parameters and boundary conditions to be adjusted during model calibration. Sensitivity analysis is used in conjunction with predictive simulations to assess the effect of parameter uncertainty on model results.

6.7.2 Sensitivity of a model parameter is often expressed as the relative rate of change of a selected model calculation with respect to that parameter **(16)**. If a small change in the input parameter or boundary condition causes a significant change in the output, the model is sensitive to that parameter or boundary condition.

6.8 Application of the groundwater flow model to a particular site or problem often includes predictive simulations. Predictive simulations are the analyses of scenarios defined as part of the study objectives. Document predictive simulations with appropriate illustrations as necessary in the model report.

6.8.1 Boundary conditions are often selected during model construction based upon existing or past groundwater flow conditions. Boundary conditions used in the calibrated model may not be appropriate for some predictive simulations **(17)**. If the model simulations result in unusually large hydrologic stresses or if new stresses are placed in proximity to model boundaries, evaluate the sensitivity of the predictions to the boundary conditions. This may produce additional iteration in the modeling process **(D5609)**.

6.9 In cases where the groundwater flow model has been used for predictive purposes, a postaudit may be performed to determine the accuracy of the predictions. While model calibration and verification demonstrate that the model accurately simulate past behavior of the system, the postaudit tests whether the model can predict future system behavior **(14)**. Post-audits are normally performed several years after submittal of the modeling report and are therefore documented in a separate report.

7. Report: Test Data Sheets/Forms

7.1 Record as a minimum the following general information:

7.1.1 The purpose of the model report is to communicate findings, to document the procedures and assumptions inherent in the study, and to provide detailed information for peer review. The report should be a complete document allowing reviewers and decision makers to formulate their own opinion as to the credibility of the model. The report should be detailed enough that an independent modeler could duplicate the model results. The model report should describe all aspects of the modeling study outlined in this guide. An example table of contents for a modeling report is presented in Appendix X1.

8. Keywords

8.1 computer model; groundwater; simulation

APPENDIX

(Nonmandatory Information)

X1. GROUNDWATER FLOW MODEL REPORT

X1.1 See Fig. X1.1.

1.0 Introduction
- 1.1 General Setting
- 1.2 Study Objectives

2.0 Conceptual Model
- 2.1 Aquifer System Framework
- 2.2 Ground-Water Flow System
- 2.3 Hydrologic Boundaries
- 2.4 Hydraulic Properties
- 2.5 Sources and Sinks
- 2.6 Water Budget
- 2.7 Modeling Results

3.0 Computer Code
- 3.1 Code Selection
- 3.2 Code Description

4.0 Ground-Water Flow Model Construction
- 4.1 Model Grid
- 4.2 Hydraulic Parameters
- 4.3 Boundary Conditions
- 4.4 Selection of Calibration Targets

5.0 Calibration
- 5.1 Residual Analysis
- 5.2 Sensitivity Analysis
- 5.3 Model Verification

6.0 Predictive Simulations

7.0 Summary and Conclusions
- 7.1 Model Assumptions and Limitations
- 7.2 Model Predictions
- 7.3 Recommendations

8.0 References

Appendices: Model Input Files

FIG. X1.1 Example Table of Contents of Groundwater Flow Model Report

REFERENCES

(1) National Research Council, *Groundwater Models: Scientific and Regulatory Applications*, National Academy Press, Washington, DC, 1990.

(2) van der Heijde, P. K. M., *Quality Assurance in Computer Simulations of Ground Water Contamination*, EPA/600/J-87/084, PB-0124524, 1987.

(3) U.S. Environmental Protection Agency, *Selection Criteria for Mathematical Models Used in Exposure Assessments: Ground-Water Models*, EPA/600/8-88/075, 1987.

(4) Silling, S. A., *Final Technical Position on Documentation of Computer Codes for High-Level Waste Management*, U.S. Nuclear Regulatory Commission, NUREG-0856, 1983.

(5) Anderson, M. P., and Woessner, W. W., *Applied Groundwater Modeling: Simulation of Flow and Advective Transport*, Academic Press, Inc., New York, NY, 2015.

(6) Trescott, P. C., Pinder, G. F., and Larson, S. P., "Finite-Difference Model for Aquifer Simulation in Two Dimensions with Results of Numerical Experiments," *U.S. Geological Survey TWRI*, Book 7, Chapter C1, 1976.

(7) Mercer, J. W., and Faust, C. R., *Ground-Water Modeling: Numerical Models, Ground Water*, Vol 18, No. 4, 1980, pp. 395–409.

(8) Franke, O. L., Reilly, T. E., and Bennett, G. D., "Definition of Boundary and Initial Conditions in the Analysis of Saturated Ground-Water Flow Systems—An Introduction," *U.S. Geological Survey, Techniques of Water Resources Investigations,* Book 3, Chapter B5, Vol 15, 1987.

(9) Konikow, I. F., "Calibration of Ground-Water Models," *Proceedings of the Specialty Conference on Verification of Mathematical and Physical Models in Hydraulic Engineering*, ASCE, College Park, MD, Aug. 9–11, 1978, pp. 87–93.

(10) Cooley, R. L., A Method of Estimating Parameters and Assessing Reliability for Models of Steady State Ground-Water Flow. I. Theory and Numerical Properties, *WRR*, Vol 13, No. 2, 1977, pp. 318–324.

(11) Faust, C. R., and Mercer, J. W., "Ground-Water Modeling: Recent Developments," *Ground Water*, Vol 18, No. 6, 1980, pp. 569–577.

(12) Yeh, W. W-G., "Review of Parameter Identification Procedures in Groundwater Hydrology: The Inverse Problem," *WRR*, Vol 22, 1986, pp. 95–108.

(13) Wang, H. F., and Anderson, M. P., *Introduction to Groundwater Modeling: Finite Difference and Finite Element Methods*, W. H. Freeman and Co., San Francisco, CA, 1982.

(14) Anderson, M. P., and Woessner, W. W., "The Role of the Postaudit in Model Validation," *Advances in Water Resources*, 18, No. 3, January 1992, pp. 167–173.

(15) U.S. Environmental Protection Agency, *Resolution on the Use of Mathematical Models by EPA for Regulatory Assessment and Decision-Making*, EPA-SAB-EEC-89-012, 1989.

(16) van der Heijde, P. K. M., *Quality Assurance and Quality Control in Groundwater Modeling*, International Ground Water Modeling Center, GWMI 89-04, 1989.

(17) Franke, O. L., and Reilly, T. E., "The Effects of Boundary Conditions on the Steady-State Response of Three Hypothetical Ground-Water Systems—Results and Implications of Numerical Experiments," *U.S. Geological Survey Water Supply Paper 2315*, 1987.

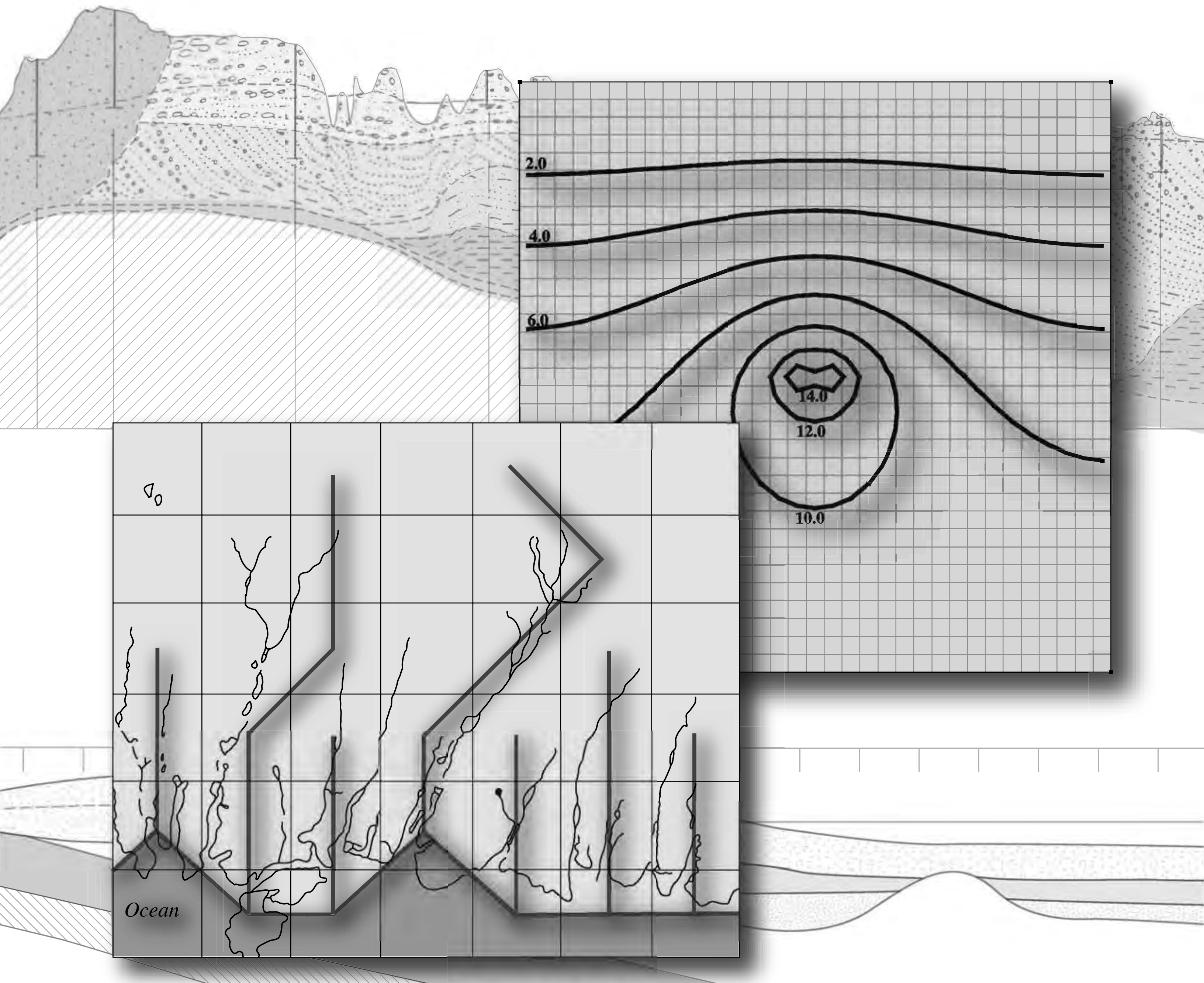
SUMMARY OF CHANGES

Committee D18 has identified the location of selected changes to this standard since the last issue (2004(2010)) that may impact the use of this standard. (December 15, 2017)

(1) Removed references to withdrawn standards Section 2.
(2) Revised Terminology Section 3 to align with current D18 procedures, removed terms that are in D653. Added section for terms that are in D653 but provided for user convenience.
(3) Added note in significance and Use Section 4 concerning the calibration and Sensitivity analyses.
(4) Removed unavailable references and renumber references in text.
(5) Removed or modified jargon and superlatives.
(6) Added references to other ASM groundwater modeling standards in Section 2 and referenced in the text.
(7) Revised title to reflect the content of the Guide.

EXHIBIT 6

Guidelines for Evaluating Ground-Water Flow Models



Scientific Investigations Report 2004-5038

U.S. Department of the Interior
U.S. Geological Survey

Cover. See figures 2 and 3, page 6.

Guidelines for Evaluating Ground-Water Flow Models

By Thomas E. Reilly and Arlen W. Harbaugh

Scientific Investigations Report 2004-5038

U.S. Department of the Interior
U.S. Geological Survey

U.S. Department of the Interior
Gale A. Norton, Secretary

U.S. Geological Survey
Charles G. Groat, Director

U.S. Geological Survey, Reston, Virginia: 2004
For sale by U.S. Geological Survey, Information Services
Box 25286, Denver Federal Center
Denver, CO 80225

For more information about the USGS and its products:
Telephone: 1-888-ASK-USGS
World Wide Web: http://www.usgs.gov/

Suggested citation:
Reilly, T.E., and Harbaugh, A.W., 2004, Guidelines for evaluating ground-water flow models: U.S. Geological Survey Scientific Investigations Report 2004-5038, 30 p.

CONTENTS

Figures

Tables

Conversion Factors

Multiply	By	To obtain
foot (ft)	0.3048	meter (m)
mile (mi)	1.609	kilometer (km)
square mile (mi^2)	2.590	square kilometer (km^2)
cubic foot per second (ft^3/s)	0.02832	cubic meter per second (m^3/s)

English units are used in all original work presented in this report. Figures and results from published studies are also presented throughout this report. The system of units that were originally used in these previously published studies are retained in this report in order not to introduce any errors and to show the level of approximation used in the investigator's estimates.

Guidelines for Evaluating Ground-Water Flow Models

By Thomas E. Reilly and Arlen W. Harbaugh

Abstract

Ground-water flow modeling is an important tool frequently used in studies of ground-water systems. Reviewers and users of these studies have a need to evaluate the accuracy or reasonableness of the ground-water flow model. This report provides some guidelines and discussion on how to evaluate complex ground-water flow models used in the investigation of ground-water systems. A consistent thread throughout these guidelines is that the objectives of the study must be specified to allow the adequacy of the model to be evaluated.

Introduction

The simulation of ground-water flow systems using computer models is standard practice in the field of hydrology. Models are used for a variety of purposes that include education, hydrologic investigation, water management, and legal determination of responsibility. In the most general terms, a model is a simplified representation of the appearance or operation of a real object or system. Ground-water flow models represent the operation of a real ground-water system with mathematical equations solved by a computer program. A difficulty that faces all individuals attempting to use the results of a model is the development of an understanding of the strengths and limitations of a model analysis without having to reproduce the entire analysis.

The primary purpose of this report is to help users of reports that document ground-water flow models evaluate the adequacy or appropriateness of a model. A secondary purpose for this report is to provide for model developers a guide to the information that should be included in model documentation. The information in this report is mainly qualitative. It reflects the views developed by the authors on the basis of over 50 years combined experience with ground-water modeling. The authors have used models, reviewed modeling studies and reports, provided modeling advice, taught modeling courses, and developed computer model programs.

It is important to distinguish among three terms we use to discuss the modeling process: conceptual model, computer model program, and model. A “conceptual model” is the hydrologist’s concept of a ground-water system. A “computer model program” is a computer program that solves ground-water equations. Computer model programs are general purpose in that they can be used to simulate a variety of specific systems by varying input data. A “model” is the application of a computer model program to simulate a specific system. Thus, a model incorporates the model program and all of the input data required to represent a ground-water system. The modeler attempts to incorporate what he or she believes to be the most important aspects of the conceptual model into a model so that the model will provide useful information about the system.

The information provided in this report is generally relevant to all types of ground-water flow model programs; however, the examples cited throughout the report use the model program MODFLOW (Harbaugh and others, 2000).

This report reviews the important aspects of simulating a ground-water flow system using a computer model program and explains the ramifications of various design decisions. An important part of the information necessary for evaluating a model is the intended use of a model, because it is impossible to develop a model that will fulfill all purposes. Further, the intended use must be specific as opposed to general. For example, saying that a model will be used to evaluate water-management alternatives is inadequate. Specific information about the alternatives to be considered also would be necessary. Thus, a consistent thread throughout this report is the need to consider the purpose of a model when evaluating the appropriateness of the model.

Appropriateness of the Computer Model Program

Many computer model programs are available for simulating ground-water systems. Each computer model program can be characterized by the mathematical method used to represent ground-water equations (Konikow and Reilly, 1999), assumptions, and the range of simulation capabilities. For example, the mathematical method in MODFLOW is finite difference in space and time, with backward difference for time. Major assumptions are (1) confined three-dimensional flow with water-table approximations, and (2) principal directions of hydraulic conductivity are aligned with the coordinate axes. A variety of hydrologic capabilities are included, for example, the simulation of wells, rivers, recharge, and ground-water evapotranspiration. There also are simple analytical models that assume homogeneous conditions for one or two dimensions that can be used to solve some problems. The tool or computer model program used can be as simple or as complex as required for the problem, but the method, assumptions, and capabilities must be evaluated to assure that the tool is appropriate and can provide scientifically defensible results.

Questions to be answered in the evaluation of the appropriateness of the modeling program are:

1. Are the objectives of the study clearly stated?
2. Is the mathematical method used in the computer model program appropriate to address the problem?
3. Does the numerical or analytical model selected for use simulate the important physical processes needed to adequately represent the system?

Different Modeling Approaches to Address a Problem

A general-purpose computer model program such as MODFLOW can be used in many ways to address a problem as illustrated in table 1. Approaches to a problem that are commonly used are: calibrated model, hypothetical system model, sensitivity analysis, superposition, and particle tracking. Frequently, several approaches are combined to address a problem.

A Calibrated Model

A model that is "calibrated" is required to address many hydrologic problems. Model calibration in its most limited meaning is the modification of model input data for the purpose of making the model more closely match observed heads and flows. Adjustment of parameters can be done manually or automatically by using nonlinear regression statistical techniques. In the broader meaning of model calibration, parameter adjustment is only one aspect of model calibration. Key aspects of the model, such as the conceptualization of the flow system, that influence the capability of the model to meet the problem objectives also are evaluated and adjusted as needed during calibration. For example, it may be noticed that some of the parameters that result in the best match to observations are not reasonable based on other knowledge of their values. This may indicate that there is a conceptualization problem with the model. Thus, the closeness of fit between the simulated and observed conditions, and the extent to which important aspects of the simulation are incorporated in the model are both important in evaluating how well a model is calibrated. In practice, calibration is conducted differently by each investigator; some examples that discuss calibrated models are Luckey and others (1986), Buxton and Smolensky (1999), and Anderson and Woessner (1992, section 8.3 and 8.4).

The amount of effort that is required in calibrating a ground-water flow model is dependent upon the intended use of the model (that is, the objective of the investigation). Most models of specific ground-water systems that are used to estimate aquifer properties, understand the past, understand the present, or to forecast the future are calibrated by matching observed heads and flows. Determining if the calibration is sufficient for the intended use of the model is very important in evaluating whether the model has been constructed appropriately. (See later section for more on evaluating the adequacy of model calibration.)

A Hypothetical Model

A hypothetical model is a model of an idealized or representative system as opposed to a model of a specific system. In an attempt to understand the basic operation of a ground-water system, the determination of whether to develop a model of a hypothetical idealized system or a model of an actual system greatly affects the amount of data needed to construct the model. Hypothetical models are not calibrated, but input data are frequently adjusted during model development to make the model fit the idealized system or to test how the model responds. The utility of hypothetical models is that the system can be defined exactly and the cause and effect processes under investigation can be clearly identified with minimal cost. The input data needed to define the hypothetical system can be as simple or as complex as required to investigate the processes of interest. No effort is required to collect and interpret data from an actual ground-water system and no uncertainty exists in the ability of the model to represent the system, which results in substantial cost savings compared to making a model of a specific system. Hypothetical models have been used to examine various processes that affect or are affected by ground-water flow, for example: boundary conditions (Franke and Reilly, 1987), contributing areas to wells (Morrissey, 1989; Reilly and Pollock, 1993), and model calibration (Hill and others, 1998).

Sensitivity Analysis

Sensitivity analysis is the evaluation of model input parameters to see how much they affect model outputs, which are heads and flows. The relative effect of the parameters helps to provide fundamental understanding of the simulated system. Sensitivity analysis also is inherently part of model calibration. The most sensitive parameters will be the most important parameters for causing the model to match observed values. For example, an area in which the model is insensitive to hydraulic conductivity generally indicates an area where there is relatively little water flowing. If the model is being calibrated, then changing the value of hydraulic conductivity in this area will

Table 1. Types of problems that may initiate a hydrologic study involving a ground-water flow model.

Problem Type	Reason for Undertaking Study	Approach to Model the Problem
Basic Understanding of Ground-Water System	Investigation of hydrologic processes	• Hypothetical system model • Superposition • Particle Tracking
	Determination of effective data collection network	• Calibrated model • Hypothetical system model • Superposition • Sensitivity analysis
	Preliminary model to determine current level of understanding	• Calibrated model • Hypothetical system model • Superposition • Sensitivity analysis
Estimation of Aquifer Properties	Aquifer test analysis	• Calibrated model • Superposition
	Determination of aquifer properties	• Calibrated model
Understanding the Past	Understanding historical development of an aquifer system	• Calibrated model
	Estimation of predevelopment conditions	• Calibrated model
Understanding the Present	Determination of the effect of ground-water pumpage on surface-water bodies	• Calibrated model • Superposition • Particle Tracking
	Determination of sources of water to wells	• Calibrated model • Particle Tracking
	Determination of responsible parties causing impacts on the system	• Calibrated model • Particle Tracking
Forecasting the Future	Management of a system	• Calibrated model • Superposition • Particle Tracking

not help much in causing the model to match observations. The calibration will not provide much certainty about the value of the parameter, but the uncertainty will not matter provided the model is not used in situations where large amounts of water will flow in that area. Such a model, however, would probably not be suitable for evaluation of recharge or withdrawal in this area because the amount of flow in the area would be much greater than it was when the model was calibrated, and the uncertainty from the calibration would be unacceptable. Anderson and Woessner (1992, p. 246-257) provide some examples of sensitivity analyses.

Sensitivity analysis can be conducted manually or automatically. In the manual approach, multiple model simulations are made in which ideally a single parameter is adjusted by an arbitrary amount. The changes to the model output for all of the parameter changes may be displayed in tables or graphs for evaluation. The automatic approach directly computes parameter sensitivity, which is the change in head or flow divided by the change in a parameter. Automatic sensitivity analysis is inherently part of automatic parameter adjustment for model calibration. The automatic parameter adjustment algorithm uses parameter sensitivity to compute the parameter values that cause the model to best match observed heads and flows.

Superposition

Superposition (Reilly and others, 1987) is a modeling approach that is useful in saving time and effort and eliminating uncertainty in some model evaluations. Models that are designed to use superposition evaluate only changes in stress and changes in responses. Most aquifer tests that analyze drawdown use superposition. Only the change in heads (the drawdown) and change in flows are analyzed, which assumes the response of the system is only due to the stress imposed and is not due to other processes in the system. The absolute value of the head and a quantification of the actual regional flows are not needed. In the past, superposition was frequently used with analog model analysis of ground-water systems because electrical simulation of areal stresses and boundary conditions was extremely difficult. As modern numerical computer models made simulation of all stress conditions easier, superposition was used less frequently in areal models. If the problem to be solved involves only the evaluation of a change due to some change in stress, however, the application of superposition can greatly simplify the data needs for model development. Superposition is strictly applicable to linear problems only, that is, constant saturated thickness and linear boundary conditions. If the system is relatively linear, however, for example the saturated thickness does not change by a significant portion (no absolute guidance can be given, but some investigators have used a 10 percent change in thickness as a rule of thumb), superposition can still provide reasonably accurate answers. Currently, superposition is used primarily in the simulation of aquifer tests, in that only changes due to the imposed change in stress (that is, the well discharge) are simulated and zero drawdowns are specified as the initial and boundary conditions; example simulations are presented in Prince and Schneider (1989) and McAda (2001).

Particle Tracking

Particle tracking (Pollock, 1989) is the determination of the path a particle will take through a three-dimensional ground-water flow system. The determination of the paths of water in the flow system aids in conceptualizing and quantifying the sources of water in a modeled system. For example, Buxton and others (1991) used particle-tracking analysis to determine recharge areas on Long Island, New York, and Modica and others (1997) made use of particle tracking in the context of a ground-water flow model to understand the patterns and age distribution of ground-water flow to streams of the Atlantic Coastal Plain. Although particle tracking is useful in determining advective transport, this report does not address the use of models to determine transport of chemicals, but rather refers to the approach of using particle tracking to understand the flow system.

Spatial and Temporal Approaches

In addition to the overall modeling approaches discussed above, many model programs can be used in one, two, or three dimensions, and they can be applied as transient or steady state. The simplification of the model domain to one or two dimensions, either in plan view or cross section, is used to minimize the cost of constructing a model. The simplification of the system to one or two dimensions, however, must be consistent with the flow field under investigation and consistent with the objectives of the study. Consistent with the flow field, means that there is no or negligible flow orthogonal to the line or plane of the one- or two-dimensional system being simulated.

Steady-state models are used widely, although true steady-state conditions do not exist in natural systems. All natural systems fluctuate in response to climatic variations that can be seasonal, annual, decadal or longer. In steady-state models, an assumption is made that a system can be represented by a state of dynamic equilibrium or an approximate equilibrium condition. If the objectives of the investigation do not require information on the time it takes for a system to respond to new stresses or the response of the system between periods of relative equilibrium, then simulation of the system as a steady-state system may be a reasonable approach. However, if the system is not at a period of equilibrium or approximate equilibrium during the periods of interest, then a transient analysis is required.

Questions to be answered in the evaluation of the appropriateness of the modeling approach to analyze the problem are:

1. Is the overall approach (calibrated model, hypothetical system model, sensitivity analysis, superposition, and particle tracking) for using simulation in addressing the objectives clearly stated and appropriate?
2. If the analysis is not three dimensional, is the representation of the system using one or two dimensions appropriate to meet the objectives of the study and justified in the report?
3. If the model is steady state, is adequate information provided to justify that the system is reasonably close to a steady-state condition?

Models of ground-water systems may be very different in their level of complexity. Whether the model design and approach are appropriate for the problem being investigated must be evaluated. This evaluation requires a clear statement of the problem to be investigated and the modeling approach. A further requirement is an understanding of the model design. The remainder of this report focuses on specific aspects of model design that should be examined in determining the worth of a particular model. These aspects are: discretization and representation of the hydrogeologic framework, boundary conditions, initial conditions, accuracy of the numerical solution, and accuracy of calibration for the intended use of the model.

Discretization and Representation of the Hydrogeologic Framework

A fundamental aspect of numerical models is the representation of the real world by discrete volumes of material. The volumes are called cells in the finite-difference method, and the volumes are called elements in the finite-element method. The accuracy of the model is limited by the size of the discrete volumes. Further, for transient models, time is represented by discrete increments of time called time steps in most model programs. The size of the time steps also has an impact on the accuracy of a model. The issue of the size of the discrete volumes and time steps is discussed for the finite-difference method.

Cell Size

The size of cells determines the extent to which hydraulic properties and stresses can vary throughout the modeled region. Hydraulic properties and stresses are specified for each cell, so the more cells in a model, the greater the ability to vary hydraulic properties and stresses. If the cell size is too large, important features of the framework may be left out or poorly represented. Accordingly, it is important to evaluate the known (or assumed) variation of hydraulic properties and stresses of the system being simulated compared to the size of the cells. For example, the differences in the representation of a confining unit in a regional ground-water flow model and a sub-regional model of Long Island, New York (Buxton and Reilly, 1987) are substantial (fig. 1), and the locations where the clay is absent is much better represented at the finer scale. In a parallel sense, the representation of the streams and shoreline are different depending on the scale (fig. 2). The intended use of the model and the importance of the features being discretized affect both the evaluation of whether the model is discretized appropriately and whether important features are missing that would cause a systematic error or bias in the simulation results.

Figure 3 shows the difference in simulated drawdown when different cell sizes are used to simulate pumping from two wells in a one-layer model. The 3,300 ft by 3,300 ft system is confined with a uniform transmissivity of 10,000 ft^2/d. No-flow boundaries surround all sides except the northern boundary, which has a specified head of 0 ft. The wells are 200 ft apart, and each is pumped at a constant rate of 100,000 ft^3/d. Figure 3A shows drawdown with a grid spacing of 300 ft. With this grid spacing, the two wells are located in a single cell, so the model “sees” the two wells as a single well pumping at 200,000 ft^3/d. Figure 3B shows the same system using a 100-ft grid spacing; this spacing allows each well to be represented separately. Both grids result in nearly identical drawdown for distances greater than 500 ft from the wells, but the drawdown is quite different close to the well.

Continuity of geologic deposits can be disrupted when cells are too large; for example, isolated cells, unintended holes in confining units, and breaks in channels with high conductivity can occur. An example of this is shown in figure 4 where a high hydraulic-conductivity channel becomes discontinuous when discretized with finite-difference cells that are too large to accurately define the important feature of the framework. The effect of the high hydraulic-conductivity channel is not adequately represented in a model with this discretization because it is not represented as a channel but rather as a set of discontinuous pockets of high hydraulic conductivity.

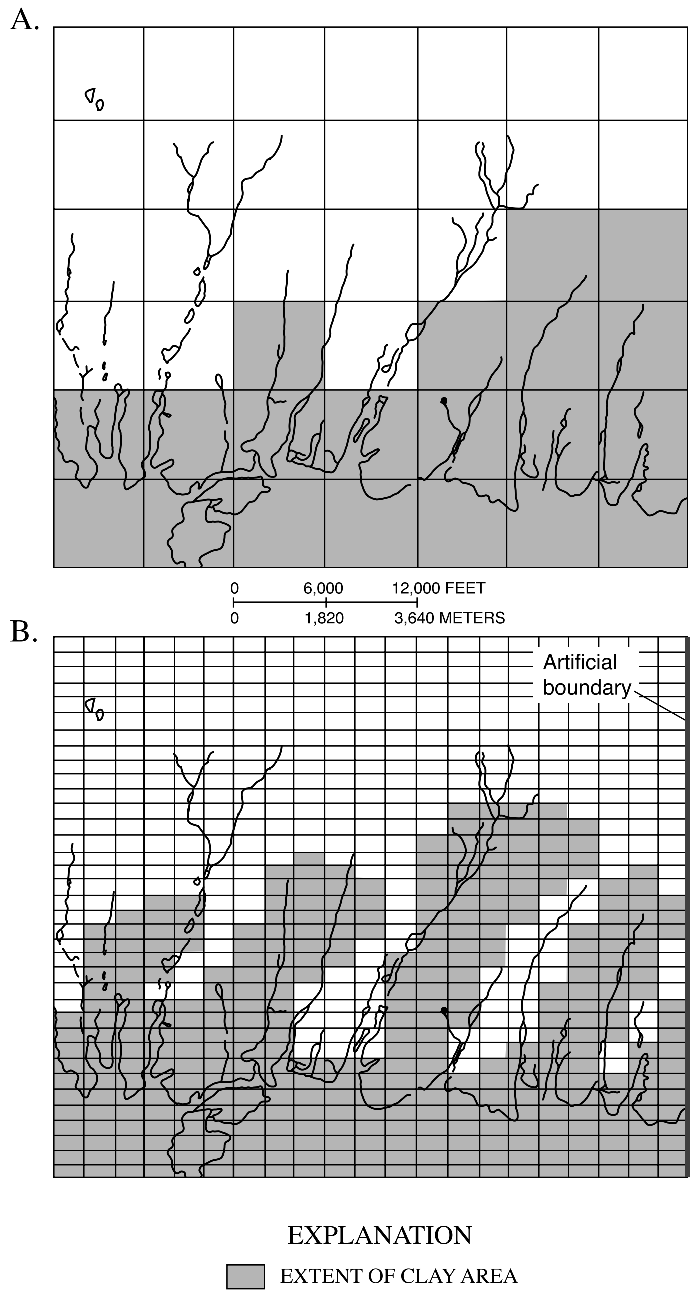


Figure 1. Extent of the south-shore confining unit on Long Island, New York, (A) as represented in a regional ground-water flow model grid, and (B) as represented in a sub-regional ground-water flow model grid. (Modified from Buxton and Reilly, 1987.)

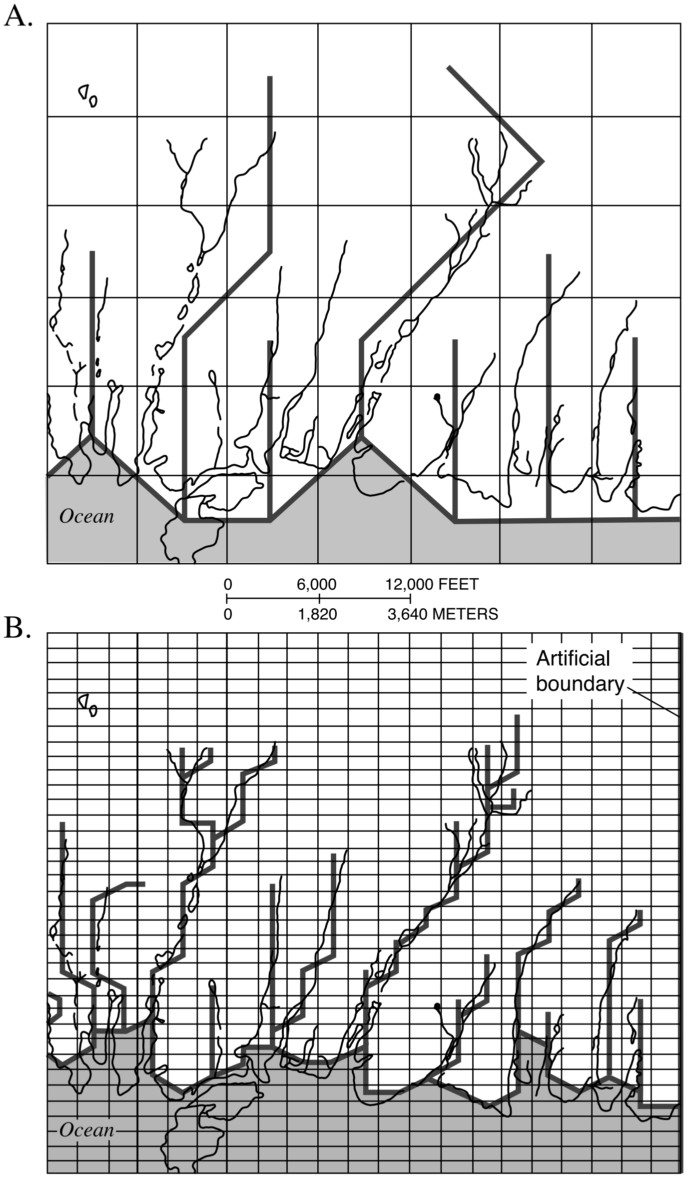


Figure 2. Representation of stream and shoreline boundaries on Long Island, New York, (A) as represented in a regional ground-water flow model grid, and (B) as represented in a sub-regional ground-water flow model grid. (Modified from Buxton and Reilly, 1987.)

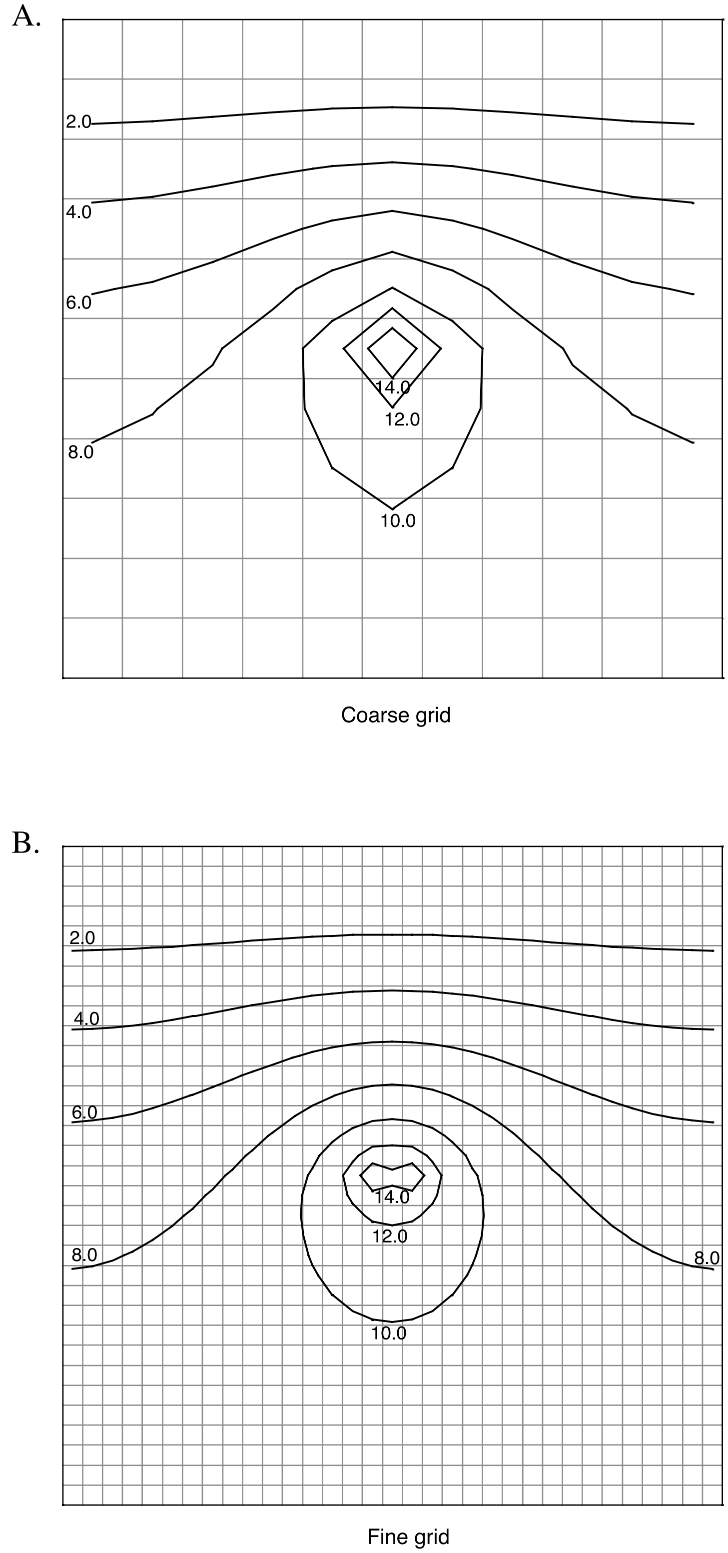


Figure 3. Simulated drawdown from two wells using different grid spacings.

Further, selecting a cell size that is just adequate to represent the variation of hydraulic properties and stresses generally is inadequate. A change in a property or stress in a system has an effect on the computed head some distance away. A complex distribution of hydraulic properties and stresses results in a complex head distribution. Many cells are needed to simulate a complex head distribution because the finite-difference method computes a single value of head for each cell. Many single values are required to approximate a complex distribution. Thus, it is important to incorporate a sufficient number of cells to allow the complexity of head distribution to be simulated. A simple example is shown in figure 5. A system is simulated with two different grid spacings, as described for figure 3, except that a single well pumping 200,000 ft^3/d is being simulated. The figure shows a cross section of head along the row containing the well. The head distribution is most complex near the well, and accordingly, there is noticeable difference in drawdown for the two grid spacings near the well. If accuracy of head near the well is not important to the problem, then the coarse grid is probably acceptable. But, if accuracy is needed near the well, then the finer grid would be necessary.

Some of the examples in this report have used uniform horizontal grid spacing; however, finite-difference models generally allow the widths of rows and columns to vary, which is called variable grid spacing. The use of variable grid spacing allows some flexibility to make cells smaller in some areas and coarser in other areas. Another approach to allowing cell sizes to vary, called telescopic refinement, is to couple a finer grid model to a subregion of a coarser grid model. This approach can avoid having the elongated cells, which are characteristic of using variable grid spacing. An approach for implementing telescopic refinement with MODFLOW is documented in Leake and Claar (1999).

In the vertical direction, two approaches commonly are used to represent the hydrogeologic framework in the model—uniform model layers (a rectilinear grid) and deformed model layers (fig. 6). Deformed model layers allow horizontal

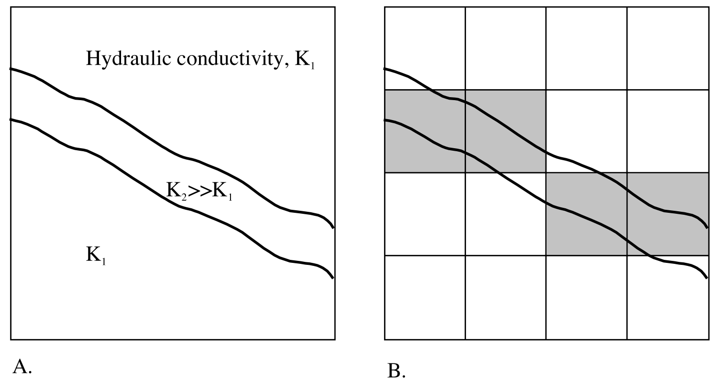


Figure 4. Large finite-difference cells may be inadequate to represent some important features of a ground-water system. (A) Map of the distribution of horizontal hydraulic conductivity showing a channel of high hydraulic conductivity. (B) Finite-difference cells representing the high hydraulic-conductivity channel are no longer continuous, because there is no direct connection between diagonal cells in the finite-difference method.

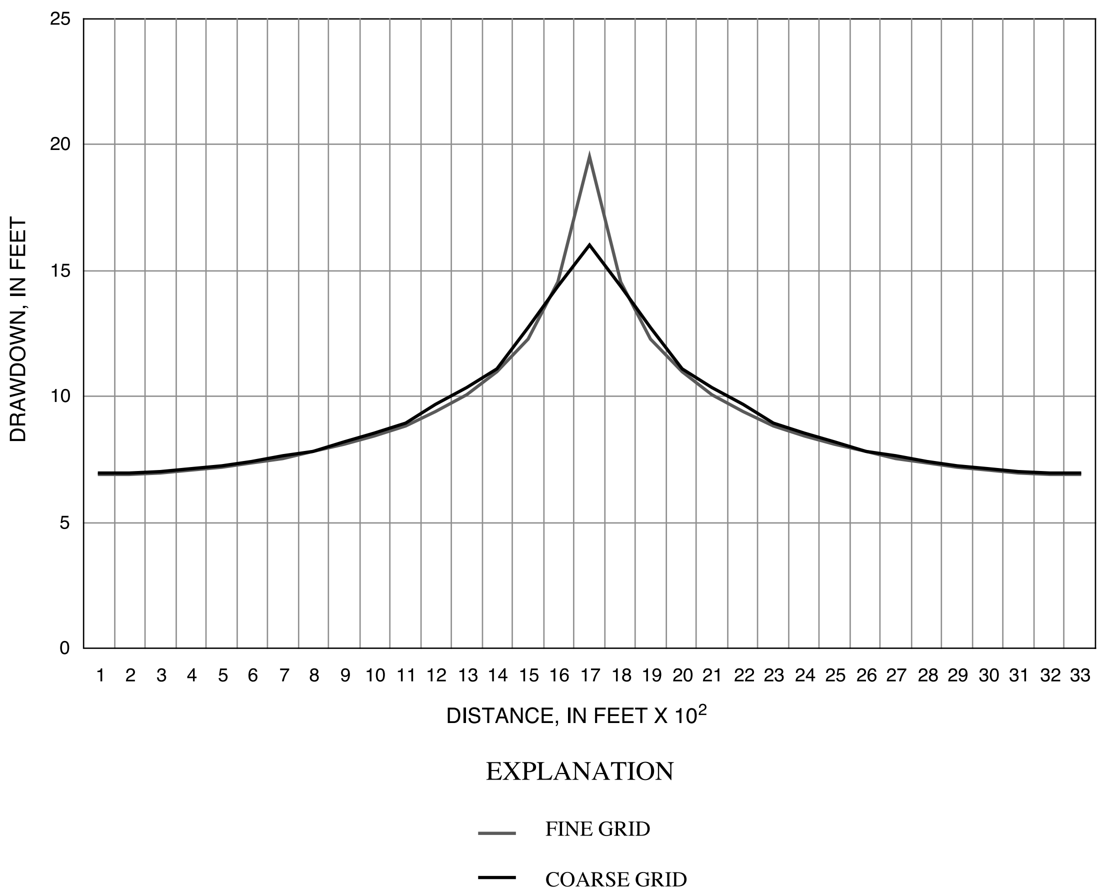


Figure 5. Cross section of drawdown showing the effect of grid spacing.

continuity to be maintained with fewer cells at the expense of introducing some error in the finite-difference method. As examples, the discretization of the geologic framework into uniform model layers was used in the simulation of ground-water flow on Cape Cod, Massachusetts as shown in figure 7 (modified from Masterson and others, 1997), and the discretization of the geologic framework by deformed or hydrogeologic model layers was used in the simulation of ground-water flow on Long Island, New York as shown in figure 8 (modified from Buxton and others, 1999).

A two-dimensional (single-layer) model and a three-dimensional (eight-layer) model of Cape Cod, Massachusetts, provide an example of the effect of vertical discretization on model results. The number of layers used to discretize the aquifer affects the resultant flow field and estimation of the area contributing recharge to pumping wells. The ground-water flow system in the example consists of a thick (250–500 ft) multilayered sequence of unconsolidated deposits or materials that range in grain size from gravel and sand to silt and clay and includes numerous overlying ponds and streams and variable

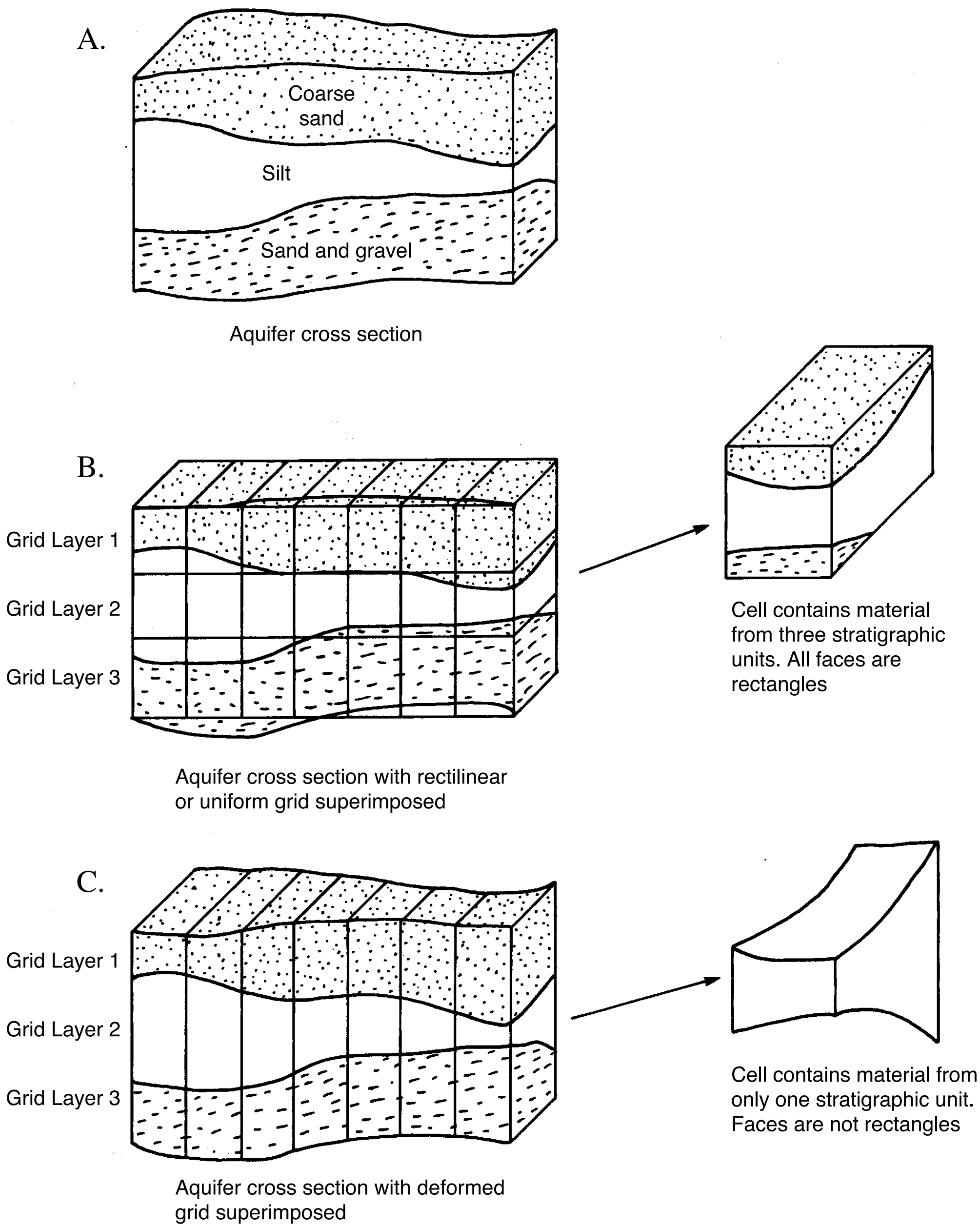


Figure 6. Schemes of vertical discretization for (A) aquifer cross section, (B) aquifer cross section with rectilinear or uniform grid superimposed, and (C) aquifer cross section with deformed grid superimposed.

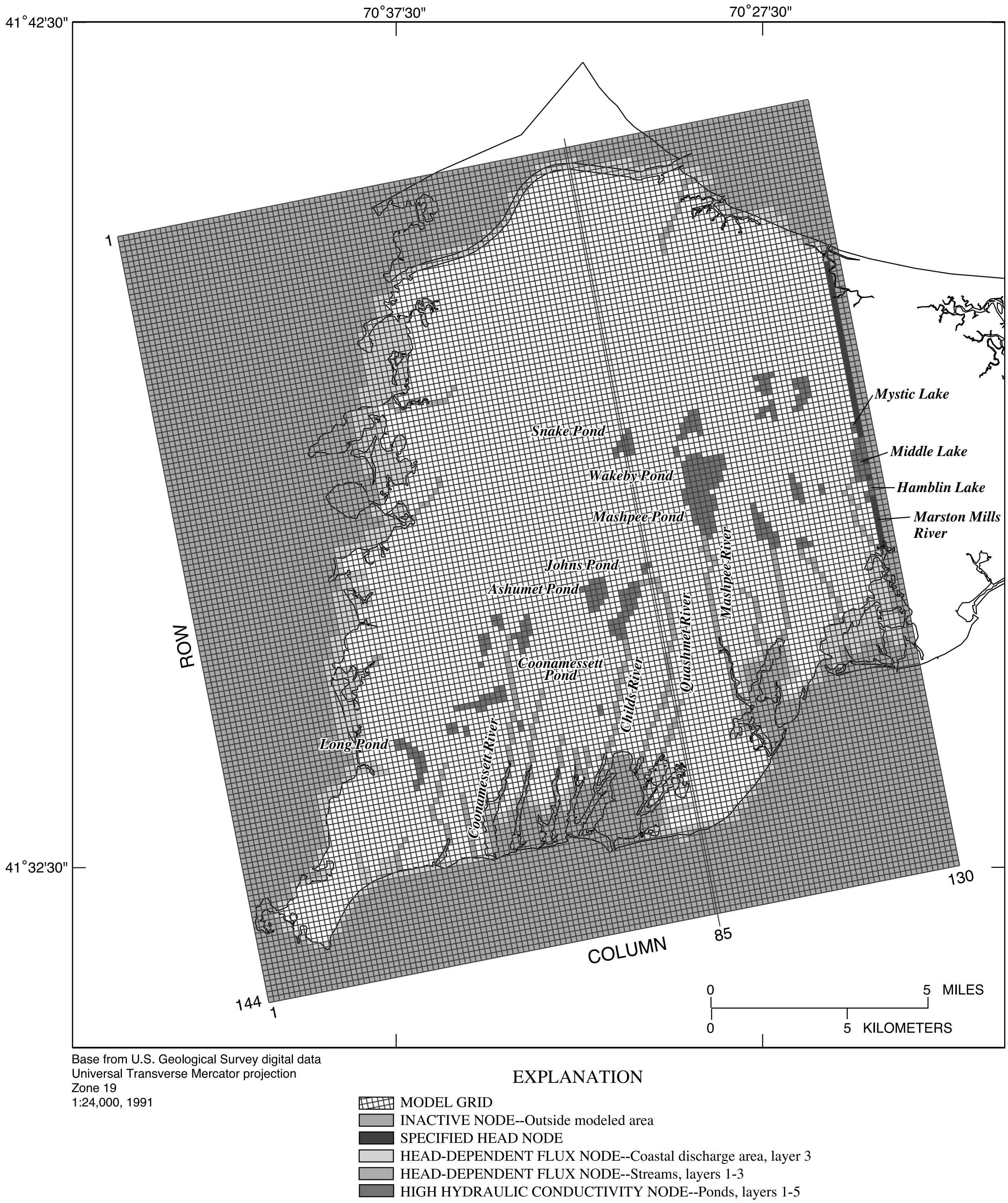


Figure 7A. Horizontal and vertical discretization using uniform layers for the model simulating ground-water flow on Cape Cod, Massachussetts. Horizontal grid. (Modified from Masterson and others, 1997.)

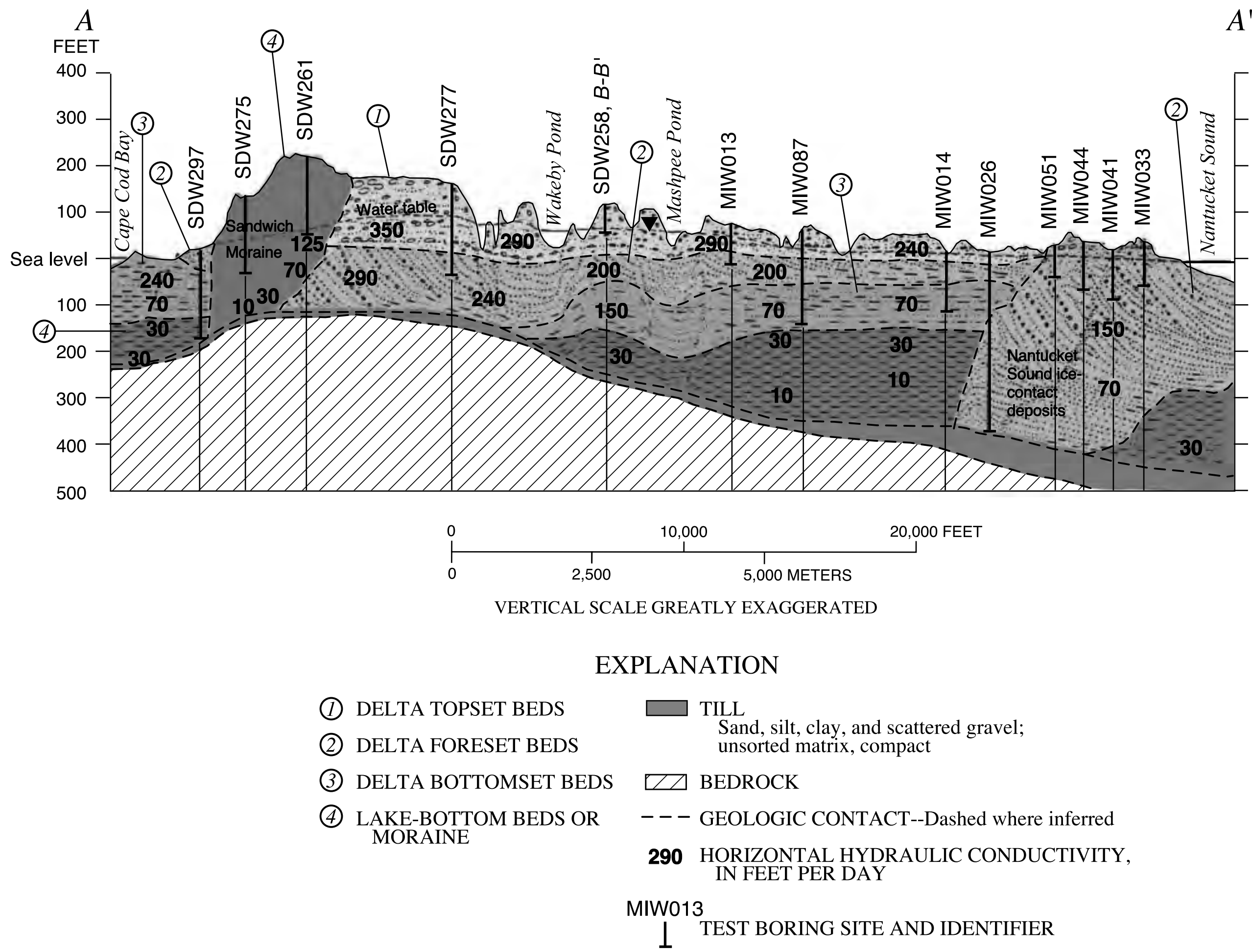


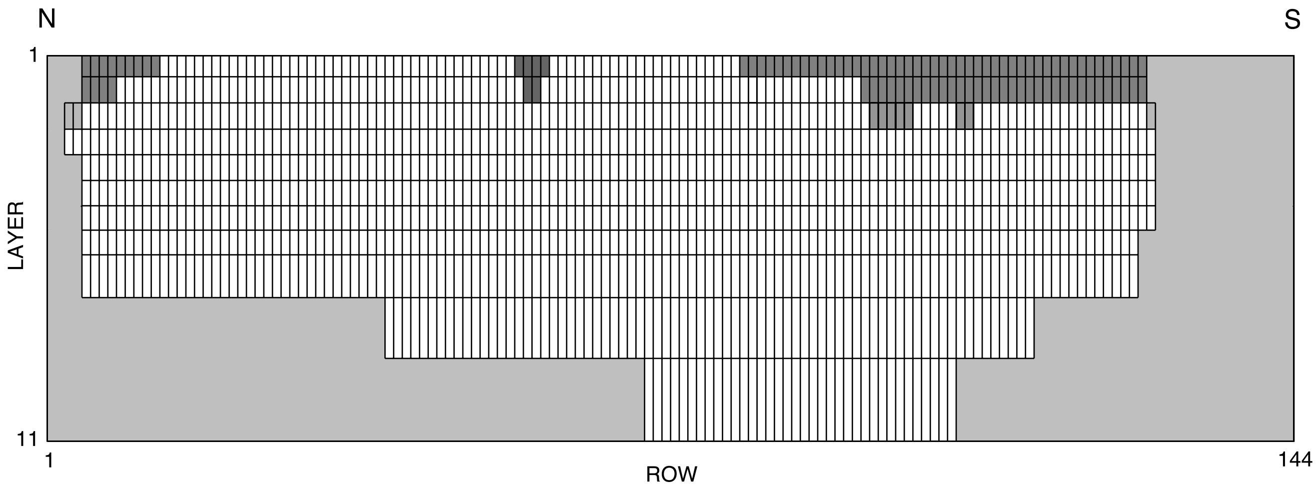
Figure 7B. Horizontal and vertical discretization using uniform layers for the model simulating ground-water flow on Cape Cod, Massachussetts. Hydrogeologic cross section near column 85. (Modified from Masterson and others, 1997.)

recharge rates from precipitation. More than 30 public-supply wells, screened at various depths, withdraw water from the system at widely differing rates. The three-dimensional model was developed first and then simplified into a two-dimensional model that was calibrated independently; consequently, the total transmissivities of the two models are not identical. The contributing recharge areas for the two-dimensional model and three-dimensional model (fig. 9) are different, however, even though both models represent the flow field on Cape Cod, Massachusetts. In the two-dimensional model (fig. 9A), the contributing areas are fairly typical of the simple ellipsoidal shapes that are delineated by two-dimensional analytical and numerical modeling techniques. In comparison, however, the shapes of the contributing recharge areas using the multilayer three-dimensional model (fig. 9B) are more complex (Barlow, 1994; Franke and others, 1998).

In evaluating a ground-water flow simulation, the proper or sufficient discretization is not straightforward to determine. Enough detail is required to represent the hydraulic properties, stresses, and complexities of the flow field for the objectives of the study; yet, the cost will be less if the model is kept as simple as possible so that data entry, computer resources, and analysis of model output are as minimal as possible. Thus, the determination of the proper discretization is always a compromise. Ideally, the modeler would test the effect of grid spacing on a model to help determine the optimal grid spacing; however, the authors have not seen this done with any frequency. The model documentation should justify the discretization that is used.

Specifying Properties of Cells

A second aspect of representing the hydrogeologic framework is the choice of the hydraulic properties assigned to the cells. When simulating an actual system (as opposed to a hypothetical system), the properties of a system are generally not known at every cell in the grid; therefore, interpolation from limited real-world data must be done. Given the uncertainty of knowledge of the distribution of hydraulic properties, groups of cells are sometimes given a uniform value rather than attempting to define an individual value for every cell. Interpolation schemes, such as distance weighting and various geostatistical



EXPLANATION

INACTIVE NODE—Outside modeled area

INACTIVE NODE—Layers 1 and 2

HEAD-DEPENDENT FLUX NODE—Coastal discharge area, layer 3

HEAD-DEPENDENT FLUX NODE—Streams, layers 1-3

HIGH HYDRAULIC CONDUCTIVITY NODE—Ponds, layers 1-5

Figure 7C. Horizontal and vertical discretization using uniform layers for the model simulating ground-water flow on Cape Cod, Massachussetts. Vertical grid using uniform layers along column 85. (Modified from Masterson and others, 1997.)

methods, also are used. The user of a model should evaluate the appropriateness of the interpolation scheme. To make such evaluation possible, the model documentation should specify the interpolation method used and include the rationale for using that interpolation method.

Three examples of interpolated hydraulic conductivity data for a hypothetical system are shown in figure 10. All three examples are based upon the assumption that values are known (presumably from aquifer tests) at four points. Figure 10A shows the use of the nearest-neighbor method. For every cell, the data point that is closest to the center of a cell is used as the cell value. An even simpler approach would be to use a single value for all the cells that is the average of the four known values. This simpler approach could be justified if the known values are not considered to be accurate. Figure 10B shows grid values determined by using a weighted average of the four known values based on the inverse distance squared from the center of a cell to the four points. Finally, figure 10C shows grid values determined from the hydraulic conductivity of the two adjacent contours. The value for a cell is the distance-weighted average of the two contour values. Contours were drawn based on the four known points plus additional geologic information about the types of sediments throughout the area (which was made up for this example). The three distributions shown in figure 10 differ significantly even though they are all based on the same four data points. There are many other methods available for interpolation that would each produce different parameter distributions.

The authors are aware of only one general guideline to help determine the best interpolation method to use in a particular situation. This guideline states that it is best to use the simplest interpolation method that is consistent with the known data. The rationale for this guideline is that unwarranted complexity in the discretized values builds a bias into a model that affects all future use. Ideally the model developer would evaluate the importance of the interpolation method by testing different methods and comparing the effect on model results. Such testing is not always practical depending on the resources available for model development.

The chosen interpolation method is often implemented by a computer program. The model documentation should reference the program that is used. Some model programs incorporate interpolation capabilities. For example, the Hydrogeologic-Unit Flow (HUF) Package (Anderman and Hill, 2000) in MODFLOW vertically averages hydraulic properties for cells based on real-world geometry of hydrogeologic units.

The discretization of the storage properties of the groundwater system has some intricacies of its own. The two main types of aquifer storativity are confined storage (specific storage) and unconfined storage (specific yield). Unconfined storage is related to the release of water as the water table lowers (dewatering of the aquifer material); thus, it occurs only along the top boundary of the saturated flow system. Confined storage is related to the release of water as the head drops because of expansion of the water itself as the pressure changes and changes in the solid framework of the aquifer (no dewatering

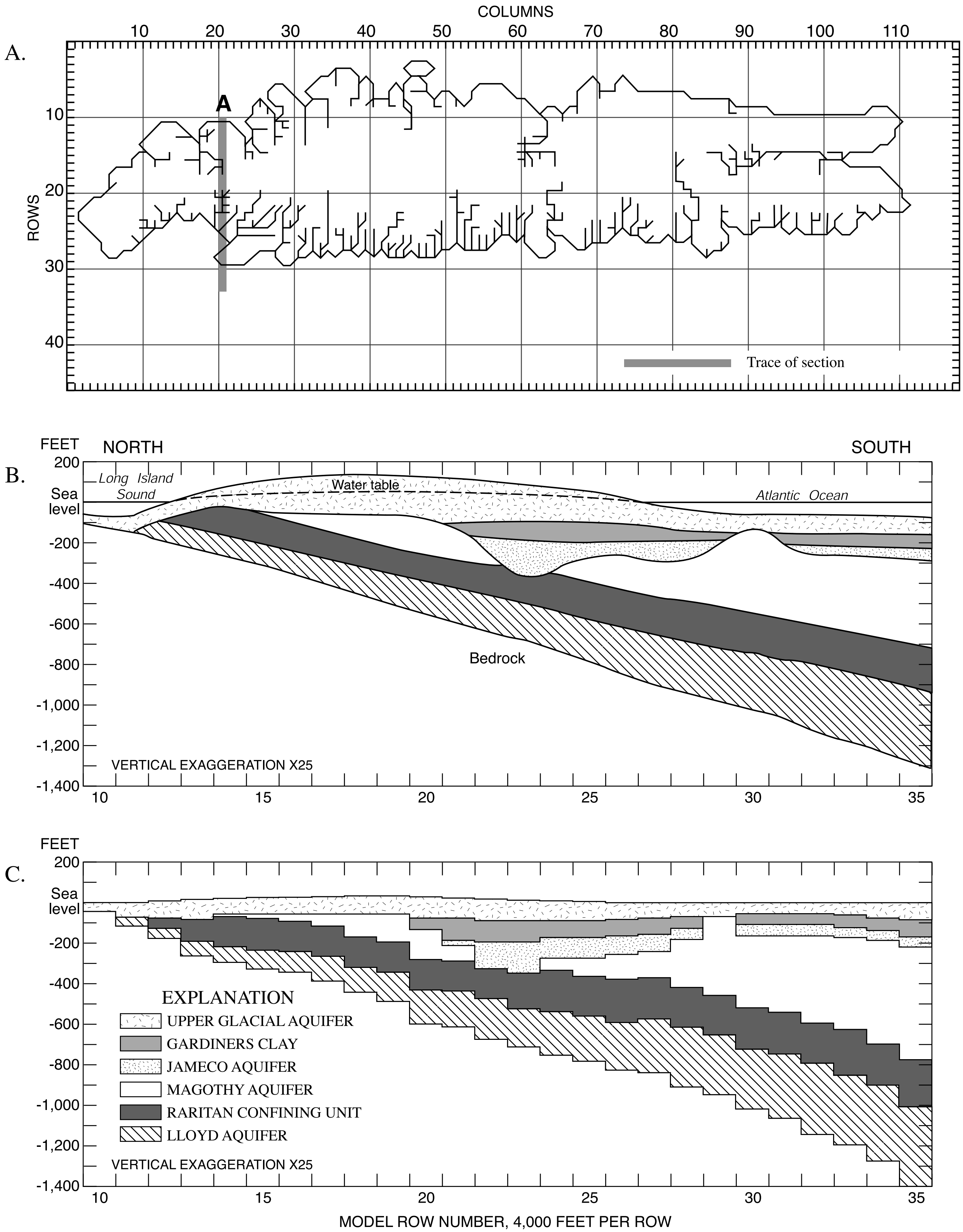


Figure 8. Horizontal and vertical discretization using deformed layers for the model simulating ground-water flow on Long Island, New York: (A) horizontal grid, (B) hydrogeologic cross section, and (C) vertical grid using deformed layers. (Modified from Buxton and others, 1999.)

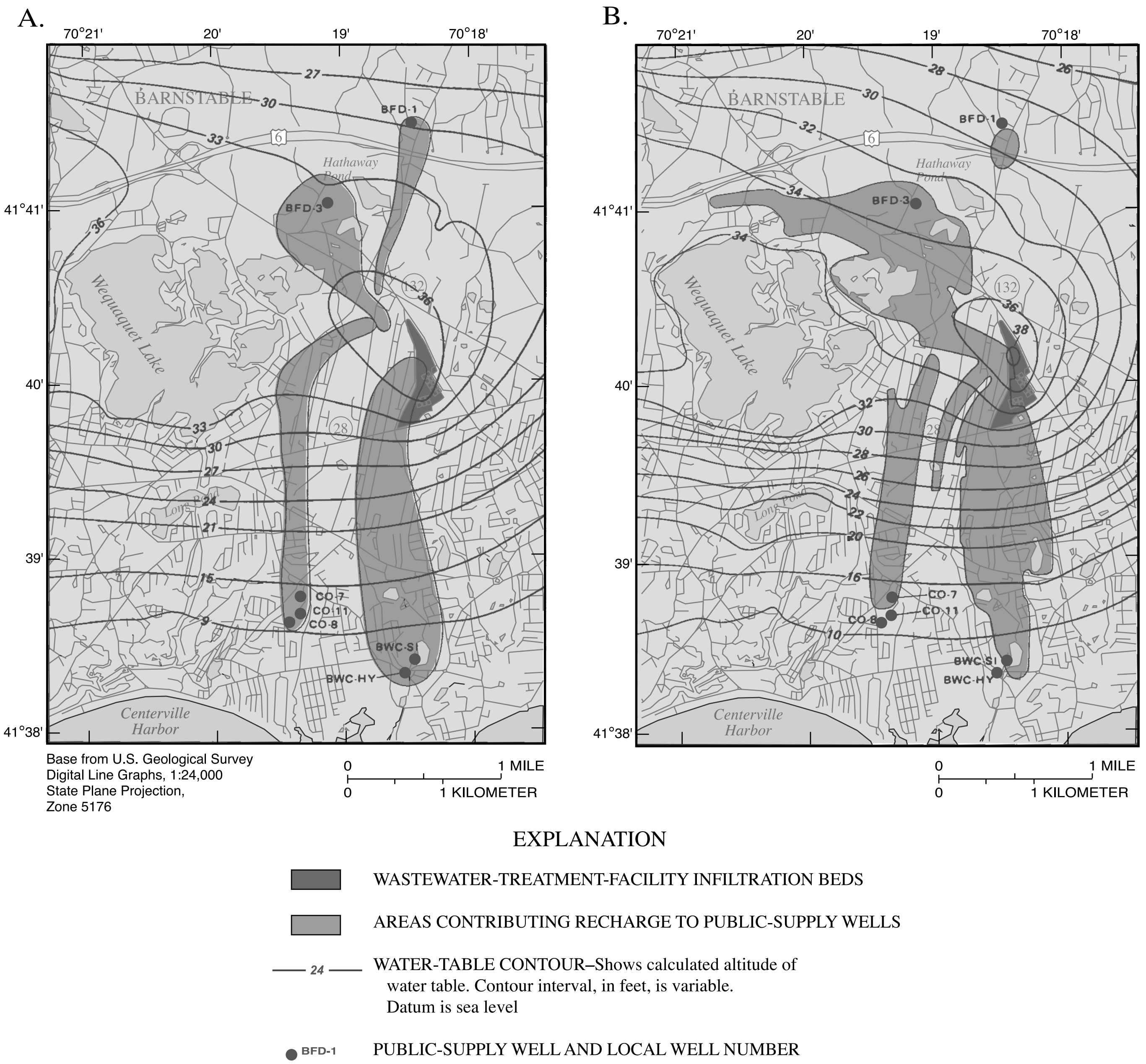
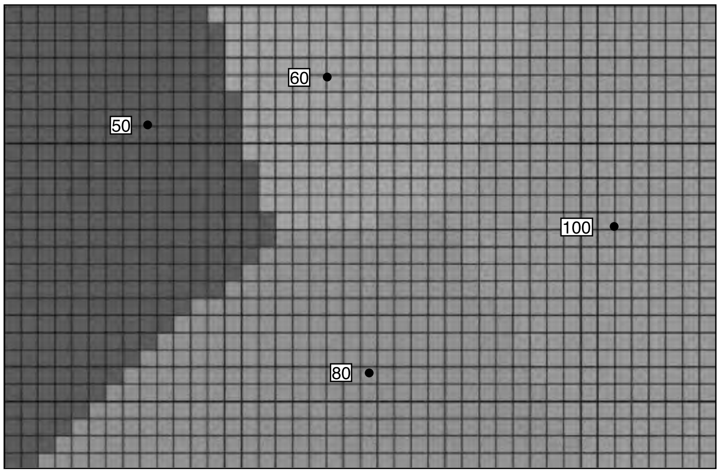


Figure 9. Comparison of areas contributing recharge to seven public-supply wells as determined by two different numerical models, Cape Cod, Massachusetts: (A) results from a two-dimensional single-layer model, and (B) results from a three-dimensional eight-layer model. (Modified from Barlow, 1994; and Franke and others, 1998.)

occurs). In simulating the changes in storage for transient systems, it is important that the unconfined storage occurs only at the top boundary (or top active layer), even if the water-table aquifer is divided into many layers. Some model programs, such as MODFLOW, control which storage coefficient is used based on the layer geometries and heads, thus ensuring that the proper (either the specific storage or the specific yield) coefficient is used. Other model programs require the user to specify the coefficient for each cell. Some investigators have erroneously specified specific yield for all layers in an unconfined aquifer, when it should be specified only for the uppermost active layer, causing incorrect quantities of water to be simulated from storage. Thus, care must be taken in determining if the proper storativity is simulated in a model.

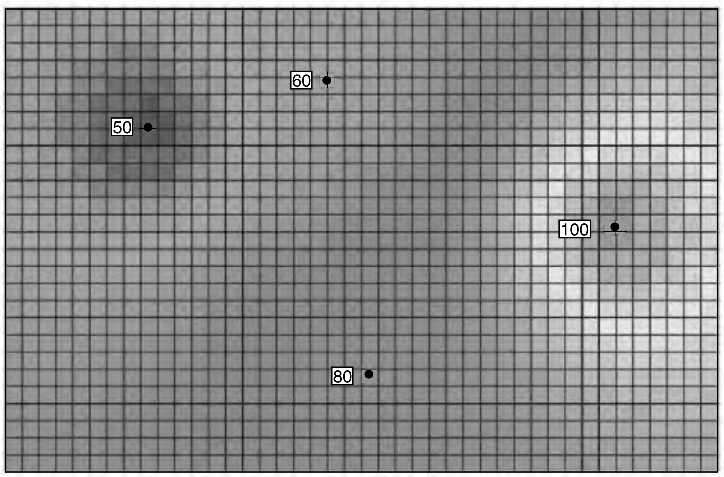
Models that simulate a water table also can have a uniqueness problem related to the representation of the hydrogeologic framework by discrete volumes. Ground-water model programs such as MODFLOW allow cells representing the water table to go dry (desaturate) so that ground-water flow is not simulated in those cells. Cells also can convert from dry to wet in some situations. Cell wetting and drying depends on a variety of factors such as initial conditions, the iterative solution process, and

A.



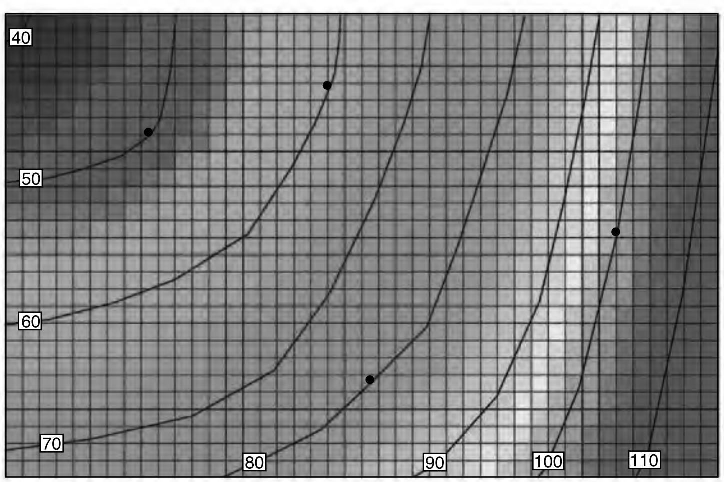
Cell value is the nearest measured value

B.



Cell value is the inverse-distance-squared weighted average of measured values

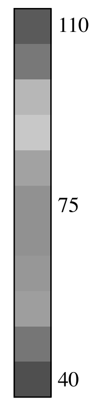
C.



Cell value is the distance-weighted average of the two adjacent contours

EXPLANATION

HYDRAULIC CONDUCTIVITY, IN FEET PER DAY



CONTOUR OF HYDRAULIC CONDUCTIVITY, IN FEET PER DAY. CONTOUR INTERVAL IS 10 FEET PER DAY

100 • DATA POINT LOCATION AND VALUE OF HYDRAULIC CONDUCTIVITY, IN FEET PER DAY

Figure 10. Examples of interpolating data for cells from measured data. (A) Cell value is the nearest measured value, (B) cell value is the inverse-distance-squared weighted average of measured values, and (C) cell value is the distance-weighted average of the two adjacent contours.

user-specified options to control wetting and drying. By varying these factors, it is possible to change the number of dry cells, and thus the head will vary. Careful evaluation is required to detect the potential for nonuniqueness and reject solutions that are unreasonable.

To avoid solver convergence problems that sometimes occur when cells can convert between wet and dry, some investigators have resorted to specifying cells representing the water table as having a constant saturated thickness. It is important to evaluate the extent to which this has been done and the degree to which the thickness represented by the simulated heads varies from the assumed specified thickness. For steady-state models, the following process can be repeated until the simulated saturated thickness is reasonably close to the specified saturated thickness:

1. Run the model.
2. Compare the simulated saturated thickness (head minus bottom elevation) to the specified saturated thickness.
3. Adjust the specified saturated thickness to match the simulated thickness.

For transient models, the changes in saturated thickness throughout the simulation can be compared to the specified saturated thickness to insure that the change is small compared to the total saturated thickness.

Time Steps

Transient models simulate the impact of stresses over time. In MODFLOW, time is divided into time steps, and head is computed at the end of each time step. Many time steps are required to simulate a complex distribution of head over time. This is similar to the need for many cells to represent the spatial distribution of head. It is important to incorporate enough time steps to allow the temporal complexity of head distribution to be simulated.

Figure 11 shows the effect of using different numbers of time steps to simulate the drawdown of a well. The system is the same as that used for the fine-grid simulation in figure 3, with a dimensionless storage coefficient of 0.01 and a well located in the cell at row 17 and column 17. The hydrographs are for the cell at row 17, column 13, which is the 4th cell directly to the left of the pumping cell. At the start of the simulation, the well is turned on with a pumping rate of 100,000 ft^3/d. Each time step is 1.5 times longer than the previous time step, which results in more time steps in early time when head is changing most rapidly. Use of six or more time steps in this model produces nearly the same results, but four or less time steps produces much different results, especially in early time.

MODFLOW also makes use of stress periods to facilitate specification of stress data. A stress period is a group of one or more time steps in which stress input data are constant. In many situations, it is appropriate to maintain the same stresses for multiple time steps, so combining time steps into a stress period for the purposes of data input minimizes the data preparation effort. A new stress period must start whenever it becomes necessary to change stress input data. If stress periods are too long, important dynamics of the stresses may be left out or poorly represented. For example, the Well Package of MODFLOW (Harbaugh and others, 2000) allows pumping rates for wells to change every stress period, and within a stress period the pumping is constant. If the simulation is broken into stress periods of one year, for example, but the actual pumping rate changes more frequently, then stress periods may need to be shorter.

The intended use of the model is also an important factor in evaluating whether the size of stress periods and time steps is appropriate. Considering again the simulation of wells, if a model is used to analyze the average response of a system over many years, then pumping might be represented as yearly averages using yearly stress periods. There would likely be multiple time steps in each yearly stress period, but the stress would remain constant for each year. Thus, hourly, daily, and seasonal variations in pumping would be ignored. But, if a model is used to simulate seasonal system response, then pumping should be represented with shorter stress periods – perhaps monthly.

Questions to be answered in evaluating the appropriateness of the discretization and the representation of the hydrogeologic framework in the simulation of the ground-water system are:

1. Does the horizontal discretization represent the important features of the hydrogeologic framework to meet the objectives of the study?

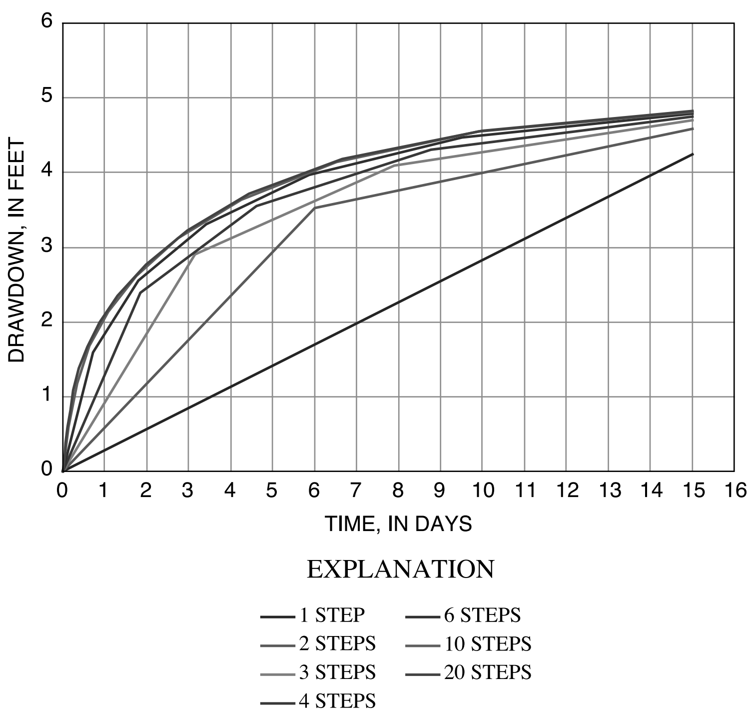


Figure 11. Drawdown versus time for different numbers of time steps.

2. Are the physical boundaries represented appropriately in space by the discretized representation?
3. Is the horizontal discretization appropriate to represent the degree of complexity in the aquifer properties and head distribution (flow system)?
4. Does the vertical discretization adequately represent the vertical connectivity and transmitting properties of the hydrogeologic framework to meet the objectives of the study? Does the method of vertical discretization, either a rectilinear grid or deformed grid, introduce any bias into the representation of the hydrogeologic framework?
5. Is the method of assigning parameter values to individual cells explicitly explained? Is the method appropriate for the objectives of the study and the geologic environment?
6. If the ground-water system is transient, then is the specification of storage coefficients appropriate?
7. If the ground-water system is unconfined in some areas, then is the treatment of changes in saturated thickness and the potential for cells to go dry explained and appropriate? If cells have gone dry, does the resultant solution seem appropriate?
8. Is the time discretization fine enough to represent the degree of complexity in stresses and head distribution over time?

The evaluation of the proper or sufficient discretization of the hydrogeologic framework of a ground-water flow simulation is not straightforward to determine. The continuity of deposits and the reasonableness of the specification of values for each cell in light of the depositional environment of the hydrogeologic framework must be considered. As always, the objectives of the study also determine which features must be represented in the model and the level of detail required to adequately represent their effect on the flow system.

Representation of Boundary Conditions

Boundary conditions are a key component of the conceptualization of a ground-water system. The topic of boundary conditions in the simulation of ground-water flow systems has been discussed in Franke and others (1987) and Reilly (2001).

As discussed in Reilly (2001), computer simulations of ground-water flow systems numerically evaluate the mathematical equation governing the flow of fluids through porous media. This equation is a second-order partial differential equation with head as the dependent variable. In order to determine a unique solution of such a mathematical problem, it is necessary to specify boundary conditions around the flow domain for head (the dependent variable) or its derivatives (Collins, 1961). These mathematical problems are referred to as boundary-value problems. Thus, a requirement for the solution of the mathematical equation that describes ground-water flow is that boundary conditions must be prescribed over the boundary of the domain. Boundary conditions also represent any flow or head constraints within the flow domain. For example, recharge from percolation of precipitation, river interaction, and pumping from wells are simulated as boundary conditions. Three types of boundary conditions—specified head, specified flow, and head-dependent flow—are commonly specified in mathematical analyses of ground-water flow systems. The values of head (the dependent function) in the flow domain must satisfy the pre-assigned boundary conditions to be a valid solution.

In solving a ground-water flow problem, however, the boundary conditions are not simply mathematical constraints; they generally represent the sources and sinks of water within the system. Furthermore, their selection is critical to the development of an accurate model (Franke and others, 1987). Not only is the location of the boundaries important, but also their numerical or mathematical representation in the model. This is because many physical features that are hydrologic boundaries can be mathematically represented in more than one way. The determination of an appropriate mathematical representation of a boundary condition is dependent upon the objectives of the study. For example, if the objective of a model study is to understand the present and no estimate of future conditions is planned, then local surface-water bodies may be simulated as known constant-head boundaries; however, if the model is intended to forecast the response of the system to additional withdrawals that may affect the stage of the surface-water bodies, then a constant head is not appropriate and a more complex boundary is required. A model of a particular area developed for one study with a particular set of objectives may not necessarily be appropriate for another study in the same area, but with different objectives. All of these aspects of boundary conditions must be considered in evaluating the strengths and weaknesses of a ground-water flow model.

In the ground-water flow modeling process (fig. 12), boundary conditions have an important influence on the areal extent of the model. Ideally in developing a conceptual model, the extent of the model is expanded outward from the area of concern both vertically and horizontally so that the physical extent coincides with physical features of the ground-water system that can be represented as boundaries. The effect of these boundaries on heads and flows must then be conceptualized, and the best or most appropriate mathematical representation of this effect is selected for use in the model.

When physical hydrologic features that can be used as boundary conditions are far from the area of interest, artificial boundaries are sometimes used. The use of an artificial boundary should be evaluated carefully to determine whether its use would cause unacceptable errors in the model. For example, a no-flow boundary might be specified along an approximated flow line at the edge of a modeled area even though the aquifer extends beyond the modeled area. The rationale might be that the artificial boundary is positioned far enough from the area of interest that whatever is simulated in the area of interest would not cause significant flow across that area of the system. The rationale for artificial boundaries can generally be tested using the model. In the example of an artificial no-flow boundary, the

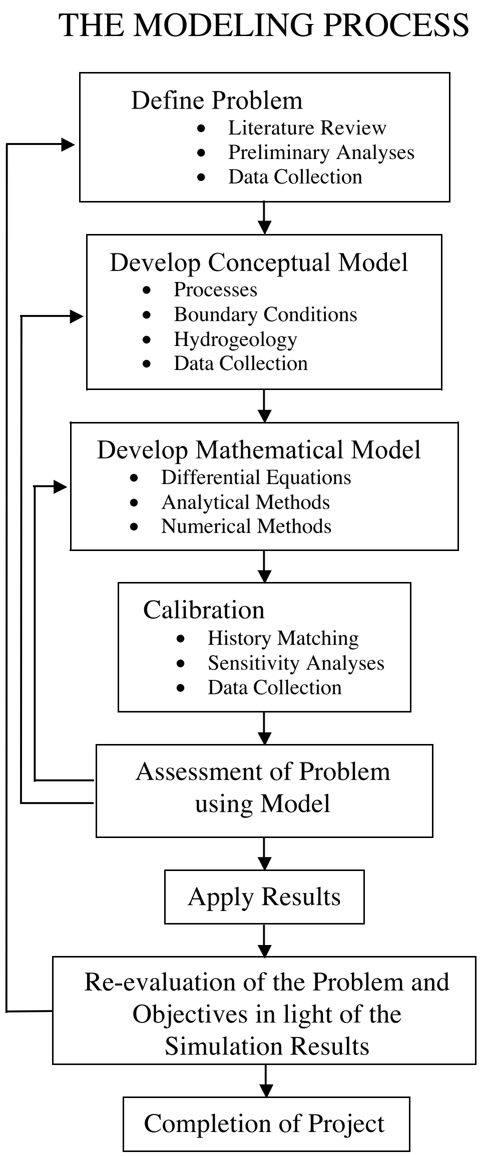


Figure 12. Flow chart of the ground-water flow modeling process. (From Reilly, 2001.)

appropriateness can be tested by looking at how much the head changes near the boundary when the model is used for its intended purpose. Substantial change in heads near the boundary is an indication that significant flow across the region would occur if the artificial boundary were not imposed.

Another example of an artificial boundary is a specified-head boundary at a location where there is no source of water to maintain the head at its specified value. The appropriateness of this boundary can be tested by evaluating the flow from the boundary and the change in flow due to changes in parameter values or stresses within the model. If a stress causes a large change in flow from the boundary, then the head would probably change at the boundary if it were not artificially fixed. Artificial boundaries, if applied improperly and not evaluated, can overly constrain the response of the system and bias the results of an analysis. A frequently observed example is when the area of interest for a study is artificially bounded by specified heads, without regard to the flow being simulated from this boundary into the study area. In this case, the model may not be sensitive to parameter values and stresses because the specified heads artificially keep the simulated heads from deviating much. For further discussion of this topic, see Franke and Reilly (1987).

The objective of the modeling analysis and the magnitude of the stresses to be simulated also influence the selection of the appropriate approach to simulate the physical features that bound the ground-water system. When ground-water systems are heavily stressed, the physical features that bound the system can change in response to the stress. Any representation of these features must account for these potential changes, either by understanding the limitations of the simulation or by representing the physical feature as realistically as possible.

In evaluating the appropriateness of a ground-water flow model, the boundary conditions are key because they determine where the water enters and leaves the system. If the boundaries are inappropriate, the model will be a poor representation of the actual ground-water flow system. Questions to be used in evaluating the boundary conditions of a ground-water flow model are:

1. Are all the external boundaries of the model associated with a definable physical feature?

If no –

A. Why not?

B. Is sufficient justification provided to warrant the use of artificial boundaries?

C. Are the effects of the “artificial” boundaries tested in the calibration of the model and documented in the report? Does the documentation of their use and their testing make a convincing argument for their reasonableness?

If yes –

A. Is the mathematical representation of the physical feature appropriate?

B. Are there conditions under which the representation of the boundary used in the model would become invalid? Are these conditions discussed?

2. Do the boundary conditions of the model overly constrain the model results so that the calibration is insensitive and the predictions are not realistic?

Representation of Initial Conditions in Transient Simulations

Initial conditions represent the heads at the beginning of a transient simulation. Thus, initial conditions serve as a boundary condition in time for the transient head response of a ground-water model solution. Initial conditions are used only in transient simulations, and are different from starting heads (or the initial guess) in steady state solutions. In steady-state solutions, the starting heads can and do affect the efficiency of the matrix solution, but the final correct solution should not be affected by different starting heads. In transient solutions, however, the initial conditions are the heads from which the model calculates changes in the system due to the stresses applied. Thus, the response of the system is directly related to the initial conditions used in the simulation.

The changes in head that occur in the transient model due to any applied stress will be a combination of the effect of the change in stress on the system and any adjustments in heads as a result of errors in the initial head configuration (the initial conditions). Adjustments in heads resulting from errors in the initial head configuration do not reflect changes that would occur in the actual system, but rather occur because the heads specified as the initial condition are not a valid solution to the numerical model. Because errors in the initial head conditions cause changes in head over time during the simulation, it is best to begin all transient simulations with a head distribution that is a valid solution for the model. This ensures that there are no discrepancies (or errors) between the specified initial conditions and a valid head solution for the model.

For simulations that start from a period when the aquifer system was in a steady-state equilibrium, the development of appropriate initial conditions is straightforward. A simulation of the steady-state period should be made. The results of this simulation should then be used as the initial conditions for the transient simulation.

Sometimes, however, it is not possible to start a simulation from a point in time where the aquifer was in steady-state equilibrium. This condition could occur if the simulation is intended to simulate seasonal or other cyclic conditions where the system is never at steady state, or in instances where there is a period of unknown stress that cannot be reproduced accurately, or when it is not feasible to simulate the entire period of record from a time of steady state because of time and money constraints. Under these conditions, it is important that the initial conditions used do not bias the results for the period of interest. Some rules of thumb for the evaluation of the appropriateness of the initial conditions in these non-ideal situations are to evaluate the time constant of the system under investigation and to test the effect of different initial conditions on the results of the model.

The time constant for a ground-water system is derived from a dimensionless form of the ground-water flow equation and is defined as (Domenico and Schwartz, 1998, p. 73):

$$T = \frac{S_s L^2}{K},$$

where T is the time constant (T), S_s is the specific storage of a confined aquifer (L^{-1}), L is a characteristic length of the system (L), and K is the hydraulic conductivity (LT^{-1}). The effect of any transient condition will not be observable if the time after the condition occurs is significantly larger than the time constant for the aquifer (T) (Domenico and Schwartz, 1998). Thus, the effect of a poor or erroneous initial condition (assuming the rest of the model including boundary conditions is correct) should not be observable in model results that are for periods of time significantly larger than the time constant for the aquifer. The time constant is developed from the ground-water flow equation for a confined system with homogeneous hydraulic conductivity. Thus, its application in actual systems is not always exact. The appropriate characteristic length (L) of the system is usually chosen to represent the distance between major boundaries. The specific storage (S_s) represents the compressible storage characteristics of the system; however, an equivalent storativity for unconfined aquifers could be calculated as the specific yield (S_y) divided by the thickness (b) of the unconfined aquifer. For unconfined aquifers, an approximate time constant would be:

$$T = \frac{S_y L^2}{bK}.$$

The determination of the importance and duration of effects of erroneous or imperfect initial conditions can also be accomplished by testing the effect of different initial conditions on the model under study. This test is accomplished by simulating the same system with the stresses and different initial conditions. When the simulations for all the different initial conditions produce the same result, then one can assume the influence of the inaccurate initial conditions is negligible at all following time periods.

A simulation of a simple transient ground-water system can illustrate some of these points. In the illustrative simulation, the simple transient ground-water system is 20,000 ft long and 20,000 ft wide with two aquifers separated by a confining unit, and bounded by no-flow boundaries with a stream along one edge. The aquifer has uniform areal recharge of 0.003 ft/d. The upper aquifer is unconfined and both aquifers have a horizontal hydraulic conductivity of 50 ft/d and a vertical hydraulic conductivity of 5 ft/d. The confining bed is 10-ft thick with a vertical hydraulic conductivity of 0.001 ft/d. The system is discretized as shown in figure 13, and simulated using the finite-difference model MODFLOW. The areal grid size is 1,000 ft by 1,000 ft, and the two aquifers are each represented by two layers; the bottom aquifer is represented by a lower layer (layer 4) 50-ft thick overlain by a 40-ft thick layer (layer 3), and the unconfined aquifer is represented by a 50-ft thick layer (layer 2) overlain by a layer (layer 1) with a uniform bottom at –50 ft, which allows changes in thickness as a function of the head. The stream is represented as a constant head of 0 ft along the right-hand boundary in the top layer. The specific yield for the top layer is 0.2 and the specific storage for the entire model domain is 1.0 x 10^{-6} 1/ft.

The steady-state head distribution for the simple system in layer 1 is symmetric perpendicular to the stream and varies from 67.94 ft at the ground-water divide to 0.0 ft at the stream (fig. 14). A transient simulation is run from the initial steady state to examine the effect of a well discharging 100,000 ft^3/d from layer 3 in cell 10, 10 (9,500 ft from the divide). The correct simulation has as the initial condition the steady-state head

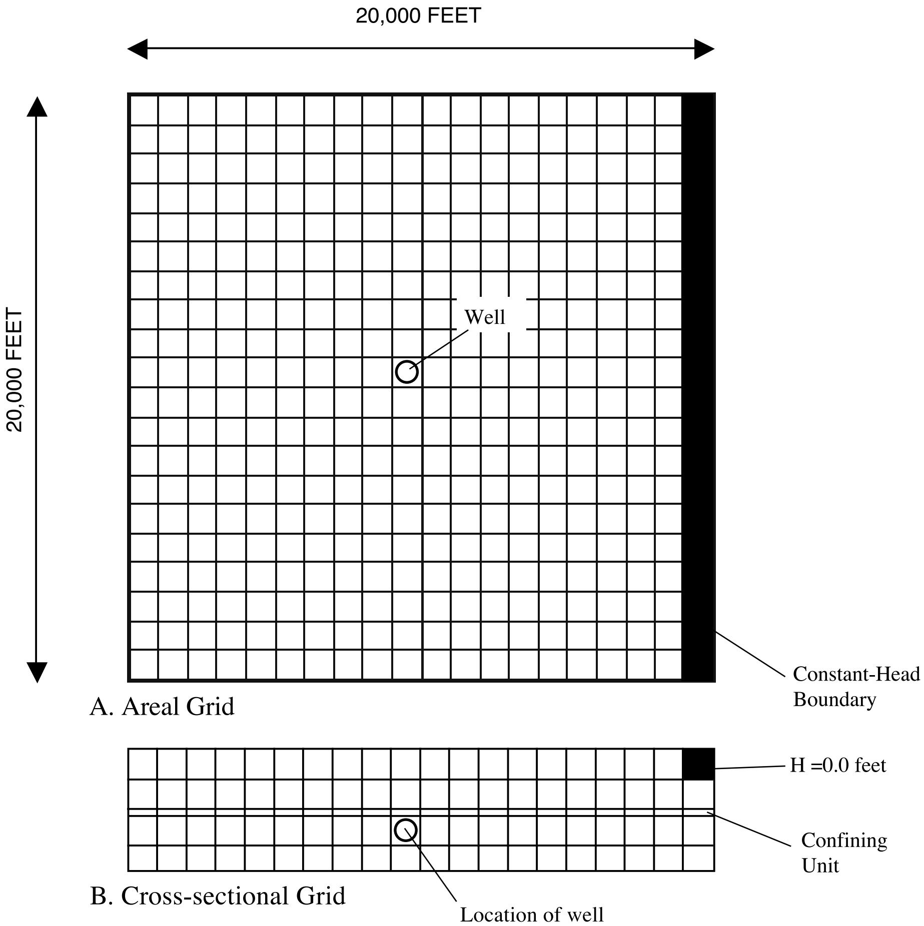


Figure 13. Extent and model grid of the finite-difference model used to illustrate initial conditions: (A) areal grid, and (B) cross-sectional grid.

distribution before the well began discharging; the response of the system through time is shown at the divide in layer 1 (fig. 15A) and at the cell containing the well in layer 3 (fig. 15B). The effect of inaccurate initial conditions can be observed in the response of the aquifer at these same locations. Two different initial conditions, as shown on figure 14, are used to test the response of the system to inaccurate initial conditions. These two other conditions are a uniform head of 100 ft everywhere (all layers), except at the stream, and a linearly changing initial head ranging from 95 ft to 0 ft at the stream. The response of the system over time in response to the pumping well compared to the correct response that used the steady-state head distribution is shown in figure 15 for a cell in layer 1 at the divide and for the cell containing the well in layer 3. The time constant can also be calculated for this system, although some approximations must be made to estimate a saturated thickness. If the saturated thickness of the unconfined aquifer is assumed to be 100 ft (the thickness at the stream), then the time constant is calculated as:

$$T = \frac{0.2(20,000\,\text{ft})^2}{100.\text{ft}(50\ \text{ft/d})} = 1.6\times 10^4 \text{ days} = 44 \text{ years}.$$

As shown in figure 15, the curves for the two inaccurate initial conditions do not approach the correct transient response until about 20 to 40 years after the start of pumping. Thus, inaccurate initial conditions can cause errors for a significant time period in transient simulations.

Examination of the simulated response through time from 0-5 years in the finite-difference cell containing the well illustrates some interesting points. The correct response of the system is simulated for the case with the steady-state heads as the initial conditions (fig. 16); the initial value for the head is 50.09 ft in the cell containing the well. The case with the linearly varying heads as initial conditions has the initial value for the cell containing the well equal to 50.0 ft, which is almost the same as the correct steady-state value. Even though the initial conditions in the individual cell are almost the same, the response is different, because the initial conditions over the entire model domain affect the head response. The response of the system with the linearly varying initial conditions is obviously in error because the response of the system shows an increase in head after the first time step in response to pumping, which is not physically reasonable.

Questions to be used in evaluating the initial conditions of a ground-water flow model are:

1. Does the transient model simulation start from a steady-state condition?

If yes –

A. Were the initial conditions generated from a steady-state simulation of the period of equilibrium, which is the preferred method?

B. If the initial conditions were not generated from a steady-state simulation of the period of equilibrium, then is there a compelling reason why they were not generated, or are the initial conditions invalid?

If no –

A. Was it possible to select a period of equilibrium to start the simulation and make the determination of initial conditions more straightforward? If it is possible, then the model should have simulated the transient period from the period of equilibrium.

B. If it was not possible to select a period of equilibrium to start the simulation, then what was the justification for selecting the starting time and the initial conditions for the simulation? How was it shown that the initial conditions used did not bias the result of the simulation?

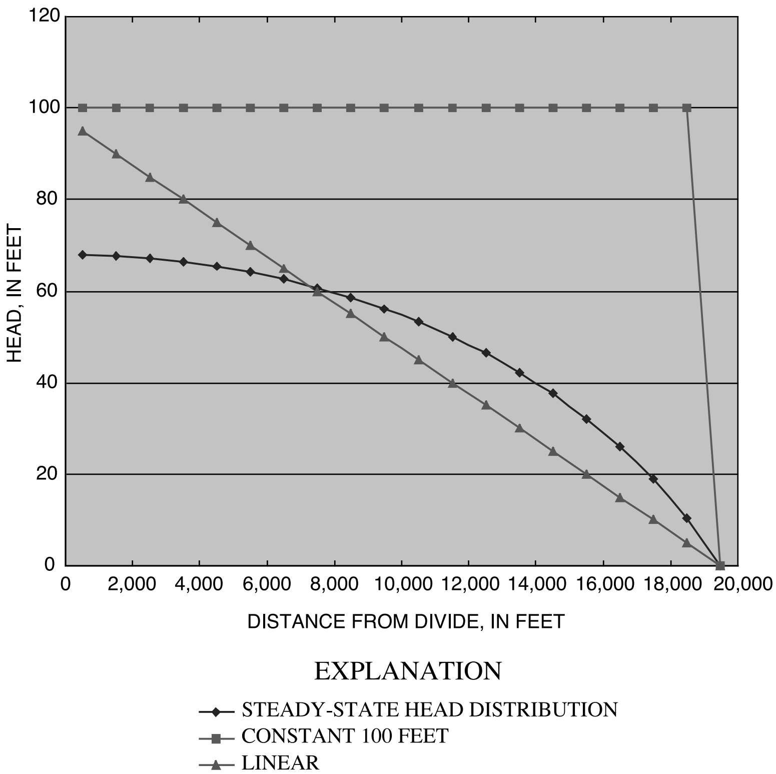


Figure 14. Head distribution along a model row from the divide to the constant-head node for three different initial conditions used for a transient simulation.

Accuracy of the Matrix Solution

Discrete numerical models involve the solution of large sets of simultaneous algebraic equations (Harbaugh and others, 2000). This solution of large sets of algebraic equations usually involves the use of sophisticated matrix solution techniques. Most of the solution techniques are iterative in nature whereby the solution is obtained through successive approximation, which is stopped when it is determined that a "good" solution has been obtained (Bennett, 1976). The criterion used in most iterative solution techniques is called the "head change criterion." When the maximum absolute value of head change from all nodes during an iteration is less than or equal to the selected head change criterion, then iteration stops.

When evaluating a ground-water flow model, even if the computer model has output results, one must check to determine if indeed a solution has been obtained by the matrix solution technique. The first check is to evaluate the head change criterion. Was the head change criterion set small enough to obtain a model solution with minimal error? One means of evaluating the head change criterion is to examine the global mass balance for the model. If the error in the mass balance (for example, total inflow minus total outflow divided by one half the sum of the inflow and outflow) over the entire model domain is small, usually less than

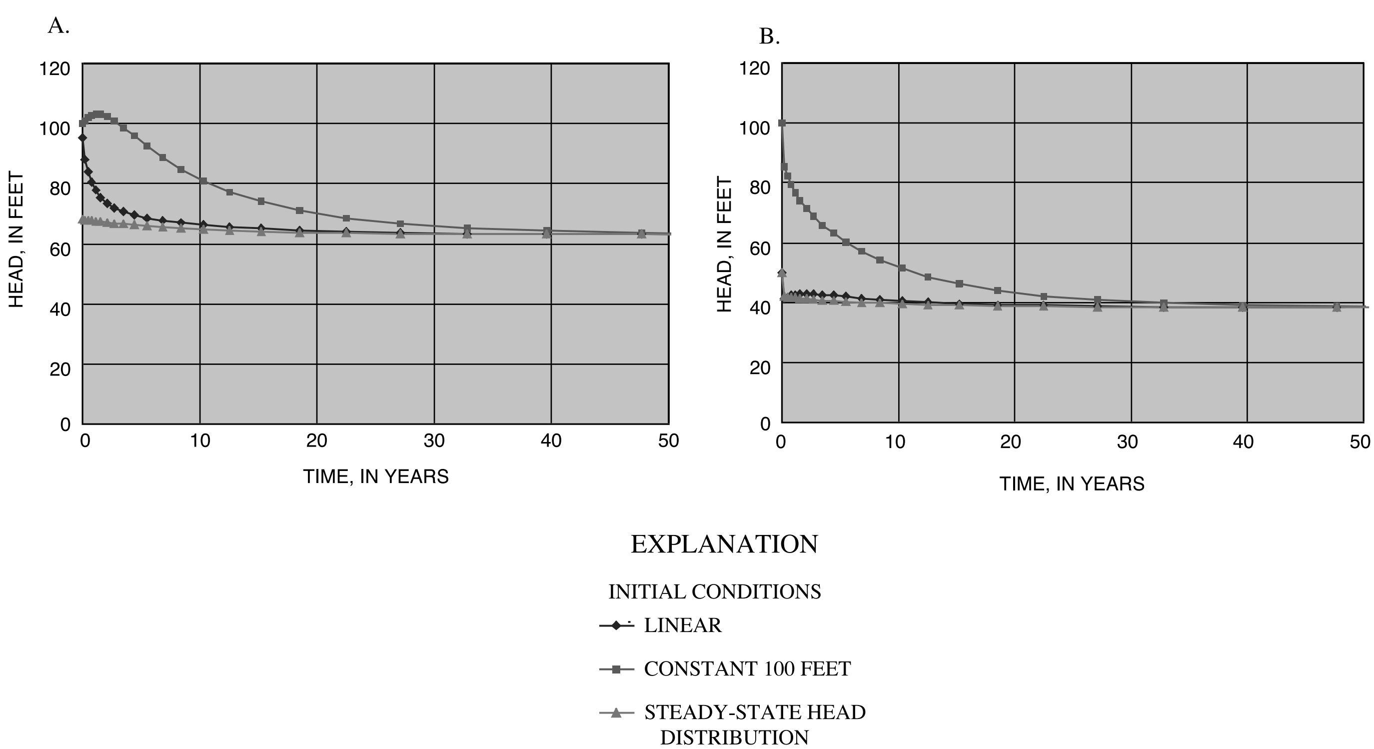


Figure 15. Head in a cell through time in response to a well discharging at a rate of 100,000 ft^3/d: (A) the head in layer 1 at the divide, and (B) the head in the cell with the discharging well in layer 3.

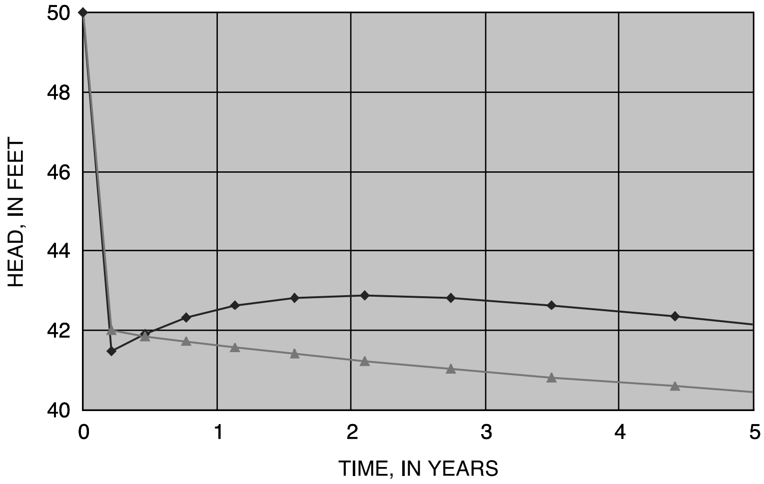


Figure 16. Head in the well for the first 5 years after the start of pumping for the cases using the initial conditions of the steady-state head distribution and the linearly varying head distribution.

0.5 percent, then the head change criterion is assumed to have been sufficient. If the error in the mass balance calculations is significant, then the matrix solution was not good and the model should be corrected by improving the matrix solution. The matrix solution can be improved by lowering the head change criterion, adjusting iteration parameters (if the solution techniques use iteration parameters), using different starting heads for steady-state simulations, or using a different solution technique.

Even if the head change criterion is met and the global mass balance error is small, the model solution may not be appropriate for the system under investigation. Two potential reasons are that some models can either be mathematically nonunique or very nonlinear. The mathematically nonunique problem usually is a poorly posed problem where a model has only specified-flow boundary conditions and no other boundary condition that specifies a head or datum (such as, constant head, river stage, general head boundary, etc.). In this type of problem, there is a family of solutions all with the same gradients but different absolute heads. The matrix solution technique may not converge or it may converge to one of the infinite number of possible solutions.

In nonlinear problems, the solution affects the coefficients of the matrix being solved; thus, the solution affects the problem being solved. As a result, the manner in which the iterative solution technique approaches a solution can affect the final solution. An example from Reilly (2001) illustrates this point. Consider a one-dimensional water-table system with a sloping impermeable bottom that contains a specified head and extends 5,000 m, with an areal recharge rate of 0.5 m/yr. The starting head for the equation solution is specified at 20 m, which is above all the bottom elevations of the cells but yet close to the magnitude of the expected results. Figure 17A is a cross-sectional view of a finite-difference representation of the steady-state solution. The cell farthest from the specified head is simulated as being dry. The total recharge flowing to the specified head cell for a 500-m width is 2,740 m^3/d. The convergence criterion of the model was met and the mass balance was excellent (showing 0.00 percent budget discrepancy). Now consider figure 17B, which is the result of a simulation of the same problem, except the starting head for the matrix solution was set at 100 m. As is shown in figure 17 and table 2, three cells are now simulated as being dry. The result is that less recharge is simulated as entering the model and the heads and water budgets are reduced accordingly, with only 2,055 m^3/d being represented as recharge entering the system for a 500-m width. Although both solutions converged and had excellent mass balances, at least one of them is incorrect. Because it is a nonlinear problem, it is not easy to determine which solution is correct. The rate of convergence and the method of making cells inactive must be considered and evaluated. After evaluating these aspects, and noting that the head in cell 7 (table 2 and fig. 17) of the second model is above the bottom elevation of cell 8, which was converted to dry during the iterative process, it seems that the first model most likely is correct. In the second model, the iterative solution, in attempting to converge, apparently overshot the bottom of some of the cells, which prematurely or erroneously truncated the area from the active model domain,

Table 2. Heads calculated for the same system with areal recharge and two different intitial heads.

[m, meters]

Cell number	Bottom elevation of cell	Head calculated with the initial head at 20 m	Head calculated with the initial head at 100 m
1	-30.0	0.00	0.00
2	-25.0	1.93	1.46
3	-20.0	3.83	2.86
4	-15.0	5.68	4.17
5	-10.0	7.49	5.38
6	-5.0	9.24	6.42
7	0.0	10.90	7.20
8	5.0	12.45	Dry
9	10.0	13.81	Dry
10	15.0	Dry	Dry

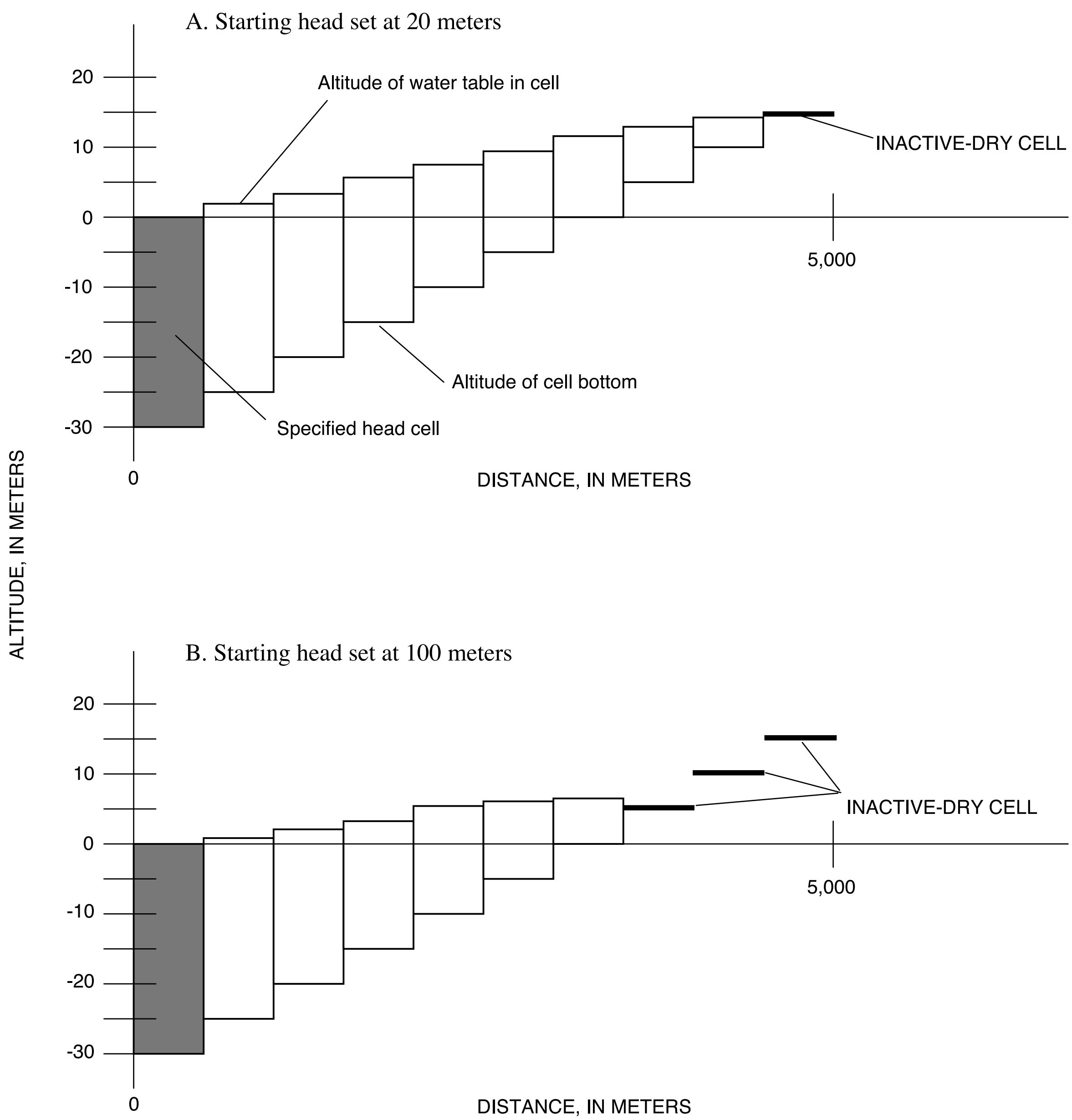


Figure 17. Cross-sectional view of a finite-difference representation simulating a variable thickness ground-water system with flow to a specified head due to areal recharge: (A) starting head set at 20 meters, and (B) starting head set at 100 meters. (From Reilly, 2001.)

and resulted in the wrong problem being solved. The model developer or user must carefully evaluate nonlinear problems and monitor the rate of convergence to ensure that cells that should be part of the active problem domain are not removed.

The accuracy of the matrix solution usually is not an issue with ground-water models that meet the head change criterion and have small mass balance errors. It is important when using models and especially nonlinear models, however, to keep in mind that the accuracy of the solution is not assured, which is another aspect for continued evaluation. Some models do not converge smoothly, and investigators use non-standard methods (tricks) to obtain a model solution. For example, some non-standard methods that have been used include: the saving of intermediate solutions that have not yet converged and changing matrix solution parameters when restarting the model; making a nonlinear water-table simulation linear by fixing the saturated thickness of the model; and obtaining a steady-state solution by using storage to slow convergence and damp the approach to the solution through simulating a long transient time period. As long as the non-standard method does not violate any important hydrologic process, they are usually transparent to the final solution and are appropriate. However, these non-standard techniques should be evaluated to determine whether they cause potential errors to be introduced to the model solution.

Questions to be addressed when evaluating the adequacy of the matrix solution in the simulation of a ground-water system are:

1. Is the ground-water system and set of matrix equations linear or nonlinear?

If linear –

A. Was the head change criterion met and was it sufficiently small to obtain an acceptable (that is, less than 0.5 percent error) global mass balance?

If nonlinear –

A. Was a nonlinear matrix solution technique used?

B. Was the head change criterion met and was it sufficiently small to obtain an acceptable (that is, less than 0.5 percent error) global mass balance?

C. Did the nonlinear terms, such as cells going dry or drains turning off, behave smoothly during the iteration process? Or were there large oscillations that would indicate a potential for convergence to an incorrect solution?

D. Were any "tricks" used to smooth convergence, such as setting saturated thickness as a constant in water-table simulations, and are the assumptions used in defining these artificially constrained features reasonable for the solution obtained?

2. Does the solution seem reasonable for the problem posed? If it is not and there are no input data errors, then another matrix solution technique should be tried to determine whether it is a matrix-solution issue or some other problem.

Adequacy of Calibration for Intended Use of Model Results

As discussed previously, not all objectives of using a ground-water model require calibration. For models that require calibration, however, an evaluation of the adequacy of the calibration is another difficult task. There are different quantitative measures that investigators use to show the accuracy of the calibration of a ground-water flow model. Some of these are: the mean error, the mean absolute error, and the root mean squared error (Anderson and Woessner, 1992). The areal distribution of residuals (differences between measured and simulated values) also is important to determine whether some areas of the model are biased either too high or too low. The difficulty that arises, however, is how to determine what is good enough.

As stated previously, key aspects of the model, such as the conceptualization of the flow system, that influence the appropriateness of the model to address the problem objectives, are often not considered during calibration by many investigators; their focus is on the quantitative measures of goodness of fit. However, the appropriateness of the conceptualization of the ground-water system and processes should always be evaluated during calibration. Thus, the method of calibration, the closeness of fit between the simulated and observed conditions, and the extent to which important aspects of the simulation were considered during the calibration process are all important in evaluating the appropriateness of the model to address the problem objectives.

Freyberg (1988) reported on a class exercise where different models were calibrated by students using the same model and identical sets of data. Freyberg's observations of the exercise showed that "success in prediction was unrelated to success in matching observed heads under premodification conditions." He concluded, "good calibration did not lead to good prediction." This is not to imply that matching heads is unimportant, only that there are other factors that need to be considered in determining the "goodness" of a model. Put in terms of logic, a good match between calculated and observed heads and flow is a necessary condition for a reasonable model, but it is not sufficient. The conceptual model and the mathematical representation of all the important processes must also be appropriate for the model to accurately represent the system under investigation. Thus, a model that matches heads and flows well must also be evaluated to determine if it is a reasonable representation of the system under study. As stated by Bredehoeft (2003), "A wrong conceptual model invariably leads to poor predictions, no matter how well the model is fit to the data."

Thus, the evaluation of the adequacy of the calibration of a model should be based more on the insight of the investigators and the appropriateness of the conceptual model rather than the exact value of the various measures of goodness of fit. For example, it would be possible to specify every cell in a model that had an observation associated with it as a specified head cell in the model. This would produce a perfect match between simulated and observed heads, however, it is conceptually unreasonable to simulate random cells as specified heads that could serve as sources and sinks of water. Thus, although the measures of calibration might make it appear to be a well-calibrated model, in effect the violation of a reasonable conceptual model makes it a poor model. A model developed according to a well-argued conceptual model with minor adjustments, in our opinion, is generally superior to a model that has a smaller discrepancy between simulated and observed heads because of unjustified manipulation of the parameter values. A reasonable representation of the conceptual model and sources of water is more important than blindly minimizing the discrepancy between simulated and observed heads.

Models can be calibrated by trial and error or by automatic parameter estimation techniques, such as nonlinear regression to minimize some measure of goodness of fit between the simulated and observed values. A key concept in automatic parameter estimation methods is that a limited set of parameters used in the model is designated to be automatically adjusted. These parameters usually are identified for specific regions (or zones) of the model that are determined before the calibration process (a priori). An example of parameter zones for hydraulic conductivity is shown in figure 18 for the top two layers of a model of the Albuquerque Basin, New Mexico (Tiedeman and others, 1998). In this example, the zones represent different hydrogeologic units. The areal extent of these units remains fixed during automatic calibration, and the conceptualization of the location and extent of these zones is part of the information specified before the automatic calibration process. The parameters and boundary conditions that are not identified for automatic calibration either remain fixed at their initial values or must be calibrated by trial and error. In addition, most automatic calibration methods weight observations according to the investigators insight into the reliability of the observations. Obviously, if the model is conceptualized incorrectly, the parameter zones are not representative of the actual parameter distribution, the fixed parameters and boundary conditions are poorly chosen, or the weighting functions are not appropriate, then the resultant estimates of the parameter values will be inaccurate even if the residual between observed and simulated conditions is automatically minimized.

If there are errors in the model conceptualization, the parameter zones selected, and the weighting functions defined for observed values, then the parameter estimation methods will provide the best parameters for the poorly defined model. This does not mean that the model will be an accurate representation of the system or will produce reasonable predictions. Perhaps the best use of the formal parameter estimation methods is to test different model, zone, and weighting function conceptualizations and determine which conceptualizations are most reasonable. In testing alternative models, Hill (1998) states that better models will have “three attributes: better fit, weighted residuals that are more randomly distributed, and more realistic optimal parameter values.” This approach was used by Yager (1996) to test three different model conceptualizations for the Niagara Falls area in New York and by Tiedeman and others (1998) to test six different system conceptualizations of the Albuquerque Basin system. This use of parameter estimation provides a quantitative means (although some subjectivity comes into determining which model is good enough) to test different conceptualizations.

In trial and error calibration, investigators have the ability to continuously change their conceptualization of the system and parameter distributions in order to improve the calibration fit, although the benefits of these changes are frequently difficult to quantify. It is the insight and skill of the investigator during a trial and error calibration that will control how well a model represents the ground-water system under investigation. In evaluating the adequacy of a model calibration, the conceptual model and the insight of the investigators generally are more important than just an evaluation of quantitative measures of goodness of fit.

Questions to be addressed in evaluating the adequacy of calibration of a model using either trial and error or automatic methods are:

1. Is the conceptual model of the system under investigation reasonable?
2. Are the mathematical representations of the boundary conditions reasonable for the objectives of the study?
3. Does the simulated head and flow distribution mimic the important aspects of the flow system, such as magnitude and direction of the head contours?
4. Does some quantitative measure of head and flow differences between the simulated and observed values seem reasonable for the objectives of the investigation?
5. Does the distribution of areas where simulated heads are too high and areas where simulated heads are too low seem randomly distributed? If they are not randomly distributed, then is there a hydrogeologic justification to change the model and make the residuals more random areally?

Just because a model is constructed and calibrated, does not ensure that it is an accurate representation of the system. The appropriateness of the boundaries and the system conceptualization is frequently more important than achieving the smallest differences between simulated and observed heads and flows.

Model Input Data, Output Listing, and Report Consistency Check

In evaluating the adequacy of a model, the input data, output listing, and report ideally should be compared with each other to ensure that they all represent the same analysis. Depending on the level of evaluation being undertaken, this comparison can vary greatly in its thoroughness. Many times the output listing and input data sets are not available to the person evaluating the model, so there is nothing that can be checked.

If the listing file is available, then it is useful as a minimum to compare some of the model output to information in the report. The simulated water budget in the output listing can be compared to budget values determined from the system conceptualization and real-world measurements provided in the report. For example, if the areal recharge rate is specified in the report, the total recharge over the modeled area can be calculated and compared to the reported recharge in the model budget. Heads or drawdowns in the model output listing can be compared to values in the report.

If a more thorough evaluation is required, then the input data can also be checked. Although it is impossible to ensure that all the preprocessor steps and manual data entry were undertaken correctly, data checking can increase confidence that the model is consistent with the description in the report. Whether the model data files were constructed by manually entering information into files or by using a graphical user interface, there is the possibility that the data files contain errors.

Figure 18. Hydraulic-conductivity zones identified for automatic parameter estimation in a ground-water flow model of the Albuquerque Basin, New Mexico: (A) zones in model layer 1, and (B) zones in model layer 2. (From Tiedeman and others, 1998.)

Examples of possible errors are: numbers scaled improperly, inconsistent data, data entered into incorrect fields, data assigned to incorrect cells, typographical errors, and many others. An example of inconsistent data is the use of inconsistent time or space units for different parts of the data. For example, pumping might be entered in cubic feet per second (ft^3/s) and hydraulic conductivity in feet per day (ft/d). An example of data assigned to incorrect cells is the specification of stress data, for example pumping wells located in inactive cells.

The extent to which the input data can be checked depends on the size of the model, available resources, and how the data were entered. Typical models vary in size from several thousand cells to over a hundred thousand cells. There are multiple data values per cell, so it is impractical to check every input value in even the smaller models. Thus, data scanning is a better term to describe the data-checking process. If data files are available, then they can be checked or scanned directly. If the output listing is available and if this listing contains an echo of the input data, then usually it is easier to examine the output listing than the input files. Also, seeing the data in the output listing provides added confirmation that the data files have been properly read by the model program.

Some checks that can be considered are:

1. Do the model water-budget quantities seem appropriate for the values described for the actual system in the report?
2. Are the input data the same as those described in the report?
3. Are data values consistent and assigned to appropriate cells?

Checking the information that is read directly by the model increases confidence that the simulation is indeed a solution to the problem described. The level of evaluation required determines the thoroughness of the consistency check that should be undertaken.

Model Reporting and Archiving

Because models are embodiments of scientific hypotheses, a clear and complete documentation of the model development is required for individuals to understand the hypotheses, to understand the methods used to represent the actual system with a mathematical counterpart, and to determine if the model is sufficiently accurate for the objectives of the investigation. As stated in U.S. Geological Survey Office of Ground Water Technical Memorandum 96.04 (see appendix), there is no rigid checklist or recipe for reporting on the use of simulation in a ground-water study. The appropriate level of documentation will vary depending on the study objectives and the complexity of the simulations. A valuable result of the ground-water modeling effort is the insight gained by the investigator during the modeling process about the functioning of the flow system. This understanding of the flow system gained during the modeling process can be an important product of the study and should be appropriately discussed and documented in the modeling report.

The general structure of a well-constructed report describing simulation is much the same as that for any investigative study. It should present (1) the objectives of the study, (2) a description of the work that was done, (3) logical arguments to convince the reader that the methods and analyses used in the study are valid, and (4) results and conclusions.

Ten specific topics that should be addressed in reports that describe studies in which simulation is used are listed and explained in U.S. Geological Survey Office of Ground Water Technical Memorandum 96.04 to aid individuals in documenting their model studies. These 10 topics are:

1. Describe the purpose of the study and the role that simulation plays in addressing that purpose.
2. Describe the hydrologic system under investigation.
3. Describe the mathematical methods used and their appropriateness to the problem being solved.
4. Describe the hydrogeologic character of the boundary conditions used in the simulation of the system.
5. If the method of simulation involves discretizing the system (finite-difference and finite-element methods for example), describe and justify the discretized network used.
6. Describe the aquifer system properties that are modeled.
7. Describe all the stresses modeled such as pumpage, evapotranspiration from ground water, recharge from infiltration, river stage changes, leakage from other aquifers, and source concentrations in transport models.
8. For transient models, describe the initial conditions that are used in the simulations.
9. If a model is calibrated, present the calibration criteria, procedure, and results.
10. Discuss the limitations of the model's representation of the actual system and the impact those limitations have on the results and conclusions presented in the report.

Once the study is finished, it is always useful to organize and archive the model files. The purpose of the archive is to ensure that the results are reproducible in the future either by the model developer or other interested parties. Thus, the archive should reference any published reports on the model and provide enough explanation in a text "readme" file for the model to be used by others. The archival of the model provides good scientific practice and reproducibility of results.

Summary

Ground-water models are designed and built to meet specific objectives. Models must be critically evaluated to ensure that there are no data input errors and that the conceptual model does indeed accurately represent the actual ground-water system sufficiently to meet the objectives of the study. The items to be evaluated are: the appropriateness of the model program, the discretization and representation of the geologic framework, the representation of the boundary conditions, the representation of the initial conditions, and the accuracy of the matrix solution.

Ground-water flow models attempt to reproduce, or simulate, the operation of a real ground-water system using a mathematical counterpart (a mathematical model). Thus, the evaluation of the model is intended to ensure that the model program and numerical representation of the important aspects of the system are sufficient to meet the objectives of the study. The guidelines presented in this report raise some of the important aspects of model evaluation.

Acknowledgments

The technical review and improvement of the report by William Alley, James Bartolino, William Cunningham, and Keith Prince are gratefully acknowledged. Sandra Cooper provided editorial review and assistance. The final report and illustrations were prepared by E.G. Baker and K.A. Waltenbaugh, and J.E. Banton, respectively.

References

Anderman, E.R., and Hill, M.C., 2000, MODFLOW-2000, the U.S. Geological Survey Modular Ground-Water Model—Documentation of the hydrogeologic-unit flow (HUF) package: U.S. Geological Survey Open-File Report 00-342, 89 p.

Anderson, M.P., and Woessner, W.W., 1992, Applied Groundwater Modeling—Simulation of flow and advective transport: Academic Press, Inc., San Diego, Calif., 381 p.

Barlow, P.M., 1994, Two- and three-dimensional pathline analysis of contributing areas to public-supply wells of Cape Cod, Massachusetts: Ground Water, v. 32, no. 3, p. 399–410.

Bennett, G.D., 1976, Introduction to ground-water hydraulics—A programmed text for self-instruction: Techniques of Water-Resources Investigations of the United States Geological Survey, Book 3, Chapter B2, 172 p.

Bredehoeft, J.D., 2003, From models to performance assessment: The conceptualization problem: Ground Water, v. 41, no. 5, p. 571-577.

Buxton, H.T., and Reilly, T.E., 1987, A technique for analysis of ground-water systems at regional and subregional scales, applied on Long Island, New York: U.S. Geological Survey Water-Supply Paper 2310, p. 129-142.

Buxton, H.T., Reilly, T.E., Pollock, D.W., and Smolensky, D.A., 1991, Particle tracking analysis of recharge areas on Long Island, New York: Ground Water, v. 29, no. 1, p. 63-71.

Buxton, H.T., and Smolensky, D.A., 1999, Simulation of the effects of development of the ground-water flow system of Long Island, New York: U.S. Geological Survey Water-Resources Investigations Report 98-4069, 57 p.

Buxton, H.T., Smolensky, D.A., and Shernoff, P.K., 1999, Feasibility of using ground water as a supplemental supply for Brooklyn and Queens, New York: U.S. Geological Survey Water-Resources Investigations Report 98-4070, 33 p.

Collins, R.E., 1961, Flow of fluids through porous materials: Reinhold Publishing Corp., N.Y., 270 p.

Domenico, P.A., and Schwartz, F.W., 1998, Physical and Chemical Hydrogeology (Second Edition): John Wiley and Sons, New York, N.Y., 506 p.

Franke, O.L., and Reilly, T.E., 1987, The effects of boundary conditions on the steady-state response of three hypothetical ground-water systems—Results and implications of numerical experiments: U.S. Geological Survey Water-Supply Paper 2315, 19 p.

Franke, O.L., Reilly, T.E., and Bennett, G.D., 1987, Definition of boundary and initial conditions in the analysis of saturated ground-water flow systems—An introduction: U.S. Geological Survey Techniques of Water-Resources Investigations 3-B5, 15 p.

Franke, O.L., Reilly, T.E., Pollock, D.W., and LaBaugh, J.W., 1998, Estimating areas contributing recharge to wells—Lessons from previous studies: U.S. Geological Survey Circular 1174, 14 p. (Third printing, 1999.)

Freyberg, David L., 1988, An exercise in ground-water model calibration and prediction: Ground Water, v. 26, no. 3, p. 350-360.

Harbaugh, A.W., Banta, E.R., Hill, M.C., and McDonald, M.G., 2000, MODFLOW-2000, The U.S. Geological Survey Modular Ground-Water Model—User guide to modularization concepts and the ground-water flow process: U.S. Geological Survey Open-File Report 00-92, 121 p.

Hill, M.C., 1998, Methods and guidelines for effective model calibration: U.S. Geological Survey Water-Resources Investigations Report 98-4005, 90 p.

Hill, M.C., Cooley, R.L., and Pollock, D.W., 1998, A controlled experiment in ground-water flow model calibration: Ground Water, v. 36, no. 3, p. 520-535.

Konikow, L.F., and Reilly, T.E., 1999, Groundwater modeling: *in* Delleur, J.W. (ed.), The handbook of groundwater engineering: CRC Press, Boca Raton, Fla., 40 p.

Leake, S.A., and Claar, D.V., 1999, Procedures and computer programs for telescopic mesh refinement using MODFLOW: U.S. Geological Survey Open-File Report 99-238, 53 p.

Luckey, R.R., Gutentag, E.D., Heimes, F.J., and Weeks, J.B., 1986, Digital simulation of ground-water flow in the High Plains aquifer in parts of Colorado, Kansas, Nebraska, New

Mexico, Oklahoma, South Dakota, Texas, and Wyoming: U.S. Geological Survey Professional Paper 1400-D, 57 p.

Masterson, J.P., Walter, D.A., and Savoie, Jennifer, 1997, Use of particle tracking to improve numerical model calibration and to analyze ground-water flow and contaminant migration, Massachusetts Military Reservation, western Cape Cod, Massachusetts: U.S. Geological Survey Water-Supply Paper 2482, 50 p.

McAda, D.P., 2001, Simulation of a long-term aquifer test conducted near the Rio Grande, Albuquerque, New Mexico: U.S. Geological Survey Water-Resources Investigations Report 99-4260, 66 p.

McDonald, M.G., and Harbaugh, A.W., 1988, A modular three-dimensional finite-difference ground-water flow model: Techniques of Water-Resources Investigations of the United States Geological Survey, Book 6, Chapter A1, 586 p.

Modica, Edward, Reilly, T.E., and Pollock, D.W., 1997, Patterns and age distribution of ground-water flow to streams: Ground Water, v. 35, no. 3, p. 523-537.

Morrissey, D.J., 1989, Estimation of the recharge area contributing water to a pumped well in a glacial-drift, river-valley aquifer: U.S. Geological Survey Water-Supply Paper 2338, 41 p.

Pollock, D.W., 1989, Documentation of computer programs to compute and display pathlines using results from the U.S. Geological Survey modular three-dimensional finite-difference ground-water flow model: U.S. Geological Survey Open-File Report 89-381, 188 p.

Prince, K.R., and Schneider, B.J., 1989, Estimation of hydraulic characteristics of the Upper Glacial and Magothy aquifers at East Meadow, New York, by use of aquifer tests: U.S. Geological Survey Water-Resources Investigations Report 87-4211, 43 p.

Reilly, T.E., 2001, System and boundary conceptualization in ground-water flow simulation: U.S. Geological Survey Techniques of Water-Resources Investigations, Book 3, Chapter B8, 26 p.

Reilly, T.E., Franke, O.L., and Bennett, G.D., 1987, The principle of superposition and its application in ground-water hydraulics: U.S. Geological Survey Techniques of Water-Resources Investigations 3-B6, 28 p.

Reilly, T.E., and Pollock, D.W., 1993, Factors affecting areas contributing recharge to wells in shallow aquifers: U.S. Geological Survey Water-Supply Paper 2412, 21 p.

Tiedeman, C.R., Kernodle, J.M., and McAda, D.P., 1998, Application of nonlinear-regression methods to a ground-water flow model of the Albuquerque Basin, New Mexico: U.S. Geological Survey Water-Resources Investigations Report 98-4172, 90 p.

Yager, R.M., 1996, Simulated three-dimensional ground-water flow in the Lockport Group, a fractured-dolomite aquifer near Niagara Falls, New York: U.S. Geological Survey Water-Supply Paper 2487, 42 p.

Appendix

April 24, 1996

OFFICE OF GROUND WATER TECHNICAL MEMORANDUM NO. 96.04

Subject: PUBLICATIONS—Policy on documenting the use of ground-water simulation in project reports

It has been more than two decades since Ground Water Branch Technical Memorandum No. 75.11 was released on the subject of documenting the use of ground-water simulation in project reports. Because of the time lapse, changes in modeling techniques, and the frequency of problems found when reports are reviewed, a revisit to policy on this subject is appropriate.

There is no rigid checklist or recipe for reporting on the use of simulation in a ground-water study. The appropriate level of documentation will vary depending on the project objectives and the complexity of the simulations. The general structure of a well-constructed report describing simulation is much the same as that for any investigative study. It should present (1) the objectives of the study, (2) a description of the work that was done, (3) logical arguments to convince the reader that the methods and analyses used in the study are valid, and (4) results and conclusions.

Specific topics that should be addressed in reports that describe studies in which simulation is used include the following.

1. Describe the purpose of the study and the role that simulation plays in addressing that purpose.

   The objective of the simulation must be clearly stated. The model should be represented as a tool to help solve specific problems or answer specific questions rather than as an end product.

2. Describe the hydrologic system under investigation.

   The extent, nature of boundaries, transmitting properties, storage properties, sources of water, discharge mechanisms and other relevant components of the ground-water system should be described as known or conceptualized. Usually this can be accomplished in part by referencing previous works, but major relevant system characteristics should be summarized in the report that describes the simulation.

3. Describe the mathematical methods used and their appropriateness to the problem being solved.

   In most cases, a reference to a readily available publication will be sufficient to document mathematical details; however, it will usually be desirable to briefly summarize the methods that are used. For a well-documented computer program, this will often require only a paragraph or two. If a documented computer program is modified such that computed values are affected, the modifications should be documented and evidence that the modifications are correct should be supplied.

4. Describe the hydrogeologic character of the boundary conditions used in the simulation of the system.

   In many cases, the model boundaries are placed where the aquifer terminates against relatively impermeable rocks or is intersected by a perennial stream whose head variation in time and space is known. In other cases, the aquifer may be so extensive relative to the area of interest that the modeled area may need to extend beyond the project area to accurately simulate the natural boundaries of the aquifer system. If the modeled area is arbitrarily truncated at some distance from the area of interest, it should be shown that the selection of the arbitrary boundary condition does not materially affect the ability of the model to simulate the system for the purposes of the study. Internal boundaries such as streams, lakes, and pinchouts of important hydrogeologic zones should be identified and their representation in the model should be described in the report. A clear, convincing argument of the appropriateness of the boundary conditions used in the model to represent the actual system should be made for the entire bounding surface of the modeled volume or cross section, as well as for any internal boundaries.

5. If the method of simulation involves discretizing the system (finite-difference and finite-element methods for example), describe and justify the discretized network used.

   The spacing and distribution of the blocks, elements, or subregions should reflect, in part, the spatial variability of the hydraulic parameters and the location of boundaries (for example streams, lakes, bed pinchouts), human-made features (for example wells and dams), and stresses. In most cases, a map showing the discretized network superimposed on the study area is required. Vertical discretization should be described and/or shown on illustrations. The manner in which time is discretized for transient models also should be described. If a steady-state model is used to simulate an average or approximate steady-state condition, discuss the errors that could be introduced in the study results as a consequence of using a steady-state model.

6. Describe the aquifer system properties that are modeled.

   Explain whatever inferences are made from field data and previous studies as to the spatial variation of hydraulic properties of aquifers and confining beds and how discretized values are computed throughout the simulated area. During model calibration (see item 9), modeled values are often changed; the final aquifer system properties that are modeled should be described in the report. This can be through maps or descriptions in the text. Lists of model arrays do not generally provide much understanding of the model and accordingly should not be included in the report unless it is expected that readers will want to repeat the simulations. If lists of arrays are included, they should usually be provided on electronic media. Note that Office of Ground Water Technical Memorandum No. 93.01 describes the separate requirement for archiving the complete model data sets used in ground-water projects.

7. Describe all the stresses modeled such as pumpage, evapotranspiration from ground water, recharge from infiltration, river stage changes, leakage from other aquifers, and source concentrations in transport models.

   The relations between observed and modeled stresses should be described. For example, it usually is desirable to provide a representative sample of actual pumping histories and the corresponding modeled pumping histories, although such information would not necessarily be provided for every pumped well. The manner in which stresses are averaged within the discretized time and space scheme should also be described. If a steady-state model is used to simulate an average or approximate steady-state condition, describe how the average stresses representing this system are calculated.

8. For transient models, describe the initial conditions that are used in the simulations.

   Ideally, a transient simulation will start from a steady-state condition, and the steady-state initial conditions will be generated by a steady-state simulation using the same model. In this case, the steady-state simulation must use the same hydraulic and stress parameters that are used in the transient simulation, except that the transient stresses are removed. In situations where it is not possible to start a transient model from a simulated steady-state condition, it is necessary to describe how the initial conditions were derived. It is also important to estimate the error in the derived values and the possible impact on the model results.

9. If a model is calibrated, present the calibration criteria, procedure, and results.

   Describe the source of the observed data to which model results are compared. Explain the appropriateness of using these data for model comparisons and the rationale for any adjustments made to actual observations when making the comparisons. For example, when steady-state models are used to simulate an approximate steady-state condition, it is important to explain to what extent the observations that have been made at specific points in time correspond to the approximate steady-state condition being simulated. Give a representative sample of the actual comparisons used for calibration, and show the locations of the observation points on maps. When the number of observations is extensive, locations of representative points can be shown. It is important to report and use as many types of data as possible for calibration. For example, in a flow model, both head and flow observations are desirable for use in calibration.

10. Discuss the limitations of the model's representation of the actual system and the impact those limitations have on the results and conclusions presented in the report.

    Evaluating the sensitivity of the computed model responses to changes in parameter values that reflect plausible parameter uncertainty helps to assess the model reliability. If the model is to be used to make specific projections, it is useful to estimate the impacts of the uncertainty of parameter values on the projections. In calibrated models, a concern is nonuniqueness, which is the extent to which other combinations of parameter values or configurations may result in an equally good fit to the observed data. Discuss the extent to which nonuniqueness may affect the use of the model in the study.

In summary, a report describing a study in which simulation is used should address the above topics; however, there is considerable flexibility in the form of such a report. The report should describe the purpose of the simulation and convince the reader that the use of simulation is credible. The report should further describe the system being simulated, the methods of simulation, and the data that are used.

William M. Alley
Chief, Office of Ground Water

Distribution: A, B, S, FO, PO

This memorandum supersedes Ground Water Branch Technical Memorandum No. 75.11

EXHIBIT 7

Addendum – Imputation of Missing Rainfall Data

On October 25, 2024, R. Jeffrey Davis and I submitted a report titled "*Tarawa Terrace Flow and Transport Model Post-Audit"* describing a set of groundwater flow and transport simulations we performed and analyzed and our resulting conclusions. As part of that process, I performed a data imputation step on the rainfall data we used. This step was not described in the report. During my deposition on February 14, 2025, the attorney for the Department of Justice presented me with some gaps in the original rainfall data and at the time I could not recall how these gaps were imputed to generate the complete rainfall data set we presented in the post-audit report. I subsequently reviewed my analysis to determine the source of those data values. The objective of this addendum is to provide a description of the data imputation step I had previously used to generate this rainfall data.

In order to extend the original Tarawa Terrace model from the original simulation period of 1953 – 1994 to include the years 1995 – 2008 required by the post-audit, one of the steps involved was to generate aquifer recharge data over this extended period. This process was described in Section 3.2 of our post-audit report. As described in this section, we followed the same process used in the original model construction where a recharge coefficient of 0.235 was applied to the annual rainfall totals to get a net recharge value that was then applied to the year in question as a constant rate over that year.

To estimate the annual rainfall values, we obtained rainfall data from three nearby rain gauge stations from a *National Oceanic and Atmospheric Administration National Weather Service* website (NOAA, 2024). The rainfall data from this website for each station was provided to the Department of Justice along with our report (files CL_PLG-EXPERT_DAVIS_0000000203- CL_PLG-EXPERT_DAVIS_0000000205). The annual rainfall totals for each of the three stations were extracted for the years 1995 – 2009 from the last column of data for each station. However, some of the years had missing annual totals, indicated by the presence of an "M" in the data files. To fill in the missing values so that we had a complete set of numbers from which we could compute an average value to use in the simulation, I imported the annual rainfall data into Python, where I treated the data from each station as a time series and imputed the gaps using the PCHIP option associated with the **interpolate** method that is part of the PANDAS package (Pandas, 2024). PCHIP stands for *Piecewise Cubic Hermite Interpolating Polynomial*; it is a common algorithm for imputing missing values in a time series because it gives a smooth interpolation that preserves the inherent shape of the data without introducing unwanted oscillations above or below the provided data values. PANDAS implements PCHIP interpolations as a wrapper around the **PchipInterpolator** method that comes from the SciPy package in Python (SciPy, 2025).

The annual rainfall values for the three neighboring rainfall stations extracted from the last column of the tables downloaded from the NOAA website are shown in Table 1 below. The yellow cells correspond to values that were missing from the NOAA tables. The numbers in the yellow cells are the values I interpolated using the PCHIP algorithm.

Year	WA	W7	NR	Avg	Effective Recharge (in/yr)	Effective Recharge (ft/day)
1995	65.11	64.35	48.56	59.34	13.96	0.00319
1996	64.42	52.69	74.96	64.02	15.06	0.00344
1997	49.59	51.02	53.63	51.41	12.10	0.00276
1998	64.20	77.16	70.10	70.49	16.59	0.00379
1999	72.06	82.14	63.19	72.46	17.05	0.00389
2000	53.82	59.17	50.37	54.45	12.81	0.00293
2001	37.98	57.40	43.46	46.28	10.89	0.00249
2002	49.32	56.85	49.39	51.85	12.20	0.00279
2003	63.62	72.79	50.54	62.32	14.66	0.00335
2004	50.73	71.69	51.73	58.05	13.66	0.00312
2005	69.33	68.35	59.18	65.62	15.44	0.00353
2006	63.80	62.72	62.47	63.00	14.82	0.00338
2007	33.35	37.31	60.39	43.68	10.28	0.00235
2008	60.80	48.38	56.35	55.18	12.98	0.00296
2009	59.73	59.44	53.63	57.60	13.55	0.00309

Table 1. Annual recharge values for rain gauge stations near Tarawa Terrace. WA = Wilmington Airport, W7 = Wilmington 7N, NR = New River Metcalf.

Once the missing numbers were imputed, I calculated the average of the values from the three stations and then applied the recharge coefficient described above to get an annual effective recharge rate in ft/year that was then converted to ft/day to match the units required by the MODFLOW model. The numbers in Table 1 above match the values shown in Table 1 from our original post-audit report. The recharge rates were provided to my colleague R. Jeffrey Davis, who entered them in the MODFLOW input files and ran the post-audit simulations.

Norman L. Jones

February 21, 2025

References

NOAA. (2024). *National Weather Service*. NOAA's National Weather Service. https://www.weather.gov/

Pandas. (2024). *pandas—Python Data Analysis Library*. https://pandas.pydata.org/

SciPy. (2025). *SciPy—Fundamental algorithms for scientific computing in Python*. https://scipy.org/

EXHIBIT 8

October 2024 Expert Report of Norman L. Jones and R. Jeffrey Davis

Reliance Materials

Revised 11/5/2024

1. Aquaveo LLC. 2024. Groundwater Modeling System, Aquaveo LLC, Provo, UT.

2. Faye, R.E., and C. Valenzuela. 2008. Analyses of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water at Tarawa Terrace and Vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina: Historical Reconstruction and Present-Day Conditions – Chapter C: Simulation of Groundwater Flow. Agency for Toxic Substances and Disease Registry U.S. Department of Health and Human Services, Atlanta, GA.

3. Faye, R.E. 2008, Analyses of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water at Tarawa Terrace and Vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina: Historical Reconstruction and Present-Day Conditions – Chapter F: Simulation of the Fate and Transport of Tetrachloroethylene (PCE). Agency for Toxic Substances and Disease Registry, U.S. Department of Health and Human Services, Atlanta, GA.

4. Harbaugh, A.W. 2005. MODFLOW-2005: The U.S. Geological Survey Modular Ground-Water Model—the Ground-Water Flow Process; Techniques and Methods. U.S. Geological Survey.

5. Harbaugh, A.W., E.R. Banta, M.C. Hill, and M.G McDonald. 2000. MODFLOW-2000, the U.S. Geological Survey Modular Ground-Water Model—User Guide to Modularization Concepts and the Ground-Water Flow Process. U.S. Geological Survey Open-File Report 00-92 2000. U.S. Geological Survey.

6. Langevin, C.D., J.D. Hughes, E.R. Banta, R.G. Niswonger, S. Panday, and A.M. Provost. 2017. Documentation for the MODFLOW 6 Groundwater Flow Model. U.S. Geological Survey.

7. Maslia, M.L., J.B. Sautner, R.E. Faye, R.J. Saurez-Soto, M.M. Aral, et al. 2007. Analyses of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water at Tarawa Terrace and Vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina: Historical Reconstruction and Present-Day Conditions – Chapter A: Summary of Findings. Agency for Toxic Substances and Disease Registry U.S. Department of Health and Human Services, Atlanta, GA.

8. McDonald, M.G., and A.W. Harbaugh. 1984. A Modular Three-Dimensional Finite-Difference Ground-Water Flow Model. Open-File Report.

9. National Weather Service. 2024. Home page. https://www.weather.gov/. Accessed on October 19, 2024. U.S. Department of Commerce and National Weather Service.

10. Owen, S.J., N.L. Jones, and J.P. Holland. 1996. A Comprehensive Modeling Environment for the Simulation of Groundwater Flow and Transport. Eng. Comput.12:235–242.

11. Panday, S., C.D. Langevin, R.G. Niswonger, M. Ibaraki, and J.D. Hughes. 2013. MODFLOW–USG Version 1: An Unstructured Grid Version of MODFLOW for Simulating Groundwater Flow and Tightly Coupled Processes Using a Control Volume Finite-Difference Formulation. U.S. Geological Survey.

12. USGS. 1996. USGS MODFLOW-96: MODular Three-Dimensional Finite-Difference Ground- Water FLOW Model with the Hydrograph Package. https://water.usgs.gov/nrp/gwsoftware/modflow/modflow-96h.htm Accessed on October 13, 2024. Available online: https://water.usgs.gov/nrp/gwsoftware/modflow/modflow-96h.htm. (Accessed on October 13, 2024). U.S. Geologic Survey.

13. Zheng, C., and P.P. Wang. 1999. MT3DMS, A Modular Three-Dimensional Multi-Species Transport Model for Simulation of Advection, Dispersion and Chemical Reactions of Contaminants in Groundwater Systems; Documentation and User's Guide. U.S. Army Engineer Research and Development Center Contract Report SERDP-99-1. Vicksburg, MS. 202 pp.

Weston ABC One-Hour Cleaners Dataset – Materials 14-98

14. ATSDR_WATERMODELING_01-0000891326-ATSDR_WATERMODELING_01-0000891327

15. CLJ127700-CLJ127815

16. CLJ197942-CLJ197952

17. CLJ198717-CLJ198821

18. CLJA_ATSDR_BOVE-0000161600-CLJA_ATSDR_BOVE-0000161600

19. CLJA_EPA01-0000126130-CLJA_EPA01-0000126716

20. CLJA_EPA01-0000142833-CLJA_EPA01-0000143291

21. CLJA_EPA01-0000188587-CLJA_EPA01-0000188603

22. CLJA_EPA01-0000189259-CLJA_EPA01-0000189527

23. CLJA_EPA01-0000189571-CLJA_EPA01-0000189661

24. CLJA_EPA01-0000189664-CLJA_EPA01-0000189807

25. CLJA_EPA01-0000193138-CLJA_EPA01-0000193158

26. CLJA_EPA01-0000193174-CLJA_EPA01-0000193947

27. CLJA_EPA01-0000194021-CLJA_EPA01-0000194041

28. CLJA_EPA01-0000194064-CLJA_EPA01-0000194698

29. CLJA_EPA01-0000194864-CLJA_EPA01-0000195595

30. CLJA_EPA01-0000195979-CLJA_EPA01-0000196267

31. CLJA_EPA01-0000196782-CLJA_EPA01-0000196868

32. CLJA_EPA01-0000200261-CLJA_EPA01-0000200456

33. CLJA_EPA01-0000202668-CLJA_EPA01-0000202674

34. CLJA_EPA01-0000246825-CLJA_EPA01-0000247456

35. CLJA_EPA01-0000202986-CLJA_EPA01-0000203009

36. CLJA_EPA01-0000203579-CLJA_EPA01-0000203847

37. CLJA_EPA01-0000208035-CLJA_EPA01-0000208258

38. CLJA_EPA01-0000208666-CLJA_EPA01-0000208922

39. CLJA_EPA01-0000209254-CLJA_EPA01-0000209947

40. CLJA_EPA01-0000211395-CLJA_EPA01-0000211548

41. CLJA_EPA01-0000213011-CLJA_EPA01-0000213047

42. CLJA_EPA01-0000213093-CLJA_EPA01-0000213416

43. CLJA_EPA01-0000214123-CLJA_EPA01-0000214973

44. CLJA_EPA01-0000216337-CLJA_EPA01-0000220965

45. CLJA_EPA01-0000221000-CLJA_EPA01-0000221001

46. CLJA_EPA01-0000221441-CLJA_EPA01-0000221576

47. CLJA_EPA01-0000221627-CLJA_EPA01-0000221909

48. CLJA_EPA01-0000222630-CLJA_EPA01-0000222686

49. CLJA_EPA01-0000222689-CLJA_EPA01-0000222701

50. CLJA_EPA01-0000222769-CLJA_EPA01-0000225748

51. CLJA_EPA01-0000227106-CLJA_EPA01-0000228053

52. CLJA_EPA01-0000228770-CLJA_EPA01-0000228910

53. CLJA_EPA01-0000228912-CLJA_EPA01-0000228953

54. CLJA_EPA01-0000229097-CLJA_EPA01-0000229331

55. CLJA_EPA01-0000229727-CLJA_EPA01-0000229778

56. CLJA_EPA01-0000229939-CLJA_EPA01-0000231046

57. CLJA_EPA01-0000232385-CLJA_EPA01-0000232400

58. CLJA_EPA01-0000232435-CLJA_EPA01-0000232469

59. CLJA_EPA01-0000233060-CLJA_EPA01-0000233410

60. CLJA_EPA01-0000233410-CLJA_EPA01-0000242081

61. CLJA_EPA01-0000233505-CLJA_EPA01-0000233563

62. CLJA_EPA01-0000234550-CLJA_EPA01-0000234690

63. CLJA_EPA01-0000236018-CLJA_EPA01-0000236062

64. CLJA_EPA01-0000237127-CLJA_EPA01-0000237400

65. CLJA_EPA01-0000237403-CLJA_EPA01-0000237510

66. CLJA_EPA01-0000237740-CLJA_EPA01-0000237920

67. CLJA_EPA01-0000239125-CLJA_EPA01-0000239214

68. CLJA_EPA01-0000239782-CLJA_EPA01-0000239806

69. CLJA_EPA01-0000240353-CLJA_EPA01-0000240366

70. CLJA_EPA01-0000241073-CLJA_EPA01-0000241230

71. CLJA_EPA01-0000241492-CLJA_EPA01-0000241650

72. CLJA_EPA01-0000241663-CLJA_EPA01-0000241792

73. CLJA_EPA01-0000244650-CLJA_EPA01-0000244659

74. CLJA_EPA01-0000245370-CLJA_EPA01-0000245405

75. CLJA_EPA01-0000245618-CLJA_EPA01-0000245659

76. CLJA_EPA01-0000247631-CLJA_EPA01-0000247713

77. CLJA_EPA01-0000249269-CLJA_EPA01-0000252201

78. CLJA_EPA01-0000253434-CLJA_EPA01-0000253444

79. CLJA_EPA01-0000254980-CLJA_EPA01-0000257235

80. CLJA_LANTDIV-0000268975-CLJA_LANTDIV-0000269398

81. CLJA_WATERMODELING_01-0000058439-CLJA_WATERMODELING_01-0000058439

82. CLJA_WATERMODELING_01-0000058440-CLJA_WATERMODELING_01-0000058448

83. CLJA_WATERMODELING_01-0000067692-CLJA_WATERMODELING_01-0000067692

84. CLJA_WATERMODELING_01-0000067693-CLJA_WATERMODELING_01-0000067695

85. CLJA_WATERMODELING_01-0000136165-CLJA_WATERMODELING_01-0000136279

86. CLJA_WATERMODELING_01-0000136286-CLJA_WATERMODELING_01-0000136319

87. CLJA_WATERMODELING_01-0000136320-CLJA_WATERMODELING_01-0000136330

88. CLJA_WATERMODELING_01-0000136346-CLJA_WATERMODELING_01-0000136416

89. CLJA_WATERMODELING_01-0000205652-CLJA_WATERMODELING_01-0000205674

90. CLJA_WATERMODELING_01-0000840243-CLJA_WATERMODELING_01-0000840246

91. CLJA_WATERMODELING_01-0000840247-CLJA_WATERMODELING_01-0000840250

92. CLJA_WATERMODELING_07-0000440066-CLJA_WATERMODELING_07-0000440439

93. CLJA_WATERMODELING_07-0000441159-CLJA_WATERMODELING_07-0000441495

94. CLJA_WATERMODELING_07-0000441791-CLJA_WATERMODELING_07-0000442145

95. CLJA_WATERMODELING_07-0000461898-CLJA_WATERMODELING_07-0000461902

96. CLJA_WATERMODELING_07-0000462245-CLJA_WATERMODELING_07-0000462249

97. CLJA_WATERMODELING_07-0001197480-CLJA_WATERMODELING_07-0001197563

98. CLJA_WATERMODELING_09-0000084196-CLJA_WATERMODELING_09-0000084557

Tarawa Terrace Model Input Files – Materials 99-123

99. CLJA_WATERMODELING_01-0000489859-CLJA_WATERMODELING_01-0000489859

100. CLJA_WATERMODELING_01-0000489861-CLJA_WATERMODELING_01-0000489861

101. CLJA_WATERMODELING_01-0000489863-CLJA_WATERMODELING_01-0000489863

102. CLJA_WATERMODELING_01-0000489862-CLJA_WATERMODELING_01-0000489862

103. CLJA_WATERMODELING_01-0000489860-CLJA_WATERMODELING_01-0000489860

104. CLJA_WATERMODELING_01-0000489864-CLJA_WATERMODELING_01-0000489864

105. CLJA_WATERMODELING_01-0000489857-CLJA_WATERMODELING_01-0000489857

106. CLJA_WATERMODELING_01-0000489858-CLJA_WATERMODELING_01-0000489858

107. CLJA_WATERMODELING_01-0000489817-CLJA_WATERMODELING_01-0000489817

108. CLJA_WATERMODELING_01-0000489819-CLJA_WATERMODELING_01-0000489819

109. CLJA_WATERMODELING_01-0000489814-CLJA_WATERMODELING_01-0000489814

110. CLJA_WATERMODELING_01-0000489815-CLJA_WATERMODELING_01-0000489815

111. CLJA_WATERMODELING_01-0000489821-CLJA_WATERMODELING_01-0000489821

112. CLJA_WATERMODELING_01-0000489848-CLJA_WATERMODELING_01-0000489848

113. CLJA_WATERMODELING_01-0000489818-CLJA_WATERMODELING_01-0000489818

114. CLJA_WATERMODELING_01-0000489820-CLJA_WATERMODELING_01-0000489820

115. CLJA_WATERMODELING_01-0000489816-CLJA_WATERMODELING_01-0000489816

116. CLJA_WATERMODELING_01-0000489852-CLJA_WATERMODELING_01-0000489852

117. CLJA_WATERMODELING_01-0000489855-CLJA_WATERMODELING_01-0000489855

118. CLJA_WATERMODELING_01-0000489851-CLJA_WATERMODELING_01-0000489851

119. CLJA_WATERMODELING_01-0000489853-CLJA_WATERMODELING_01-0000489853

120. CLJA_WATERMODELING_01-0000489854-CLJA_WATERMODELING_01-0000489854

121. CLJA_WATERMODELING_01-0000489850-CLJA_WATERMODELING_01-0000489850

122. CLJA_WATERMODELING_01-0000489849-CLJA_WATERMODELING_01-0000489849

123. CLJA_WATERMODELING_01-0000489856-CLJA_WATERMODELING_01-0000489856

Post-Audit Tarawa Terrace Model Files – Materials 124-145

124. TTerrace_1951-2008.adv (CL_PLG-EXPERT_DAVIS_0000000001)

125. TTerrace_1951-2008.ba6 (CL_PLG-EXPERT_DAVIS_0000000002)

126. TTerrace_1951-2008.bc6 (CL_PLG-EXPERT_DAVIS_0000000003)

127. TTerrace_1951-2008.btn (CL_PLG-EXPERT_DAVIS_0000000004)

128. TTerrace_1951-2008.dis (CL_PLG-EXPERT_DAVIS_0000000005)

129. TTerrace_1951-2008.drn (CL_PLG-EXPERT_DAVIS_0000000006)

130. TTerrace_1951-2008.dsp (CL_PLG-EXPERT_DAVIS_0000000007)

131. TTerrace_1951-2008.gcg (CL_PLG-EXPERT_DAVIS_0000000008)

132. TTerrace_1951-2008.ghb (CL_PLG-EXPERT_DAVIS_0000000009)

133. TTerrace_1951-2008.lmt6 (CL_PLG-EXPERT_DAVIS_0000000010)

134. TTerrace_1951-2008.mfn (CL_PLG-EXPERT_DAVIS_0000000011)

135. TTerrace_1951-2008.mfw (CL_PLG-EXPERT_DAVIS_0000000012)

136. TTerrace_1951-2008.mtr (CL_PLG-EXPERT_DAVIS_0000000013)

137. TTerrace_1951-2008.mts (CL_PLG-EXPERT_DAVIS_0000000014)

138. TTerrace_1951-2008.oc (CL_PLG-EXPERT_DAVIS_0000000015)

139. TTerrace_1951-2008.pcg (CL_PLG-EXPERT_DAVIS_0000000016)

140. TTerrace_1951-2008.prj (CL_PLG-EXPERT_DAVIS_0000000017)

141. TTerrace_1951-2008.rch (CL_PLG-EXPERT_DAVIS_0000000018)

142. TTerrace_1951-2008.rct (CL_PLG-EXPERT_DAVIS_0000000019)

143. TTerrace_1951-2008.ssm (CL_PLG-EXPERT_DAVIS_0000000020)

144. TTerrace_1951-2008.tob (CL_PLG-EXPERT_DAVIS_0000000021)

145. TTerrace_1951-2008.wel (CL_PLG-EXPERT_DAVIS_0000000022)

EXHIBIT 9

. W E I T Z
&
L U X E N B E R G
A PROFESSIONAL CORPORATION
• LAW OFFICES •
700 BROADWAY • NEW YORK, NY 10003
TEL. 212-558-5500 FAX 212-344-5461
WWW.WEITZLUX.COM

November 5, 2024

VIA EMAIL ONLY
Haroon Anwar
Adam Bain, Esquire
Bridget Lipscomb, Esquire
U.S. Department of Justice
Civil Division, Torts Branch
P.O. Box 340, Ben Franklin Station
Washington, D.C. 20044

IN RE: Camp Lejeune Water Litigation – Expert Reliance File Production
Case No: 7:23-cv-897

Dear Haroon:

On behalf of the Track 1 Trail Plaintiffs, the Plaintiffs' Leadership Group ("PLG") produces a revised reliance materials list for experts Norman Jones and Jeffrey Davis that includes their post-audit model files for Tarawa Terrace. These files–items 124-145– are also being produced pursuant to the Parties' ESI protocol as CL_PLG-EXPERT_DAVIS_0000000001-CL_PLG-EXPERT_DAVIS_0000000022. The document production has been uploaded to the Parties' shared CL - Plaintiffs' Productions folder on JEFS under 2024-11-05 Track 1 Trial Plaintiffs Phase I Expert File Production. Plaintiffs are producing these files with the understanding that the United States will also produce any model files relied upon by its experts.

Should you have any questions, or if you require assistance with accessing the files, please do not hesitate to contact me.

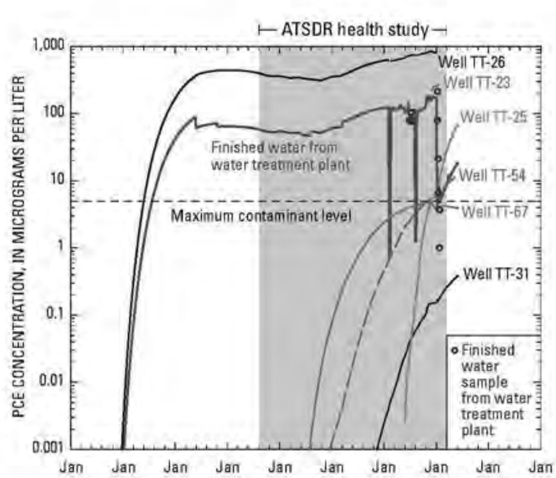
Sincerely,

Devin Bolton

EXHIBIT 10

Analyses of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water at Tarawa Terrace and Vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina: Historical Reconstruction and Present-Day Conditions

Chapter A: Summary of Findings



DEPARTMENT OF HEALTH & HUMAN SERVICES · USA

ATSDR
AGENCY FOR TOXIC SUBSTANCES AND DISEASE REGISTRY

Atlanta, Georgia–July 2007

Front cover: Historical reconstruction process using data, information sources, and water-modeling techniques to estimate historical exposures

Maps: U.S. Marine Corps Base Camp Lejeune, North Carolina; Tarawa Terrace area showing historical water-supply wells and site of ABC One-Hour Cleaners

Photographs on left: Ground storage tank STT-39 and four high-lift pumps used to deliver finished water from tank STT-39 to Tarawa Terrace water-distribution system

Photograph on right: Equipment used to measure flow and pressure at a hydrant during field test of the present-day (2004) water-distribution system

Graph: Reconstructed historical concentrations of tetrachloroethylene (PCE) at selected water-supply wells and in finished water at Tarawa Terrace water treatment plant

Analyses of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water at Tarawa Terrace and Vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina: Historical Reconstruction and Present-Day Conditions

Chapter A: Summary of Findings

By Morris L. Maslia, Jason B. Sautner, Robert E. Faye, René J. Suárez-Soto, Mustafa M. Aral, Walter M. Grayman, Wonyong Jang, Jinjun Wang, Frank J. Bove, Perri Z. Ruckart, Claudia Valenzuela, Joseph W. Green, Jr., and Amy L. Krueger

Agency for Toxic Substances and Disease Registry
U.S. Department of Health and Human Services
Atlanta, Georgia

July 2007

Authors

Morris L. Maslia, MSCE, PE, D.WRE, DEE
Research Environmental Engineer and Project Officer
Exposure-Dose Reconstruction Project
Agency for Toxic Substances and Disease Registry
Atlanta, Georgia

Jason B. Sautner, MSCE, EIT
Environmental Health Scientist
Division of Health Assessment and Consultation
Agency for Toxic Substances and Disease Registry
Atlanta, Georgia

Robert E. Faye, MSCE, PE
Hydrologist
Robert E. Faye and Associates
Consultant to Eastern Research Group, Inc.
Lexington, Massachusetts

René J. Suárez-Soto, MSCE, EIT
Environmental Health Scientist
Division of Health Assessment and Consultation
Agency for Toxic Substances and Disease Registry
Atlanta, Georgia

Mustafa M. Aral, PhD, PE, Phy
Director and Professor
Multimedia Environmental Simulations Laboratory
School of Civil and Environmental Engineering
Georgia Institute of Technology
Atlanta, Georgia

Walter M. Grayman, PhD, PE
Consulting Engineer
W.M. Grayman Consulting Engineer
Cincinnati, Ohio

Wonyong Jang, PhD
Post Doctoral Fellow
Multimedia Environmental Simulations Laboratory
School of Civil and Environmental Engineering
Georgia Institute of Technology
Atlanta, Georgia

Jinjun Wang, MSCE
Ph.D. Candidate
Multimedia Environmental Simulations Laboratory
School of Civil and Environmental Engineering
Georgia Institute of Technology
Atlanta, Georgia

Frank J. Bove, ScD
Senior Epidemiologist
Division of Health Studies
Agency for Toxic Substances and Disease Registry
Atlanta, Georgia

Perri Z. Ruckart, MPH
Epidemiologist and Principal Investigator
Division of Health Studies
Agency for Toxic Substances and Disease Registry
Atlanta, Georgia

Claudia Valenzuela, MSCE
Post Graduate Research Fellow
Oak Ridge Institute for Science and Education
Agency for Toxic Substances and Disease Registry
Atlanta, Georgia

Joseph W. Green, Jr., MA
Post Graduate Research Fellow
Oak Ridge Institute for Science and Education
Agency for Toxic Substances and Disease Registry
Atlanta, Georgia

Amy L. Krueger, MPH
Post Graduate Research Fellow
Oak Ridge Institute for Science and Education
Agency for Toxic Substances and Disease Registry
Atlanta, Georgia

For additional information write to:

Project Officer
Exposure-Dose Reconstruction Project
Division of Health Assessment and Consultation
Agency for Toxic Substances and Disease Registry
1600 Clifton Road, Mail Stop E-32
Atlanta, Georgia 30333

Suggested citation: Maslia ML, Sautner JB, Faye RE, Suárez-Soto RJ, Aral MM, Grayman WM, Jang W, Wang J, Bove FJ, Ruckart PZ, Valenzuela C, Green JW Jr, and Krueger AL. Analyses of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water at Tarawa Terrace and Vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina: Historical Reconstruction and Present-Day Conditions—Chapter A: Summary of Findings. Atlanta, GA: Agency for Toxic Substances and Disease Registry; 2007.

Foreword

The Agency for Toxic Substances and Disease Registry (ATSDR), an agency of the U.S. Department of Health and Human Services, is conducting an epidemiological study to evaluate whether in utero and infant (up to 1 year of age) exposures to volatile organic compounds in contaminated drinking water at U.S. Marine Corps Base Camp Lejeune, North Carolina, were associated with specific birth defects and childhood cancers. The study includes births occurring during the period 1968–1985 to women who were pregnant while they resided in family housing at the base. During 2004, the study protocol received approval from the Centers for Disease Control and Prevention Institutional Review Board and the U.S. Office of Management and Budget.

Historical exposure data needed for the epidemiological case-control study are limited. To obtain estimates of historical exposure, ATSDR is using water-modeling techniques and the process of historical reconstruction. These methods are used to quantify concentrations of particular contaminants in finished water and to compute the level and duration of human exposure to contaminated drinking water.

Final interpretive results for Tarawa Terrace and vicinity—based on information gathering, data interpretations, and water-modeling analyses—are presented as a series of ATSDR reports. These reports provide comprehensive descriptions of information, data analyses and interpretations, and modeling results used to reconstruct historical contaminant levels in drinking water at Tarawa Terrace and vicinity. Each topical subject within the water-modeling analysis and historical reconstruction process is assigned a chapter letter. Specific topics for each chapter report are listed below:

- **Chapter A**: Summary of Findings
- **Chapter B**: Geohydrologic Framework of the Castle Hayne Aquifer System
- **Chapter C**: Simulation of Groundwater Flow
- **Chapter D**: Properties and Degradation Pathways of Common Organic Compounds in Groundwater
- **Chapter E**: Occurrence of Contaminants in Groundwater
- **Chapter F**: Simulation of the Fate and Transport of Tetrachloroethylene (PCE) in Groundwater
- **Chapter G**: Simulation of Three-Dimensional Multispecies, Multiphase Mass Transport of Tetrachloroethylene (PCE) and Associated Degradation By-Products
- **Chapter H**: Effect of Groundwater Pumping Schedule Variation on Arrival of Tetrachloroethylene (PCE) at Water-Supply Wells and the Water Treatment Plant
- **Chapter I**: Parameter Sensitivity, Uncertainty, and Variability Associated with Model Simulations of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water
- **Chapter J**: Field Tests, Data Analyses, and Simulation of the Distribution of Drinking Water
- **Chapter K**: Supplemental Information

Electronic versions of these reports and their supporting information and data will be made available on the ATSDR Camp Lejeune Web site at *http://www.atsdr.cdc.gov/sites/lejeune/index.html*.

Contents

Figures

Tables

Conversion Factors

Multiply	By	To obtain
	Length	
inch	2.54	centimeter (cm)
foot (ft)	0.3048	meter (m)
mile (mi)	1.609	kilometer (km)
	Volume	
gallon (gal)	3.785	liter (L)
gallon (gal)	0.003785	cubic meter (m^3)
million gallons (MG)	3,785	cubic meter (m^3)
	Flow rate	
foot per day (ft/d)	0.3048	meter per day (m/d)
million gallons per day (MGD)	0.04381	cubic meter per second (m^3/s)
inch per year (in/yr)	25.4	millimeter per year (mm/yr)
	Hydraulic conductivity	
foot per day (ft/d)	0.3048	meter per day (m/d)

Concentration Conversion Factors

Unit	To convert to	Multiply by
microgram per liter (µg/L)	milligram per liter (mg/L)	0.001
microgram per liter (µg/L)	milligram per cubic meter (mg/m^3)	1
microgram per liter (µg/L)	microgram per cubic meter (µg/m^3)	1,000
parts per billion by volume (ppbv)	parts per million by volume (ppmv)	1,000

Vertical coordinate information is referenced to the National Geodetic Vertical Datum of 1929 (NGVD 29).

Horizontal coordinate information is referenced to the North American Datum of 1983 (NAD 83).

Altitude, as used in this report, refers to distance above the vertical datum.

Glossary and Abbreviations

Definitions of terms and abbreviations used throughout this report are listed below.

A

aerobic conditions Conditions for growth or metabolism in which the organism is sufficiently supplied with oxygen (IUPAC 2006)

anaerobic process A biologically-mediated process or condition not requiring molecular or free oxygen (IUPAC 2006)

ATSDR Agency for Toxic Substances and Disease Registry

B

biodegradation Transformation of substances into new compounds through biochemical reactions or the actions of microorganisms, such as bacteria. Typically expressed in terms of a rate constant or half-life (USEPA 2004). The new compounds are referred to as degradation by-products (for example, TCE, 1,2-tDCE, and VC are degradation by-products of PCE)

BTEX Benzene, toluene, ethylbenzene, and xylene; a group of VOCs found in petroleum hydrocarbons, such as gasoline, and other common environmental contaminants

C

calibration *See* model calibration

CERCLA The Comprehensive Environmental Response, Compensation, and Liability Act of 1980, also know as Superfund

CRWQME Continuous recording water-quality monitoring equipment; equipment that can be connected to hydraulic devices such as hydrants to continuously record water-quality parameters such as temperature, pH, and fluoride. For the Camp Lejeune analyses, the Horiba W-23XD continuous recording, dual probe ion detector data logger was used

D

DCE 1,1-dichloroethylene or 1,1-dichloroethene

1,2-DCE *cis*-1,2- dichloroethylene or *trans*-1,2-dichloroethylene

1,2-cDCE *cis*-1,2- dichloroethylene or *cis*-1,2-dichloroethene

1,2-tDCE *trans*-1,2-dichloroethylene or *trans*-1,2-dichloroethene

degradation *See* biodegradation

degradation by-product *See* biodegradation

density The mass per unit volume of material, expressed in terms of kilograms per cubic meter or grams per cubic centimeter

direct measurement or observation A method of obtaining data that is based on measuring or observation of the parameter of interest

diurnal pattern The temporal variations in water usage for a water system that typically follow a 24-hour cycle (Haestad Methods et al. 2003)

DNAPL Dense nonaqueous phase liquids; a class of environmental contaminants that have a specific gravity greater than water (Huling and Weaver 1991). Immiscible (nonmixing)DNAPLs exit in the subsurface as a separate fluid phase in the presence of air and water. DNAPLs can vaporize into air and slowly dissolve into flowing groundwater. Examples of DNAPLs include chlorinated solvents, creosote, coal tar,
and PCBs (Kueper et al. 2003)

DVD Digital video disc

E

EPANET 2 A water-distribution system model developed by USEPA

epidemiological study A study to determine whether a relation exists between the occurrence and frequency of a disease and a specific factor such as exposure to a toxic compound found in the environment

EPS Extended period simulation; a simulation method used to analyze a water-distribution system that is characterized by time-varying demand and operating conditions

exposure Pollutants or contaminants that come in contact with the body and present a potential health threat

F

fate and transport Also known as mass transport; a process that refers to how contaminants move through, and are transformed in, the environment

finished water Groundwater that has undergone treatment at a water treatment plant and is delivered to a person's home. For this study, the concentration of treated water at the water treatment plant is considered the same as the concentration of water delivered to a person's home

ft Foot or feet

G

gal Gallon or gallons

gal/min Gallons per minute

H

historical reconstruction A diagnostic analysis used to examine historical characteristics of groundwater flow, contaminant fate and transport, water-distribution systems, and exposure

I

interconnection The continuous flow of water in a pipeline from one water-distribution system to another

inverse distance weighting A process of assigning values to unknown points by using values from known points; a method used to contour data or simulation results

IUPAC International Union of Pure and Applied Chemistry

K

K_{oc} Organic carbon partition coefficient

K_{ow} Octanol-water partition coefficient

M

MCL Maximum contaminant level; a legal threshold limit set by the USEPA on the amount of a hazardous substance that is allowed in drinking water under the Safe Drinking Water Act; usually expressed as a concentration in milligrams or micrograms per liter. Effective dates for MCLs are as follows: trichloroethylene (TCE) and vinyl chloride (VC), January 9, 1989; tetrachloroethylene (PCE) and *trans*-1,2-dichloroethylene (1,2-tDCE), July 6, 1992 (40 CFR, Section 141.60, Effective Dates, July 1, 2002, ed.)

MCS Monte Carlo simulation; *see* Monte Carlo analysis

MESL Multimedia Environmental Simulations Laboratory, School of Civil and Environmental Engineering, Georgia Institute of Technology, Atlanta, Georgia; an ATSDR cooperative agreement partner

μg/L Microgram per liter; 1 part per billion, a unit of concentration

MG Million gallons

MGD Million gallons per day

mg/L Milligram per liter; 1 part per million (ppm), a unit of concentration

mL Milliliter; 1/1000th of a liter

model calibration The process of adjusting model input parameter values until reasonable agreement is achieved between model-predicted outputs or behavior and field observations

MODFLOW-96 A three-dimensional groundwater-flow model, 1996 version, developed by the U.S. Geological Survey

MODFLOW-2K A three-dimensional groundwater-flow model, 2000 version, developed by the U.S. Geological Survey

Monte Carlo analysis Also referred to as Monte Carlo simulation; a computer-based method of analysis that uses statistical sampling techniques to obtain a probabilistic approximation to the solution of a mathematical equation or model (USEPA 1997)

MT3DMS A three-dimensional mass transport, multispecies model developed by C. Zheng and P. Wang on behalf of the U.S. Army Engineer Research and Development Center in Vicksburg, Mississippi

N

NPL National Priorities List; the USEPA's official list of uncontrolled hazardous waste sites which are to be cleaned up under the Superfund legislation

P

paired data point A location with observed data (for example, water level or concentration) that is associated with a model location for the purpose of comparing observed data with model results

PCE Tetrachloroethene, tetrachloroethylene, 1,1,2,2-tetrachloroethylene, or perchloroethylene; also known as PERC® or PERK®

PDF Probability density function; also known as the probability function or the frequency function. A mathematical function that expresses the probability of a random variable falling within some interval

PHA Public health assessment; an evaluation conducted by ATSDR of data and information on the release of hazardous substances into the environment in order to assess any past, present, or future impact on public health

potentiometric level A level to which water will rise in a tightly cased well

potentiometric surface An imaginary surface defined by the levels to which water will rise in a tightly cased wells. The water table is a particular potentiometric surface

probabilistic analysis An analysis in which frequency (or probability) distributions are assigned to represent variability (or uncertainty) in quantities. The output of a probabilistic analysis is a distribution (Cullen and Frey 1999)

pseudo-random number generator A deterministic algorithm used to generate a sequence of numbers with little or no discernable pattern in the numbers except for broad statistical properties

PSOpS A pumping schedule optimization system simulation tool used to assess impacts of unknown and uncertain historical groundwater well operations. The simulation tool was developed by the Multimedia Environmental Simulations Laboratory at the Georgia Institute of Technology, Atlanta, Georgia

Q

qualitative description A method of estimating data that is based on inference

quantitative estimate A method of estimating data that is based on the application of computational techniques

R

rank-and-assign method An optimization method uniquely developed for the pumping schedule optimization system (PSOpS) simulation tool . This procedure updates the pumping schedule for maximum and minimum contaminant concentration levels in finished water of the WTP based on derivative, pumping capacity, and total pumping demand information

RMS Root-mean-square; a statistical measure of the magnitude of a varying quantity

S

saturated zone Zone at or below the water table

SCADA Supervisory control and data acquisition; a computerized data collection system used to collect hydraulic data and information in water-distribution systems at specified time intervals such as every 1, 5, 15, etc., minutes

sensitivity analysis An analysis method used to ascertain how a given model output (for example, concentration) depends upon the input parameters (for example, pumping rate, mass loading rate). Sensitivity analysis is an important method for checking the quality of a given model, as well as a powerful tool for checking the robustness and reliability of its analysis

sequential biodegradation Degradation of a volatile organic compound as a result of a biological process that occurs in a progression, for example, the biodegradation of PCE ⟶ TCE ⟶ 1,2-tDCE ⟶ VC

SGA Small for gestational age; a term used to describe when an infant's weight is very low given their gestational week of birth

SGS Sequential Gaussian simulation; a process in which a field of values (such as hydraulic conductivity) is obtained multiple times assuming the spatially interpolated values follow a Gaussian (normal) distribution

skeletonization The reduction or aggregation of a water-distribution system network so that only the major hydraulic characteristics need be represented by a model. Skeletonization is often used to reduce the computational requirements of modeling an all-pipes network

SR Highway or state route

standard deviation Square root of the variance or the root-mean-square (RMS) deviation of values from their arithmetic mean

T

TCE 1,1,2-trichloroethene, or 1,1,2-trichloroethylene, or trichloroethylene

TechFlowMP A three-dimensional multispecies, multiphase mass transport model developed by the Multimedia Environmental Simulations Laboratory at the Georgia Institute of Technology, Atlanta, Georgia

trihalomethane A chemical compound in which three of the four hydrogen atoms of methane (CH_4) are replaced by halogen atoms. Many trihalomethanes are used in industry as solvents or refrigerants. They also are environmental pollutants, and many are considered carcinogenic

U

uncertainty The lack of knowledge about specific factors, parameters, or models (for example, one is uncertain about the mean value of the concentration of PCE at the source)

unsaturated zone Zone or area above the water table; also known as the vadose zone

USEPA U.S. Environmental Protection Agency

USGS U.S. Geological Survey

V

variability Observed differences attributable to heterogeneity or diversity in a model parameter, an exposure parameter, or a population

VC Vinyl chloride or chloroethene

Venn diagram A diagram that shows the mathematical or logical relationship between different groups or sets; the diagram shows all the possible logical relations between the sets

venturi meter A device used to measure the flow rate or velocity of a fluid through a pipe

VOC Volatile organic compound; an organic chemical compound (chlorinated solvent) that has a high enough vapor pressure under normal circumstances to significantly vaporize and enter the atmosphere. VOCs are considered environmental pollutants and some may be carcinogenic

W

water-distribution system A water-conveyance network consisting of hydraulic facilities such as wells, reservoirs, storage tanks, high-service and booster pumps, and a network of pipelines for delivering drinking water

water table Also known as the phreatic surface; the surface where the water pressure is equal to atmospheric pressure

WTP Water treatment plant

Analyses of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water at Tarawa Terrace and Vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina: Historical Reconstruction and Present-Day Conditions

Chapter A: Summary of Findings

By Morris L. Maslia,[1] Jason B. Sautner,[1] Robert E. Faye,[2] René J. Suárez-Soto,[1] Mustafa M. Aral,[3] Walter M. Grayman,[4] Wonyong Jang,[3] Jinjun Wang,[3] Frank J. Bove,[1] Perri Z. Ruckart,[1] Claudia Valenzuela,[5] Joseph W. Green, Jr.,[5] and Amy L. Krueger [5]

Abstract

Two of three water-distribution systems that have historically supplied drinking water to family housing at U.S. Marine Corps Base Camp Lejeune, North Carolina, were contaminated with volatile organic compounds (VOCs). Tarawa Terrace was contaminated mostly with tetrachloroethylene (PCE), and Hadnot Point was contaminated mostly with trichloroethylene (TCE). Because scientific data relating to the harmful effects of VOCs on a child or fetus are limited, the Agency for Toxic Substances and Disease Registry (ATSDR), an agency of the U.S. Department of Health and Human Services, is conducting an epidemiological study to evaluate potential associations between in utero and infant (up to 1 year of age) exposures to VOCs in contaminated drinking water at Camp Lejeune and specific birth defects and childhood cancers. The study includes births occurring during the period 1968–1985 to women who were pregnant while they resided in family housing at Camp Lejeune. Because limited measurements of contaminant and exposure data are available to support the epidemiological study, ATSDR is using modeling techniques to reconstruct historical conditions of groundwater flow, contaminant fate and transport, and the distribution of drinking water contaminated with VOCs delivered to family housing areas. The analyses and results presented in this Summary of Findings, and in reports described herein, refer solely to Tarawa Terrace and vicinity. Future analyses and reports will present information and data about contamination of the Hadnot Point water-distribution system.

Models and methods used as part of the historical reconstruction process for Tarawa Terrace and vicinity included: (1) MODFLOW-96, used for simulating steady-state (predevelopment) and transient groundwater flow; (2) MT3DMS, used for simulating three-dimensional, single-specie contaminant fate and transport; (3) a materials mass balance model (simple mixing) used to compute the flow-weighted average concentration of PCE assigned to the finished water at the Tarawa Terrace water treatment plant (WTP); (4) TechFlowMP, used for simulating three-dimensional, multispecies, multiphase mass transport; (5) PSOpS, used for simulating the impacts of unknown and uncertain historical well operations; (6) Monte Carlo simulation and sequential Gaussian simulation used to conduct probabilistic analyses to assess uncertainty and variability of concentrations

[1] Agency for Toxic Substances and Disease Registry, Atlanta, Georgia.

[2] Robert E. Faye and Associates, consultant to Eastern Research Group, Inc., Lexington, Massachusetts.

[3] School of Civil and Environmental Engineering, Georgia Institute of Technology, Atlanta, Georgia.

[4] W.M. Grayman Consulting Engineer, Cincinnati, Ohio.

[5] Oak Ridge Institute for Science and Education, Oak Ridge, Tennessee.

of PCE-contaminated groundwater and drinking water; and (7) EPANET 2, used to conduct extended-period hydraulic and water-quality simulations of the Tarawa Terrace water-distribution system. Through historical reconstruction, monthly concentrations of PCE in groundwater and in finished water distributed from the Tarawa Terrace WTP to residents of Tarawa Terrace were determined.

Based on field data, modeling results, and the historical reconstruction process, the following conclusions are made:

- Simulated PCE concentrations exceeded the current maximum contaminant level (MCL) of 5 micrograms per liter (μg/L) at water-supply well TT-26 for 333 months—January 1957–January 1985.
- The maximum simulated PCE concentration at well TT-26 was 851 μg/L during July 1984; the maximum measured PCE concentration was 1,580 μg/L during January 1985.
- Simulated PCE concentrations exceeded the current MCL of 5 μg/L in finished water at the Tarawa Terrace WTP for 346 months—November 1957–February 1987.
- The maximum simulated PCE concentration in finished water at the Tarawa Terrace WTP was 183 μg/L during March 1984; the maximum measured PCE concentration was 215 μg/L during February 1985.
- Simulation of PCE degradation by-products—TCE, *trans*-1,2-dichloroethylene (1,2-tDCE), and vinyl chloride—indicated that maximum concentrations of the degradation by-products generally were in the range of 10–100 μg/L at water-supply well TT-26; measured concentrations of TCE and 1,2-tDCE on January 16, 1985, were 57 and 92 μg/L, respectively.
- Maximum concentrations of degradation by-products in finished water at the Tarawa Terrace WTP generally were in the range of 2–15 μg/L; measured concentrations of TCE and 1,2-tDCE on February 11, 1985, were 8 and 12 μg/L, respectively.
- Based on water-supply well scheduling analyses, finished water exceeding the current MCL for PCE (5 μg/L) at the Tarawa Terrace WTP could have been delivered as early as December 1956 and no later than June 1960.
- Based on probabilistic analyses, the most likely dates that finished water first exceeded the current MCL for PCE ranged from October 1957 to August 1958 (95 percent probability), with an average first exceedance date of November 1957.
- Exposure to drinking water contaminated with PCE and PCE degradation by-products ceased after February 1987 when the Tarawa Terrace WTP was closed.

Introduction

The Agency for Toxic Substances and Disease Registry (ATSDR), an agency of the U.S. Department of Health and Human Services, is conducting an epidemiological study to evaluate whether in utero and infant (up to 1 year of age) exposures to drinking water contaminated with volatile organic compounds (VOCs) at U.S. Marine Corps Base Camp Lejeune, North Carolina (Plate 1), were associated with specific birth defects and childhood cancers. The study includes births occurring during the period 1968–1985 to women who resided in family housing at Camp Lejeune. The first year of the study, 1968, was chosen because North Carolina computerized its birth certificates starting that year. The last year of the study, 1985, was chosen because the most contaminated water-supply wells were removed from regular service that year. ATSDR is using water-modeling techniques to provide the epidemiological study with quantitative estimates of monthly contaminant concentrations in finished drinking water[6] because contaminant concentration data and exposure information are limited. Results obtained by using water-modeling techniques, along with information from the mother on her water use, can be used by the epidemiological study to estimate the level and duration of exposures to the mother during her pregnancy and to the infant (up to 1 year of age). Using water-modeling techniques in such a process is referred to as historical reconstruction (Maslia et al. 2001).

Three water-distribution systems have historically supplied drinking water to family housing at U.S. Marine Corps Base Camp Lejeune—Tarawa Terrace, Holcomb Boulevard, and Hadnot Point (Plate 1, Figure A1).

[6] For this study, finished drinking water is defined as groundwater that has undergone treatment at a water treatment plant and is delivered to a person's home. The concentration of contaminants in treated water at the water treatment plant is considered the same as the concentrations in the water delivered to a person's home. This assumption is tested and verified in the Chapter J report (Sautner et al. In press 2007). Hereafter, the term "finished water" will be used.

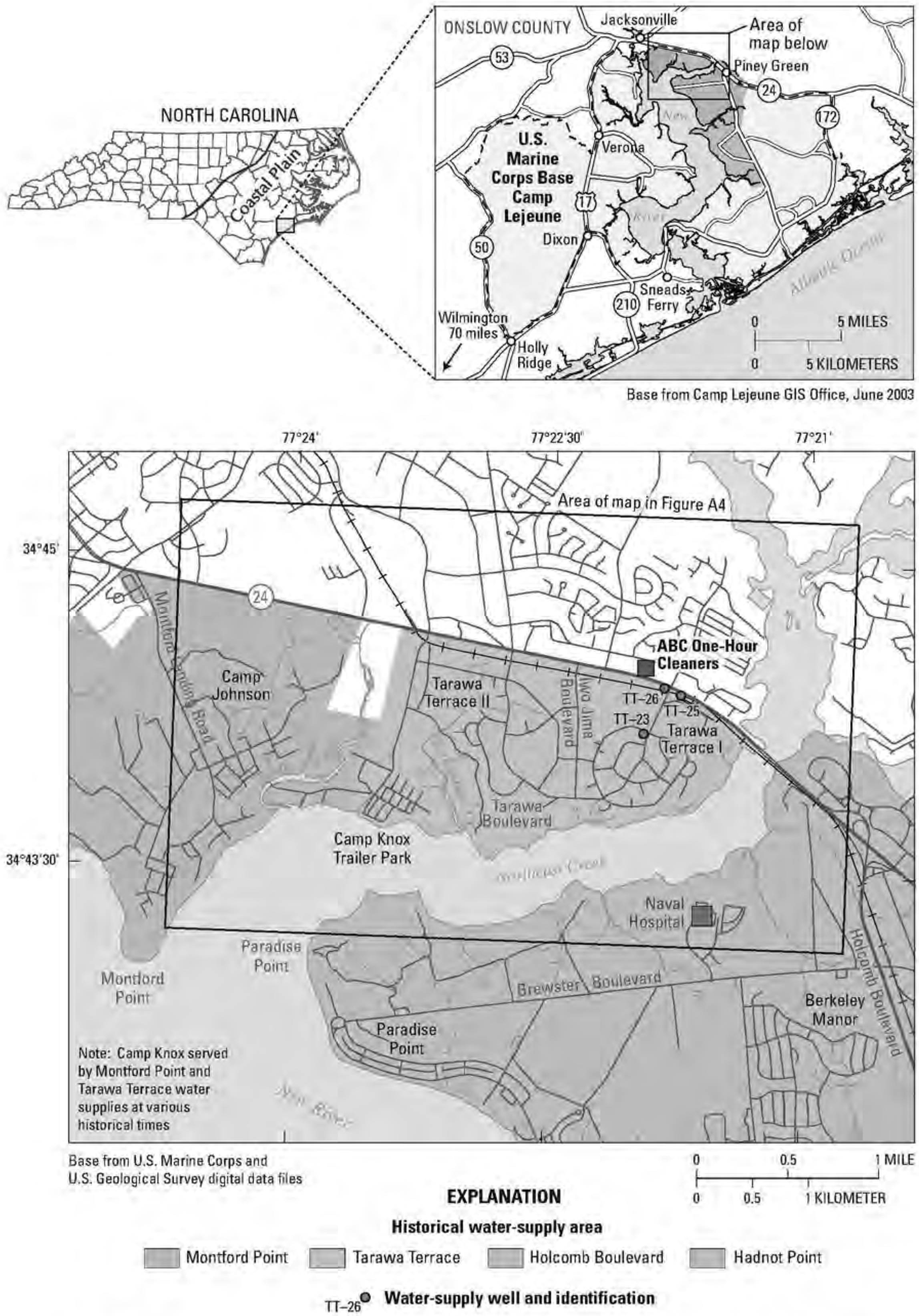


Figure A1. Selected base housing and historical water-supply areas, Tarawa Terrace and vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina.

Two of the water-distribution systems were contaminated with VOCs. Tarawa Terrace was contaminated mostly with tetrachloroethylene (PCE), and Hadnot Point was contaminated mostly with trichloroethylene (TCE). Historical information and data have indicated that one source of contamination—ABC One-Hour Cleaners (Figure A1)—was responsible for contaminating Tarawa Terrace water-supply wells (Shiver 1985). Water-supply data and operational information indicate that Tarawa Terrace wells supplied water solely to the Tarawa Terrace water treatment plant (WTP). Additionally, the Tarawa Terrace water-distribution system was operated independently of the other two water-distribution systems (Holcomb Boulevard and Hadnot Point). Therefore, analyses presented in this Summary of Findings and in reports described herein refer solely to Tarawa Terrace and vicinity. Future analyses and reports will present information and data about contamination of the Hadnot Point water-distribution system.

Previous Studies and Purpose of the Current Investigation

Only a small number of studies have evaluated the risk of birth defects and childhood cancers from exposures to drinking water contaminated with VOCs. These include, for example, studies by Cohn et al. (1994), Bove et al. (1995, 2002), Costas et al. (2002), Massachusetts Department of Public Health (1996), and the New Jersey Department of Health and Senior Services (2003). Five studies that have evaluated exposures to TCE and PCE in drinking water and adverse birth outcomes are summarized in Table A1. Compared to

Table A1. Summary of trichloroethylene and tetrachloroethylene study characteristics and results.[1]

[OR, odds ratio; TCE, trichloroethylene; PCE, tetrachloroethylene; SGA, small for gestational age; LBW, low birth weight; NTD, neural tube defects; MBW, mean birth weight; MBWD, mean birth weight difference; VLBW, very low birth weight; GIS, geographic information system; =, equal; ≤, less than or equal to; –, negative; g, gram; yr, year]

Study site and period	Outcome	Number of subjects	Exposure	Results (OR)[2]
Arizona 1969–1981 (Goldberg et al. 1990)	Cardiac defects	365 cases	1st trimester residence (or employment) in area of TCE contamination	Prevalence ratio = 2.58
Woburn, Massachusetts 1975–1979 (MDPH,CDC 1996)	SGA preterm birth birth defects fetal death	2,211 births 19 fetal deaths	Modeled distribution system to estimate monthly exposures; address at delivery	SGA = 1.55; LBW ≤1.0; preterm delivery ≤ 1.0; **fetal death = 2.57; NTD = 2.21; cleft palate = 2.21; heart defects = 0.40; eye defects = 4.41;** cluster of choanal atresia
1969–1979	LBW	5,347 births		
Northern New Jersey 1985–1988 (Bove et al. 1995)	SGA preterm birth birth defects fetal death	80,938 live births, 594 fetal deaths	Estimated average monthly levels of solvents based on tap water sample data and address at delivery	TCE: SGA ≤1.0; preterm birth = 1.02; NTD = 2.53; oral clefts = 2.24; heart defects = 1.24; fetal death ≤ 1.0 PCE: SGA ≤ 1.0; preterm birth ≤ 1.0; NTD = 1.16; oral clefts = 3.54; heart defects = 1.13; fetal death ≤ 1.0
Camp Lejeune, North Carolina 1968–1985 (ATSDR 1998)	MBW SGA preterm birth	31 births exposed to TCE, 997 unexposed; 6,117 births exposed to PCE, 5,681 births unexposed	Residence in a base housing area known to have received contaminated water	TCE: SGA = 1.5; MBWD = –139 g; preterm birth = 0.0; males: SGA = 3.9; MBWD = –312 g PCE: SGA = 1.2; MBWD = –24 g; preterm birth = 1.0; women > 35 yr: SGA = 4.0; MBWD = –205 g; women with ≥2 fetal losses: SGA = 2.5
Arizona 1979–1981 (high exposure) and 1983–1985 (post exposure) (Rodenbeck et al. 2000)	LBW VLBW full-term LBW	1,099 exposed births, 877 unexposed births	Maternal residence in target or comparison census tracts at delivery; GIS modeling of groundwater plume	TCE: LBW = 0.90; VLBW = 3.30; full-term LBW = 0.81

[1]Bove et al. (2002)
[2]Results in bold type indicate those that were calculated by the reviewing authors (Bove et al. 2002)

the aforementioned studies, the current study at Camp Lejeune is unique in that it will examine the associations between well-defined, quantitative levels of PCE and TCE in drinking water and the risk of developing specific birth defects—spina bifida, anencephaly, cleft lip, and cleft palate—childhood leukemia, and non-Hodgkin's lymphoma. The current study includes parent interviews conducted to obtain residential history, information on water consumption habits, and risk factors. Using model-derived drinking-water concentrations and interview data, associations between exposure to PCE and TCE during various time periods of interest—preconception, trimesters, entire pregnancy, and infancy (up to 1 year of age)—and the risk of particular health outcomes can be thoroughly examined.

The purpose of the analyses described in this report and associated chapter reports is to provide epidemiologists with historical monthly concentrations of contaminants in drinking water to facilitate the estimation of exposures. Because historical contaminant concentration data are limited, the process of historical reconstruction—which included water-modeling analyses—was used to synthesize information and quantify estimates of contaminant occurrences in groundwater and the water-distribution system at Tarawa Terrace.

Tarawa Terrace Chapter Reports

Owing to the complexity, uniqueness, and the number of topical subjects included in the historical reconstruction process, a number of reports were prepared that provide comprehensive descriptions of information, data, and methods used to conduct historical and present-day analyses at Tarawa Terrace and vicinity. Table A2 lists the 11 chapters (A–K) and chapter titles of reports that compose the complete description and details of the historical reconstruction process used for the Tarawa Terrace analyses. Also included in Table A2 are listings of the authors and a topical summary of each chapter report. Figure A2 shows the relation among the Chapter A report (Summary of Findings—this report), Chapters B–K reports, and the overall process of historical reconstruction as it relates to quantifying exposures and the ATSDR case-control epidemiological study. Reports for chapters B–K present detailed information, data, and analyses. Summaries of results from each chapter report are provided in Appendix A1. Readers interested in details of a specific topic, for example, numerical model development, model-calibration procedures, synoptic maps showing groundwater migration of PCE at Tarawa Terrace, or probabilistic analyses, should consult the appropriate chapter report (Table A2, Appendix A1). Also provided with the Chapter A report is a searchable electronic database—on digital video disc (DVD) format—of information and data sources used to conduct the historical reconstruction analysis. Electronic versions of each chapter report—summarized in Appendix A1—and supporting information and data will be made available on the ATSDR Camp Lejeune Web site at *http://www.atsdr.cdc.gov/sites/lejeune/index.html.*

External Peer Review

Throughout this investigation, ATSDR has sought independent external expert scientific input and review of project methods, approaches, and interpretations to assure scientific credibility of the analyses described in the Tarawa Terrace reports. The review process has included convening an expert peer review panel and submitting individual chapter reports to outside experts for technical reviews. On March 28–29, 2005, ATSDR convened an external expert panel to review the approach used in conducting the historical reconstruction analysis and to provide input and recommendations on preliminary analyses and modeling results (Maslia 2005). The panel was composed of experts with professional backgrounds from government and academia, as well as the private sector. Areas of expertise included numerical model development and simulation, groundwater-flow and contaminant fate and transport analyses and model calibration, hydraulic and water-quality analysis of water-distribution systems, epidemiology, and public health. After reviewing data and initial approaches and analyses provided by ATSDR, panel members made the following recommendations:

- *Data discovery:* ATSDR should expend additional effort and resources in the area of conducting more rigorous data discovery activities. To the extent possible, the agency should augment, enhance, and refine data it is relying on to conduct water-modeling activities.
- *Chronology of events:* ATSDR should focus efforts on refining its understanding of chronological events. These need to include documenting periods of known contamination, times when water-distribution systems were interconnected, and the start of operations of the Holcomb Boulevard WTP.

Table A2. Summary of ATSDR chapter reports on topical subjects of water-modeling analyses and the historical reconstruction process, Tarawa Terrace and vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina.

[ATSDR, Agency for Toxic Substances and Disease Registry; VOC, volatile organic compound; PCE, tetrachloroethylene; WTP, water treatment plant]

Report chapter	Author(s)	Chapter title and reference citation	Topical summary
A	Maslia ML, Sautner JB, Faye RE, Suárez-Soto RJ, Aral MM, Grayman WM, Jang W, Wang J, Bove FJ, Ruckart PZ, Valenzuela C, Green JW Jr, and Krueger AL	Summary of Findings; Maslia et al. 2007 (this report)	Summary of detailed technical findings (found in Chapters B–K) focusing on the historical reconstruction analysis and present-day conditions of groundwater flow, contaminant fate and transport, and distribution of drinking water
B	Faye RE	Geohydrologic Framework of the Castle Hayne Aquifer System; Faye (In press 2007a)	Analyses of well and geohydrologic data used to develop the geohydrologic framework of the Castle Hayne aquifer system at Tarawa Terrace and vicinity
C	Faye RE, and Valenzuela C	Simulation of Groundwater Flow; Faye and Valenzuela (In press 2007)	Analyses of groundwater flow including developing a predevelopment (steady state) and transient groundwater-flow model
D	Lawrence SJ	Properties of Degradation Pathways of Common Organic Compounds in Groundwater; Lawrence (In press 2007)	Describes and summarizes the properties, degradation pathways, and degradation by-products of VOCs (non-trihalomethane) commonly detected in groundwater
E	Faye RE, and Green JW Jr	Occurrence of Contaminants in Groundwater; Faye and Green (In press 2007)	Describes the occurrence and distribution of PCE and related contaminants within the Tarawa Terrace aquifer and the Upper Castle Hayne aquifer system at and in the vicinity of the Tarawa Terrace housing area
F	Faye RE	Simulation of the Fate and Transport of Tetrachloroethylene (PCE); Faye (In press 2007b)	Historical reconstruction of the fate and transport of PCE in groundwater from the vicinity of ABC One-Hour Cleaners to individual water-supply wells and the Tarawa Terrace WTP
G	Jang W, and Aral MM	Simulation of Three-Dimensional Multi-species, Multiphase Mass Transport of Tetrachloroethylene (PCE) and Associated Degradation By-Products; Jang and Aral (In press 2007)	Descriptions about the development and application of a model capable of simulating three-dimensional, multispecies, and multiphase transport of PCE and associated degradation by-products
H	Wang J, and Aral MM	Effect of Groundwater Pumping Schedule Variation on Arrival of Tetrachloroethylene (PCE) at Water-Supply Wells and the Water Treatment Plant; Wang and Aral (In press 2007)	Analysis of the effect of groundwater pumping schedule variation on the arrival of PCE at water-supply wells and the Tarawa Terrace WTP
I	Maslia ML, Suárez-Soto RJ, Wang J, Aral MM, Sautner JB, and Valenzuela C	Parameter Sensitivity, Uncertainty, and Variability Associated with Model Simulations of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water; Maslia et al. (In press 2007b)	Assessment of parameter sensitivity, uncertainty, and variability associated with model simulations of groundwater flow, contaminant fate and transport, and the distribution of drinking water
J	Sautner JB, Valenzuela C, Maslia ML, and Grayman WM	Field Tests, Data Analyses, and Simulation of the Distribution of Drinking Water; Sautner et al. (In press 2007)	Field tests, data analyses, and simulation of the distribution of drinking water at Tarawa Terrace and vicinity
K	Maslia ML, Sautner JB, Faye RE, Suárez-Soto RJ, Aral MM, Grayman WM, Jang W, Wang J, Bove FJ, Ruckart PZ, Valenzuela C, Green JW Jr, and Krueger AL	Supplemental Information; Maslia et al. (In press 2007a)	Additional information such as synoptic maps showing groundwater levels, directions of groundwater flow, and the distribution of PCE based on simulation; a complete list of references; and other ancillary information and data that were used as the basis of this study

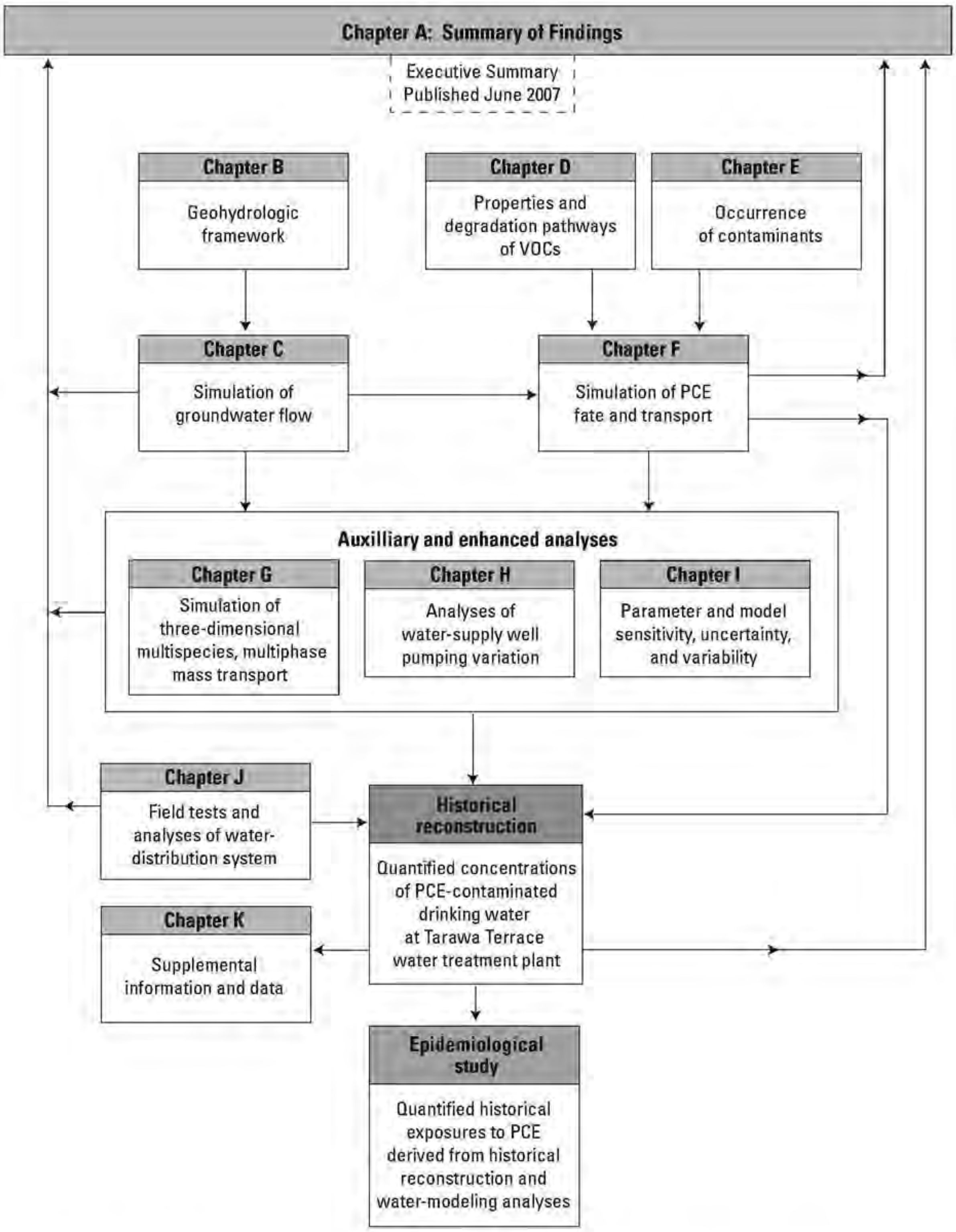


Figure A2. Relation among Chapter A report (Summary of Findings), Chapters B–K reports, historical reconstruction process, and the ATSDR epidemiological case-control study, Tarawa Terrace and vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina. [VOCs, volatile organic compounds; PCE, tetrachloroethylene]

- *Groundwater modeling, Tarawa Terrace area:* Several recommendations were made with respect to groundwater modeling and associated activities for the Tarawa Terrace area, and these included: (1) refine operational schedules of water-supply wells, (2) conduct fate and dispersive transport analyses, (3) conduct sensitivity and uncertainty analyses to refine initial estimates of model parameter values, and (4) determine sensitivity of model to cell sizes and boundary conditions.[7]
- *Water-distribution system analyses:* In light of available data, the ATSDR water-modeling team should consider using more simplified mixing models (rather than complex water-distribution system models) to quantify historical exposures to drinking-water supplies. More complex modeling might be warranted only if data discovery shows that the water-distribution systems had a greater frequency of interconnectivity.

The recommendations of the external expert panel were implemented as part of the historical reconstruction analysis efforts. Results of these efforts are presented in conjunction with specific data needs, descriptions of the historical reconstruction simulations, and sensitivity analyses that are summarized in this report (Chapter A) and discussed in detail in subsequent chapter reports (B–J).

Chlorinated Solvents and Volatile Organic Compounds (VOCs)

The compounds and contaminants discussed in this report and other Tarawa Terrace chapter reports belong to a class of chemicals referred to as chlorinated solvents. The denser-than-water characteristic of liquid chlorinated solvents has led to their being called "dense nonaqueous phase liquids" (DNAPLs[8]) (Pankow and Cherry 1996). The significant volatility that characterizes chlorinated solvents also has led to these compounds being referred to as "volatile organic compounds" (VOCs). It is the property of significant volatility that has led to the greatest lack of understanding of their potential for causing groundwater contamination (Schwille 1988). Thus, VOCs are organic compounds that have a high enough vapor pressure under normal circumstances to significantly vaporize and enter the atmosphere.

In the United States, the production of chlorinated solvents, and more generally, synthetic organic chemicals, was most probably a direct result of World War I. As of 1914, PCE was manufactured as a by-product of carbon tetrachloride, and domestic production of TCE is reported to have begun during the 1920s (Doherty 2000a, b). Contamination of groundwater systems by chlorinated solvents, however, was not recognized in North America until the late 1970s.[9] The lateness of this recognition was due in part because monitoring for VOCs and nearly all other organic compounds was not common until that time. Research into the properties of chlorinated solvents and how their properties, such as density (DNAPLs) and significant volatility (VOCs), were capable of leading to severe groundwater problems was first recognized by Schwille in West Germany during the 1970s (Schwille 1988). Thus, VOCs are considered environmental pollutants, and some may be carcinogenic. Briefly described next are naming conventions used for VOCs and maximum contaminant levels (MCLs) established by the U.S. Environmental Protection Agency (USEPA) for selected VOCs.

Naming Conventions

It is common to find a confusing variety of names used to identify VOCs. For example, tetrachloroethene also is known as perchloroethylene, PCE, PERC®, and tetrachloroethylene (Table A3). The variety of different names for VOCs depends on (1) the brand name under which the product is sold, (2) the region where the compound is used, (3) the type of publication referring to the compound, (4) the popularity of the name in recently published literature, (5) the profession of the person using the name, or (6) a combination of all or part of the above. As early as the late 1800s, chemists and others recognized the need to have a consistent naming convention for chemical compounds. The International Union of Pure and Applied Chemistry (IUPAC) is an organization responsible for formal naming conventions

[7] Detailed discussions related to specific model characteristics such as geometry, cell size, boundary conditions, and more, are provided in Chapter C (Faye and Valenzuela In press 2007) and Chapter F (Faye In press 2007b) reports.

[8] Dense nonaqueous phase liquids (DNAPLs) have a specific gravity greater than water (> 1.0), and are immiscible (nonmixing) in water.

[9] Contaminants were detected in groundwater sampling by the New Jersey Department of Environmental Protection during 1978 (Cohn et al. 1994) and at Woburn, Massachusetts, during May 1979 (Massachusetts Department of Public Health 1996).

and corresponding names assigned to chemical compounds. Table A3, obtained from Lawrence (2006), lists the IUPAC names and synonyms (associated common, alternate, and other possible names) for selected VOCs detected in groundwater. The common or alternate names are used in this and all of the Tarawa Terrace reports for ease of reference to, and recognition of, previously published reports, documents, and laboratory analyses that pertain to the Tarawa Terrace area.[10]

Maximum Contaminant Levels

The maximum contaminant level or MCL is a legal threshold set by the USEPA to quantify the amount of a hazardous substance allowed in drinking water under the Safe Drinking Water Act. For example, the MCL for PCE was set at 5 micrograms per liter (μg/L) during 1992 because, given the technology at that time, 5 μg/L was the lowest level that water systems could be required to achieve. Effective dates for MCLs presented in this report are as follows: TCE and vinyl chloride (VC), January 9, 1989; PCE and *trans*-1,2-dichloroethylene (1,2-tDCE), July 6, 1992 (40 CFR, Section 141.60, Effective Dates, July 1, 2002, ed.). In this report and other Tarawa Terrace chapter reports, the current MCL for a specific VOC—for example, 5 μg/L for PCE—is used as a reference concentration to compare historically measured data and computer simulation results. These comparisons are not intended to imply (1) that the MCL was in effect at the time of sample measurement or simulated historical time or (2) that a measured or simulated concentration above an MCL was necessarily unsafe. Hereafter, the use of the term MCL should be understood to mean the current MCL associated with a particular contaminant. A complete list of MCLs for common VOCs can be found in USEPA report EPA 816-F-03-016 (2003). A complete list of effective dates for MCLs can be found in 40 CFR, Section 141.60, Effective Dates, July 1, 2002, edition.

[10]A detailed discussion and description of selected volatile organic compounds and associated degradation pathways is presented in the Chapter D report (Lawrence In press 2007).

Table A3. Names and synonyms of selected volatile organic compounds detected in groundwater.[1]

[IUPAC, International Union of Pure and Applied Chemistry; CAS, Chemical Abstract Services; —, not applicable]

IUPAC name[2]	Common or alternate name (synonym)[3]	Other possible names[3]	CAS number[2]
benzene	—	The B in BTEX, coal naptha, 1,3,5-cyclohexatriene, mineral naptha	71-43-2
1,2-dimethylbenzene	*o*-xylene	The X in BTEX, dimethyltoluene, Xylol	95-47-6
1,3-dimethylbenzene	*m*-xylene		108-38-3
1,4-dimethylbenzene	*p*-xylene		106-42-3
ethylbenzene	—	The E in BTEX, Ethylbenzol, phenylethane	100-41-4
methylbenzene	toluene	The T in BTEX, phenylmethane, Methacide, Toluol, Antisal 1A	108-88-3
chloroethene	vinyl chloride	chloroethylene, VC, monochloroethylene, monovinyl chloride, MVC	75-01-4
1,1-dichloroethene	1,1-dichloroethylene, DCE	vinylidene chloride	75-35-4
cis-1,2-dichloroethene	*cis*-1,2-dichloroethylene	1,2 DCE, Z-1,2-dichloroethene	156-59-2
trans-1,2-dichloroethene	*trans*-1,2-dichloroethylene	1,2 DCE, E-1,2-dichloroethene	156-60-2
tetrachloroethene	perchloroethylene, PCE, 1,1,2,2-tetrachloroethylene	ethylene tetrachloride, carbon dichloride, PERC®, PERK®, tetrachloroethylene	127-18-4
1,1,2-trichloroethene	1,1,2-trichloroethylene, TCE	acetylene trichloroethylene, trichloroethylene	79-01-6

[1]Lawrence (modified from 2006, In press 2007)

[2]International Union of Pure and Applied Chemistry (2006)

[3]USEPA (1995)

Historical Background

U.S. Marine Corps Base Camp Lejeune is located in the Coastal Plain of North Carolina, in Onslow County, southeast of the City of Jacksonville and about 70 miles northeast of the City of Wilmington, North Carolina (Figure A1). Operations began at Camp Lejeune during the 1940s. Today, nearly 150,000 people work and live on base, including active-duty personnel, dependents, retirees, and civilian employees. About two-thirds of the active-duty personnel and their dependents are less than 25 years of age.

Camp Lejeune consists of 15 different housing areas; families live in base housing for an average of 2 years. During the 1970s and 1980s, family housing areas were served by three water-distribution systems, all of which used groundwater as the source for drinking water—Hadnot Point, Tarawa Terrace, and Holcomb Boulevard (Plate 1). Hadnot Point was the original water-distribution system serving the entire base with drinking water during the 1940s. The Tarawa Terrace WTP began delivering drinking water during 1952–1953, and the Holcomb Boulevard WTP began delivering drinking water during June 1972 (S.A. Brewer, U.S. Marine Corps Base Camp Lejeune, written communication, September 29, 2005).

The Tarawa Terrace housing area was constructed during 1951 and was subdivided into housing areas I and II (Figure A1). Originally, areas I and II contained a total of 1,846 housing units and accommodated a resident population of about 6,000 persons (Sheet 3 of 18, Map of Tarawa Terrace II Quarters, June 30, 1961; Sheet 7 of 34, Tarawa Terrace I Quarters, July 31, 1984). The general area of Tarawa Terrace is bounded on the east by Northeast Creek, to the south by New River and Northeast Creek, to the west by New River, and to the north by North Carolina Highway 24 (SR 24).

The documented onset of pumping at Tarawa Terrace is unknown but is estimated to have begun during 1952. Water-supply well TT-26, located about 900 feet southeast of ABC One-Hour Cleaners (Figure A1), began operations during 1952. ABC One-Hour Cleaners—an off-base dry-cleaning facility that used PCE in the dry-cleaning process (Melts 2001)—is the only documented source of PCE contamination of groundwater resources at Tarawa Terrace (Shiver 1985). The first occurrence of PCE contamination at a Tarawa Terrace water-supply well probably occurred at well TT-26 after the onset of dry-cleaning operations at ABC One-Hour Cleaners during 1953.

The Camp Knox trailer park area was constructed during 1976 with 112 trailer spaces. An additional 75 spaces were added during 1989 allowing for a total of 187 housing units, which could accommodate a population of 629 persons (Sheet 5 of 34, Map of Knox Trailer Park Area, July 31, 1984). The Camp Knox trailer park area is located in the southwestern part of the Tarawa Terrace area and is bounded on the south by Northeast Creek (Figure A1). Camp Johnson and Montford Point are located to the west and southwest of Tarawa Terrace, respectively. Historically, the Camp Knox trailer park was served by both Tarawa Terrace and Montford Point water supplies.

During 1989, the USEPA placed U.S. Marine Corps Base Camp Lejeune and ABC One-Hour Cleaners on its National Priorities List (NPL) of sites requiring environmental investigation (also known as the list of Superfund sites). During August 1990, ATSDR conducted a public health assessment (PHA) at ABC One-Hour Cleaners. The PHA found that PCE, detected in onsite and offsite wells, was the primary contaminant of concern. Other detected contaminants included TCE, 1,2-dichloroethylene (1,2-DCE), 1,2-tDCE, 1,1-dichloroethylene (DCE), VC, benzene, and toluene (ATSDR 1990).

During 1997, ATSDR completed a PHA for Camp Lejeune which concluded that estimated exposures to VOCs in drinking water were significantly below the levels shown to be of concern in animal studies. Thus, ATSDR determined that exposure to VOCs in on-base drinking water was unlikely to result in cancer and noncancer health effects in adults. However, because scientific data relating to the harmful effects of VOCs on a child or a fetus were limited, ATSDR recommended conducting an epidemiological study to assess the risks to infants and children during in utero exposure to chlorinated solvents (for example, PCE and TCE) contained in on-base drinking water (ATSDR 1997).

Following this recommendation, during 1998 ATSDR published a study of adverse birth outcomes (ATSDR 1998). ATSDR used various databases to evaluate possible associations between maternal exposure to contaminants contained in drinking water on the base and mean birth weight deficit, preterm birth (less than 37 weeks gestational age), and small for gestational age (SGA). To identify women living in base housing when they delivered, birth certificates were collected for live births that occurred January 1, 1968—December 31, 1985. The study found that exposure to PCE in drinking water was related to an elevated risk of SGA for mothers older than 35 years or who experienced two or more prior fetal losses (ATSDR 1998; Sonnenfeld et al. 2001). The study could not, however, evaluate childhood cancers and birth defects because the study relied solely on birth certificates to ascertain adverse birth outcomes.[11] However, because this study used incorrect information on the start-up date for the Holcomb Boulevard WTP,[12] errors were made in assigning exposures to the mothers. Therefore, this study is being re-analyzed using the results from the historical reconstruction process and water-modeling analyses.

During 1999, ATSDR began an epidemiological study to evaluate whether in utero and infant (up to 1 year of age) exposure to VOC-contaminated drinking water was associated with specific birth defects and childhood cancers. The study includes births during 1968–1985 to women who resided at the base anytime during their pregnancy. The first year of the study, 1968, was chosen because North Carolina computerized its birth certificates starting that year. The last year of the study, 1985, was chosen because the most contaminated Tarawa Terrace water-supply wells (TT-23 and TT-26, Figure A1) were removed from regular service that year (February 1985). The study is evaluating the central nervous system defects known as neural tube defects (for example, spina bifida and anencephaly), cleft lip and cleft palate, and childhood leukemia and non-Hodgkin's lymphoma. The study consists of a multistep process that includes:

- a scientific literature review to identify particular childhood cancers and birth defects associated with exposure to VOC-contaminated drinking water,
- a telephone survey to identify potential cases,
- a medical records search to confirm the diagnoses of the reported cases, and
- a case-control study to interview parents (collect information on a mother's residential history and water use as well as potential risk factors such as a mother's occupation and illnesses during pregnancy) and obtain exposure estimates through water-modeling analyses and the historical reconstruction process.

[11] Birth defects are only poorly ascertained using birth certificates; childhood cancers are not included on birth certificates.

[12] Current information from the Camp Lejeune Public Works Department Utilities Section indicates that the Holcomb Boulevard WTP began supplying finished water to areas serviced by the Holcomb Boulevard WTP (Plate 1) during June 1972 (S.A. Brewer, U.S. Marine Corps Base Camp Lejeune, written communication, September 29, 2005).

During 2004, the study protocol received approval from the Centers for Disease Control and Prevention Institutional Review Board and the U.S. Office of Management and Budget.

Water-Distribution Investigation

Given the paucity of measured historical contaminant-specific data and the lack of historical exposure data during most of the period relevant to the epidemiological study (January 1968–December 1985), ATSDR decided to apply the concepts of historical reconstruction to synthesize and estimate the spatial and temporal distributions of contaminant-specific concentrations in the drinking-water supply at Tarawa Terrace. Historical reconstruction typically includes the application of simulation tools, such as models, to recreate (or synthesize) past conditions. For this study, historical reconstruction included the linking of groundwater fate and transport models with materials mass balance (simple mixing) and water-distribution system models (Table A4). The primary focus for the investigation of the Tarawa Terrace historical reconstruction analyses was the fate and transport of, and exposure to, a single constituent—PCE. Additional and enhanced analyses that relate to degradation by-products of PCE—TCE, 1,2-tDCE, and VC—also are presented (Figure A2). Based on groundwater and water-quality data collection and analyses by Shiver (1985), PCE originating from the site of ABC One-Hour Cleaners is considered the primary VOC compound responsible for contaminating the Tarawa Terrace water-supply wells.

Models Used for Water-Distribution Investigation

Applying simulation tools or models to reconstruct historical contamination and exposure events at Tarawa Terrace and vicinity required the development of databases from diverse sources of information such as well and geohydrologic analyses, computations of PCE mass at the ABC One-Hour Cleaners site and within the Tarawa Terrace and Upper Castle Hayne aquifers, and analyses and assessment of

Table A4. Analyses and simulation tools (models) used to reconstruct historical contamination events at Tarawa Terrace and vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina.

[VOC, volatile organic compound; PCE, tetrachloroethylene; GIS, geographic information system; WTP, water treatment plant; TCE, trichloroethylene; 1,2-tDCE, *trans*-1,2-dichloroethylene; VC, vinyl chloride]

Analysis	Description	Analysis or simulation tool and type	Reference
Geohydrologic framework	Detailed analyses of well and geohydrologic data used to develop framework of the Castle Hayne aquifer system at Tarawa Terrace and vicinity	Data analysis	Faye (In press 2007a)
Predevelopment groundwater flow	Steady-state groundwater flow, occurring prior to initiation of water-supply well activities (1951) or after recovery of water levels from cessation of pumping activities (1994)	MODFLOW-96—numerical model	Harbaugh and McDonald (1996); Faye and Valenzuela (In press 2007)
Transient groundwater flow	Unsteady-state groundwater flow occurring primarily because of the initiation and continued operation of water-supply wells (January 1951–December 1994)	MODFLOW-96—numerical model	Harbaugh and McDonald (1996); Faye and Valenzuela (In press 2007)
Properties of VOCs in groundwater	Properties of degradation pathways of common organic compounds in groundwater	Literature survey	Lawrence (2006, In press 2007)
Computation of PCE mass	Estimates of mass (volume) of PCE: (a) unsaturated zone (above water table) in vicinity of ABC One-Hour Cleaners based on 1987–1993 data; (b) within Tarawa Terrace and Upper Castle Hayne aquifers based on 1991–1993 data	Site investigation data, GIS, and spatial analyses	Roy F. Weston, Inc. (1992, 1994); Pankow and Cherry (1996); Faye and Green (In press 2007)
Fate and transport of PCE	Simulation of the fate and migration of PCE from its source (ABC One-Hour Cleaners) to Tarawa Terrace water-supply wells (January 1951–December 1994)	MT3DMS—numerical model	Zheng and Wang (1999); Faye (In press 2007b)
PCE concentration in WTP finished water	Computation of concentration of PCE in drinking water from the Tarawa Terrace WTP using results from fate and transport modeling	Materials mass balance model using principles of conservation of mass and continuity—algebraic	Masters (1998); Faye (In press 2007b)
Fate and transport of PCE and degradation by-products in groundwater and vapor phase	Three-dimensional, multiphase simulation of the fate, degradation, and transport of PCE degradation by-products: TCE, 1,2-tDCE, and VC	TechFlowMP—numerical	Jang and Aral (2005, 2007, In press 2007)
Early and late arrival of PCE at WTP	Analysis to assess impact of schedule variation of water-supply well operations on arrival of PCE at wells and the Tarawa Terrace WTP	PSOpS—numerical; optimization	Wang and Aral (2007, In press 2007)
Parameter uncertainty and variability	Assessment of parameter sensitivity, uncertainty, and variability associated with model simulations of ground-water flow, fate and transport, and water distribution	PEST; Monte Carlo simulation—probabilistic	Doherty (2005); Maslia et al. (In press 2007b)
Distribution of PCE in drinking water	Simulation of hydraulics and water quality in water-distribution system serving Tarawa Terrace based on present-day (2004) conditions	EPANET 2—numerical	Rossman (2000); Sautner et al. (In press 2007)

historical and present-day (2002) operations of the water-distribution system serving Tarawa Terrace.[13] A complete list of analysis and simulation tools used to reconstruct historical contamination and exposure events at Tarawa Terrace and vicinity is provided in Table A4. Information and data were applied to the models in the following sequence:

1. Geohydrologic framework information, aquifer and confining unit hydraulic data, and climatic data were used to determine predevelopment (prior to 1951) groundwater-flow characteristics.[14] To simulate predevelopment groundwater-flow conditions, the public-domain code MODFLOW-96 (Harbaugh and McDonald 1996)—a three-dimensional groundwater-flow model code—was used.

2. Transient groundwater conditions occurring primarily because of the initiation and continued operation of water-supply wells at Tarawa Terrace also were simulated using the three-dimensional model code MODFLOW-96; well operations were accounted for and could vary on a monthly basis.

3. Groundwater velocities or specific discharges derived from the transient groundwater-flow model were used in conjunction with PCE source, fate, and transport data to develop a fate and transport model. To simulate the fate and transport of PCE as a single specie from its source at ABC One-Hour Cleaners to Tarawa Terrace water-supply wells, the public domain code MT3DMS (Zheng and Wang 1999) was used. MT3DMS is a model capable of simulating three-dimensional fate and transport. Simulations describe PCE concentrations on a monthly basis during January 1951–December 1994.

4. The monthly concentrations of PCE assigned to finished water at the Tarawa Terrace WTP were determined using a materials mass balance model (simple mixing) to compute the flow-weighted average concentration of PCE. The model is based on the principles of continuity and conservation of mass (Masters 1998).

5. To analyze the degradation of PCE into degradation by-products (TCE, 1,2-tDCE, and VC) and to simulate the fate and transport of these contaminants in the unsaturated zone (zone above the water table), a three-dimensional, multispecies, and multiphase mass transport model was developed by the Multimedia Simulations Laboratory (MESL) at the Georgia Institute of Technology (Jang and Aral 2005, 2007, In press 2007) .

6. To analyze and understand the impacts of unknown and uncertain historical pumping schedule variations of water-supply wells on arrival of PCE at the Tarawa Terrace water-supply wells and WTP, a pumping and schedule optimization system tool (PSOpS) was used. This model was also developed by the MESL (Wang and Aral 2007, In press 2007).

7. To assess parameter sensitivity, uncertainty, and variability associated with model simulations of flow, fate and transport, and computed PCE concentrations in finished water at the Tarawa Terrace WTP, sensitivity and probabilistic analyses were conducted. Sensitivity analyses were conducted using a one-at-a-time approach; the probabilistic analyses applied the Monte Carlo simulation (MCS) and sequential Gaussian simulation (SGS) methods to results previously obtained using MODFLOW-96, MT3DMS, and the drinking-water mixing model.

8. The initial approach for estimating the concentration of PCE delivered to residences of Tarawa Terrace used the public domain model, EPANET 2 (Rossman 2000)—a water-distribution system model used to simulate street-by-street PCE concentrations (Sautner et al. 2005, 2007). Based on expert peer review of this approach (Maslia 2005) and exhaustive reviews of historical data—including water-supply well and WTP operational data when available—study staff concluded that the Tarawa Terrace WTP and water-distribution system was not interconnected with other water-distribution systems at Camp Lejeune for any substantial time periods (greater than 2 weeks).[15] Thus, all water

[13] A comprehensive list of references used to gather, analyze, and assemble information and data for the Tarawa Terrace water-distribution investigation is provided on the electronic media (DVD) accompanying this report and in the Chapter K report (Maslia et al. In press 2007a).

[14] Predevelopment or steady-state refers to groundwater conditions prior to or after the cessation of all water-supply well pumping activity.

[15] The term "interconnection" is defined in this study as the continuous flow of water in a pipeline from one water-distribution system to another for periods exceeding two weeks. Pipelines did connect two or more water-distribution systems, but unless continuous flow was documented, the water-distribution systems were assumed not to be interconnected.

arriving at the WTP was assumed to originate solely from Tarawa Terrace water-supply wells (Faye and Valenzuela In press 2007; Faye In press 2007b) and to be completely and uniformly mixed prior to delivery to residents of Tarawa Terrace through the network of distribution system pipelines and storage tanks. Based on these information and data, study staff concluded that a simple mixing model approach, based on the principles of continuity and conservation of mass, would provide a sufficient level of detail and accuracy to estimate monthly PCE exposure concentrations at Tarawa Terrace.[16] Thus, results of the monthly flow-weighted average PCE-concentration computations were provided to agency health scientists and epidemiologists to assess population exposure to PCE.

Data Needs and Availability

The historical reconstruction process required information and data describing the functional and physical characteristics of the groundwater-flow system, the chemical specific contaminant (PCE) and its degradation by-products, and the water-distribution system. Required for the successful completion of the historical reconstruction process, specific data can be categorized into four generalized information types that relate to: (1) aquifer geometry and hydraulic characteristics (for example, horizontal hydraulic conductivity, effective porosity, and dispersivity); (2) well-construction, capacity, and pumpage data (for example, drilling dates, well depth, operational dates, and quantities of pumped groundwater by month); (3) chemical properties and transport parameters (for example, partition coefficients, sorption rate, solubility, and biodegradation rate); and (4) water-distribution system design and operation data (for example, monthly delivery of finished water from the Tarawa Terrace WTP, network geometry and materials of pipelines, and size and location of storage tanks). Availability of specific data, methods of obtaining data, assessment of the reliability of the data, and implications with respect to model assumptions and simulations are discussed in detail in chapter reports B–J (Table A2 and Appendix A1).

[16] This assumption is tested and verified in the Chapter J report (Sautner et al. In press 2007) of this study.

Ideally, data collection in support of the historical reconstruction process is through direct measurement and observation. In reality, however, data collected are not routinely available by direct measurement and must be recreated or synthesized using generally accepted engineering analyses and methods (for example, modeling analyses). Additionally, the reliability of data obtained by direct measurement or observation must be assessed in accordance with methods used to obtain the data. Issues of data sources and the methods used to obtain data that cannot be directly measured, or are based on methods of less accuracy, ultimately reflect on the credibility of simulation results. The methods for obtaining the necessary data for the historical reconstruction analysis were grouped into three categories (ATSDR 2001):

• *Direct measurement or observation*—Data included in this category were obtained by direct measurement or observation of historical data and are verifiable by independent means. Data obtained by direct measurement or observation still must be assessed as to the methods used in measuring the data. For example, in the Chapter C report, Faye and Valenzuela (In press 2007) discuss that water-level data obtained from properly constructed monitor wells using electric- or steel-tape measurements are more reliable than water-level data obtained from water-supply wells using airline measurements. Of the three data categories discussed, data obtained by direct measurement were the most preferred in terms of reliability and least affected by issues of uncertainty. Examples of such data included aquifer water levels, PCE concentrations in water-supply wells and in finished water at the WTP, and PCE concentration at the location of the contaminant source (ABC One-Hour Cleaners).

• *Quantitative estimates*—Data included in this category were estimated or quantified using generally accepted computational methods and analyses, for example, monthly infiltration or recharge rates to the Castle Hayne aquifer system and estimates of contaminant mass in the vicinity of ABC One-Hour Cleaners and the Tarawa Terrace and Upper Castle Hayne aquifers.

• *Qualitative description*—Data included in this category were based on inference or were synthesized using surrogate information, for example, water-supply well operational information, retardation factors, and aquifer dispersivity. Of the three data categories described, data derived by qualitative description were the least preferred in terms of reliability and the most affected by issues of uncertainty.

Chronology of Events

To reconstruct historical exposures, a reliable chronology related to operations of the identified source of the PCE contamination, ABC One-Hour Cleaners, and of water-supply facilities (wells and the WTP) is of utmost importance. This information has a direct impact on the reliability and accuracy of estimates derived for the levels and duration of exposure to contaminated drinking water. Using a variety of information sources and references, events related to water supply and contamination of groundwater and drinking water at Tarawa Terrace and vicinity are shown graphically and explained in Figure A3. Examples of information sources and references used to develop the chronology of events shown in Figure A3 include: (1) capacity and operational histories of Tarawa Terrace water-supply wells and the WTP (Faye and Valenzuela In press 2007), (2) depositions from the owners of ABC One-Hour Cleaners (Melts 2001), (3) identification and characterization of the source of PCE contamination (Shiver 1985), and (4) laboratory analyses of samples from water-supply wells (Granger Laboratories 1982) and the WTP (CLW 3298-3305).

One of the purposes of Figure A3 is to present, in a graphical manner, the relation among water supply, contamination events, exposure to contaminated drinking water in family housing areas, selected simulation results, and the time frame of the epidemiological case-control study. For the first time, all of these different types of information and data sources are summarized in one document that is believed to be an accurate reconciliation of chronological events that relate to Tarawa Terrace and vicinity. Three events are noteworthy: (1) the year shown for the start of operations of ABC One-Hour Cleaners (1953) is used as the starting time for PCE contamination of groundwater in the fate and transport modeling of PCE, (2) sampling events and PCE concentration values of tap water are shown for 1982, and (3) the closure of the Tarawa Terrace WTP is shown as occurring during March 1987. Care has been taken to assure that chronological event information and data required for modeling analyses and the historical reconstruction process (1) honor original data and information sources, (2) are consistent and in agreement with all Tarawa Terrace chapter reports, and (3) reflect the most up-to-date information.

Occurrence of Contaminants in Groundwater[17]

Detailed analyses of concentrations of PCE at groundwater sampling locations and at Tarawa Terrace water-supply wells during the period 1991–1993 were sufficient to estimate the mass, or amount, of PCE remaining in the Tarawa Terrace and Upper Castle Hayne aquifers. Similar methods were applied to compute the mass of PCE in the unsaturated zone (zone above the water table) at and in the vicinity of ABC One-Hour Cleaners using concentration-depth data determined from soil borings during field investigations of 1987–1993. These analyses are presented in Faye and Green (In press 2007) and are summarized in Table A5. This information and data were necessary to develop accurate and reliable databases to conduct model simulations of the fate and transport of PCE from its source—ABC One-Hour Cleaners—to Tarawa Terrace water-supply wells and WTP. The total mass of PCE computed in groundwater and within the unsaturated zone during the period 1953–1985 equals about 6,000 pounds and equates to a volume of about 430 gallons (gal).[18] This volume represents an average minimum loss rate of PCE to the

Table A5. Computed volume and mass of tetrachloroethylene in the unsaturated and saturated zones, Tarawa Terrace and vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina.[1]

[PCE, tetrachloroethylene]

Zone	Dates of computation	Volume, in gallons[2]	Average annual contribution of PCE, 1953–1985	
			In gallons	In grams
Unsaturated[3]	1987–1993	190	6	36,340
Saturated[4]	1991–1993	240	7	42,397
Total		**430**	**13**	**78,737**

[1]Refer to Chapter E report (Faye and Green In press 2007) for specific computational details

[2]Density of PCE is 1.6 grams per cubic centimeter, or about 101 pounds per cubic foot

[3]Zone above water table in vicinity of ABC One-Hour Cleaners

[4]Tarawa Terrace and Upper Castle Hayne aquifers

[17] For detailed analyses and discussions of occurrence of contaminants in groundwater at Tarawa Terrace and vicinity, refer to the Chapter E report (Faye and Green In press 2007).

[18] Typically, such volumes also are expressed in terms of 55-gal drums. The aforementioned volume of 430 gal of PCE is equivalent to 7.8 drums of PCE.

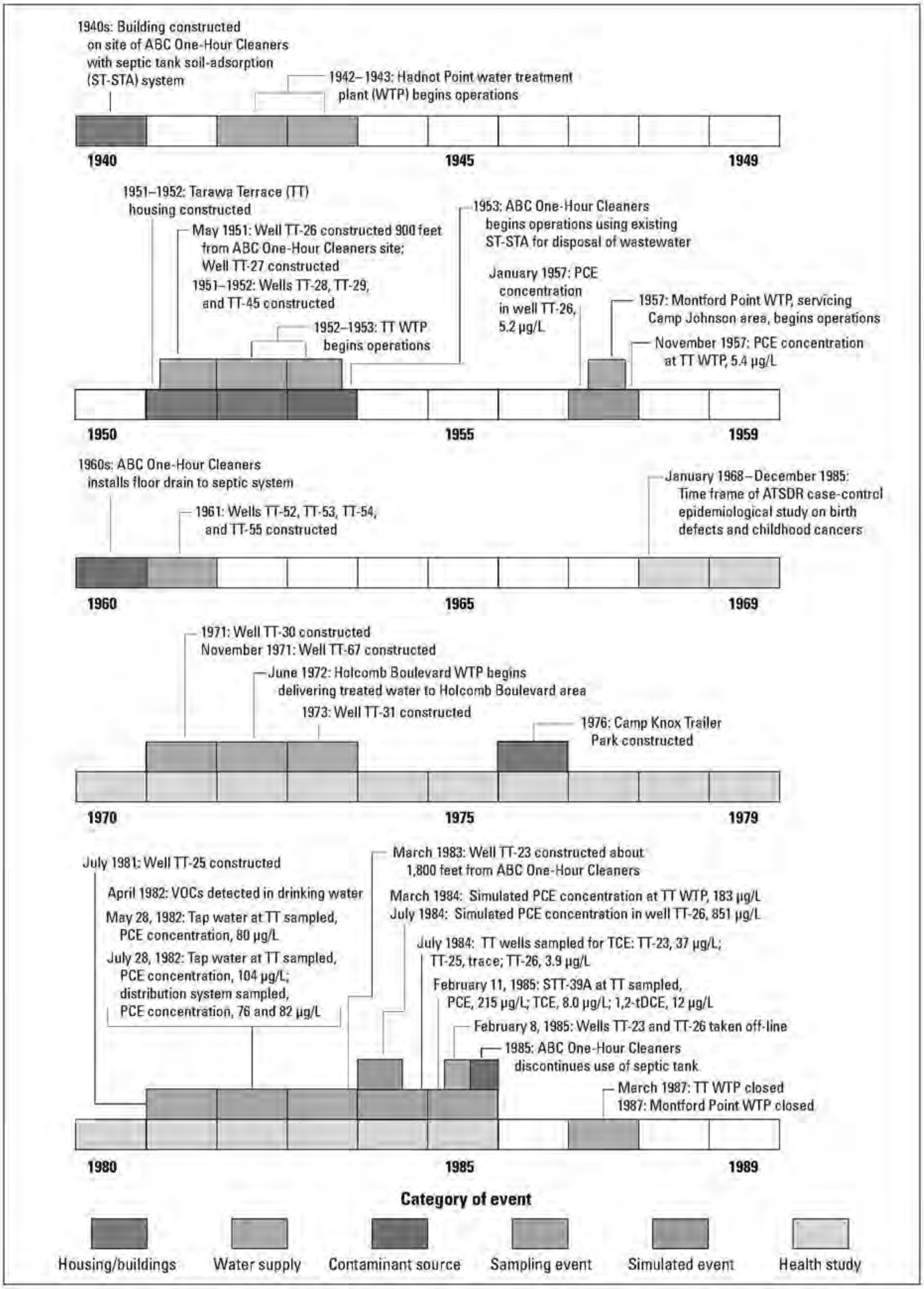


Figure A3. Chronology of events related to supply and contamination of drinking water, Tarawa Terrace and vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina. (STT-39A is the pump house associated with storage tank STT-39.) [ft, foot; µg/L, microgram per liter; VOC, volatile organic compound; PCE, tetrachloroethylene; TCE, trichloroethylene; 1,2-tDCE, *trans*-1,2-dichloroethylene; current maximum contaminant levels: PCE 5 µg/L, TCE 5 µg/L, 1,2-tDCE 100 µg/L] subsurface at ABC One-Hour Cleaners of about 13 gallons per year during the period 1953–1985. This PCE loss rate should be considered a minimum because (1) the quantity of PCE removed from the aquifers at Tarawa Terrace water-supply wells during 1953–1985 is unknown, (2) biodegradation of PCE to daughter products of TCE, 1,2-tDCE, and VC was probably occurring in the aquifers during and prior to 1991, and (3) PCE mass adsorbed to the sands and clays of the aquifer porous media and was not accounted for during the PCE mass computations. Pankow and Cherry (1996) indicate that computations of contaminant mass similar to those summarized here and described in detail in Faye and Green (In press 2007) represent only a small fraction of the total contaminant mass in the subsurface. Comparing the estimated volume of 430 gal of PCE (7.8 55-gal drums) computed by Faye and Green (In press 2007) with documented contaminant plumes in sand-gravel aquifers indicates that the contaminant mass in the subsurface at Tarawa Terrace would have been ranked as the third greatest volume of contaminant mass among seven contamination sites in the United States listed in a table provided in Mackay and Cherry (Table 1, 1989).

Relation of Contamination to Water Supply, Production, and Distribution

Historically, groundwater was used as the sole source of water supply for Camp Lejeune, and in particular, Tarawa Terrace. Of critical need in terms of historical reconstruction analysis, was information and data on the monthly raw water production of supply wells (to enable computations of flow-weighted drinking-water concentrations), and the distribution of finished water to family housing areas. The supply of drinking water to Tarawa Terrace was composed of two components: (1) the supply of water from groundwater wells to the Tarawa Terrace WTP and (2) the delivery of finished water from the WTP through the network of pipelines and storage tanks of the water-distribution system. The placement of water-supply wells into service and their permanent removal from service are critical to the analysis and simulation of contamination events. For example, water-supply well TT-26 was constructed during May 1951, probably placed into service during 1952, and was permanently taken off-line (service terminated) February 8, 1985. The Tarawa Terrace WTP began operations during 1952–1953 and was closed during March 1987 (Figure A3). All groundwater wells in the Tarawa Terrace area supplied untreated (or raw) water to a central treatment facility—the Tarawa Terrace WTP (Figure A4). Information pertaining to well-capacity histories, including construction, termination of service, and abandonment dates and spatial coordinate data are described in detail in Chapter C (Faye and Valenzuela In press 2007).

After treatment at the Tarawa Terrace WTP, finished water was distributed through pipelines to storage tanks, residential housing, military facility buildings, and shopping centers.[19] Information and data related to the water-distribution system (Plate 1; Figure A4) were gathered as part of data discovery and field investigation activities in support of the ATSDR epidemiological case-control study. The network of pipelines and storage tanks shown on Plate 1 and in Figure A4 represents present-day (2004) conditions, described in detail in Chapter J (Sautner et al. In press 2007). Based on a review of historical operating and housing information, the historical water-distribution system serving Tarawa Terrace was considered very similar and nearly identical to the present-day (2004) water-distribution system—the exception being two pipelines that were put into service during 1987 after the closing of the Tarawa Terrace and Camp Johnson WTPs. One pipeline, constructed during 1984, follows SR 24 northwest from the Holcomb Boulevard WTP and presently is used to supply ground storage tank STT-39 with finished water (Plate 1, Figure A4). The other pipeline, constructed during 1986, trends east-west from the Tarawa Terrace II area to storage tank SM-623 and presently is used to supply finished water from Tarawa Terrace to elevated storage tank SM-623. Historically (1952–1987), the Tarawa Terrace water-distribution system was operated independently of, and was not interconnected with, the Montford Point or Holcomb Boulevard water-distribution systems.[20]

Based on epidemiological considerations, historical reconstruction results were provided at monthly intervals. Ideally, these analyses require monthly groundwater pumpage data for the historical period. However, pumpage data were limited and were available on a monthly basis solely for 1978 and intermittently during the period of 1981–1985. Faye and Valenzuela (In press 2007)

[19] Based on an analysis of building type and usage in Tarawa Terrace, greater than 90% of the buildings were used for residential housing.

[20] Although the two pipelines discussed were constructed during 1984 and 1986, historical records such as water plant operator notes indicate that the pipelines did not convey finished water on a continuous basis prior to 1987.

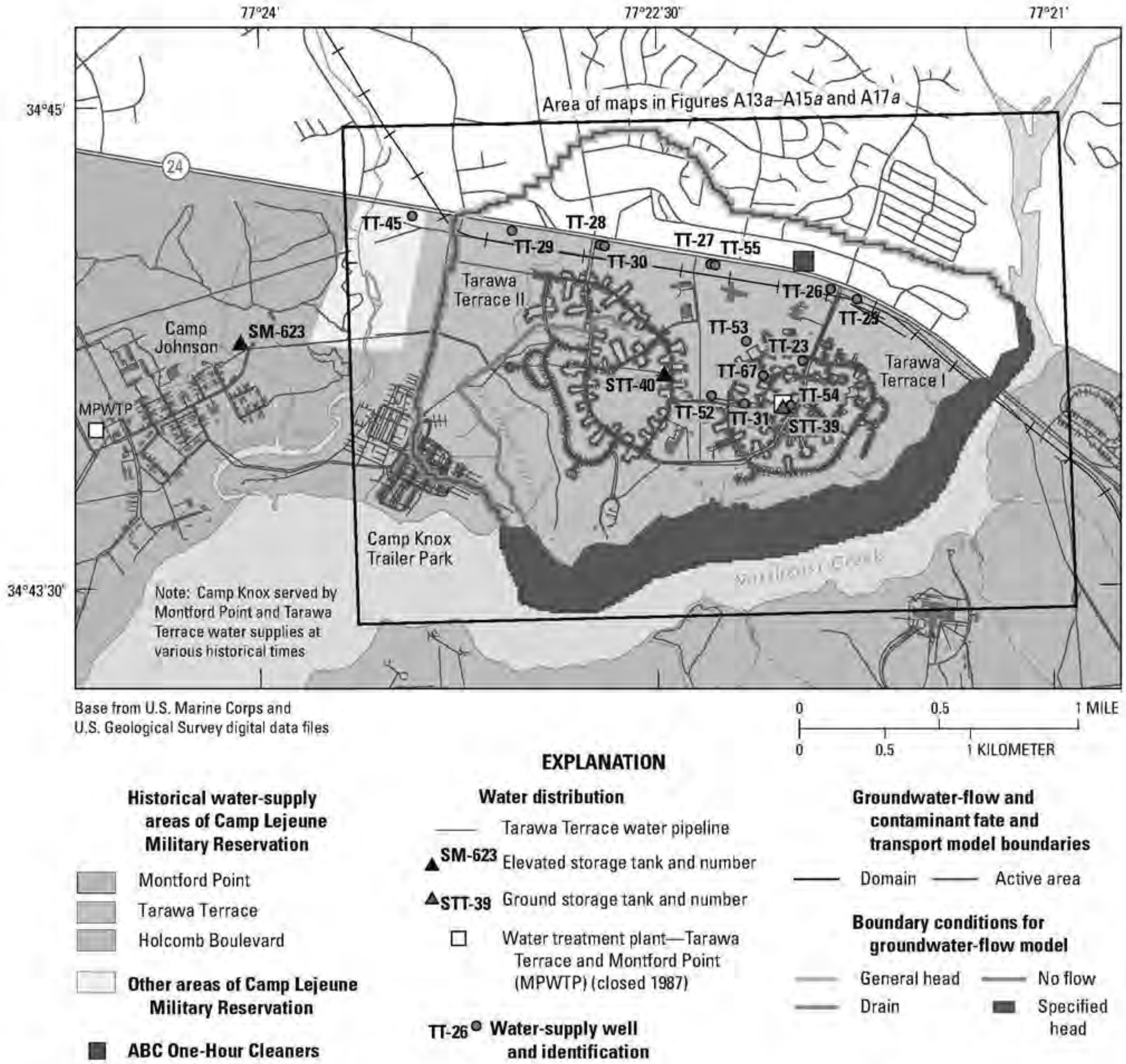


Figure A4. Location of groundwater-flow and contaminant fate and transport modeling areas and water-supply facilities used for historical reconstruction analyses, Tarawa Terrace and vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina.

provide details regarding groundwater pumpage including sources and capacity history. Where pumpage data were missing or incomplete, aquifer water-level and water-supply data, in conjunction with model simulation, were used to synthesize and reconstruct monthly water-supply well operations. Tarawa Terrace water-supply well operations—in terms of online dates and off-line dates for water supply—are presented graphically in Figure A5. Once a well was put in service, it was assumed to operate continuously for modeling purposes until it was permanently taken off-line—the exception being temporary shut downs for long-term maintenance. Breaks in continuous operations, such as those for wells TT-26 and TT-53, also are shown in Figure A5 and are based on documented information detailing periods of maintenance for specific wells. For example, water-supply well TT-26 was shut down for maintenance during July–August 1980 and January–February 1983 (Faye and Valenzuela In press 2007). Table A6 lists the specific month and year for the start of service for all Tarawa Terrace water-supply wells and the specific month and year for the end of service. Because raw water from all groundwater wells was

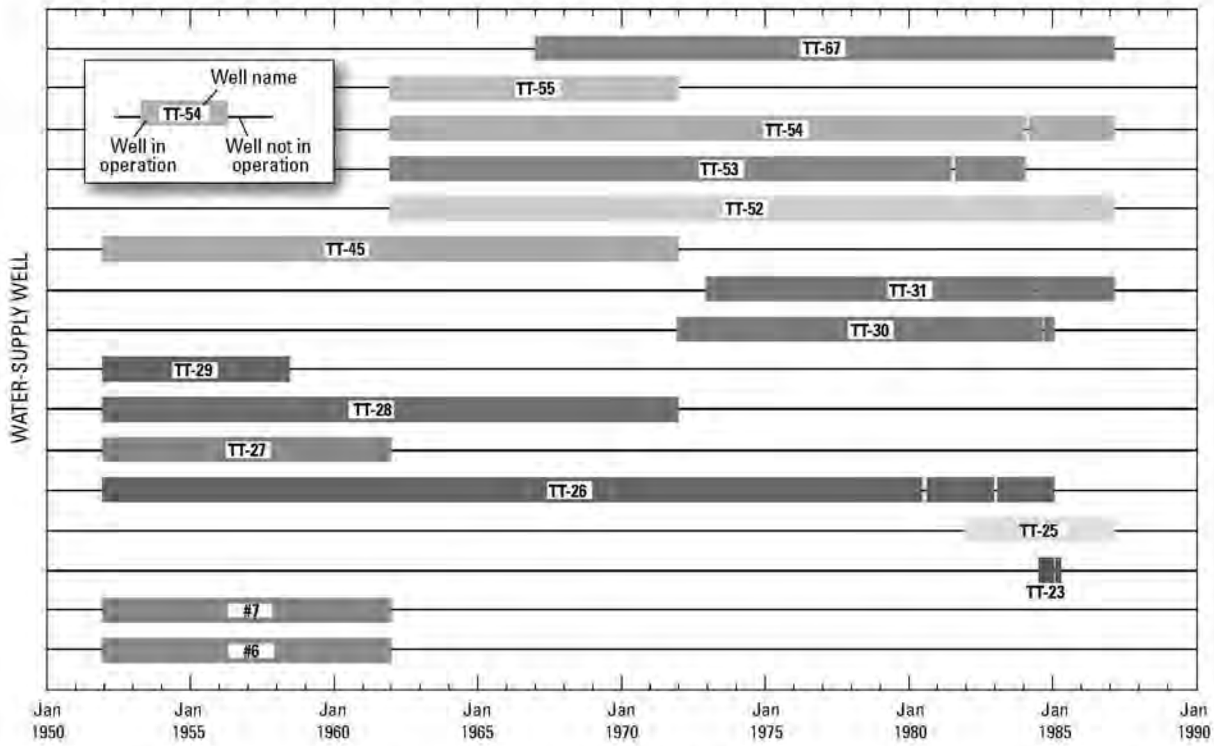


Figure A5. Historical operations of water-supply wells, 1952–87, Tarawa Terrace and vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina.

Table A6. Historical operations for water-supply wells, 1952–1987, Tarawa Terrace and vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina.[1]

[—, not applicable]

Well identification	In service	Off-line	Service terminated
#6	January 1952	—	January 1962
#7	January 1952	—	January 1962
TT-23	August 1984	February 1985	May 1985
TT-25	January 1982	—	March 1987
TT-26	January 1952	July–August 1980; January–February 1983	February 1985
TT-27	January 1952	—	January 1962
TT-28	January 1952	—	January 1972
TT-29	January 1952	—	July 1958
TT-30	January 1972	September 1984	February 1985
TT-31	January 1973	June 1984	March 1987
TT-45	January 1952	—	January 1972
TT-52	January 1962	March 1986	March 1987
TT-53	January 1962	July–August 1981	February 1984
TT-54	January 1962	February–March 1984	March 1987
TT-55	January 1962	—	January 1972
TT-67	January 1967	—	March 1987

[1]Refer to the Chapter C report (Faye and Valenzuela In press 2007) for additional details

mixed at the Tarawa Terrace WTP prior to treatment and distribution to Tarawa Terrace housing areas, the start-up and shut-down dates of specific water-supply wells, such as TT-26 and TT-23, were critical to accurately determining the concentration of contaminants in finished water delivered from the Tarawa Terrace WTP.

Total annual groundwater pumpage by well for all Tarawa Terrace water-supply wells is shown graphically in Figure A6. Refer to the Chapter C report (Faye and Valenzuela In Press 2007) for data sources used to derive Figure A6. This illustration also shows the contribution to pumpage by individual wells on an annual basis. For example, during 1978 total annual groundwater pumpage was 327 million gallons (MG) contributed by wells TT-26 (64.7 MG), TT-30 (25.9 MG), TT-31 (46.2 MG), TT-52 (48.1 MG), TT-53 (27.7 MG), TT-54 (62.8 MG), and TT-67 (51.7 MG) (Faye and Valenzuela In press 2007). Thus, well TT-26 and TT-54 contributed about 20 percent (%) each to the total annual pumpage for 1978, and well TT-30 contributed about 8%. This total annual groundwater pumpage is in agreement with the average rate of water delivered to the Tarawa Terrace WTP in 1978 of 0.90 million gallons per day, reported by Henry Von Oesen and Associates Inc. (1979).

The historical Tarawa Terrace water-distribution system was probably nearly identical to the present-day (2004) water-distribution system. Operational characteristics of the present-day water-distribution system were used for historical reconstruction analyses and were based on data gathered during field investigations (Sautner et al. 2005, Maslia et al. 2005). Delivery rates of finished water on a monthly basis during 2000–2004 are listed in Table A7 and shown graphically in Figure A7. For the 5-year period 2000–2004, the mean monthly delivery of finished water to the Tarawa Terrace water-distribution system was estimated to be 18.5 MG.[21] Monthly variations were most probably due to troop deployments. Monthly delivery data indicate that relatively high rates of finished water were delivered during the months of April, May, June, and July of 2000 and 2001. In addition, May and June of 2000 were the months of greatest delivery of finished water to the Tarawa Terrace water-distribution system—an estimated 30.9 MG of finished water during each month (Figure A7, Table A7).

[21] Since March 1987, finished water for the Tarawa Terrace water-distribution system has been provided by the Holcomb Boulevard WTP and delivered to ground storage tank STT-39 (Plate 1). See section on Field Tests and Analyses of the Water-Distribution System or the Chapter J report (Sautner et al. In press 2007).

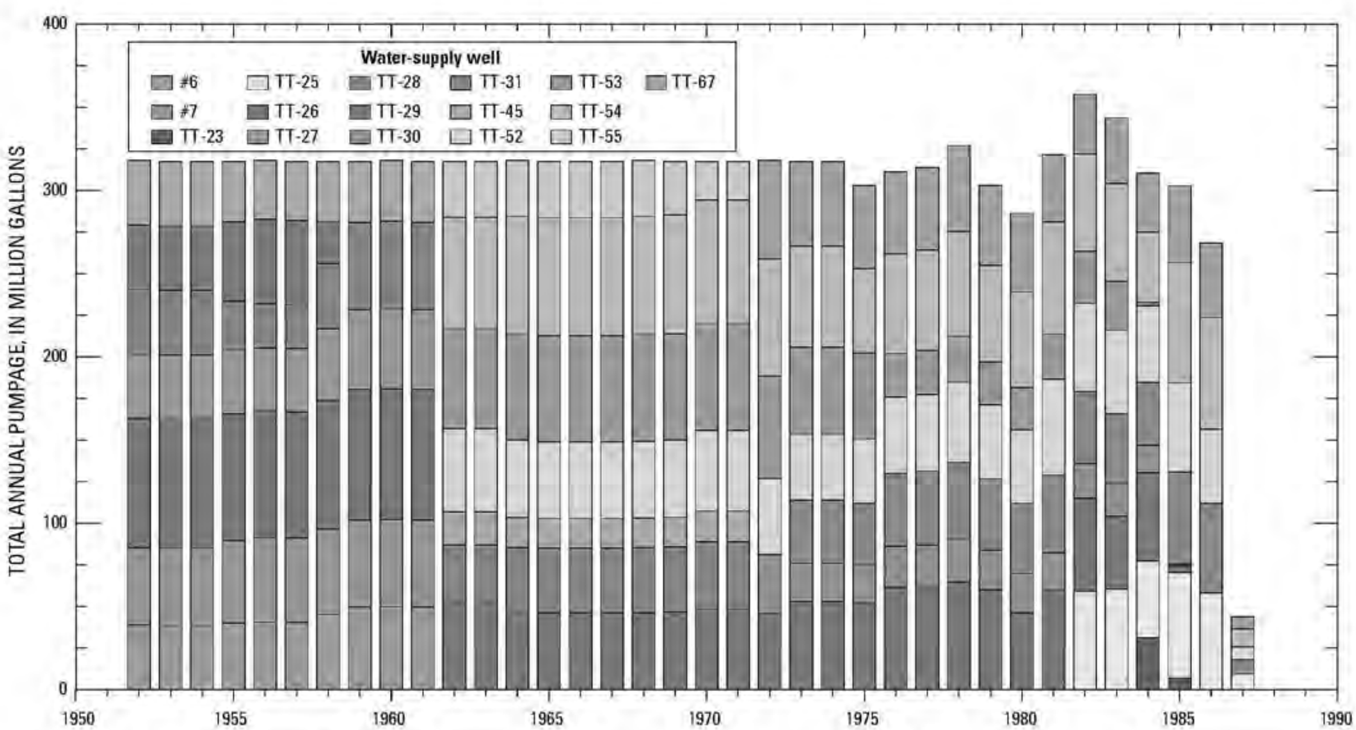


Figure A6. Total annual groundwater pumpage at water-supply wells, 1952–1987, Tarawa Terrace and vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina.

Table A7. Estimated monthly delivery of finished water to the Tarawa Terrace water-distribution system, 2000–2004, U.S. Marine Corps Base Camp Lejeune, North Carolina.[1,2]

[MG, million gallons; MGD, million gallons per day]

Month	Delivered finished water[3]									
	2000		2001		2002		2003		2004	
	MG	MGD	MG	MGD	MG	MGD	MG	MGD	MG	MGD
January	23.500	0.758	19.028	0.613	21.017	0.678	21.775	0.702	14.238	0.459
February	20.937	0.722	18.557	0.663	17.320	0.619	14.960	0.534	13.715	0.473
March	22.847	0.737	19.338	0.624	18.300	0.590	15.735	0.508	11.721	0.378
April	26.371	0.879	27.060	0.902	18.549	0.618	14.060	0.469	12.805	0.427
May	30.924	0.998	19.468	0.628	16.974	0.548	13.365	0.431	14.088	0.454
June	30.907	1.030	25.156	0.839	17.163	0.570	13.629	0.454	12.763	0.425
July	24.297	0.784	23.984	0.774	16.440	0.530	13.604	0.439	13.945	0.450
August	22.145	0.714	17.931	0.578	18.020	0.581	18.539	0.598	12.106	0.391
September	19.732	0.658	16.469	0.549	16.900	0.563	19.916	0.664	12.135	0.405
October	18.274	0.589	16.619	0.536	15.907	0.513	21.798	0.703	16.435	0.548
November	20.663	0.689	17.240	0.575	16.807	0.560	20.607	0.687	16.982	0.566
December	25.785	0.832	17.101	0.552	17.082	0.551	20.939	0.675	16.861	0.544

[1]Since March 1987, finished water for the Tarawa Terrace water-distribution system has been provided by the Holcomb Boulevard WTP and delivered to ground storage tank STT-39 (Plate 1)

[2]Data from Joel Hartsoe, Camp Lejeune Public Works Department Utilities Section, December 6, 2006

[3]Flow data measured at venturi meter located in building STT-39A (Tarawa Terrace pump house)

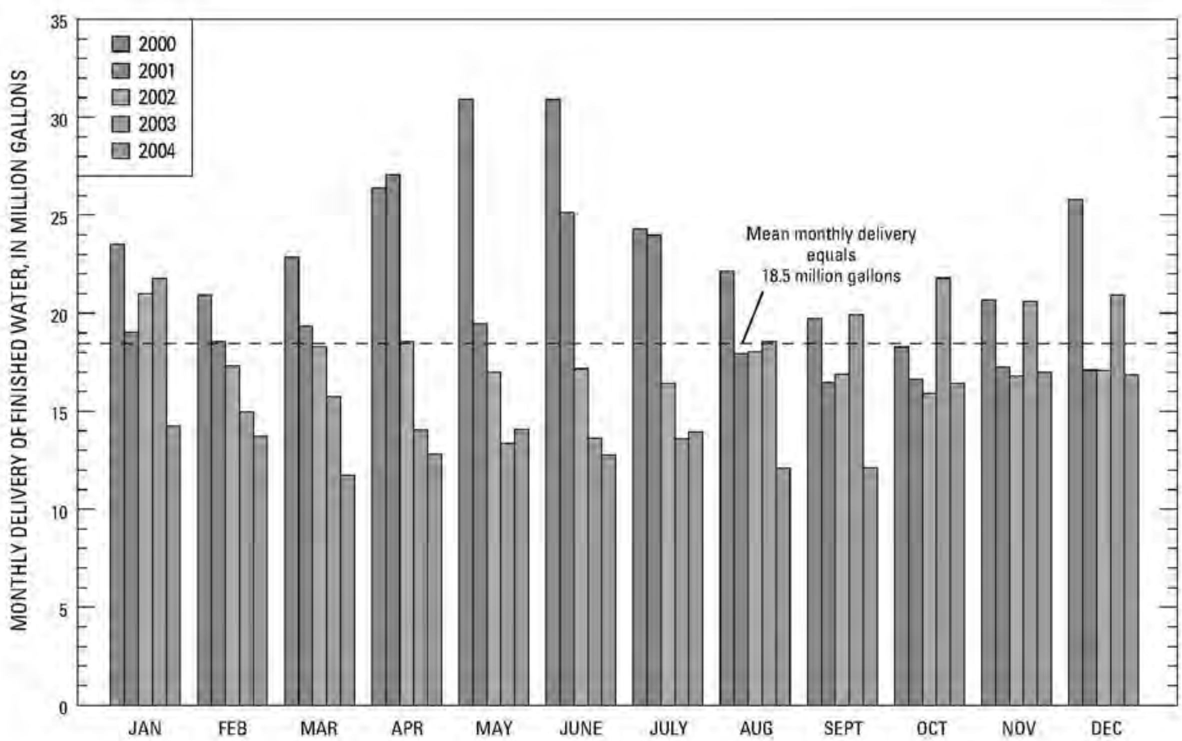


Figure A7. Estimated monthly delivery of finished water to the Tarawa Terrace water-distribution system, 2000–2004, U.S. Marine Corps Base Camp Lejeune, North Carolina. [Data from Joel Hartsoe, Camp Lejeune Public Works Department Utilities Section, December 6, 2006; flow data measured at venturi meter located in building STT-39A (Tarawa Terrace pump house)]

Additional information gathered during a field investigation of the Tarawa Terrace water-distribution system included hourly delivery rates of finished water. These hourly data were used in conjunction with water-distribution system model simulation (see section on Field Tests and Analyses of the Water-Distribution System) to determine a diurnal pattern of water use for Tarawa Terrace (Figure A8). Data from the field test show a gradually increasing demand for water occurring during 0200–0700 hours. Peak demand occurs between 1000–1400 hours, at 1800 hours, and at 2200 hours. Thus, greater amounts of water were delivered (and presumably consumed) during these time periods than during other hours of the day.

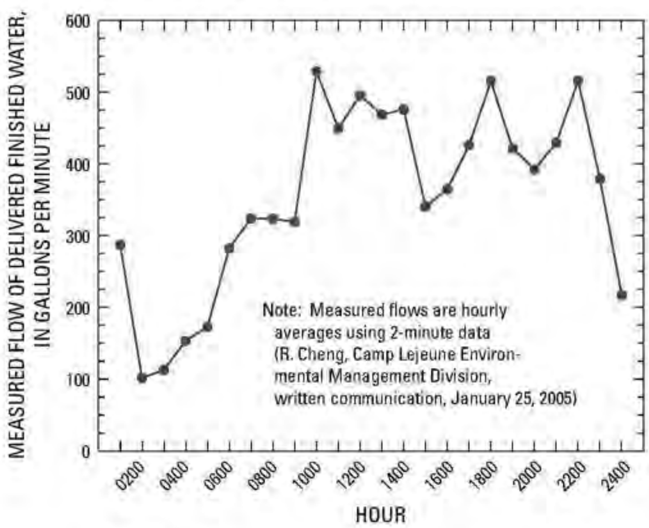


Figure A8. Measured diurnal pattern (24 hours) of delivered finished water during field test, September 22–October 12, 2004, Tarawa Terrace water-distribution system, U.S. Marine Corps Base Camp Lejeune, North Carolina.

Hierarchical Approach for Quantifying Exposure

A simulation or modeling approach was used to reconstruct and estimate (quantify) historical concentrations of PCE in finished water delivered to residents of Tarawa Terrace. In using a simulation approach, a calibration process is used so that the combination of various model parameters—regardless of whether a model is simple or complex—appropriately reproduces the behavior of real-world systems (for example, migration of PCE) as closely as possible. The American Water Works Association Engineering Computer Applications Committee indicates that "true model calibration is achieved by adjusting whatever parameter values need adjusting until a reasonable agreement is achieved between model-predicted behavior and actual field behavior" (AWWA Engineering Computer Applications Committee 1999). A model modified in this manner is called a calibrated model (Hill and Tiedeman 2007). Calibration of models used for the Tarawa Terrace analyses was accomplished in a hierarchical or step-wise approach consisting of four successive stages or levels. Simulation results achieved for each calibration level were refined by adjusting model parameter values and comparing these results with simulation results of previous levels until results at all levels were within ranges of preselected calibration targets or measures. The step-wise order of model-calibration levels consisted of simulating (1) predevelopment (steady or nonpumping) ground-water-flow conditions, (2) transient (time varying or pumping) groundwater-flow conditions, (3) the fate and transport (migration) of PCE from its source at ABC One-Hour Cleaners to water-supply wells, and (4) the concentration of PCE in finished water at the Tarawa Terrace WTP—water from the Tarawa Terrace WTP that was delivered to residents living in family housing.

Conceptual Description of Model Calibration

The hierarchical approach to estimating the concentration of PCE in finished water from the Tarawa Terrace WTP can be conceptually described in terms of Venn or set diagrams (Borowski and Borwein 1991). Such diagrams are useful for showing logical relations between sets or groups of like items and are shown in Figure A9 for each hierarchical calibration level. At level 1 (Figure A9*a*), there may be a large number of combinations of parameters that yield solutions to predevelopment groundwater-flow conditions. However, only a smaller set—the subset of solutions indicated by circle "A" in Figure A9*a*—yields acceptable combinations of parameters for a calibrated predevelopment groundwater-flow model. For transient groundwater-flow conditions, viable solutions are indicated by circle "B" (Figure A9*b*). Only those solutions that successfully simulate both predevelopment and transient groundwater-flow conditions can be accepted and classified as resulting in calibrated transient and predevelopment groundwater-flow models. These

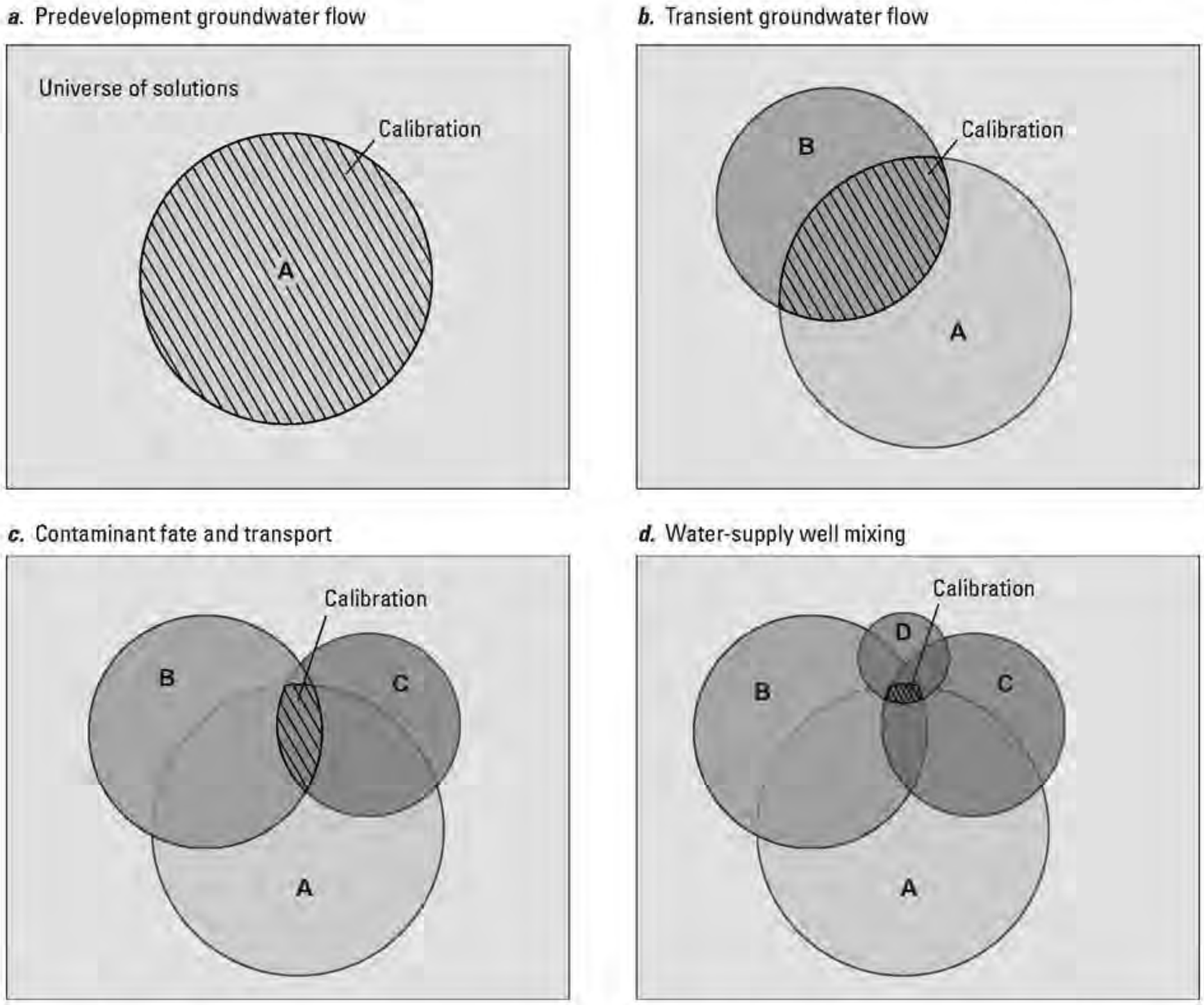


Figure A9. Venn diagrams showing hierarchical approach of model calibration used to estimate concentration of finished water: *(a)* predevelopment groundwater flow, *(b)* transient groundwater flow, *(c)* contaminant fate and transport, and *(d)* water-supply well mixing, Tarawa Terrace and vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina.

select and fewer solutions are indicated by the intersection of circles "A" and "B." The transient groundwater-flow simulations provide velocity information (specific discharge) required to conduct a fate and transport simulation. Viable solutions for the fate and transport problem are indicated by circle "C" (Figure A9*c*). Only those solutions that satisfy: (a) predevelopment groundwater-flow, (b) transient groundwater-flow, and (c) contaminant fate and transport calibration criteria are accepted and classified as resulting in a calibrated contaminant fate and transport model. These solutions are even fewer than for predevelopment and transient groundwater flow and are indicated by the intersection of circles "A," "B," and "C." The fourth hierarchical level used to reconstruct PCE concentrations in drinking water was the development of a calibrated mixing model (using the materials mass balance approach and mixing PCE-contaminated and uncontaminated groundwater from supply wells). Viable calibrated solutions depend on calibrated solutions for the previous three hierarchical levels of model calibration, thereby resulting in even fewer calibrated solutions to the mixing problem—circle "D" in Figure A9*d*. Thus, only solutions that satisfy all four levels of model calibration, indicated by the intersection of circles "A," "B," "C," and "D," provide reasonable estimates for the concentration of PCE in finished water at the Tarawa Terrace WTP. The final calibrated models were the end product of this hierarchical process.

Quantitative Assessment of Model Calibration

Specific details of the calibration process for each hierarchical level are described in the Chapter C report for levels 1 and 2 (Faye and Valenzuela In press 2007) and the Chapter F report for levels 3 and 4 (Faye In press 2007b). To summarize, at each hierarchical level, an initial calibration target or "goodness of fit" criterion was selected based on the availability, method of measurement or observation, and overall reliability of field data and related information. Once model-specific parameters were calibrated, statistical and graphical analyses were conducted to determine if selected parameters met calibration criteria targets. Summaries of calibration targets and resulting calibration statistics for each of the four hierarchical levels are listed in Table A8. Graphs of observed and simulated water levels using paired data points[22] are shown in Figure A10 for predevelopment and transient groundwater-flow calibrations (hierarchical levels 1 and 2). Of special note are calibration targets and resulting calibration statistics for hierarchal level 2—transient groundwater flow (Figure A10*b* and Table A8). The calibration targets were divided into those reflective of monitor well data and those reflective of water-supply well data. As listed in Table A8, calibration targets for water-level data derived from monitor well data were assigned a smaller head difference (±3 ft) when compared with calibration targets derived from water-supply well data (±12 ft). This difference in the calibration targets—and resulting calibration statistics—reflects the more accurate measurement method used to determine monitor well water levels (steel-tape measurements) when compared with the method used to determine water-supply well water levels (airline measurements). The resulting calibration statistics and paired data point graphs also demonstrate a better agreement between monitor well data and model simulation (average magnitude of head difference of 1.4 ft) than between water-supply well data and model simulation results (average magnitude of head difference of 7.1 ft).[23] Detailed discussion and analyses of calibration procedures and results are provided in the Chapter C report (Faye and Valenzuela In press 2007).

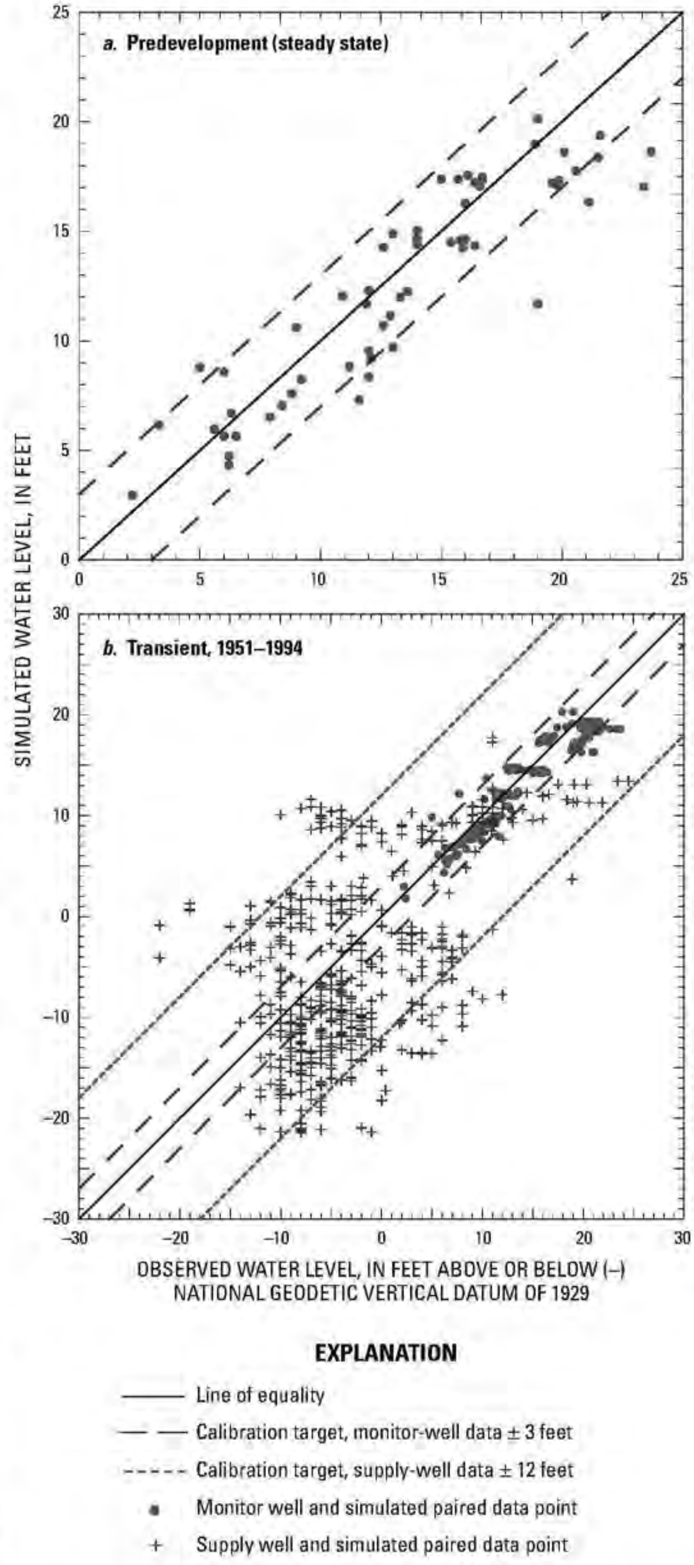


Figure A10. Observed and simulated water levels, model layer 1, and calibration targets for *(a)* predevelopment (steady-state) conditions and *(b)* transient conditions, 1951–1994, Tarawa Terrace and vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina.

[22] A location with observed data (for example, water level or concentration) that is associated with a model location for the purpose of comparing observed data with model results.

[23] Definitions of head difference, average magnitude of head difference, and other calibration targets and statistics are provided in Table A8.

To assess the calibration of the fate and transport simulation of PCE and the mixing model computations for finished water at the Tarawa Terrace WTP (hierarchical levels 3 and 4), a statistic referred to as the model bias was computed (B_m, Table A8). Model bias allows one to test the accuracy of a model by expressing the bias in terms of a simulated-to-observed (or measured) ratio (Maslia et al. 2000, Rogers et al. 1999). Model bias, defined as the ratio of simulated PCE concentration to observed PCE concentration (C_{sim}/C_{obs}), is characterized by the following properties:

when $C_{sim}/C_{obs} < 1$, there is underprediction by the model,
when $C_{sim}/C_{obs} = 1$, there is exact agreement, and
when $C_{sim}/C_{obs} > 1$, there is overprediction by the model.

Data used to compute model bias are spatially and temporally disparate and are listed in Table A9 for water-supply wells and Table A10 for the Tarawa Terrace WTP. The geometric bias (B_g) is the geometric mean of the individual C_{sim}/C_{obs} ratios and is a measure of model bias ($B_{m,i}$). Geometric bias, (B_g), is computed using the following equation:

$$B_g = \exp\left[\frac{\sum_{i=1}^{N} \ln\left(B_{m,i}\right)}{N}\right], \qquad (1)$$

where

$B_{m,i}$ is the model bias defined as the ratio of simulated PCE concentration to observed PCE concentration (C_{sim}/C_{obs}),
N is the number of observation points,
ln ( ) is the Naperian or natural logarithm, and
B_g is the geometric bias.

The geometric bias is used because the distribution of C_{sim}/C_{obs} ratios is skewed like a lognormal distribution. That is, the values are restricted for underprediction (0–1), but are unrestricted for overprediction (anything greater than 1).

Water-supply well data included 17 of 36 samples recorded as nondetect (Table A9), and these samples were not used in the computation of the geometric bias (B_g). In addition, the computation of geometric bias was accomplished twice; an inclusive bias computation that included all water-supply well data and a selected bias computation that omitted data for water-supply well TT-23. The inclusive geometric bias, using data for water-supply well TT-23, was 5.9. The selected geometric bias, omitting data for supply well TT-23, was 3.9 (Table A8). Both results, however, indicate overprediction by the model. The rationale for computing the selected geometric bias is based on data, observations, and discussions provided in Chapter E of this report series (Faye and Green In press 2007). Briefly, enhanced biodegradation possibly occurred in the vicinity of water-supply well TT-23 during 1984 and 1985. A biodegradation rate for PCE of 0.5/d was computed using analytical results and sample collection dates reported for water-supply well TT-23. This rate probably was not representative of biodegradation occurring in contaminated aquifer media at other wells and was significantly greater than the calibrated reaction rate of 5.0 x 10^{-4}/d (Table A11). Such greatly enhanced biodegradation would result in much lower PCE concentrations in water samples obtained from supply well TT-23. A second reason for computing a selected geometric bias—omitting data from water-supply well TT-23—is bias introduced into analytical results caused by incomplete or inadequate sampling methodology. As noted in Table A9, four sequential sampling events took place during March 11–12, 1985, at water-supply well TT-23. Each sampling event resulted in increased PCE concentrations compared to the preceding sample. Thus, sampling methodology at water-supply well TT-23 may not have included a sufficient volume of water discharged from the well bore prior to sampling, and samples obtained did not represent PCE concentration within the entire volume of aquifer material contributing to the well.

For the Tarawa Terrace WTP, 15 of 25 samples were recorded as nondetect (Table A10). The nondetect samples were not used in the computation of the geometric bias (B_g). The resulting geometric bias computed for measured data at the Tarawa Terrace WTP is 1.5, which indicates a slight overprediction by the model.

All data, measured and nondetect, and simulated values are displayed in Figures A11 and A12 for water-supply wells and the WTP, respectively. The sample numbers shown on the horizontal (x-) axis of each graph correspond to the sample numbers listed in Table A9 for water-supply wells and Table A10 for the WTP. The data in Figures A11 and A12 are compared with the corresponding PCE concentration calibration targets for water-supply wells and the WTP listed in Table A8.

Table A8. Summary of calibration targets and resulting calibration statistics for simulation models used to reconstruct historical contamination events at Tarawa Terrace and vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina.

Calibration level[1, 2]	Analysis type	Calibration target[3]	Resulting calibration statistics[4]	[5]Number of paired data points (N)
1	Predevelopment (no pumping) groundwater flow	Magnitude of head difference: 3 feet	$\lvert\overline{\Delta h}\rvert = 1.9$ ft $\sigma = 1.5$ ft $RMS = 2.1$ ft	59
2	Transient groundwater flow—monitor wells	Magnitude of head difference: 3 feet	$\lvert\overline{\Delta h}\rvert = 1.4$ ft $\sigma = 0.9$ ft $RMS = 1.7$ ft	263
	Transient groundwater flow—supply wells	Magnitude of head difference: 12 feet	$\lvert\overline{\Delta h}\rvert = 7.1$ ft $\sigma = 4.6$ ft $RMS = 8.5$ ft	526
3	Contaminant fate and transport—supply wells	Concentration difference: ± one-half order of magnitude or model bias (B_m) ranging from 0.3 to 3	Geometric bias [6]$B_g = 5.8/3.9$	[7]36
4	Mixing model—treated water at water treatment plant	Concentration difference: ± one-half order of magnitude or model bias (B_m) ranging from 0.3 to 3	Geometric bias $B_g = 1.5$	[8]25

[1]Refer to the Chapter C report (Faye and Valenzuela In press 2007) for calibration procedures and details on levels 1 and 2

[2]Refer to the Chapter F report (Faye In press 2007b) for calibration procedures and details on levels 3 and 4

[3]Head difference is defined as observed water level (h_{obs}) minus simulated water level (h_{sim}); Magnitude of head difference is defined as: $|\Delta h| = |h_{obs} - h_{sim}|$; a concentration difference of ± one-half order of magnitude equates to a model bias of 0.3 to 3, where, B_m = model bias and is defined as: $B_m = C_{sim}/C_{obs}$, where C_{sim} is the simulated concentration and C_{obs} is the observed concentration; when $B_m = 1$, the model exactly predicts the observed concentration, when $B_m > 1$, the model overpredicts the concentration, and when $B_m < 1$, the model underpredicts the concentration

[4]Average magnitude of head difference is defined as: $\left|\overline{\Delta h}\right| = \frac{1}{N}\sum_{i=1}^{N}\left|\Delta h_i\right|$; standard deviation of head difference is defined as: $\sigma = \sqrt{\frac{\sum_{i=1}^{N}\left(\Delta h_i - \overline{\Delta h}\right)^2}{N-1}}$, where $\overline{\Delta h}$ is the mean or average of head difference; root-mean-square of head difference is defined as: $RMS = \left[\frac{1}{N}\sum_{i=1}^{N}\Delta h_i^2\right]^{\frac{1}{2}}$; geometric bias, B_g, is defined as: $B_g = \exp\left[\frac{\sum_{i=1}^{N}\ln\left(B_{m,i}\right)}{N}\right]$, where ln ( ) is the Naperian logarithm

[5]A paired data point is defined as any location with observed data that is associated with a model location for the purpose of comparing observed data with model results for water level or concentration

[6]$B_g = 5.8$ computed using all water-supply wells listed in table A9; $B_g = 3.9$ computed without considering water-supply well TT-23—See text for explanation

[7]Observed concentration of 17 samples recorded as nondetect (see Table A9) and are not used in computation of geometric bias

[8]Observed concentration of 15 samples recorded as nondetect (see Table A10) and are not used in computation of geometric bias

For the nondetect sample data, the upper calibration target was selected as the detection limit for the sample (Tables A9 and A10), and the lower calibration target was selected as 1 μg/L. The statistical analyses summarized in Table A8 and comparisons of observed data, simulated values, and calibration targets shown in Figures A10*a*, A10*b*, A11, and A12 for the four hierarchical levels of model analyses provide evidence that the models of groundwater flow (predevelopment and transient—Figure A10), contaminant fate and transport (Figure A11), and water-supply well mixing at the Tarawa Terrace WTP (Figure A12) presented herein: (1) are reasonably calibrated and (2) provide an acceptable representation of the groundwater-flow system, the fate and transport of PCE, and the distribution of PCE-contaminated finished water to residences of Tarawa Terrace. A listing of calibrated model parameter values for the predevelopment (hierarchical level 1), transient (hierarchical level 2), and fate and transport (hierarchical level 3) models is presented in Table A11.

Table A9. Summary of model-derived values and observed data of tetrachloroethylene at water-supply wells, Tarawa Terrace, U.S. Marine Corps Base Camp Lejeune, North Carolina.[1]

[PCE, tetrachloroethylene; µg/L, microgram per liter; J, estimated; ND, nondetect]

Model-derived value		Observed data				
Month and year	PCE concentration, in µg/L	Sample date	PCE concentration, in µg/L	Detection limit, in µg/L	Calibration targets[2], in µg/L	Sample number[3]
		Supply well TT-23				
January 1985	254	1/16/1985	132	10	41.7–417	1
February 1985	253	2/12/1985	37	10	11.7–117	2
February 1985	253	2/19/1985	26.2	2	8.3–82.9	3
February 1985	253	2/19/1985	ND	10	1–10	4
March 1985	265	3/11/1985	14.9	10	4.7–47.1	5
March 1985	265	3/11/1985	16.6	2	5.2–52.5	6
March 1985	265	3/12/1985	40.6	10	12.8–128	7
March 1985	265	3/12/1985	48.8	10	15.4–154	8
April 1985	274	4/9/1985	ND	10	1–10	9
September 1985	279	9/25/1985	4J	2	1.3–12.6	10
July 1991	191	7/11/1991	ND	10	1–10	11
		Supply well TT-25				
February 1985	7.3	2/5/1985	ND	10	1–10	12
April 1985	9.6	4/9/1985	ND	10	1–10	13
September 1985	18.1	9/25/1985	0.43J	10	0.14–1.4	14
October 1985	20.4	10/29/1985	ND	10	1–10	15
November 1985	22.8	11/4/1985	ND	10	1–10	16
November 1985	22.8	11/12/1985	ND	10	1–10	17
December 1985	25.5	12/3/1985	ND	10	1–10	18
July 1991	72.7	7/11/1991	23	10	7.3–72.7	19
		Supply well TT-26				
January 1985	804	1/16/1985	1,580.0	10	500–4,996	20
January 1985	804	2/12/1985	3.8	10	1.2–12	21
February 1985	798	2/19/1985	64.0	10	20.2–202	22
February 1985	798	2/19/1985	55.2	10	17.5–175	23
April 1985	801	4/9/1985	630.0	10	199–1,992	24
June 1985	799	6/24/1985	1,160.0	10	367–3,668	25
September 1985	788	9/25/1985	1,100.0	10	348–3,478	26
July 1991	670	7/11/1991	350.0	10	111–1,107	27
		Supply well TT-30				
February 1985	0.0	2/6/1985	ND	10	1–10	28
		Supply well TT-31				
February 1985	0.17	2/6/1985	ND	10	1–10	29
		Supply well TT-52				
February 1985	0.0	2/6/1985	ND	10	1–10	30
		Supply well TT-54				
February 1985	6.0	2/6/1985	ND	10	1–10	31
July 1991	30.4	7/11/1991	ND	5	1–5	32
		Supply well TT-67				
February 1985	4.1	2/6/1985	ND	10	1–10	33
		Supply well RW1				
July 1991	0.0	7/12/1991	ND	2	1–2	34
		Supply well RW2				
July 1991	879	7/12/1991	760	2	240–2,403	35
		Supply well RW3				
July 1991	0.0	7/12/1991	ND	2	1–2	36

[1]Model-derived values for water-supply wells based on simulation results obtained from the fate and transport model MT3DMS (Zheng and Wang 1999); see the Chapter F report (Faye In press 2007b) for details

[2]Calibration targets are ±½-order of magnitude for observed data; when observed data are indicated as ND, upper calibration target is detection limit and lower calibration target is 1 µg/L

[3]See Figure A11

Table A10. Summary of model-derived values and observed data of tetrachloroethylene at the water treatment plant, Tarawa Terrace, U.S. Marine Corps Base Camp Lejeune, North Carolina.[1]

[PCE, tetrachloroethylene; µg/L, microgram per liter; ND, nondetect]

Model-derived value		Observed data				
Month and year	PCE concentration, in µg/L	Sample date	PCE concentration, in µg/L	Detection limit, in µg/L	Calibration targets, in µg/L[2]	Sample number[3]
May 1982	148	5/27/1982	80	10	25–253	1
July 1982	112	7/28/1982	104	10	33–329	2
July 1982	112	7/28/1982	76	10	24–240	3
July 1982	112	7/28/1982	82	10	26–259	4
January 1985	176	2/5/1985	80	10	25–253	5
January 1985	176	2/11/1985	215	10	68–680	6
February 1985	3.6	2/13/1985	ND	10	1–10	7
February 1985	3.6	2/19/1985	ND	2	1–2	8
February 1985	3.6	2/22/1985	ND	10	1–10	9
March 1985	8.7	3/11/1985	ND	2	1–2	10
March 1985	8.7	3/12/1985	6.6	10	2.1–21	11
March 1985	8.7	3/12/1985	21.3	10	6.7–67	12
April 1985	8.1	4/22/1985	1	10	0.3–3.2	13
April 1985	8.1	4/23/1985	ND	10	1–10	14
April 1985	8.1	4/29/1985	3.7	10	1.2–11.7	15
May 1985	4.8	5/15/1985	ND	10	1–10	16
July 1985	5.5	7/1/1985	ND	10	1–10	17
July 1985	5.5	7/8/1985	ND	10	1–10	18
July1985	5.5	7/23/1985	ND	10	1–10	19
July 1985	5.5	7/31/1985	ND	10	1–10	20
August 1985	6.0	8/19/1985	ND	10	1–10	21
September 1985	6.5	9/11/1985	ND	10	1–10	22
September 1985	6.5	9/17/1985	ND	10	1–10	23
September 1985	6.5	9/24/1985	ND	10	1–10	24
October 1985	7.1	10/29/1985	ND	10	1–10	25

[1]Model-derived values for water treatment plant based on simulation results obtained from the fate and transport model MT3DMS (Zheng and Wang 1999) and application of a materials mass balance (mixing) model; see the Chapter F report (Faye In press 2007b) for details

[2]Calibration targets are ±½-order of magnitude for observed data; when observed data are indicated as ND, upper calibration target is detection limit and lower calibration target is 1 µg/L

[3]See Figure A12

Table A11. Calibrated model parameter values used for simulating groundwater flow and contaminant fate and transport, Tarawa Terrace and vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina.

[ft/d, foot per day; ft^3/d, cubic foot per day; ft^3/g, cubic foot per gram; g/ft^3, gram per cubic foot; d^{-1}, 1/day; g/d, gram per day; ft, foot; ft^2/d, square foot per day; —, not applicable]

Model parameter[1]	Model layer number[2]						
	1	2	3	4	5	6	7
Predevelopment groundwater-flow model (conditions prior to 1951)							
Horizontal hydraulic conductivity, K_H (ft/d)	12.2–53.4	1.0	4.3–20.0	1.0	6.4–9.0	1.0	5.0
Ratio of vertical to horizontal hydraulic conductivity, K_V/K_H[3]	1:7.3	1:10	1:8.3	1:10	1:10	1:10	1:10
Infiltration (recharge), I_R (inches per year)	13.2	—	—	—	—	—	—
Transient groundwater-flow model, January 1951–December 1994							
Specific yield, S_y	0.05	—	—	—	—	—	—
Storage coefficient, S	—	4.0×10^{-4}	4.0×10^{-4}	4.0×10^{-4}	4.0×10^{-4}	4.0×10^{-4}	4.0×10^{-4}
Infiltration (recharge), I_R (inches per year)	6.6–19.3	—	—	—	—	—	—
Pumpage, Q_k (ft^3/d)	See footnote[4]	—	See footnote[4]	—	0	—	0
Fate and transport of tetrachloroethylene (PCE) model, January 1951–December 1994							
Distribution coefficient, K_d (ft^3/g)	5.0×10^{-6}	5.0×10^{-6}	5.0×10^{-6}	5.0×10^{-6}	5.0×10^{-6}	5.0×10^{-6}	5.0×10^{-6}
Bulk density, ρ_b (g/ft^3)	77,112	77,112	77,112	77,112	77,112	77,112	77,112
Effective porosity, n_E	0.2	0.2	0.2	0.2	0.2	0.2	0.2
Reaction rate, r (d^{-1})	5.0×10^{-4}	5.0×10^{-4}	5.0×10^{-4}	5.0×10^{-4}	5.0×10^{-4}	5.0×10^{-4}	5.0×10^{-4}
Mass-loading rate[5], q_SC_S (g/d)	1,200	—	—	—	—	—	—
Longitudinal dispersivity, α_L (ft)	25	25	25	25	25	25	25
Transverse dispersivity, α_T (ft)	2.5	2.5	2.5	2.5	2.5	2.5	2.5
Vertical dispersivity, α_V (ft)	0.25	0.25	0.25	0.25	0.25	0.25	0.25
Molecular diffusion coefficient, D* (ft^2/d)	8.5×10^{-4}	8.5×10^{-4}	8.5×10^{-4}	8.5×10^{-4}	8.5×10^{-4}	8.5×10^{-4}	8.5×10^{-4}

[1] Symbolic notation used to describe model parameters obtained from Chiang and Kinzelbach (2001)

[2] Refer to Chapter B (Faye In press 2007a) and Chapter C (Faye and Valenzuela In press 2007) reports for geohydrologic framework corresponding to appropriate model layers; aquifers are model layers 1, 3, 5, and 7; semiconfining units are model layers 2, 4, and 6

[3] For model cells simulating water-supply wells, vertical hydraulic conductivity (K_V) equals 100 feet per day to approximate the gravel pack around the well

[4] Pumpage varies by month, year, and model layer; refer to Chapter K report (Maslia et al. In press 2007a) for specific pumpage data

[5] Introduction of contaminant mass began January 1953 and terminated December 1984

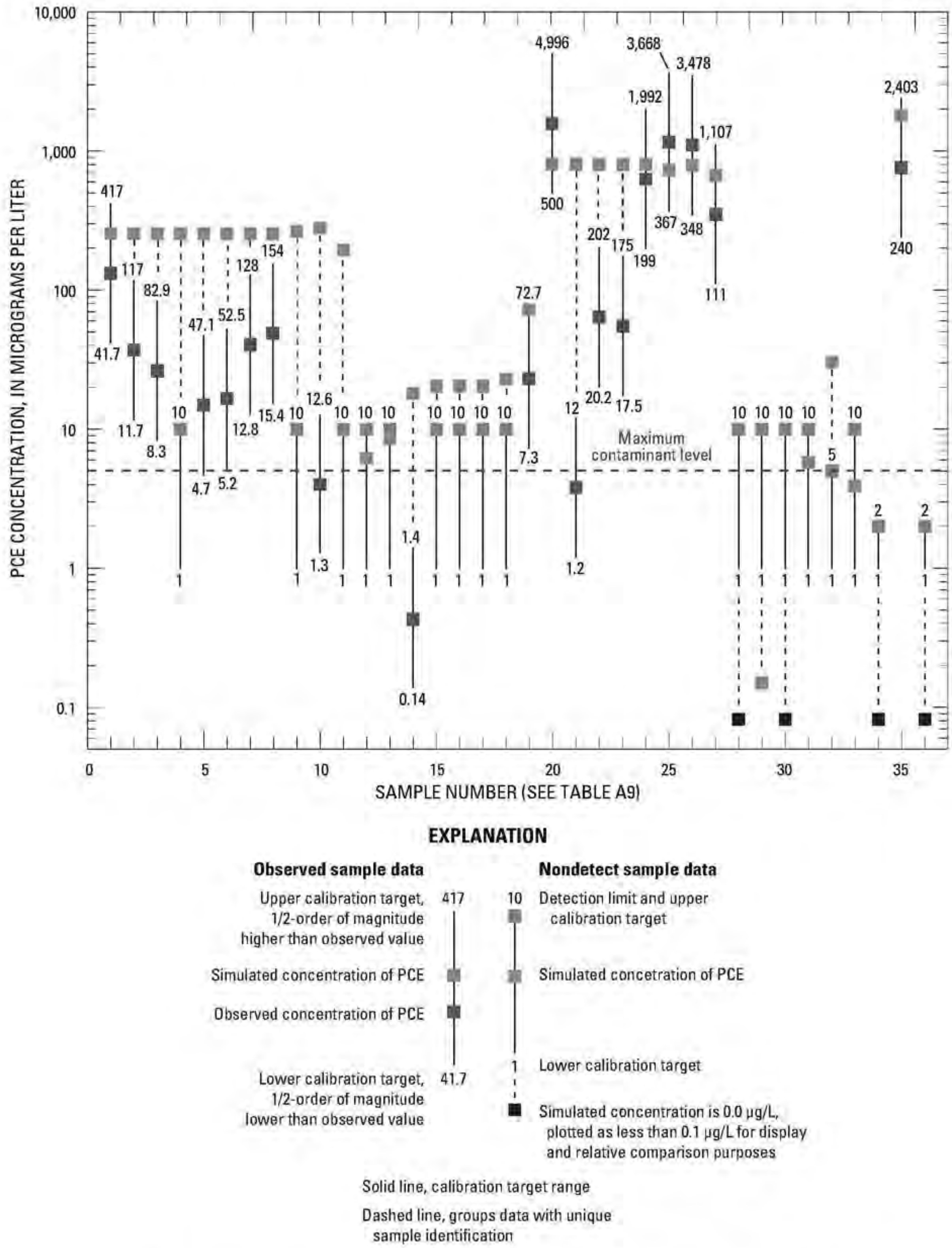


Figure A11. Comparison of observed and nondetect tetrachloroethylene sample data with calibration targets and simulated concentrations at water-supply wells, Tarawa Terrace, U.S. Marine Corps Base Camp Lejeune, North Carolina. [PCE, tetrachloroethylene; µg/L, microgram per liter]

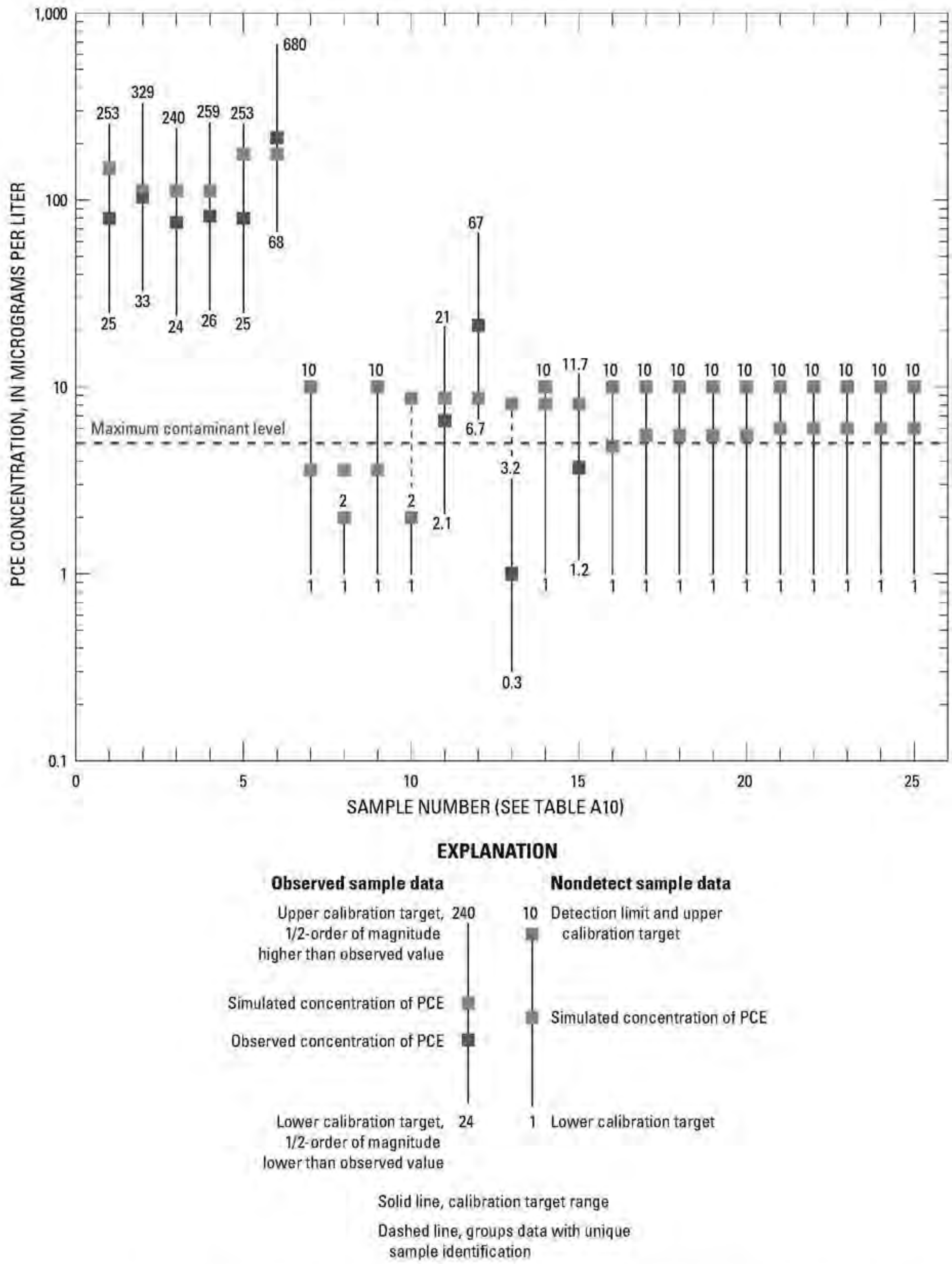


Figure A12. Comparison of observed and nondetect tetrachloroethylene sample data with calibration targets and simulated concentrations at the water treatment plant, Tarawa Terrace, U.S. Marine Corps Base Camp Lejeune, North Carolina. [PCE, tetrachloroethylene]

Selected Simulation Results

Examples of simulation results showing the distribution of PCE in groundwater and the concentration of PCE in finished water at the Tarawa Terrace WTP are presented in the form of maps and graphs. Maps show simulated water levels, directions of groundwater flow, and the areal distribution of PCE. The concentrations of PCE at specific water-supply wells and in finished water at the WTP are shown as graphs in the form of time versus concentration.

Distribution of Tetrachloroethylene (PCE) in Groundwater

Simulation results of groundwater flow and the fate and transport of PCE are shown as a series of maps for January 1958 (Figure A13), January 1968 (Figure A14), December 1984 (Figure A15), and December 1994 (Figure A17).[24] Each illustration is composed of two maps. The upper map shows simulated potentiometric levels (or water levels) and directions of groundwater flow for model layer 1 throughout the entire active model domain (for example, Figure A13*a*). Groundwater flow is from highest to lowest potentiometric level. The lower map (for example, Figure A13*b*) shows an enlarged area of the Tarawa Terrace housing area and the site of ABC One-Hour Cleaners. This map shows simulated potentiometric levels and the areal distribution of PCE-contaminated groundwater. The lower maps show simulated PCE values ranging from 5 μg/L to greater than 1,500 μg/L. The values of PCE shown on the maps—assigned a specific color to represent a concentration range—are values of PCE that were simulated at the center of a finite-difference cell that was part of the numerical model's finite-difference grid.[25] The simulated PCE values shown in Figures A13–A17 were derived by applying the inverse-distance weighting method to simulated PCE-concentration values at the center of finite-difference cells.

January 1958

With the onset of simulated pumping at water-supply well TT-26 during January 1952, local cones of depression are shown around all active supply wells. In general, however, flow is toward Northeast Creek and Frenchmans Creek (A13*a*). Under these flow conditions, PCE migrated southeast from its source at the site of ABC One-Hour Cleaners in the direction of water-supply well TT-26 (Figure A13*b*). The simulated PCE concentration at water-supply well TT-26 during January 1958 was about 29 μg/L.[26]

January 1968

During January 1968, the designated start date of the epidemiological case-control study (Figure A3), groundwater flow in the northern half of the model domain was little changed from January 1958 conditions (Figure A14*a*). In the immediate vicinity of the Tarawa Terrace I housing area, groundwater flow and water levels are affected by pumpage from water-supply wells TT-52, TT-53 and TT-54. Groundwater flow from the vicinity of TT-26 toward well TT-54 is particularly evident. Under these flow conditions, PCE has migrated in a more southwardly direction from its source at the site of ABC One-Hour Cleaners toward water-supply well TT-54 (Figure A14*b*) and covers a greater spatial extent than during January 1958. By January 1968, the simulated concentration of PCE in water-supply well TT-26 was 402 μg/L.

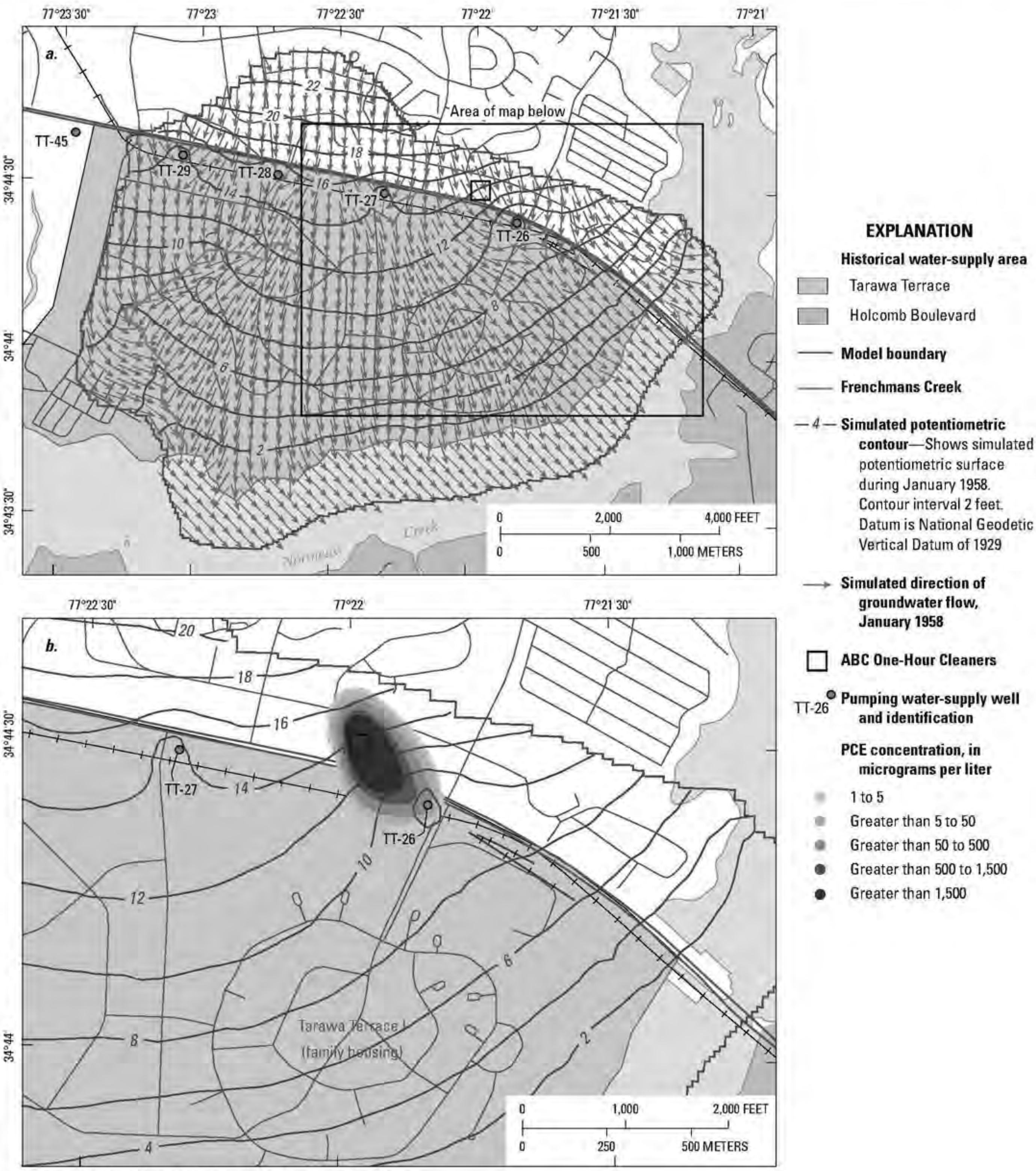
December 1984

Groundwater pumpage increased water-level declines during December 1984 in the vicinity of the Tarawa Terrace I housing area and probably accelerated the migration of PCE toward the vicinity of well TT-54 (Figure A15*a*). Between January 1968 and December 1984, the center of mass of PCE migrated generally southeastward from its source at the site of ABC One-Hour Cleaners, and the arm of the PCE plume migrated southwestward toward water-supply wells TT-23, TT-67, and TT-54 (Figure A15*b*). The areal extent of simulated

[24] For synoptic maps of model layer 1 (1951–1994), refer to the Chapter K report (Maslia et al. In press 2007a).

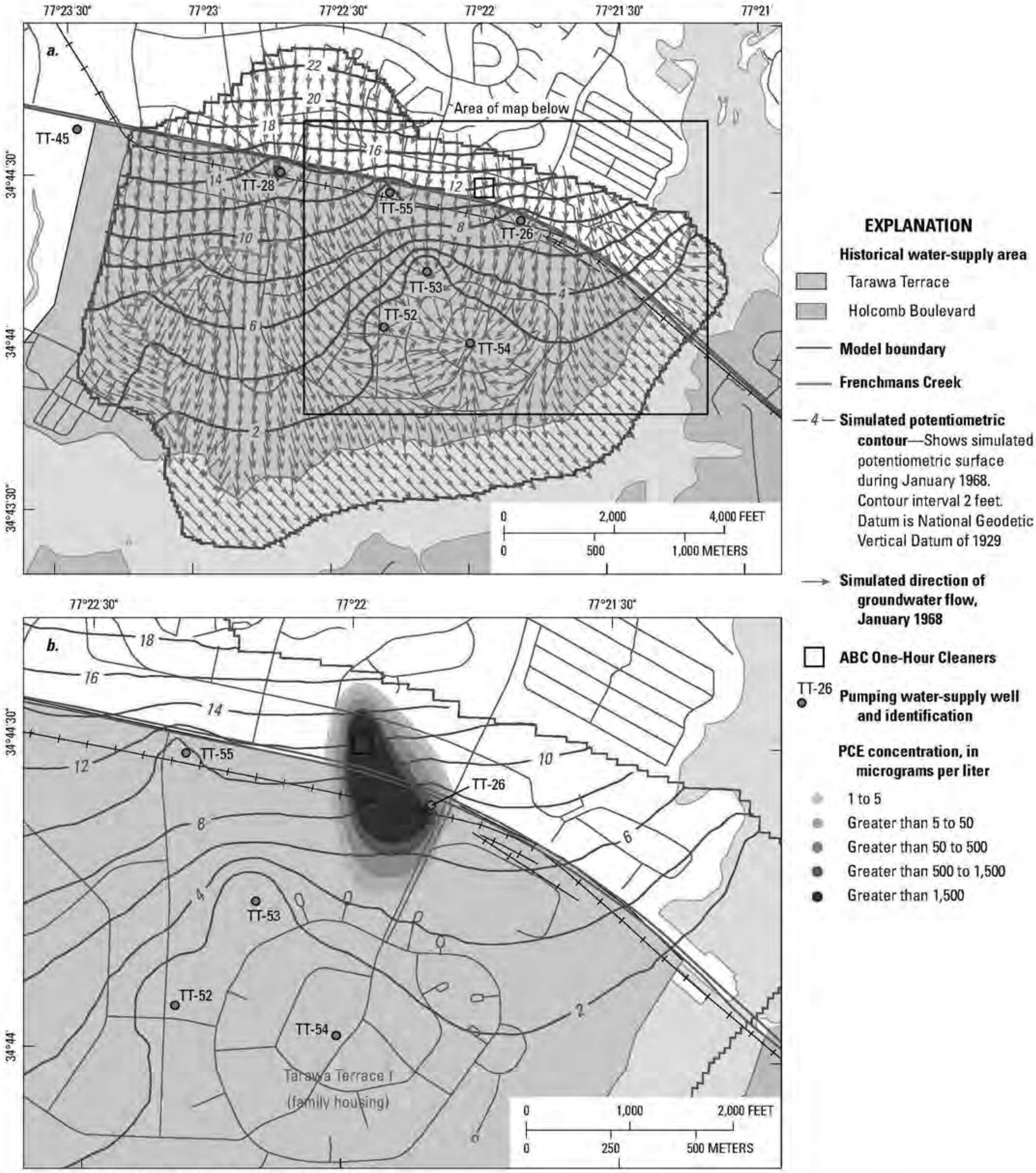
[25] Refer to report Chapter C (Faye and Valenzuela In press 2007) and Chapter F (Faye In press 2007b) reports for details specific to the computational grid and model boundaries used to simulate groundwater flow and contaminant fate and transport.

[26] Refer to the Chapter K report (Maslia et al. In press 2007a) for a monthly listing of simulated PCE concentrations at water-supply wells during January 1952–February 1987.



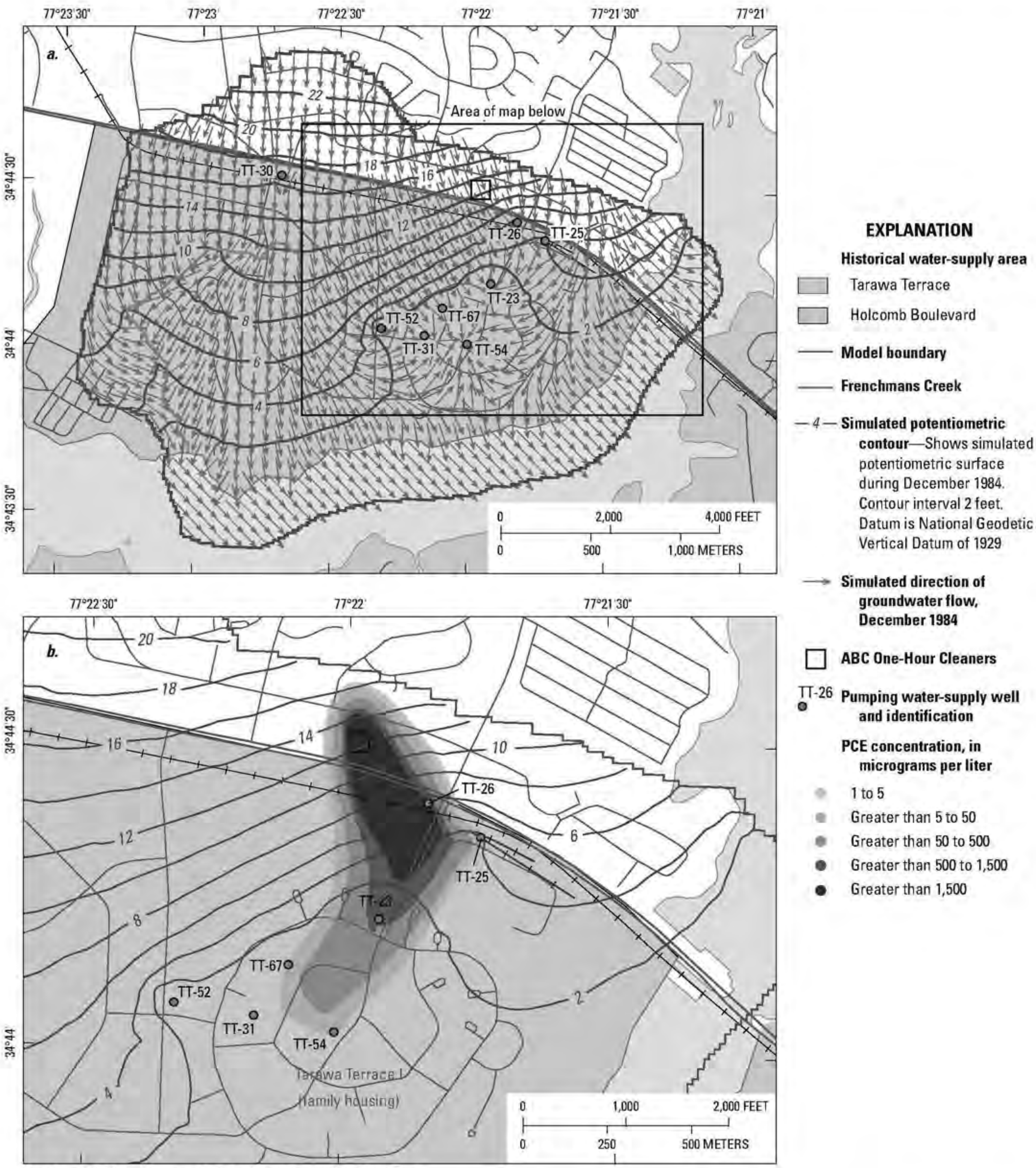
Base from U.S. Marine Corps and U.S. Geological Survey digital data files

Figure A13. Simulated *(a)* water level and direction of groundwater flow and *(b)* distribution of tetrachloroethylene, model layer 1, January 1958, Tarawa Terrace and vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina. [PCE, tetrachloroethylene]



Base from U.S. Marine Corps and U.S. Geological Survey digital data files

Figure A14. Simulated *(a)* water level and direction of groundwater flow and *(b)* distribution of tetrachloroethylene, model layer 1, January 1968, Tarawa Terrace and vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina. [PCE, tetrachloroethylene]



Base from U.S. Marine Corps and U.S. Geological Survey digital data files

Figure A15. Simulated *(a)* water level and direction of groundwater flow and *(b)* distribution of tetrachloroethylene, model layer 1, December 1984, Tarawa Terrace and vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina. [PCE, tetrachloroethylene]

PCE contamination has increased significantly from the areal extent of January 1958 and January 1968 (Figures A13*b* and A14*b*, respectively). By December 1984, the simulated concentration of PCE in water-supply wells TT-23, TT-25, and TT-26 was 255 μg/L, 6 μg/L, and 805 μg/L, respectively. These and other water-supply wells were pumping from model layer 3. Therefore, simulated concentrations for these water-supply wells are lower than the simulated PCE concentrations shown in Figure A15*b*. For maps showing simulated PCE concentration in model layer 3, refer to the Chapter F report (Faye In Press 2007b). For information on model layers that water-supply wells pumping from, refer to the Chapter K report (Maslia et al. In Press 2007a).

Some water-supply wells were constructed to obtain water from multiple water-bearing zones. Therefore, in the model representation of these wells, groundwater can be withdrawn from more than one model layer. For example, water-supply wells TT-31, TT-52, and TT-54 withdraw groundwater from model layers 1 and 3, whereas water-supply wells TT-23, TT-25, TT-26, TT-27, and TT-67 withdraw groundwater solely from model layer 3 (Faye and Valenzuela In press 2007; Maslia et al. In press 2007a). Consequently, the distribution of PCE will differ by model layer and by time, depending on groundwater-flow velocities, the number of water-supply wells withdrawing groundwater from a particular model layer, and the volume of groundwater being withdrawn. An example of the multilayer distribution of PCE by model layer for December 1984 is shown as a perspective diagram in Figure A16. In this diagram, water-supply wells are shown penetrating the model layer or layers from which they withdraw groundwater. Because no water-supply wells withdraw groundwater directly from model layer 5, the distribution of PCE in layer 5 covers a smaller area and is of lower concentration compared to model layers 1 and 3.

December 1994

Owing to documented PCE contamination in water samples obtained from the Tarawa Terrace water-supply wells and the WTP (Tables A9 and A10), wells TT-23 and TT-26 were taken off-line during February 1985. The Tarawa Terrace WTP was closed and pumping at all Tarawa Terrace water-supply wells was discontinued during March 1987 (Figures A3 and A5, Table A6). As a result, potentiometric levels began to recover. By December 1994, the simulated potentiometric levels (Figure A17*a*), were nearly identical to predevelopment conditions of 1951 (Faye and Valenzuela In press 2007). Groundwater flow was from the north and northwest to the south and east, discharging to Northeast Creek. Groundwater discharge also occurs to Frenchmans Creek in the westernmost area of the model domain (Figure A17*a*). Water-supply wells shown in Figure A17 were not operating during December 1994, but are shown on this illustration for reference purposes.

A graph showing simulated concentrations of PCE at Tarawa Terrace water-supply wells from the beginning of operations at ABC One-Hour Cleaners through the closure of the wells and the WTP is shown in Figure A18. Simulated PCE concentrations in water-supply well TT-26 exceeded the current MCL of 5 μg/L during January 1957 (simulated value is 5.2 μg/L) and reached a maximum simulated value of 851 μg/L during July 1984. The mean simulated PCE concentration in water-supply well TT-26 for its entire period of operation was 351 μg/L. The mean simulated PCE concentration for the period exceeding the current MCL of 5 μg/L—January 1957 to January 1985—was 414 μg/L. This represents a duration of 333 months (27.7 years). These results are summarized in Table A12 along with simulated results for water-supply wells TT-23 and TT-25. It should be noted that although simulation results indicate several water-supply wells were contaminated with PCE (wells TT-23, TT-25, TT-31, TT-54, and TT-67), by far, the highest concentration of PCE and the longest duration of contamination occurred in water-supply well TT-26 (Figure A18).

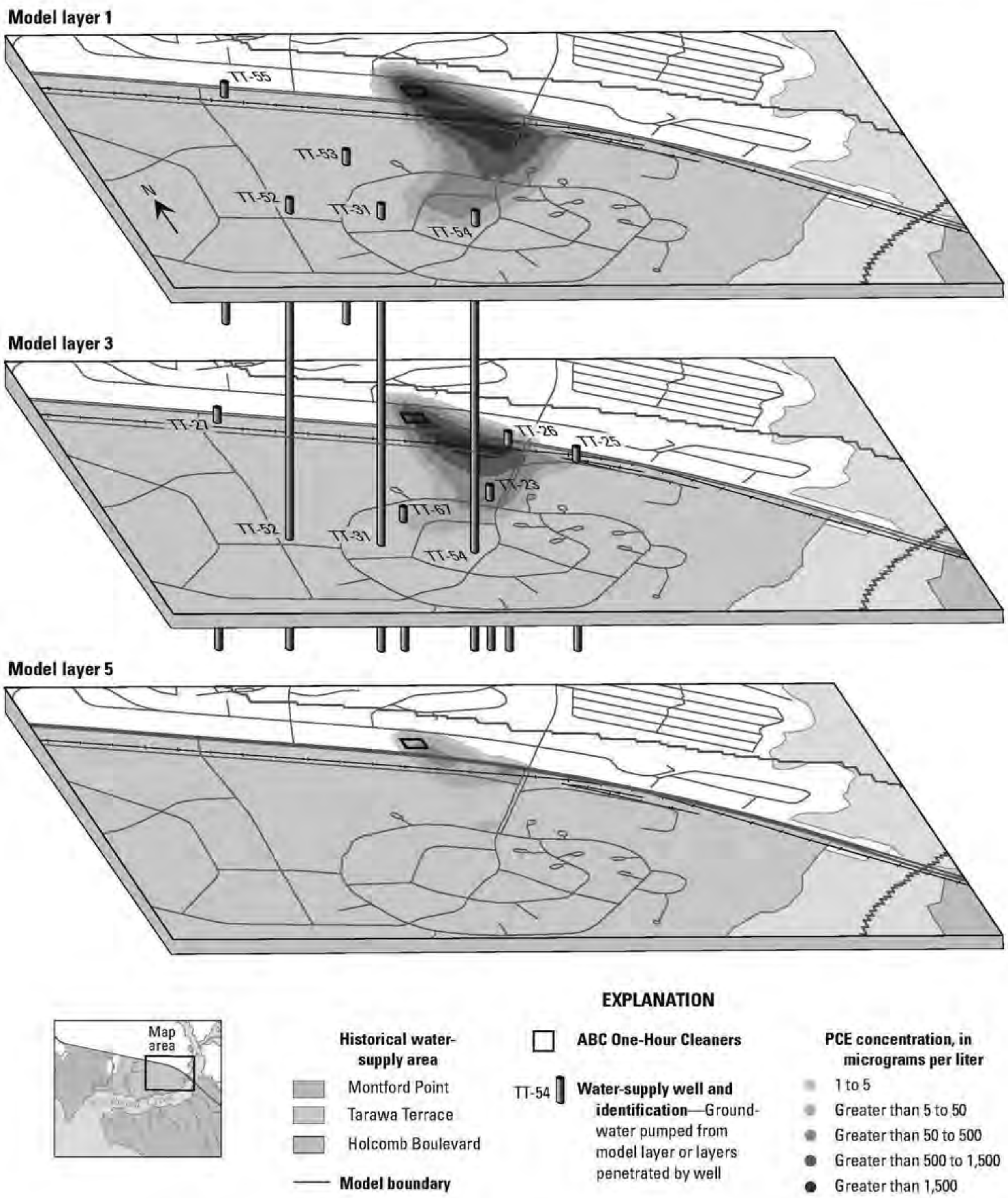
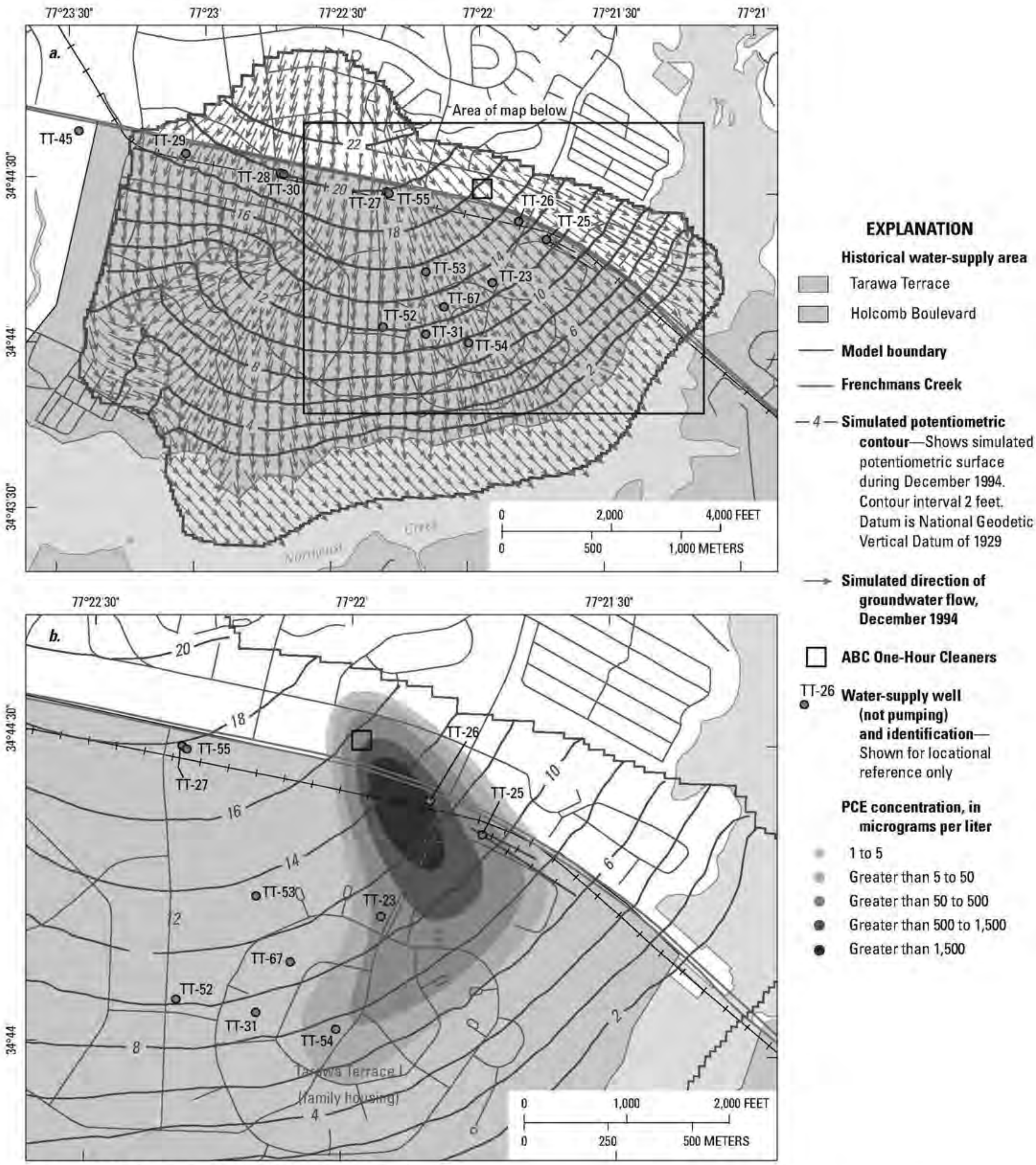


Figure A16. Diagram showing perspective views of the simulated distribution of tetrachloroethylene, model layers 1, 3, and 5, December 1984, Tarawa Terrace and vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina. [PCE, tetrachloroethylene; thickness and vertical separation of layers not to scale]



Base from U.S. Marine Corps and U.S. Geological Survey digital data files

Figure A17. Simulated *(a)* water level and direction of groundwater flow and *(b)* distribution of tetrachloroethylene, model layer 1, December 1994, Tarawa Terrace and vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina. [PCE, tetrachloroethylene]

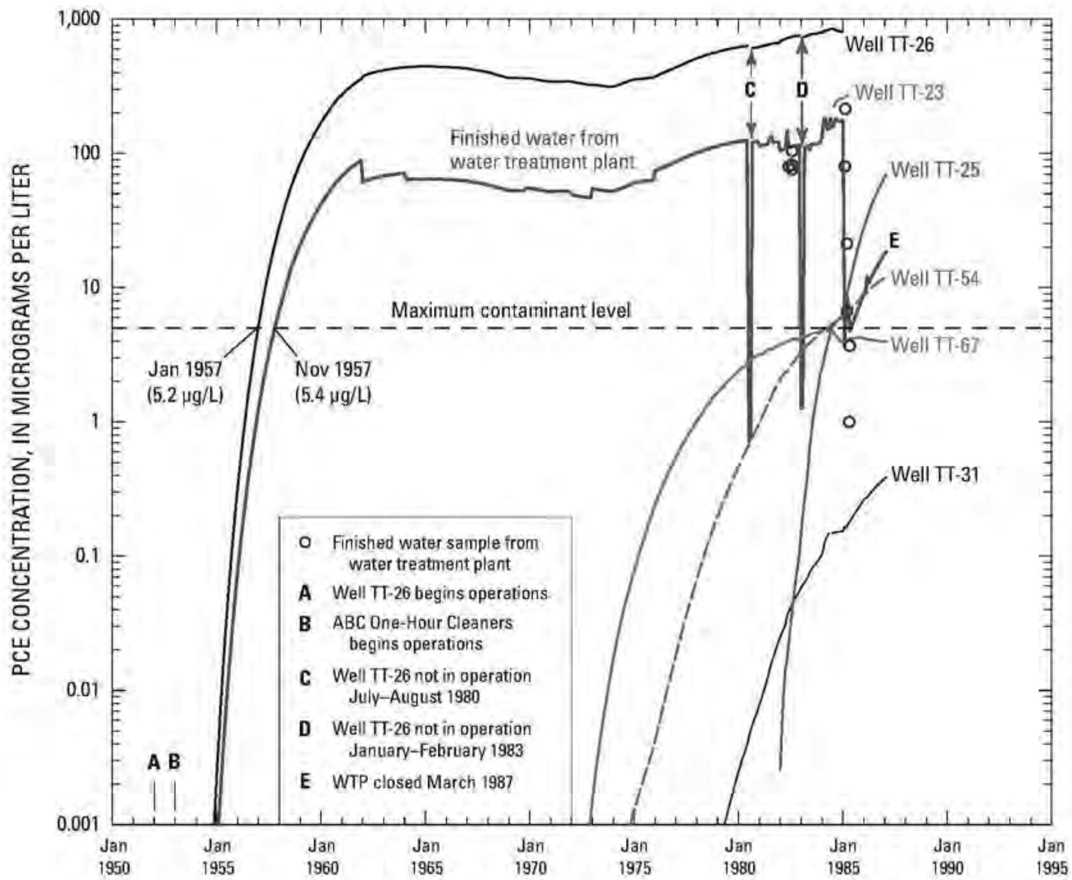


Figure A18. Concentration of tetrachloroethylene: simulated at selected water-supply wells and in finished water at the water treatment plant, and measured in finished water at the water treatment plant, Tarawa Terrace, U.S. Marine Corps Base Camp Lejeune, North Carolina. [PCE, tetrachloroethylene; µg/L, microgram per liter]

Table A12. Summary statistics for simulated tetrachloroethylene contamination of selected water-supply wells and the water treatment plant based on calibrated model simulation, Tarawa Terrace, U.S. Marine Corps Base Camp Lejeune, North Carolina.

[MCL, maximum contaminant level; µg/L, microgram per liter; WTP, water treatment plant; PCE, tetrachloroethylene]

Water supply	Month and year and duration exceeding MCL[1]	Month and year of maximum value and maximum concentration, in µg/L	Average concentration,[2] in µg/L
TT-23	August 1984–April 1985 8 months[3]	April 1985 274	252
TT-25	July 1984–February 1987 32 months	February 1987 69	27
TT-26	January 1957–January 1985 333 months[4]	July 1984 851	414
WTP	November 1957–February 1987 346 months	March 1984 183	70

[1] Current MCL for PCE is 5 µg/L, effective date July 6, 1992 (40 CFR, Section 141.60, Effective Dates, July 1, 2002, ed.)

[2] For periods exceeding 5 µg/L when water-supply well was operating

[3] Water-supply well TT-23 was not operating during February 1985

[4] Water-supply well TT-26 was not operating July–August 1980 and January–February 1983

Concentration of Tetrachloroethylene (PCE) in Finished Water

Figure A18 shows simulated PCE concentrations in finished water delivered by the Tarawa Terrace WTP. A monthly listing of simulated PCE concentrations also is provided in Appendix A2. PCE concentrations for the water-supply wells depicted in Figure A18 are based on simulated monthly results for the period of well operations (Figure A5, Table A6). PCE contamination of water-supply well TT-26 was the primary contributor to contamination in the finished water of the WTP. When water-supply well TT-26 was temporarily shut down during July–August 1980 and January–February 1983, the PCE concentration in finished water at the WTP was significantly lower (Figure A18). For example, during June 1980, the simulated PCE concentration in finished water at the Tarawa Terrace WTP was 126 μg/L, but during July–August 1980, the simulated PCE concentration in finished water at the Tarawa Terrace WTP did not exceed 0.8 μg/L. Furthermore, during December 1982, the simulated PCE concentration in finished water at the Tarawa Terrace WTP was 115 μg/L, but during January–February 1983, the simulated PCE concentration in finished water at the Tarawa Terrace WTP was 1.3 μg/L. The PCE concentration of finished water at the Tarawa Terrace WTP is less than the PCE concentration of water-supply well TT-26 because the mixing model uses water supplied to the WTP from all wells—contaminated and uncontaminated.

For any given month during the historical reconstruction period, the PCE concentration of finished water at the Tarawa Terrace WTP was computed using the following equations:

$$Q_T = \sum_{i=1}^{NWP} Q_i \qquad (2)$$

and

$$C_{WTP} = \frac{\sum_{i=1}^{NWP} C_i Q_i}{Q_T}, \qquad (3)$$

where

- NWP is the number of water-supply wells simulated as operating (pumping) during the month of interest,
- Q_i is the simulated groundwater pumping rate of water-supply well i,
- Q_T is the total simulated groundwater pumping rate from all operating water-supply wells during the month of interest,
- C_i is the simulated concentration for water-supply well i, and
- C_{WTP} is the concentration of finished water delivered from the Tarawa Terrace WTP for the month of interest.

Equation 2 is known as the continuity equation, and Equation 3 describes the conservation of mass.

The simulated concentration of PCE in finished water delivered by the Tarawa Terrace WTP first exceeded the current MCL of 5 μg/L during November 1957—10 months after the PCE concentration in water-supply well TT-26 exceeded the MCL (Figure A18). Using simulated water-supply well concentrations and mixing model computations (Equations 2 and 3), exposure to PCE-contaminated drinking water that exceeded the current MCL of 5 μg/L occurred for a duration of 346 months (28.8 years)—November 1957–February 1987. A summary of dates and durations of PCE concentrations at selected water-supply wells and in finished water at the Tarawa Terrace WTP is provided in Table A12. Simulated values of PCE concentration in finished water of the WTP compare well with available measured data shown in Figures A12 and A18 and listed in Table A10.

Analysis of Degradation By-Products

Although exposure to contaminated drinking water was eliminated after February 1987 due to the closure of the Tarawa Terrace WTP during March 1987 (Figures A3 and A18; Table A12), measurable quantities of PCE remained in the subsurface—at the source (ABC One-Hour Dry Cleaners) and distributed within the aquifer (Figure A17*b*). For example, during July 1991, the PCE concentrations in water samples obtained from off-line water-supply wells TT-25 and TT-26 were 23 μg/L and 350 μg/L, respectively (Table A9). This mass of PCE in the subsurface continued to migrate and undergo transformation through physical and biochemical processes such as volatilization and biodegradation. As such, the potential for exposure to PCE and its degradation by-products TCE,[27] 1,2-tDCE, and VC from a route other than ingestion and inhalation of drinking water—such as inhalation of soil vapors—continued beyond cessation of exposure to drinking water after the closure of the Tarawa Terrace WTP in March 1987 (Figure A3). To quantify historical concentrations of PCE degradation by-products in groundwater and in soil (vapor phase) requires a model capable of simulating multiphase flow and multispecies mass transport. For PCE, this complex analysis is summarized herein.[28]

The degradation of VOCs in groundwater is a transformation process from a parent compound (for example, PCE) to degradation by-products such as TCE, 1,2-tDCE, and VC (Lawrence 2006, In press 2007). Evidence of the transformation of PCE to degradation by-products of TCE and 1,2-tDCE can be found in water samples obtained January 16, 1985, from Tarawa Terrace water-supply wells TT-23 and TT-26. Laboratory analyses of the water samples indicated concentrations of PCE, TCE, and 1,2-tDCE of 132, 5.8, and 11.0 μg/L, respectively, for water-supply well TT-23 and concentrations of PCE, TCE, and 1,2-tDCE of 1,580, 57.0, and 92.0 μg/L, respectively, for water-supply well TT-26 (Faye and Green In press 2007). The simulation of the fate and transport of PCE in groundwater, described in the Chapter F report (Faye In press 2007b), accounted for the degradation of PCE by applying a biodegradation rate to PCE during the simulation process. (The biodegradation rate was determined from field data and the calibration process [Faye In press 2007b].) This transformation process typically is expressed in terms of a rate constant or half-life. For example, in the fate and transport simulations of PCE, the calibrated biodegradation (or reaction) rate for PCE was 5.0×10^{-4}/day (Table A11). It is important to note, however, that the basic chemical reaction package that is contained in the MT3DMS model was used to simulate a single-specie and single-phase system (Zheng and Wang 1999). Thus, as described in Faye (In press 2007b), MT3DMS was used to simulate the transport and fate (biodegradation) solely of PCE. To account for sequential biodegradation of VOCs, parent-daughter chain reactions must be taken into account in a multiphase environment (Zheng and Bennett 2002). For example, in a four-species system, the source (ABC One-Hour Cleaners) contains only a single specie—PCE. As PCE migrates from the source, it undergoes decay, and the decay product is TCE. TCE in turn undergoes decay, and the decay product can be 1,2-tDCE. 1,2-tDCE is again biologically transformed into VC (Lawrence 2006, In press 2007).[29] Thus, to account for and to simulate (1) parent-daughter chain reactions, (2) multiphase environments (water and vapor), and (3) fate and transport in the unsaturated (above the water table) and saturated (in groundwater) zones, a multispecies, multiphase modeling approach was required. For this purpose, the TechFlowMP model code was used to simulate the sequential biodegradation and transport of PCE and its associated daughter by-products (TCE, 1,2-tDCE, and VC) at Tarawa Terrace and vicinity.[30]

Using TechFlowMP, three-dimensional multispecies, and multiphase simulations were conducted to quantify the fate and transport of PCE and its degradation by-products from the source of the PCE contamination—ABC One-Hour Cleaners. The same model domain used for the MODFLOW-96 and MT3DMS model simulations (Faye and Valenzuela In press 2007, Faye In press 2007b) was used for the

[27] TCE also is used in some dry-cleaning processes. However, based on the deposition from the owner of ABC One-Hour Cleaners (Melts 2001), only PCE was used at ABC One-Hour Cleaners. Therefore, any TCE detected in Tarawa Terrace water-supply wells or in WTP finished water occurred because of the degradation of PCE.

[28] For a detailed discussion of the analysis and simulation of PCE degradation by-products at Tarawa Terrace and vicinity, refer to the Chapter G report (Jang and Aral In press 2007).

[29] Degradation pathways are very complex processes that depend on availability of microorganisms and environmental conditions. Details are provided in Lawrence (2006 In press 2007).

[30] TechFlowMP is a three-dimensional multispecies, multiphase mass transport model developed by the Multimedia Environmental Simulations Laboratory at the Georgia Institute of Technology, Atlanta, Georgia (Jang and Aral 2005).

TechFlowMP model. Contaminants simulated using this more complex model formulation were PCE and its degradation by-products TCE, 1,2-tDCE, and VC. Parameter values calibrated using the MODFLOW-96 and MT3DMS models (for example, water-supply well pumping rates, infiltration [recharge] rate, porosity, dispersivity, and PCE biodegradation [reaction] rate) were used in the TechFlowMP model simulations (Table A11). However, owing to the more complex set of mathematical equations approximated by this model, and because the contaminant source was applied to both the unsaturated and saturated zones (zones above and below the water table, respectively), additional model parameters were determined and assigned. Examples of these parameters include: moisture content; partitioning coefficients for TCE, 1,2-tDCE, and VC; and aerobic (unsaturated zone) and anaerobic (saturated zone) biodegradation rates for PCE, TCE, 1,2-tDCE, and VC. Details on specific TechFlowMP model parameters and their calibrated values are described in the Chapter G report (Jang and Aral In press 2007).

Results obtained by conducting three-dimensional, multispecies, and multiphase simulations are presented herein in terms of (1) graphs of time versus concentration of PCE and its degradation by-products (Figure A19), (2) a table listing summary statistics for PCE and its degradation by-products (Table A13), (3) maps showing the distribution of vapor-phase PCE (Figure A20), and (4) a table listing monthly PCE and PCE degradation by-products in finished water at the Tarawa Terrace WTP (Appendix A2). Figure A19 shows graphs of simulated concentrations of PCE and its degradation by-products—obtained by using the TechFlowMP model—at water-supply well TT-26 and at the Tarawa Terrace WTP. Also shown on the graphs is the concentration of PCE simulated using the MT3DMS single-specie and single-phase model (compare Figure A18 and Figure A19). Simulated concentrations of PCE at water-supply well TT-26 obtained using the TechFlowMP model are slightly lower in value than PCE concentrations obtained using the MT3DMS model (Figure A19*a*). This is to be expected because the TechFlowMP simulations take into account flow and transport in both the unsaturated zone (zone above the water table) and saturated zone (zone at and below the water table) and loss of PCE into the vapor phase, whereas the MODFLOW-96 and MT3DMS models consider groundwater flow and contaminant fate and transport solely in the saturated zone and in the water phase. Given the same total mass of PCE loaded into each of these models, the PCE concentration at water-supply well TT-26 (and other water-supply wells) will be simulated as a lesser amount in the saturated zone by the TechFlowMP model because a fraction of the mass is allocated to the unsaturated zone, as well as being partitioned into the vapor phase. Because water-supply well TT-26 was the primary contributor of PCE contamination in finished water at the Tarawa Terrace WTP (Figure A18), the resulting PCE concentrations in finished water at the Tarawa Terrace WTP computed using results from the TechFlowMP model also were lower (Figure A19*b* and Appendix A2).

Based on the TechFlowMP model simulations, TCE, 1,2-tDCE, and VC concentrations at water-supply well TT-26 generally ranged from about 10 μg/L to 100 μg/L (Figure A19*a*). Simulated concentrations of TCE, 1,2-tDCE, and VC in finished water at the Tarawa Terrace WTP generally ranged from about 2 μg/L to 15 μg/L (Figure A19*b* and Appendix A2). Comparison of the simulated concentrations of PCE degradation by-products in finished water at the Tarawa Terrace WTP indicate the following (Figure A19*b*):

1. TCE was below the current MCL value of 5 μg/L[31] for nearly the entire historical period except during January 1984–January 1985 when it ranged between 5 and 6 μg/L;
2. 1,2-tDCE was below the current MCL value of 100 μg/L[31] for the entire historical period;
3. VC was at or above the current MCL value of 2 μg/L[31] from May 1958 through February 1985 at which time water-supply well TT-26 was shut down.

Simulated concentration values of TCE in water-supply well TT-26 and in finished water delivered by the Tarawa Terrace WTP are less than simulated concentrations of VC and 1,2-tDCE. This is in agreement with measured data obtained from water samples in well TT-26 which shows a TCE concentration less than that of 1,2-tDCE. Summary statistics of PCE and degradation by-product contamination of selected water-supply wells (TT-23, TT-25, and TT-26) and at the Tarawa Terrace WTP derived from simulations of the TechFlowMP model (based on three-dimensional multispecies and multiphase simulation) are listed in Table A13.

[31] 40 CFR, Section 141.60, Effective Dates, July 1, 2002, ed.

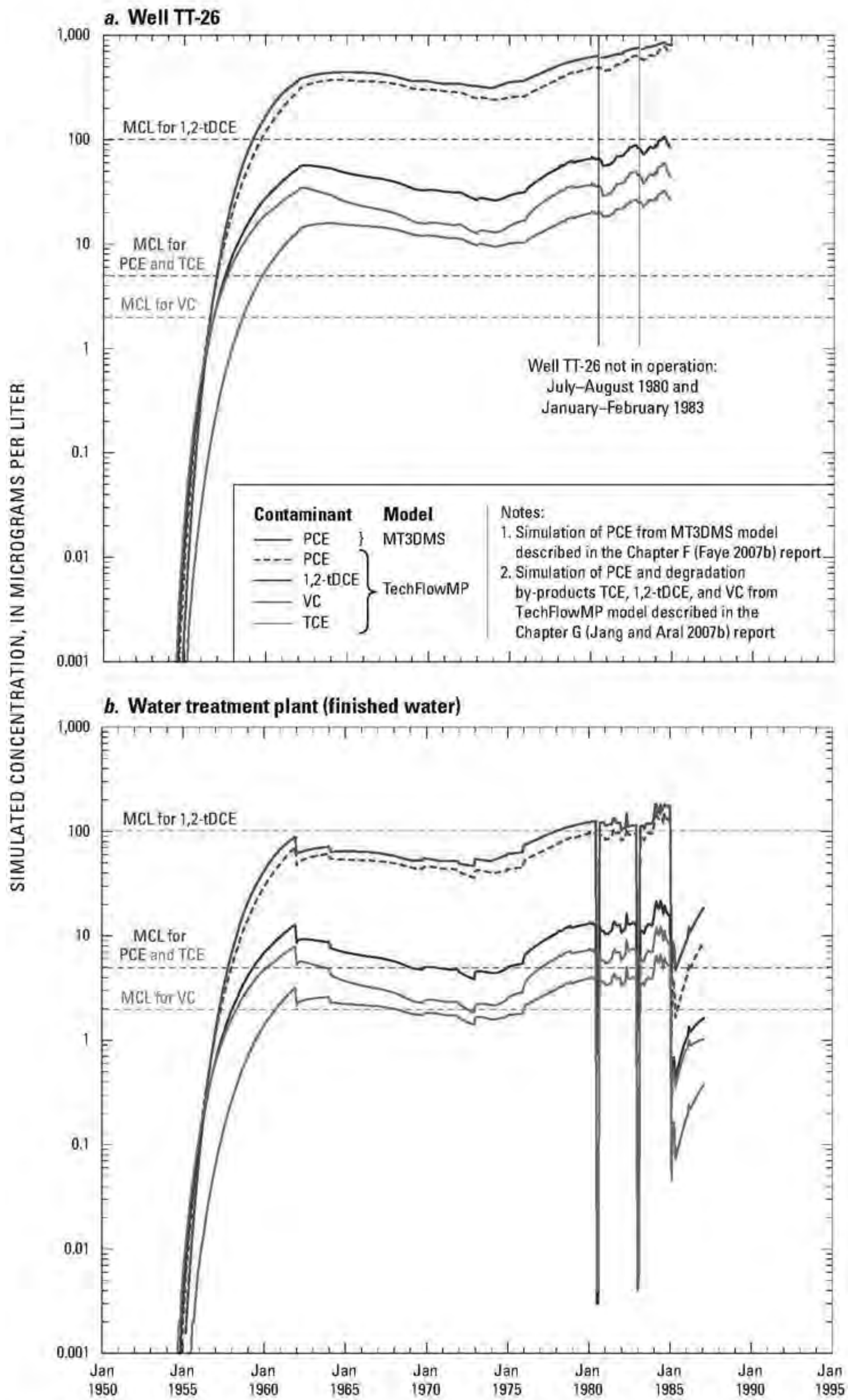


Figure A19. Simulated concentration of tetrachloroethylene (PCE) and degradation by-products trichloroethylene (TCE), *trans*-1,2-dichloroethylene (1,2-tDCE), and vinyl chloride (VC) *(a)* at water-supply well TT-26 and *(b)* in finished water from water treatment plant, Tarawa Terrace, U.S. Marine Corps Base Camp Lejeune, North Carolina. [MCL, maximum contaminant level]

Table A13. Summary statistics for simulated tetrachloroethylene and degradation by-product contamination of selected water-supply wells and the water treatment plant based on three-dimensional multispecies and multiphase model simulation, Tarawa Terrace, U.S. Marine Corps Base Camp Lejeune, North Carolina.[1]

[MCL, maximum contaminant level; µg/L, microgram per liter; PCE, tetrachloroethylene; TCE, trichloroethylene; 1,2-tDCE, *trans*-1,2-dichloroethylene; VC, vinyl chloride; Aug, August; Sept, September; Nov, November; Mar, March; Feb, February; Jan, January; WTP, water treatment plant]

Water supply	Month and year exceeding MCL,[2] in µg/L				Maximum concentration, in µg/L				Average concentration,[3] in µg/L				Duration exceeding MCL, in months			
	PCE	TCE	1,2-tDCE	VC	PCE	TCE	1,2-tDCE	VC	PCE	TCE	1,2-tDCE	VC	PCE	TCE	1,2-tDCE	VC
[4]TT-23	Aug 1984	Sept 1984	—[6]	Aug 1984	167	7	21	13	143	7	—[6]	10	8	7	—[6]	8
TT-25	Mar 1985	—[6]	—[6]	July 1985	40	2	7	5	21	—[6]	—[6]	4	24	—[6]	—[6]	20
[5]TT-26	Feb 1957	Nov 1959	June 1984	Nov 1956	775	33	107	60	332	15	105	24	332	299	3	335
WTP	Jan 1958	Feb 1984	—[6]	May 1958	158	7	22	12	57	6	—[6]	5	332	11	—[6]	311

[1]All simulations conducted using the TechFlowMP model. See text and the Chapter G report (Jang and Aral In press 2007) for details

[2]Current MCLs are: PCE and TCE, 5 µg/L; 1,2-tDCE, 100 µg/L; and VC, 2 µg/L (USEPA, 2003); effective dates for MCLs are as follows: TCE and VC, January 9, 1989; PCE and 1,2-tDCE, July 6, 1992 (40 CFR, Section 141.60, Effective Dates, July 1, 2002, ed.)

[3]For periods exceeding MCL when water-supply well operating

[4]Water-supply well TT-23 was not operating February 1985

[5]Water-supply well TT-26 was not operating July–August 1980 and January–February 1983

[6]MCL never exceeded during simulation

Maps of the areal distributions of vapor-phase PCE for December 1984 and December 1994 are shown in Figure A20. The maps depict simulated vapor-phase PCE concentrations in soil to a depth of about 10 ft. Concentration units for the vapor-phase PCE distributions shown in Figure A20 are in micrograms per liter of air.[32] Comparing these maps with similar maps for dissolved-phase PCE in groundwater for model layer 1 (Figures A15*b* and A17*b*, respectively) indicates that vapor-phase concentrations are lower than dissolved-phase PCE concentrations by about a factor of 10–15 for December 1984 and December 1994. The following examples are noteworthy.

1. During December 1984:
   a. the maximum simulated PCE concentration in groundwater at family housing (model layer 1) was 638 µg/L (Figure A15*b*), whereas the maximum simulated vapor-phase PCE (in the top 10 ft of soil) was 20 µg/L (Figure A20*a*); and
   b. the maximum simulated PCE concentration in groundwater (model layer 1) at the Tarawa Terrace elementary school was 1,418 µg/L (Figure A15*b*), whereas the maximum simulated vapor-phase PCE (in the top 10 ft of soil) was 137 µg/L (Figure A20*a*);

[32] To obtain air concentration units of micrograms per cubic meter (mg/m^3) that are typically used for indoor air studies, multiply micrograms per liter by 1000 (refer to Conversion Factors in Contents section of this report.

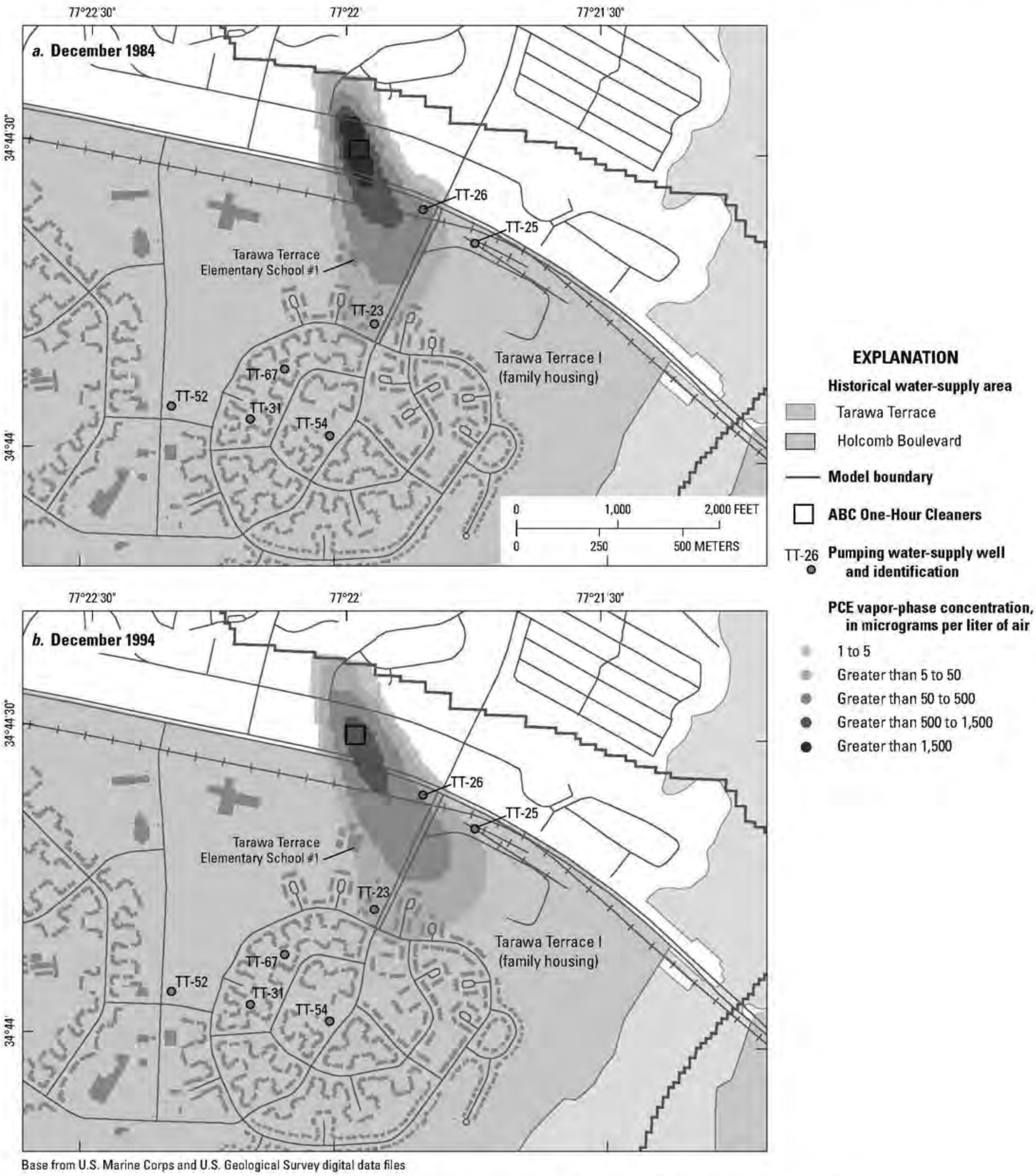


Figure A20. Simulated distribution of vapor-phase tetrachloroethylene to a depth of 10 feet below land surface, *(a)* December 1984 and *(b)* December 1994, Tarawa Terrace and vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina. [PCE, tetrachloroethylene]

2. During December 1994:

    a. the maximum simulated PCE concentration in groundwater at family housing (model layer 1) was 688 µg/L (Figure A17*b*), whereas the maximum simulated vapor-phase PCE (in the top 10 ft of soil) was 44 µg/L (Figure A20*b*); and

    b. the maximum simulated PCE concentration in groundwater (model layer 1) at the Tarawa Terrace elementary school was 688 µg/L (Figure A17*b*), whereas the maximum simulated vapor-phase PCE (in the top 10 ft of soil) was 56 µg/L (Figure A20*b*).

Due to sandy soils found at Camp Lejeune (including Tarawa Terrace), there is potential for vapors from these plumes (for example, Figure A20) to enter buildings, thereby providing a potential exposure pathway from inhalation of PCE and PCE degradation by-product vapors. At Tarawa Terrace, these buildings would include some family housing and the elementary school.

It is important to note that historical measurements of soil vapor (soil gas) were not available. Therefore, the TechFlowMP model parameters related to the simulation of vapor-phase PCE and PCE degradation by-products could not be calibrated against field conditions. For example, an assumption was made that homogeneous vapor exit conditions exist at land surface throughout the entire Tarawa Terrace area. Realistically, housing built on concrete slabs, streets and parking lots paved with asphalt, bare playground areas, and lawns will each have different vapor exit conditions requiring adjustment of model parameters to those specific conditions. This may seem like a limitation of the reliability of vapor-phase modeling results (for example, Figure A20). However, the focus of the current investigation is on drinking-water contamination and the historical reconstruction of PCE and PCE degradation by-product contamination of groundwater (water phase) and drinking water at Tarawa Terrace. The concentration of PCE and PCE degradation by-products in groundwater significantly impacts the vapor-phase simulation results. Because simulated groundwater concentrations are based on calibrated groundwater-flow and contaminant fate and transport models, the results presented for vapor-phase simulations should be viewed as reliable historical estimates of generalized vapor-phase conditions in soil during December 1984 and December 1994 at a depth of about 10 ft (Figure A20). For present-day soil-gas conditions or to obtain a more refined historical vapor-phase calibration for Tarawa Terrace, field studies, including the collection of unsaturated zone, soil gas, and indoor air concentration data would have to be undertaken as a separate detailed study. Details regarding the development of the TechFlowMP model are provided in Jang and Aral (2005). Assumptions, parameter values specific to three-dimensional multiphase flow and multispecies mass transport, and resulting simulations of PCE and PCE degradation by-products in groundwater and vapor-phase specific to Tarawa Terrace and vicinity are provided in Jang and Aral (2007) and in the Chapter G report (Jang and Aral In Press 2007).

Confidence in Simulation Results

Models and associated calibrated parameters described previously are inherently uncertain because they are based on limited data. Under such circumstances, good modeling practice requires that evaluations be conducted to ascertain the confidence in models by assessing uncertainties associated with the modeling process and with the outcomes attributed to models (Saltelli et al. 2000). With respect to model simulations at Tarawa Terrace, the availability of data to thoroughly characterize and describe model parameters and operations of water-supply wells was considerably limited, as described in the section on Water-Distribution Investigation. Such limitations give rise to the following questions:

1. Could alternative water-supply well operating schedules or combinations of model parameter values provide acceptable simulation results when compared to observed data and previously established calibration targets?

2. What is the reliability of the historically reconstructed estimates of PCE concentration determined using the calibrated models (for example, results shown in Figure A18)?

To answer these questions and address the overarching issues of model and parameter variability and uncertainty, three analyses were conducted using the calibrated groundwater-flow and contaminant fate and transport models described in Faye and Valenzuela (In press 2007) and Faye (In press 2007b), respectively. These analyses were: (1) an assessment of pumping schedule variation at Tarawa Terrace water-supply wells with respect to contaminant arrival times and concentrations,[33] (2) sensitivity analysis,[34] and (3) probabilistic analysis.[34] All of the additional analyses were conducted using PCE dissolved in groundwater as a single specie. MODFLOW-96 and MT3DMS calibrated models are described in the Chapter C (Faye and Valenzuela In press 2007) and Chapter F (Faye In press 2007b) reports.

[33] A detailed description and discussion of the effect of water-supply well schedule variation on the arrival of PCE at water-supply wells and the Tarawa Terrace WTP is presented in the Chapter H report (Wang and Aral In press 2007).

[34] A detailed description and discussion of sensitivity and uncertainty analysis, including the use of Monte Carlo simulation is presented in the Chapter I report (Maslia et al. In press 2007b).

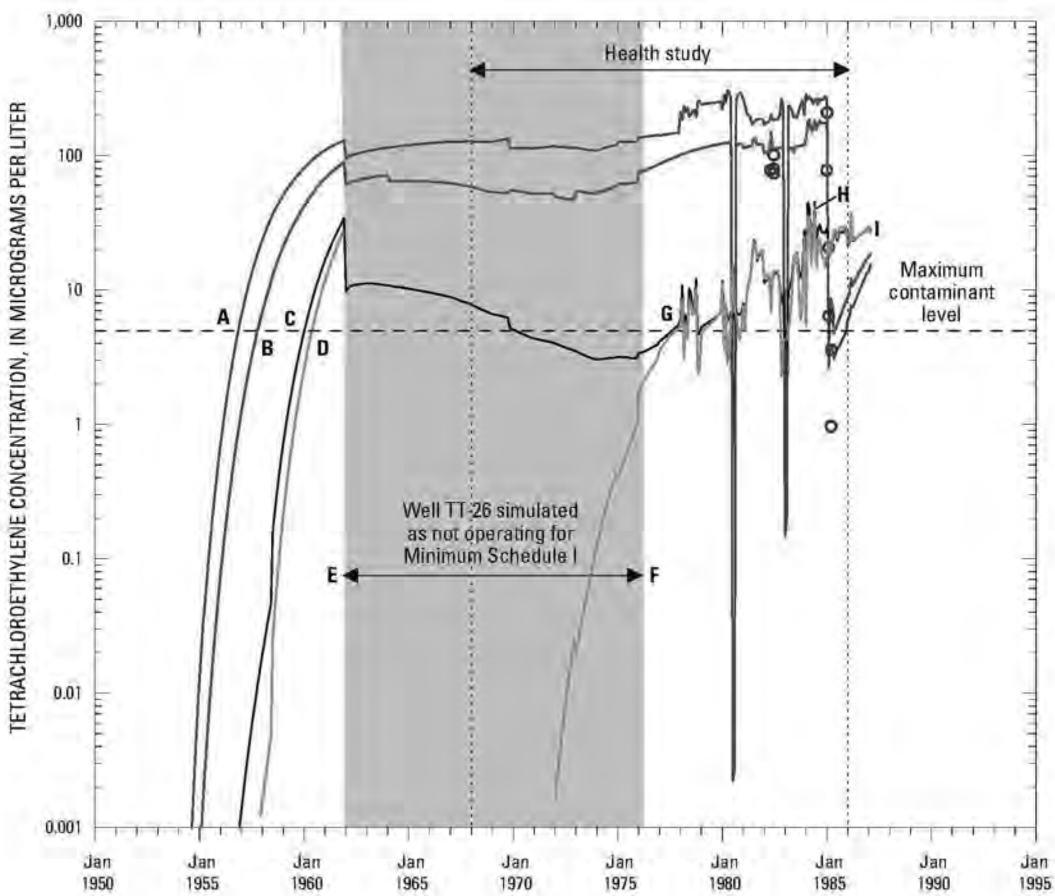
Water-Supply Well Scheduling Analysis

The scheduling and operation histories of Tarawa Terrace water-supply wells directly affected times and concentrations of PCE in groundwater at wells and at the WTP during 1952–1987. Thus, simulated water-supply well operations could be a major cause and contributor to uncertainty and variability with respect to PCE arrival and PCE concentration at water-supply wells and in finished water at the Tarawa Terrace WTP. To assess the impact of pumping schedule variability and uncertainty on groundwater-flow, contaminant fate and transport, and WTP mixing models, a procedure was developed that combined groundwater simulation models and optimization methods. This procedure is described in detail in the Chapter H report (Wang and Aral In press 2007). The simulation tool developed for this analysis—PSOpS (Table A4)—combines the MODFLOW-96 and MT3DMS groundwater simulators with a rank-and-assign optimization method developed specifically for the Tarawa Terrace analysis. This tool optimizes pumping (operational) schedules to minimize or maximize the arrival time of contaminants at water-supply wells. Based on the optimized operational schedules, the concentration of a contaminant is recalculated, and the effect of pumping schedule variation on contaminant concentration and the arrival time of groundwater exceeding the current MCL of PCE (5 μg/L) are evaluated. It is important to note that in this analysis, with the exception of pumping rates, groundwater-flow and contaminant transport model parameters were not varied from their calibrated values (Table A11; Faye and Valenzuela [In press 2007]; Faye [In press 2007b]).

Results of analyses using the PSOpS simulation tool to assess the effects of water-supply well pumping variation are presented graphically as a series of curves of simulated PCE concentration in finished water at the Tarawa Terrace WTP versus time (Figure A21).[35] The calibration curve in Figure A21 represents the same data presented in Figure A18 and represents the simulated concentration of finished drinking water delivered from the Tarawa Terrace WTP—derived from analyses described in the Chapter F report (Faye In press 2007b). Calibrated model results indicate that PCE exceeding the

[35] In the following discussion, reference is made to locations shown in Figure A21. These locations are labeled points A–I. Thus, in the ensuing discussion for the section on "Water-Supply Well Scheduling Analysis," a reference to a specific location on the graph, for example, point A, refers solely to Figure A21.

current MCL of 5 µg/L in finished water was delivered from the WTP during November 1957 (point B). By determining an optimal combination of water-supply well pumping in terms of on-off operations and the volumetric pumping rate, it would have been possible for PCE at the 5 µg/L concentration to arrive at the WTP at a date earlier than that reported for the calibrated MT3DMS model. These optimized arrival times are shown as "Earliest arrival" in Figure A21 and are defined as the "Maximum Schedule" in the Chapter H report (Wang and Aral In press 2007). The results show an arrival date 11 months earlier—December 1956 (point A)—than the



EXPLANATION

Calibration—As described in Chapter F (Faye 2007b)

Arrival—As described in Chapter H (Wang and Aral In press 2007),

Late—Defined as *Minimum Schedule I*, well TT-26 not operated January 1962–February 1976

Earliest—Defined as *Maximum Schedule*

Late—Defined as *Minimum Schedule II*, well TT-26 operated at least at 25 percent of capacity

o **Measured at water treatment plant**

Simulation time

Location on graph	Month and year
A	December 1956
B	November 1957
C	February 1960
D	June 1960
E	January 1962
F	February 1976
G	November 1977
H	June 1984
I	February 1987

Figure A21. Sensitivity of tetrachloroethylene concentration in finished water at the water treatment plant to variation in water-supply well operations, Tarawa Terrace, U.S. Marine Corps Base Camp Lejeune, North Carolina. [PCE, tetrachloroethylene; see text for discussion of points A–I] calibrated arrival date of November 1957. Also notable is the simulated concentration for January–February 1985 of 262 μg/L. This value (262 μg/L) exceeds the observed value of 215 μg/L by 47 μg/L compared with the calibrated value of 176 μg/L (Table A10) that underestimates the observed value by 39 μg/L. Overall, the "Earliest arrival" simulation shows a higher concentration of PCE in finished water delivered from the Tarawa Terrace WTP with a maximum value of 305 μg/L and an average (for concentrations exceeding 5 μg/L) of 132 μg/L. The period during which the current MCL of 5 μg/L for PCE was exceeded under the "Early arrival" scenario was 348 months (29 years).

The PSOpS simulation tool also was used to investigate a variety of other pumping scenarios by specifying limiting values for such well properties as the maximum or minimum pumping rate for a specific water-supply well or group of wells. Two additional results are presented in Figure A21 for simulations that specify minimum operating rates for water-supply well TT-26—25% and 0% of total capacity.[36] The results of these simulations show that when water-supply well TT-26 operated at least at 25% of its capacity—identified as "Minimum Schedule II" in Figure A21 and in the Chapter H report—the arrival of groundwater contaminated with PCE exceeding the current MCL (5 μg/L) was delayed by 27 months—February 1960 (point C)—when compared with the calibrated arrival time of November 1957 (point B). A notable result occurs, however, when water-supply well TT-26 is simulated as being shut down for a period of time—identified as "Minimum Schedule I" in Figure A21 and in the Chapter H report. Based on simulation results, water-supply well TT-26 could have been taken out of service in January 1962 (point E) and kept out of service until February 1976 (point F) with the remaining water-supply wells still capable of meeting all of the water demand during this period for Tarawa Terrace and vicinity. During this time, water-supply well TT-26 was modeled as being off-line, and the resulting simulated concentration of PCE in finished water from the Tarawa Terrace WTP ranged from 0 to less than 2 μg/L. After February 1976 (point F), water-supply well TT-26 had to be simulated as operating to meet increasing demand. Thus, using the PSOpS simulation tool, it was possible to simulate the operation of water-supply well TT-26 in such a manner that the PCE concentration of finished water delivered from the Tarawa Terrace WTP was below 5 μg/L from January 1962 (point E) through February 1976 (point F). Under this simulation scenario—"Minimum Schedule I"—the current MCL was exceeded during the period June 1960 (point D)–December 1961 and for most months during the period November 1977–February 1987 (points G and I, respectively).[37] Under the "Minimum Schedule I" scenario, the maximum PCE concentration in finished water at the Tarawa Terrace WTP was simulated as 41 μg/L during June 1984 (point H).

In summary, analyses of the variation in water-supply well scheduling demonstrate that the current MCL for PCE (5 μg/L) could have been exceeded in finished drinking water delivered from the Tarawa Terrace WTP as early as December 1956 (point A) and no later than June 1960 (point D). Because Tarawa Terrace WTP records indicate that water-supply well TT-26 was most likely operated routinely, the analysis also demonstrates that the earliest time that finished water at the Tarawa Terrace WTP exceeded the current MCL for PCE of 5 μg/L most likely occurred between December 1956 ("Earliest arrival" scenario, point A) and November 1957 (calibrated arrival time, point B). The most likely maximum concentration of PCE in finished water ranged between the "Earliest arrival" scenario maximum of 305 μg/L and the calibrated maximum of 183 μg/L. The mean concentration of PCE in finished water exceeding the current MCL of 5 μg/L most likely ranged between the "Earliest arrival" scenario mean of 131 μg/L and the calibrated mean of 70 μg/L. The analyses conducted using the PSOpS simulation tool provide further evidence that drinking water contaminated with PCE exceeding the current MCL of 5 μg/L was delivered to residents of Tarawa Terrace for a period ranging between the "Earliest arrival" duration of 348 months and the calibrated model duration of 346 months. This analysis further indicates that the concentration of PCE in finished water delivered to residents of Tarawa Terrace, determined from the contaminant fate and transport and mixing model analyses (Faye In press 2007b), are reasonable estimates of historical concentrations.

[36] Using the PSOpS simulation tool, the operation of water-supply well TT-26 was simulated as being shut down for a period of time—0% capacity—and it was allowed to operate as low as 25% of its rated capacity at times. A complete listing of water-supply well capacity data is provided in the Chapter C report (Faye and Valenzuela In press 2007).

[37] There were 103 months during the period November 1977–February 1987. For 14 different months during this period, the PCE concentration in finished water at the Tarawa Terrace WTP was below the current MCL of 5 μg/L, ranging in value from 2.3 to 4.9 μg/L.

Sensitivity Analysis

Sensitivity analysis is a method used to ascertain the dependency of a given model output (for example, water level or concentration) upon model input parameters (for example, hydraulic conductivity, pumping rate, and mass loading rate). Sensitivity analysis is important for checking the quality of the calibration of a given model, as well as a powerful tool for checking the robustness and reliability of model simulations. Thus, sensitivity analysis provides a method for assessing relations between information provided as input to a model—in the form of model input parameters—and information produced as output from the model. Numerous methods are described in the literature for conducting sensitivity analysis (Saltelli et al. 2000). For the Tarawa Terrace models, selected model parameters were varied one at a time from their respective calibrated values (Table A11), and the corresponding effect of this variation on the change in the PCE concentration of finished drinking water at the Tarawa Terrace WTP was assessed.[38] In conducting the sensitivity analysis, all calibrated model parameters—with the exception of pumpage—were increased and decreased by factors ranging from 50% to 400% of their calibrated values (Table A14).[39] For example, horizontal hydraulic conductivity for model layer 1 was varied by 90%, 110%, 150%, and 250% of its calibrated value; dispersivity was varied by 50%, 200%, and 400% of its calibrated value. Groundwater-flow model parameters that were subjected to the sensitivity analysis were:

- horizontal hydraulic conductivity of the aquifers (model layers 1, 3, 5, and 7),
- vertical hydraulic conductivity of the semi-confining units (model layers 2, 4, and 6),
- infiltration (recharge) rate, and
- storage coefficients (includes specific yield for model layer 1).

[38] This particular approach to sensitivity analysis is referred to as one-at-a-time (OAT) designs or experiments; details can be found in Saltelli et al. (2000).

[39] Table A14 is a list of selected parameters varied during the sensitivity analysis. For a complete list and discussion of all parameters varied, see the Chapter I report (Maslia et al. In press 2007b).

Contaminant fate and transport model parameters that were subjected to the sensitivity analysis were:

- distribution coefficient,
- bulk density,
- effective porosity,
- reaction rate,
- mass-loading rate,
- longitudinal dispersivity, and
- molecular diffusion.

Measures of the effect of varying the groundwater-flow and contaminant fate and transport model parameters were quantified in terms of five computations: (1) the date (month and year) when finished drinking water at the Tarawa Terrace WTP first exceeded the current MCL for PCE (5 µg/L), (2) the duration (in months) that finished drinking water at the WTP exceeded the current MCL, (3) the relative change in these durations (percent) caused by varying the calibrated parameter values, (4) the maximum PCE concentration in finished water at the Tarawa Terrace WTP, and (5) the relative change (percent) in the maximum concentration. Results for selected sensitivity analyses are listed in Table A14. Recall that for calibrated model parameters, the date that the PCE in finished water at the WTP first exceeded the current MCL was simulated as November 1957, and the duration that finished water exceeded the MCL for PCE was 346 months (Figure A18, Table A12). Results of the sensitivity analysis show that some parameters are insensitive to change, even when varied by factors of 10 and 20. For example, large changes in specific yield, storage coefficient, and molecular diffusion resulted in very little change in simulated results (Table A14). Changes in other parameters—for example, horizontal hydraulic conductivity for model layer 1 and infiltration, using values that were less than calibrated values—resulted in wells going dry during the simulation process. Generally, increasing or decreasing a calibrated parameter value by 10% (ratio of varied to calibrated parameter value of 0.9–1.1) resulted in changes of 6 months or less to the date that finished water first exceeded the MCL for PCE (5 µg/L). Complete details pertaining to the use of the sensitivity analysis in relation to calibrated model parameter values and results obtained from the sensitivity analysis are discussed in the Chapter I report (Maslia et al. In press 2007b).

Table A14. Summary of selected sensitivity analyses conducted on calibrated groundwater-flow and contaminant fate and transport model parameters, Tarawa Terrace and vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina.[1]

[PCE, tetrachloroethylene; MCL, maximum contaminant level; µg/L, microgram per liter; ft/d, foot per day; ft³/g, cubic foot per gram; g/ft³, grams per cubic foot; d⁻¹, 1/day; g/d, grams per day; ft²/d, square foot per day; —, not applicable; WTP, water treatment plant]

Model parameter[2]	Calibrated value	Ratio of varied to calibrated parameter value	Simulated PCE in finished water at the water treatment plant[3]				
			Date first exceeding MCL[4]	Duration exceeding MCL, in months	Relative change in duration, percent[5]	Maximum concentration, in µg/L	Relative change in maximum concentration, percent[6]
Groundwater-flow model parameters							
Horizontal hydraulic conductivity, layer 1, K_H (ft/d)	12.2–53.4	0.9	—[7]	—[7]	—[7]	—[7]	—[7]
		1.1	Aug. 1957	351	1.4	196	7.0
		1.5	Oct. 1956	365	5.5	223	22.0
		2.5	Oct. 1955	377	9.0	209	14.1
Horizontal hydraulic conductivity, layer 3, K_H (ft/d)	4.3–20.0	0.9	Oct. 1957	348	0.6	184	0.5
		1.1	Nov. 1957	345	–0.3	182	–0.5
		1.5	Feb. 1958	341	–1.4	179	–2.3
		2.5	Jul. 1958	339	–2.0	187	2.1
Horizontal hydraulic conductivity, layer 5, K_H (ft/d)	6.4–9.0	0.9	Oct. 1957	347	0.3	185	1.2
		1.1	Nov. 1957	346	0.0	181	–1.0
Horizontal hydraulic conductivity, layer 7, K_H (ft/d)	5.0	0.9	Nov. 1957	346	0.0	183	–0.1
		1.1	Nov. 1957	346	0.0	183	0.1
Infiltration (recharge), I_R (inches per year)	6.6–19.3	0.75	—[7]	—[7]	—[7]	—[7]	—[7]
		1.25	Dec. 1957	343	–0.9	210	14.8
Specific yield, S_y	0.05	10.0	Nov. 1957	342	–1.2	182	–0.6
		20.0	Nov. 1957	338	–2.3	178	–2.6
Storage coefficient, S	4.0×10^{-4}	10.0	Nov. 1957	346	0.0	183	–0.2
		20.0	Nov. 1957	346	0.0	182	–0.3
Fate and transport model parameters							
Distribution coefficient, K_d (ft³/g)	5.0×10^{-6}	0.5	Apr. 1956	371	7.2	214	16.7
		0.9	Jul. 1957	352	1.7	191	4.2
		1.5	Jun. 1959	310	–10.4	165	–10.0
		2.0	Dec. 1960	286	–17.3	143	–21.7
Bulk density, ρ_b (g/ft³)	77,112	0.9	Jul. 1957	352	1.7	191	4.2
		1.1	Mar. 1958	338	–2.3	180	–1.8
Effective porosity, n_E	0.2	0.5	Dec. 1956	363	4.9	349	90.9
		2.0	Sep. 1959	301	–13.0	86	–53.0
Reaction rate, r (d⁻¹)	5.0×10^{-4}	0.5	Oct. 1957	349	0.9	294	60.4
		2.0	Jan. 1958	326	–5.8	94	–48.7
Mass-loading rate[5], $q_S C_S$ (g/d)	1,200	0.5	May 1958	329	–4.9	92	–50.0
		1.5	Aug. 1957	351	1.4	275	50.0
Longitudinal dispersivity, α_L (foot)	25	0.5	Apr. 1958	337	–2.6	184	0.3
		2.0	Mar. 1957	356	2.9	181	–1.0
		4.0	Jun. 1956	367	6.1	176	–3.7
Molecular diffusion coefficient, D* (ft²/d)	8.5×10^{-4}	5.0	Nov. 1957	346	0.0	183	–0.1
		10.0	Nov. 1957	346	0.0	183	–0.1
		20.0	Nov. 1957	346	0.0	182	–0.3

[1] See the Chapter I report (Maslia et al. In press 2007b) for a complete listing of parameters that were subjected to variation in the sensitivity analysis

[2] Symbolic notation used to describe model parameters obtained from Chiang and Kinzelbach (2001)

[3] For calibrated model, date finished water at WTP exceeded MCL for PCE is November 1957, duration of exceeding MCL is 346 months, and maximum PCE concentration is 183 µg/L—see Table A12

[4] Current MCL for PCE is 5 µg/L (USEPA, 2003); effective date for MCL is July 6, 1992 (40 CFR, Section 141.60, Effective Dates, July 1, 2002, ed.)

[5] Relative change in duration (R_{D_i}) of finished water at the WTP exceeding the MCL for PCE is defined as: $R_{D_i} = \frac{D_i - D_0}{D_0} \times 100\%$, where D_0 is the calibrated duration in months (346) and D_i is the duration in months for the sensitivity analysis using a varied parameter

[6] Relative change in concentration (R_{C_i}) of finished water at Tarawa Terrace WTP exceeding MCL for PCE is defined as: $R_{C_i} = \frac{C_i - C_0}{C_0} \times 100\%$, where C_0 is the calibrated concentration in µg/L (183) and C_i is the PCE concentration for the sensitivity analysis using a varied parameter

[7] Dry wells simulated for this sensitivity analysis

Probabilistic Analysis[40]

A probabilistic analysis is used to generate uncertainties in model inputs (for example, hydraulic conductivity or contaminant source mass loading rate) so that estimates of uncertainties in model outputs (for example water level or PCE concentration in groundwater) can be made. Although the sensitivity analysis provided some insight into the relative importance of selected model parameters, a probabilistic analysis provides quantitative insight about the range and likelihood (probability) of model outputs. Thus, one purpose of a probabilistic analysis is to assist with understanding and characterizing variability and uncertainty of model output (Cullen and Frey 1999). A number of methods are available for conducting a probabilistic analysis. These methods can be grouped as follows: (1) analytical solutions for moments, (2) analytical solutions for distributions, (3) approximation methods for moments, and (4) numerical methods. The probabilistic analysis conducted on the Tarawa Terrace models used numerical methods—Monte Carlo simulation (MCS) and sequential Gaussian simulation (SGS)—to assess model uncertainty and parameter variability. Readers interested in specific details about these methods and about probabilistic analysis in general should refer to the following references: Cullen and Frey (1999), Deutsch and Journel (1998), Doherty (2005), USEPA (1997), and Tung and Yen (2005).

It is important to understand the conceptual difference between the deterministic modeling analysis approach used to calibrate model parameter values by Faye and Valenzuela (In press 2007) and Faye (In press 2007b) and a probabilistic analysis. As described in Maslia and Aral (2004), with respect to the approach referred to as a deterministic modeling analysis, single-point values are specified for model input parameters and results are obtained in terms of single-valued output, for example, the concentration of PCE. This approach is shown conceptually in Figure A22*a*. In a probabilistic analysis, input parameters (all or a selected subset) of a particular model (for example, contaminant fate and transport) may be characterized in terms of statistical distributions that can be generated using the MCS method (USEPA 1997, Tung and Yen 2005) or the SGS method (Deutsch and Journel 1998, Doherty 2005). Results are obtained in terms of distributed-value output that can be used to assess model uncertainty and parameter variability as part of the probabilistic analysis (Figure A22*b*). MCS is a computer-based (numerical) method of analysis that uses statistical sampling techniques to obtain a probabilistic approximation to the solution of a mathematical equation or model (USEPA 1997). The MCS method is used to simulate probability density functions (PDFs). PDFs are mathematical functions that express the probability of a random variable (or model input) falling within some interval. SGS is a process in which a field of values (such as horizontal hydraulic conductivity) is obtained multiple times assuming the spatially interpolated values follow a Gaussian (normal) distribution. Additional details pertaining to the SGS methodology are provided in Deutsch and Journel (1998) and Doherty (2005).

For the groundwater-flow and contaminant fate and transport models (Faye and Valenzuela In press 2007, Faye In press 2007b), eight parameters were assumed to be uncertain and variable: (1) horizontal hydraulic conductivity, (2) recharge rate, (3) effective porosity, (4) bulk density, (5) distribution coefficient, (6) dispersivity, (7) reaction rate, and (8) the PCE mass loading rate. With the exception of dispersivity, these parameters were selected for the probabilistic analysis because the sensitivity analysis indicated that variation from the calibrated value of the seven parameters resulted in the greatest percentage change in the simulated concentration of PCE in finished water at the Tarawa Terrace WTP (Table A14). Dispersivity was selected for the probabilistic analysis because it is a characteristic aquifer property and represents the effect of aquifer heterogeneity on the spreading of a dissolved contaminant mass (Schwartz and Zhang 2003). Each of the aforementioned model parameters can be represented by a PDF such as a normal, lognormal, triangular, or uniform distribution (Cullen and Frey 1999). In the current analysis, a normal distribution was chosen to represent each uncertain parameter (or variant) with the exception of dispersivity. This variant was represented by a lognormal distribution. Statistics associated with the normal and lognormal distributions for the variants, such as the mean, standard deviation, minimum, and maximum, are listed in Table A15. The calibrated value associated with each variant—derived from model calibrations described in Chapter C (Faye and Valenzuela In press 2007) and Chapter F reports (Faye In press 2007b)—was assigned as the

[40] A probabilistic analysis is defined as an analysis in which frequency (or probability) distributions are assigned to represent variability (or uncertainty) in quantities. The output of a probabilistic analysis is a distribution (Cullen and Frey 1999).

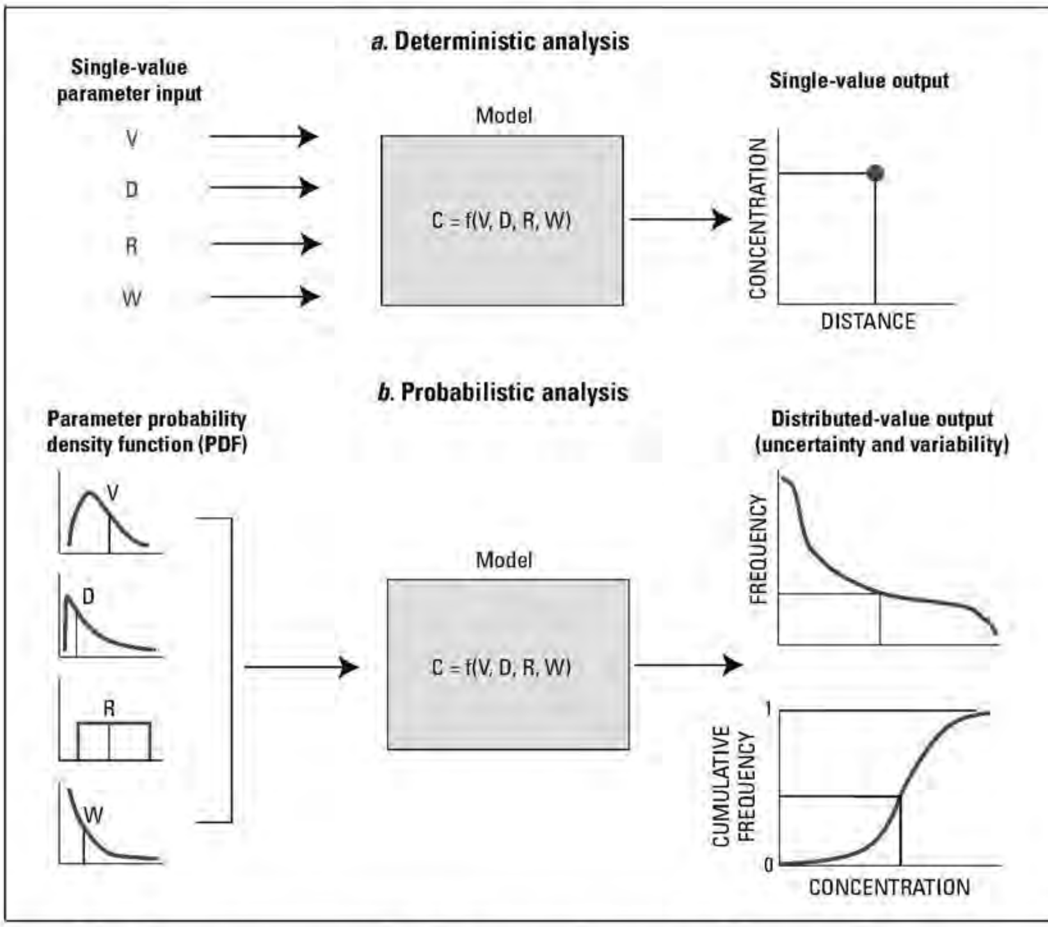


Figure A22. Conceptual framework for *(a)* a deterministic analysis and *(b)* a probabilistic analysis (from Maslia and Aral 2004).

mean value of the distribution associated with each variant. Examples of PDFs generated for recharge, mass loading rate, and dispersivity compared with the appropriate theoretical distribution are shown in Figure A23*a*, A23*b*, and A23*c*, respectively. Two points are noteworthy: (1) for a normal distribution (Figure A23*a* and A23*b*), values for the mean, mode, and median are equal, whereas for a lognormal distribution (Figure A23*c*), the values for the mean, mode, and median are not equal; and (2) because the mean value of recharge varies yearly, the generated values of recharge associated with the PDF also will vary yearly, but the type of PDF will always be the same—in this case, a normal distribution (Figure A23*a*). These types of PDFs were generated for seven of the aforementioned variants[41] with the exception of horizontal hydraulic conductivity.

[41] See the Chapter I report (Maslia et al. In press 2007b) for additional discussion on PDFs for all varied parameters.

Horizontal hydraulic conductivity is a parameter for which field values were spatially distributed. For example, in model layers 1, 3, and 5, there were 18, 22, and 5, respectively, spatially distributed values of horizontal hydraulic conductivity (Faye and Valenzuela In press 2007). Using these field values, spatially distributed values of horizontal hydraulic conductivity were generated using Shepard's inverse distance method to approximate values throughout the entire model domain (Chiang and Kinzelbach 2001). This approach resulted in cell by cell and layer by layer spatial variations of horizontal hydraulic conductivity. In this situation, an alternative method, SGS, was used to estimate the distribution of horizontal hydraulic conductivity. The specific code using the SGS methodology, FIELDGEN (Doherty 2005), is advantageous in this situation because it allows the statistical samples or realizations to be representative of field observations. Examples of spatial

Table A15. Model parameters subjected to probabilistic analysis, Tarawa Terrace and vicinity, U.S. Marine Corp Base Camp Lejeune, North Carolina.[1]

[ft/d, foot per day; ft^3/g, cubic foot per gram; g/ft^3, gram per cubic foot; d^{-1}, 1/day; g/d, grams per day; ft, foot; SGS, sequential Gaussian simulation; MCS, Monte Carlo simulation; PDF, probability density function; —, not applicable]

Model parameter or variant[2]	Calibrated value	Statistical descriptions of input parameter probabilistic distributions[3]				
		Mean	Minimum	Maximum	Standard deviation	Comment
Groundwater-flow model parameters						
Horizontal hydraulic conductivity, layer 1, K_H (ft/d)	12.2–53.4	12.2–53.4	—	—	—	SGS used to generate hydraulic conductivity under a normal distribution[4]
Horizontal hydraulic conductivity, layer 3, K_H (ft/d)	4.3–20.0	4.3–20.0	—	—	—	SGS used to generate hydraulic conductivity under a normal distribution
Horizontal hydraulic conductivity, layer 5, K_H (ft/d)	6.4–9.0	6.4–9.0	—	—	—	SGS used to generate hydraulic conductivity under a normal distribution
Infiltration (recharge), I_R (inches per year)	6.6–19.3	6.6–19.3	4.4	21.9	2.2	MCS used to generate the PDF using a normal distribution; PDF generated for each stress period
Fate and transport model parameters						
Distribution coefficient, K_d (ft^3/g)	5.0×10^{-6}	5.0×10^{-6}	3.53×10^{-6}	2.68×10^{-6}	1.77×10^{-6}	MCS used to generate the PDF using a normal distribution
Bulk density, ρ_b (g/ft^3)	77,112	77,112	69,943	79,004	1,100	MCS used to generate the PDF using a normal distribution
Effective porosity, n_E	0.2	0.2	0.1	0.3	0.05	MCS used to generate the PDF using a normal distribution
Reaction rate, r (d^{-1})	5.0×10^{-4}	5.0×10^{-4}	2.30×10^{-4}	7.70×10^{-4}	1.35×10^{-4}	MCS used to generate the PDF using a normal distribution
Mass-loading rate[5], q_SC_S (g/d)	1,200	1,200	200	2,200	100	MCS used to generate the PDF using a normal distribution
Longitudinal dispersivity, α_L (ft)	25	3.2189	5	125	0.8047	MCS used to generate the PDF using a log-normal distribution[5]

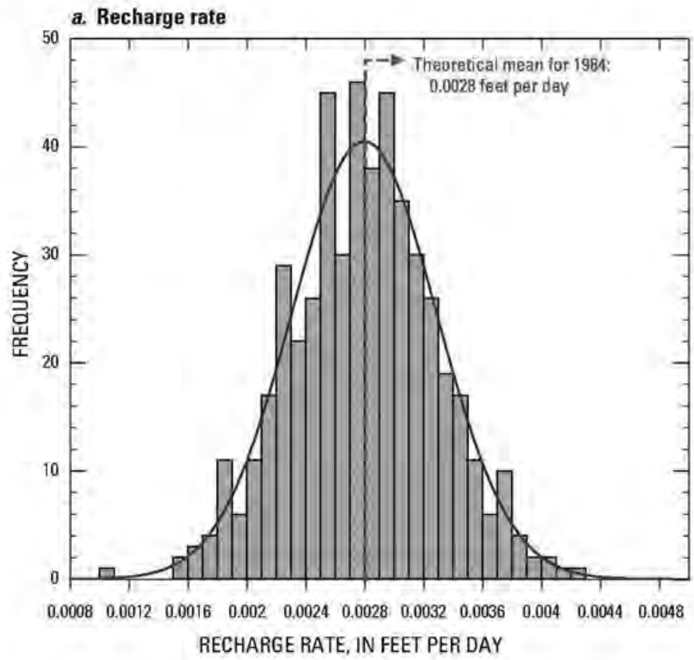
[1]See the Chapter I report (Maslia et al. In press 2007b) for a complete listing of parameters that were subjected to variation in the uncertainty analysis

[2]Symbolic notation used to describe model parameters obtained from Chiang and Kinzelbach (2001)

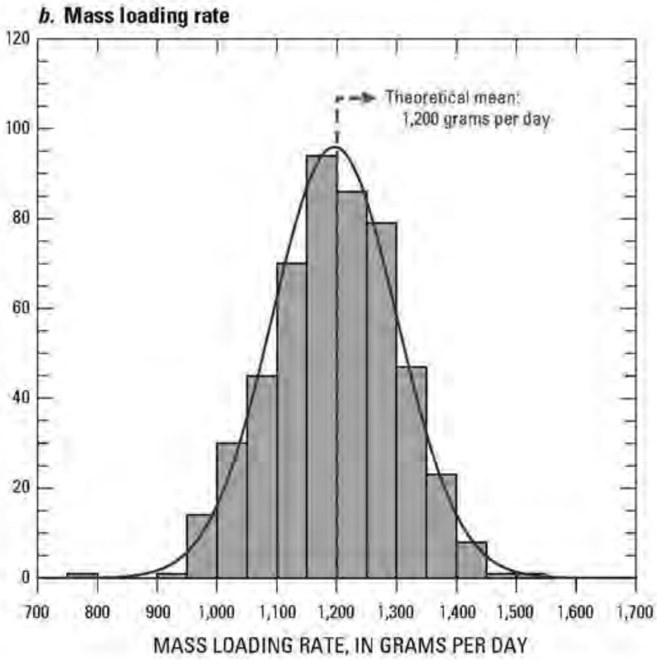
[3]Input values used to seed the pseudo-random number generator

[4]The FIELDGEN model code described in Doherty (2005) was used to generate the random, spatially varying fields of hydraulic conductivity

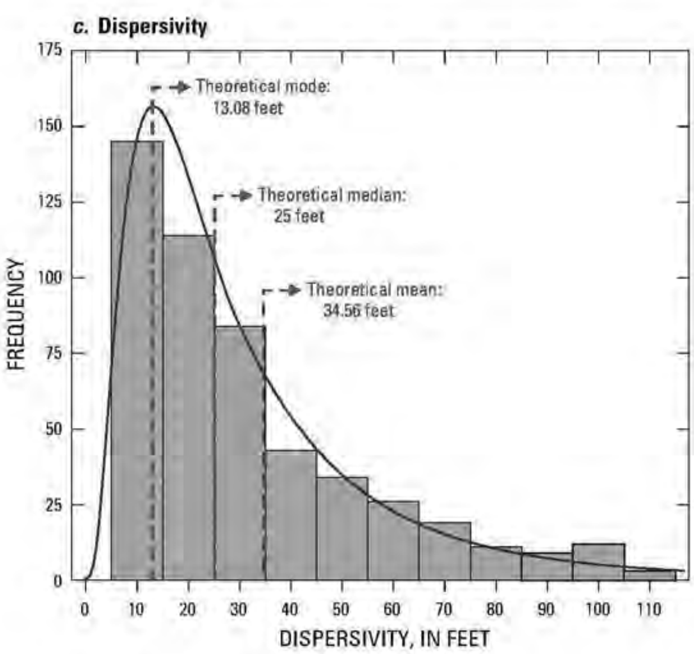
[5]The mean value derived from ln (25); standard deviation derived from ln (5)/2, where ln ( ) is the Naperian logarithm



STATISTICS		
	Theoretical	Monte Carlo simulation
Distribution	Normal	Normal
Number of realizations	Not applicable	500
Minimum	– Infinity	0.001
Maximum	+ Infinity	0.005
Mean	0.00280	0.00280
Mode	0.00280	0.00260
Median	0.00280	0.00279
Standard deviation	0.00050	0.00049



STATISTICS		
	Theoretical	Monte Carlo simulation
Distribution	Normal	Normal
Number of realizations	Not applicable	500
Minimum	– Infinity	200
Maximum	+ Infinity	2,200
Mean	1,200	1,196.1993
Mode	1,200	1,256.5000
Median	1,200	1,198.0200
Standard deviation	100	104.0659



STATISTICS		
	Theoretical	Monte Carlo simulation
Distribution	Lognormal	Lognormal
Number of realizations	Not applicable	500
Minimum	0	5
Maximum	Infinity	125
Mean	34.56	31.32
Mode	13.08	Not available
Median	25	23.85
Standard deviation	32.98	23.59

Figure A23. Probability density functions for *(a)* recharge rate, *(b)* mass loading rate (source concentration), and *(c)* dispersivity used to conduct probabilistic analyses. [–, minus; +, plus] distributions of horizontal hydraulic conductivity derived by using the SGS process are discussed in greater detail in the Chapter I report (Maslia et al. In press 2007b).

Once the variant PDFs and the multiple spatial distributions of horizontal hydraulic conductivity were generated as previously described, they were used by the MODFLOW-2K (Harbaugh et al. 2000)[42] and MT3DMS groundwater-flow and contaminant fate and transport models, respectively, instead of single-valued input data used in the deterministic approach (Figure A22*a*). This process is shown conceptually in Figure A22*b*. Approximately 500 realizations or Monte Carlo simulations were conducted using a procedure developed specifically for the Tarawa Terrace analyses.[43] This procedure included using MODFLOW-2K, MT3DMS, and mixing models previously described. Each realization randomly selected values from PDFs of the variants derived from MCS and from the random distributions of horizontal hydraulic conductivity derived from the SGS. Specific details about the procedures developed to conduct the probabilistic analysis using the MODFLOW-2K, MT3DMS, and mixing models are described in the Chapter I report (Maslia et al. In press 2007b).

[42] MODFLOW-2K is an updated version of the MODFLOW-96 model code developed by the U.S. Geological Survey. Because of programming requirements associated with conducting the MCS, it was programmatically more efficient to use the MODFLOW-2K model code. Model parameter values for MODFLOW-2K were identical and equivalent to the calibrated model parameter values derived using MODFLOW-96 (Table A11; Faye and Valenzuela In press 2007), thereby resulting in equivalent groundwater-flow simulation results for both MODFLOW-96 and MODFLOW-2K.

[43] Initially, 840 MCS realizations were conducted. However, every simulation did not necessarily result in a set of parameter values that yielded a physically viable groundwater-flow or fate and transport solution. For example, some combinations of parameter values resulted in wells drying. Therefore, out of an initial 840 MCS realizations, 510 yielded physically viable solutions.

Probabilistic analysis results of finished water for the Tarawa Terrace WTP are shown as a series of histograms for selected times: January 1958 (Figure A24*a*), January 1968 (A24*b*), January 1979 (A24*c*), and January 1985 (A24*d*). These histograms show the probability of a range of PCE-concentration values occurring during a specific month and year. For example, the probability of a PCE concentration of about 100 μg/L occurring in finished water at the Tarawa Terrace WTP during January 1979 can be identified according to the following procedure:

1. Locate the nearest concentration range that includes the 100 μg/L PCE concentration value along the x-axis of the graph in Figure A24*c*, (in this example, the different shaded histogram bar between 96 and 105 μg/L)
2. Move vertically upward until intersecting the top of the histogram bar derived from the Monte Carlo simulation results, and
3. Move horizontally to the left until intersecting the y-axis—for Figure A24*c*, about 15%.

In this example, therefore, the value on the y-axis of Figure A24*c* at the point of intersection—about 15%—is the probability that finished water at the Tarawa Terrace WTP was contaminated with a PCE concentration of about 100 μg/L during January 1979. As a comparison, the same procedure described above is used to determine the probability that finished water was contaminated with the same concentration of PCE (100 μg/L) during January 1985 (Figure A24*d*). For this situation, the probability that finished water at the Tarawa Terrace WTP was contaminated with a PCE concentration of about 100 μg/L during January 1985 is determined to be less than 2%. In other words, for conditions occurring during January 1985, a PCE concentration in the range of 100 μg/L is on the lower end (or "tail") of the normal distribution curve (Figure A24*d*).

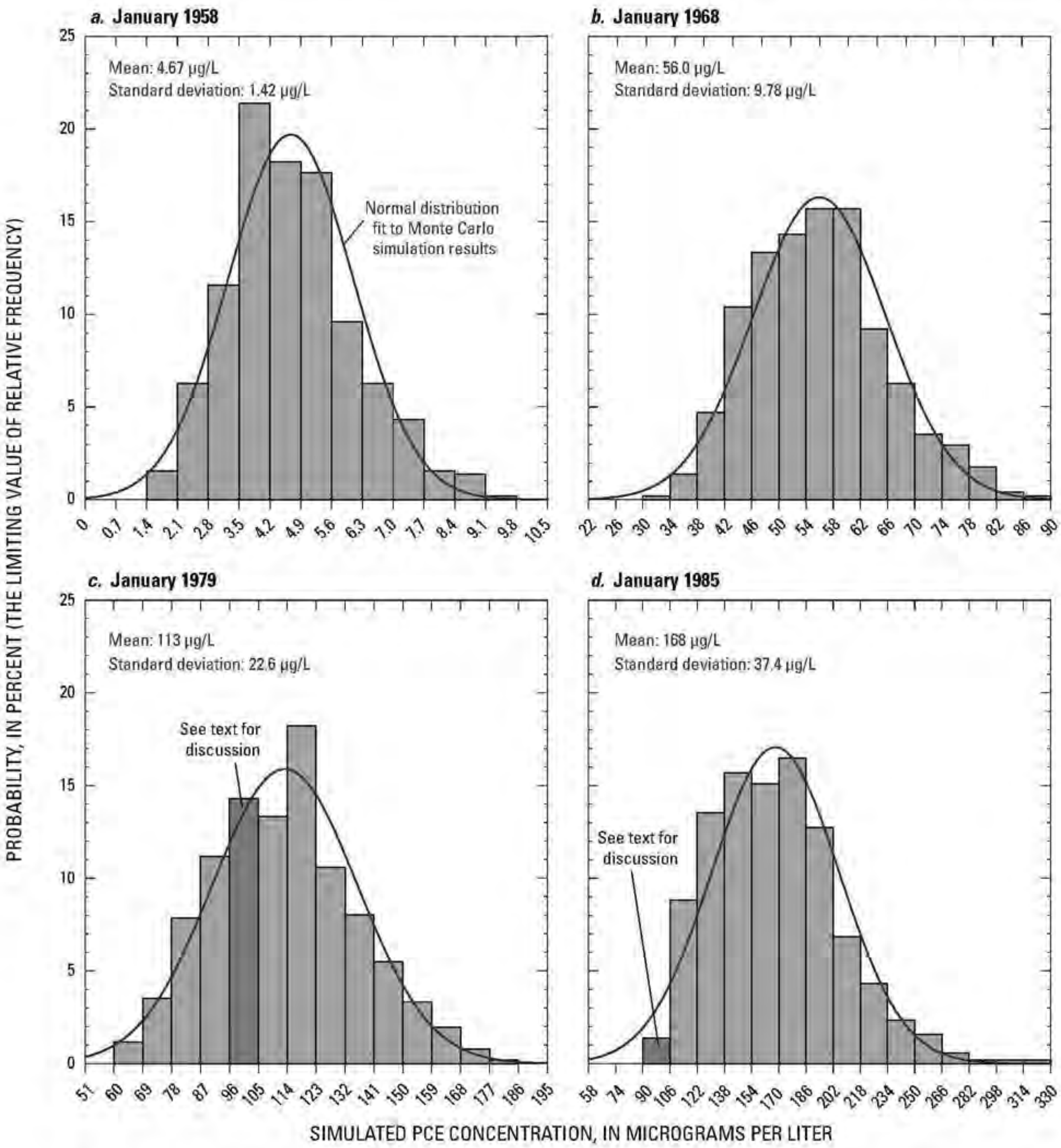


Figure A24. Probability of occurrence of tetrachloroethylene contamination in finished water at the water treatment plant derived from probabilistic analysis using Monte Carlo simulation for *(a)* January 1958, *(b)* January 1968, *(c)* January 1979, and *(d)* January 1985, Tarawa Terrace, U.S. Marine Corps Base Camp Lejeune, North Carolina. [PCE, tetrachloroethylene; µg/L, micrograms per liter]

For purposes of a health study or exposure assessment, epidemiologists and health scientists are interested in obtaining information on the probability that a person or population was exposed to a contaminant exceeding a given health guideline or criteria. For example, the probability that residents of Tarawa Terrace were exposed to drinking water contaminated with PCE exceeding an MCL of 5 µg/L. To address this issue, the MCS results described above can be presented in the form of the complementary cumulative probability function and plotted as a series of probability "type curves" (Figure A25). The complementary cumulative probability function describes the probability of exceeding a certain value or answers the question: how often is a random variable (for example, the concentration of PCE in finished water) above a certain value? Using results shown in figure A25, the probability that the PCE concentration in finished water at the Tarawa Terrace WTP exceeded a value of 5 µg/L during January 1958 is determined in the following manner:

1. Locate the probabilistic type curve for January 1958 in Figure A25*a*,
2. Locate the 5 µg/L PCE concentration along the x-axis of the graph in Figure A25*a*,
3. Follow the vertical line until it intersects with the January 1958 complementary cumulative probability function type curve (point A, Figure A25*a*), and
4. Follow the horizontal line until it intersects the y-axis—for this example, 39%.

In this case, there is a probability of 39% that the PCE concentration in finished water at the Tarawa Terrace WTP exceeded the current MCL of 5 µg/L during January 1958. Because the MCL does not intersect with any other type curves on the graph (Figure A25*a*), this can be interpreted that for other years shown in Figure A25*a* and until water-supply well TT-26 was removed from regular service during February 1985, the probability of exceeding the MCL for PCE is at least 99.8%, or a near certainty.[44]

As discussed previously, because of contaminated groundwater, water-supply well TT-26 was removed from regular service during February 1985 (Figure A5, Table A6). This caused an immediate reduction in the PCE concentration in finished water at the Tarawa Terrace WTP because of the dilution of contaminated WTP water with water from other water-supply wells that were not contaminated or were contaminated with much lower concentrations of PCE than water-supply well TT-26 (Figure A18; Appendix A2). As a result, PCE concentrations in finished water at the Tarawa Terrace WTP during February 1985–February 1987 (when the WTP was permanently closed) were significantly reduced compared with January 1985 concentrations (Figure A18; Appendix A2). Probabilistic type curves representing the complementary cumulative probability function for selected months during January 1985–February 1987 shown in Figure A25*b* also confirm this observation. For example, using the procedure described previously—for February 1985—the probability of exceeding the current MCL for PCE of 5 µg/L is 10% (point F in Figure A25*b*), compared to a probability of 39% during January 1958 and a probability of greater than 99.8% during January 1985.

The probability type curves shown in Figure A25 also can be used to ascertain uncertainty and variability associated with simulated PCE concentrations in finished water at the Tarawa Terrace WTP. For example, referring to points B and C in Figure A25*a*, during January 1958, there is a 97.5% probability that the concentration of PCE in finished water at the Tarawa Terrace WTP exceeded 2 µg/L (point B), and correspondingly, a 2.5% probability that the concentration exceeded 8 µg/L (point C). Thus, during January 1958, 95% of MCS results[45] indicate that the concentration of PCE in finished water at the Tarawa Terrace WTP was in the range of 2–8 µg/L. Stated in terms of uncertainty and variability, during January 1958, the uncertainty is 5% (100% minus 95% of all MCS results), and the corresponding variability in PCE concentration in finished water at the Tarawa Terrace WTP is 2–8 µg/L. As a comparison, this same analysis is conducted for January 1968 (points D and E). For the conditions during January 1968 (the start of the epidemiological case-control study), 95% of MCS results indicate that the concentration of PCE in finished water at the Tarawa Terrace WTP was in the range of 40–80 µg/L. Stated in terms of uncertainty and variability, during January 1968, the uncertainty is 5% (100% minus 95% of all MCS results), and the corresponding variability in PCE concentration in finished water at the Tarawa Terrace WTP is 40–80 µg/L.

[44] Except during July and August 1980 and January and February 1983 when water-supply well TT-26 was out of service—see Figure A18.

[45] In this example, point B (Figure A25*a*) represents 97.5 percentile of Monte Carlo simulations, and point C represents 2.5 percentile of Monte Carlo simulations. Thus, the range of results representing 95 percentile of Monte Carlo simulations is obtained by subtracting the probability-axis value of point C from point B or 97.5%–2.5%.

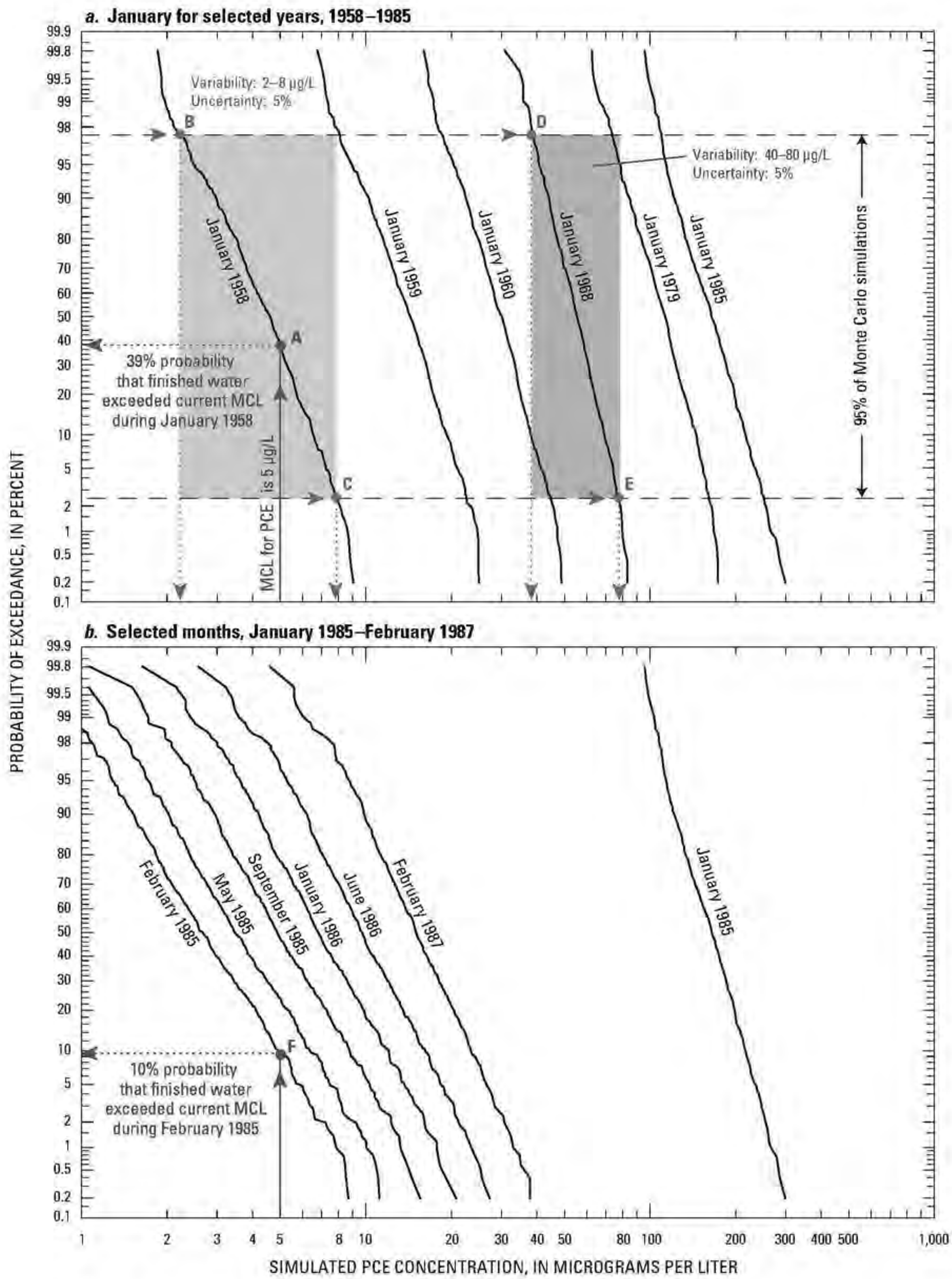


Figure A25. Probabilities of exceeding tetrachloroethylene concentrations in finished water at the water treatment plant derived from probabilistic analysis using Monte Carlo simulation for *(a)* selected years, 1958–1985, and *(b)* selected months, January 1985–February 1987, Tarawa Terrace, U.S. Marine Corps Base Camp Lejeune, North Carolina (see text for discussion of points A–F). [PCE, tetrachloroethylene; MCL, maximum contaminant level; µg/L, micrograms per liter; %, percent]

The probabilistic analysis conducted using MCS was applied to the entire period of operation of the Tarawa Terrace WTP (January 1953–February 1987). The PCE concentration in finished water determined using the deterministic analysis (single-value parameter input and output; Figure A18) also can be expressed and presented in terms of a range of probabilities for the entire duration of WTP operations. Figure A26 shows the concentration of PCE in finished water at the Tarawa Terrace WTP in terms of the MCS results. Several results shown on this graph are worthy of further explanation:

1. The range of PCE concentrations derived from the probabilistic analysis using MCS is shown as a band of solutions in Figure A26 and represents 95% of all possible results.

2. The current MCL for PCE (5 μg/L) was first exceeded in finished water during October 1957–August 1958; these solutions include November 1957, the date determined using the calibrated fate and transport model (Faye In press 2007b)—a deterministic modeling analysis approach.

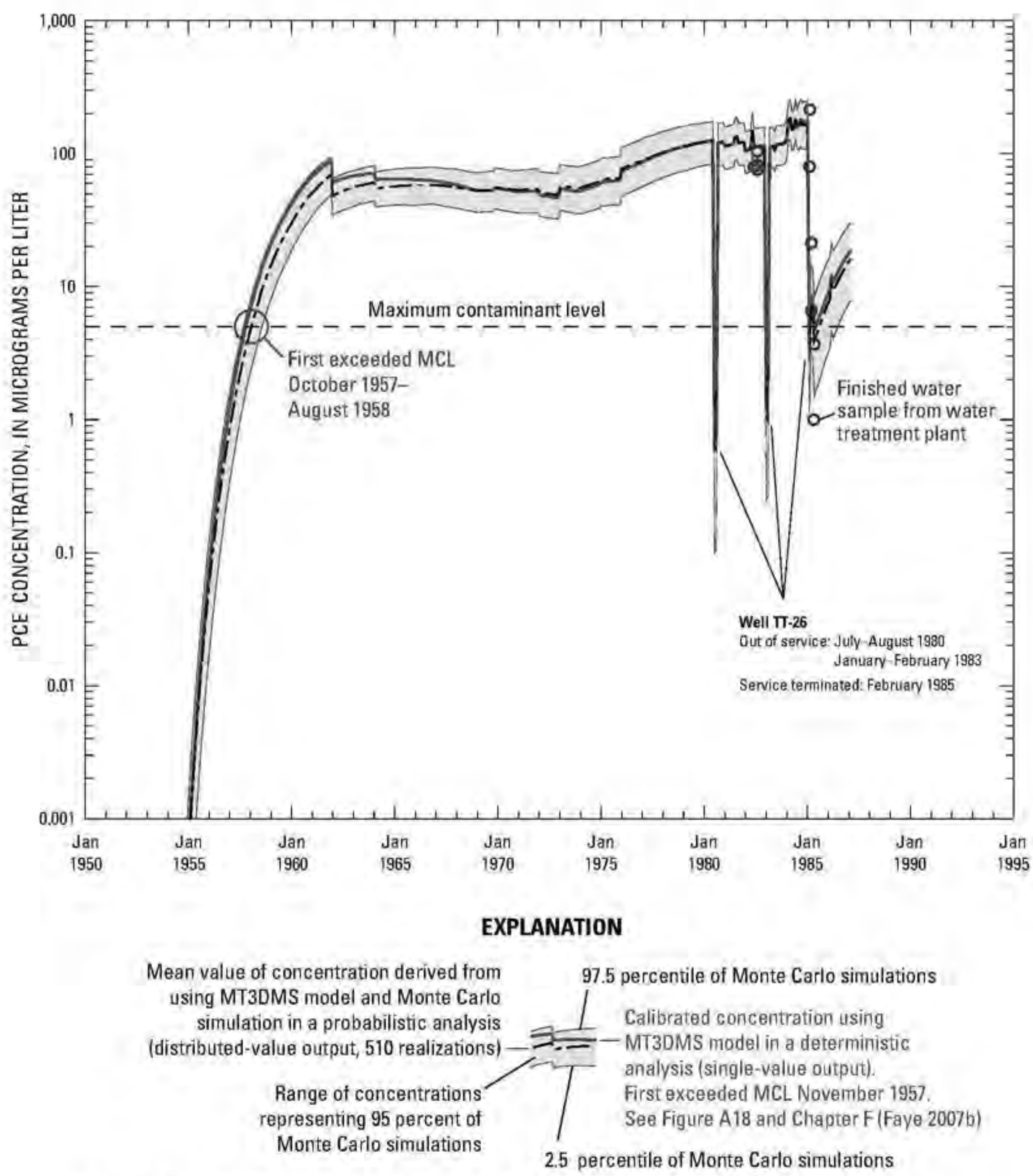


Figure A26. Concentrations of tetrachloroethylene in finished water at the water treatment plant derived from probabilistic analysis using Monte Carlo simulation, Tarawa Terrace, U.S. Marine Corps Base Camp Lejeune, North Carolina. [PCE, tetrachloroethylene; MCL, maximum contaminant level]

3. The PCE concentration in Tarawa Terrace WTP finished water during January 1985, simulated using the probabilistic analysis, ranges from 110–251 μg/L (95 percent of Monte Carlo simulations). This range includes the maximum calibrated value of 183 μg/L (derived without considering uncertainty and variability using MT3DMS [Faye In press 2007b]) and the maximum measured value of 215 μg/L (Table A10).

Therefore, these probabilistic analysis results—obtained by using Monte Carlo simulation—provide a sense of confidence in the historically reconstructed PCE concentrations that were delivered to residents of Tarawa Terrace in finished water from the WTP.

In summary, effects of parameter uncertainty and variability have been analyzed using three approaches—water-supply well scheduling analysis, sensitivity analysis, and probabilistic analysis. Individually and combined, these analyses demonstrate the high reliability of and confidence in results determined using the calibrated MODFLOW-96 and MT3DMS models (for example, Figure A18), described in the Chapter C (Faye and Valenzuela In press 2007) and Chapter F (In press Faye 2007b) reports. The probabilistic analysis, conducted using the combination of MODFLOW-2K, MT3DMS, MCS, and SGS, provides a tool (probability type curves, Figure A25) to address issues of parameter uncertainty and variability with respect to the concentration of PCE in finished water delivered from the Tarawa Terrace WTP to residents of family housing at Tarawa Terrace and vicinity.

Field Tests and Analyses of the Water-Distribution System

As discussed previously in the section on Water-Distribution Investigation, the initial approach for quantifying the concentration of PCE delivered to residences of Tarawa Terrace was to develop and calibrate a model representation of the water-distribution system using the public domain model EPANET 2 (Rossman 2000). With this approach, street-by-street concentrations of PCE could be simulated and reconstructed. Although using this rigorous approach was replaced with a simpler mixing model approach, field studies were conducted early in the project to gather information needed to develop and calibrate a model of the Tarawa Terrace water-distribution system. A summary of this information and comparison of PCE concentration results using the street-by-street water-distribution system model with the mixing model results are presented herein. A detailed description and discussion of the use and application of water-distribution system modeling with respect to the Tarawa Terrace water-distribution system is provided in the Chapter J report (Sautner et al. In press 2007).

Based on reviews of historical WTP operations as well as housing information, the authors concluded that the historical water-distribution system serving Tarawa Terrace was nearly identical to the present-day (2004) water-distribution system. Thus, information and data collected to characterize the present-day water-distribution system also would be useful in characterizing the historical water-distribution system. The network of pipelines and storage tanks, shown in Figure A27 represents the present-day water-distribution systems serving the Tarawa Terrace and Holcomb Boulevard areas, are nearly identical to historical water-distribution systems serving these areas with the following exceptions:

1. The Holcomb Boulevard WTP came online during June 1972 (Figure A3); prior to that date, the Holcomb Boulevard area received finished water from the Hadnot Point WTP (Plate 1);
2. The Tarawa Terrace and Montford Point WTPs were closed during 1987 (Figure A3) and presently, the Holcomb Boulevard WTP provides finished water to these areas;
3. A pipeline, constructed during 1984, follows SR 24 northwest from the Holcomb Boulevard WTP to ground storage tank STT-39 and presently is used to supply STT-39 in the Tarawa Terrace water-distribution system with finished water (Figure A27); and
4. A pipeline, constructed during 1986, trends east-west from the Tarawa Terrace II area to storage tank SM-623 and presently is used to supply the storage tank with finished water.

Two types of field tests were conducted to determine the hydraulic and water-quality parameter values needed to develop and calibrate a water-distribution system model for Tarawa Terrace: (1) fire-flow tests, conducted during August 2004, in the Tarawa Terrace and Camp Johnson areas; and (2) a fluoride tracer test, conducted during September and October 2004, in the Tarawa Terrace and Holcomb Boulevard areas. Detailed descriptions of the test procedures and results of the field tests are described in the Chapter J report (Sautner et al. In press 2007) and in a number of related papers.

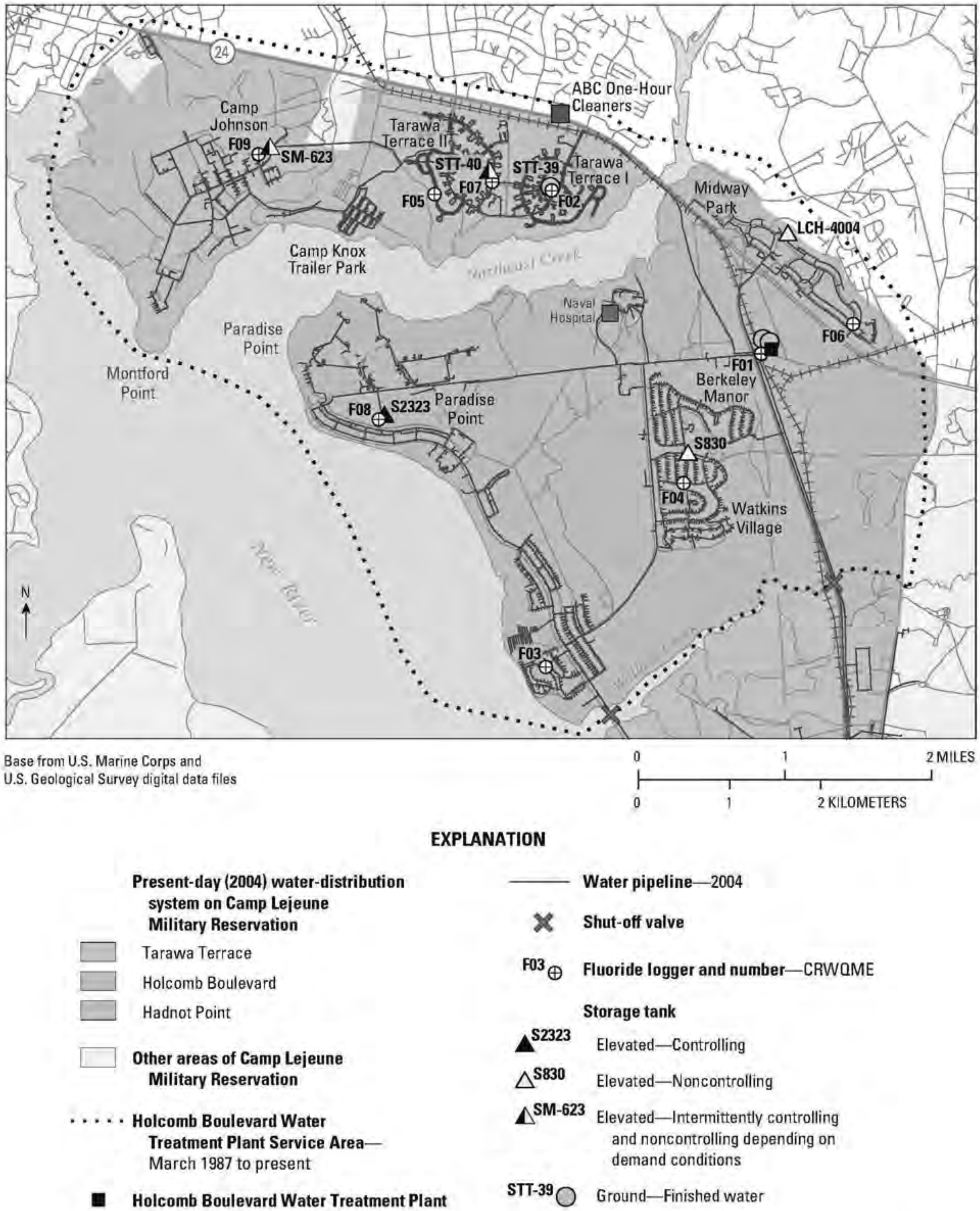


Figure A27. Locations of continuous recording water-quality monitoring equipment (CRWQME; F01–F09) and present-day (2004) Tarawa Terrace and Holcomb Boulevard water-distribution systems used for conducting a fluoride tracer test, September 22–October 12, 2004, U.S. Marine Corps Base Camp Lejeune, North Carolina.

For example, fire-flow tests are described in Sautner et al. (2005) and Grayman et al. (2006). A fluoride tracer test is described in Maslia et al. (2005) and Sautner et al. (2005, 2007).

The use of a fluoride tracer test to characterize a water-distribution system is of particular importance because results obtained from the test—the impact of storage tank operation, travel times, and dilution rates of constituents in the water-distribution system—assist with determining parameter values needed to calibrate a water-distribution system model using extended period simulation (EPS). Additionally, the movement and distribution of fluoride through the Tarawa Terrace water-distribution system would be similar to the movement and distribution of a contaminant, such as PCE through the water-distribution system. Since March 1987, the Holcomb Boulevard WTP has supplied finished water to two water-distribution systems at Camp Lejeune (Figure A27): (1) Holcomb Boulevard[46] and (2) Tarawa Terrace.[47] Therefore, the fluoride tracer test included the collection of data at selected locations within the Tarawa Terrace and Holcomb Boulevard water-distribution systems.

The fluoride tracer test was conducted September 22–October 12, 2004. The test consisted of monitoring fluoride dilution and re-injection (shutoff and startup of the sodium fluoride feed at the Holcomb Boulevard WTP). Nine locations in the Tarawa Terrace and Holcomb Boulevard water-distribution systems were equipped with continuous recording water-quality monitoring equipment (CRWQME). Monitor locations are shown in Figure A27 and are designated as F01–F09. A list of the monitoring locations and the water-distribution system location being monitored is provided in Table A16. Monitoring locations included the main transmission line from the Holcomb Boulevard WTP to the water-distribution system (F01), the Tarawa Terrace finished water reservoir (F02), two controlling elevated storage tanks (Paradise Point [S2323] and

[46] The Holcomb Boulevard WTP provides finished water to the following areas within the Holcomb Boulevard water-distribution system: Berkeley Manor, Watkins Village, Paradise Point, and Midway Park (Figure A27).

[47] Based on present-day operations (2004), the Tarawa Terrace water-distribution system includes the following areas: Tarawa Terrace housing areas I and II, Camp Knox Trailer Park, Camp Johnson, and Montford Point (Figure A27).

Table A16. Description of locations equipped with continuous recording water-quality monitoring equipment used to conduct a fluoride tracer test of the Tarawa Terrace and Holcomb Boulevard water-distribution systems, September 22–October 12, 2004, U.S. Marine Corps Base Camp Lejeune, North Carolina.

Monitoring station identification[1]	Location of continuous recording water-quality monitoring equipment[2] North	East	Water-distribution system location or area	Description of hydraulic device being monitored
F01	356478.25	2498392.43	Holcomb Boulevard	Water treatment plant, main transmission line, fluoride source
F02	362057.78	2490580.75	Tarawa Terrace	Ground storage tank, source for Tarawa Terrace water-distribution system
F03	344823.33	2491037.83	Holcomb Boulevard	Distribution system hydrant
F04	351648.84	2495750.35	Holcomb Boulevard, Berkeley Manor	Distribution system hydrant and elevated storage tank
F05	362270.35	2488417.94	Tarawa Terrace, housing area II	Distribution system hydrant
F06	357638.42	2501665.36	Holcomb Boulevard, Midway Park	Distribution system hydrant
F07	361760.20	2486365.30	Tarawa Terrace, housing area II	Distribution system hydrant and elevated storage tank
F08	353489.91	2484738.57	Holcomb Boulevard, Paradise Point	Controlling elevated storage tank
F09	362945.52	2479935.36	Tarawa Terrace, Camp Johnson	Controlling elevated storage tank

[1]See Figure A27 for station locations

[2]Coordinates are in North Carolina State Plane coordinate system, North American Datum 1983, National Geodetic Vertical Datum of 1929

Camp Johnson [SM623]—F08 and F09, respectively), and five hydrants located throughout housing areas (F03, F04, F05, F06, and F07). The fluoride at the Holcomb Boulevard WTP was shut off at 1600 hours on September 22. A background concentration of about 0.2 milligram per liter (mg/L) in the water-distribution system was reached by September 28. At 1200 hours on September 29, the fluoride was turned back on at the Holcomb Boulevard WTP, and the test continued until loggers were removed and data downloaded on October 12. In addition to CRWQME, grab samples were collected and analyzed for quality-assurance and quality-control purposes. Nine rounds of water samples were collected at each monitoring location during the test. For each round, the Holcomb Boulevard WTP water-quality lab analyzed 25 milliliters (mL) of the sampled water, and the Federal Occupational Health (FOH) laboratory, located in Chicago, Illinois, analyzed the remaining 225 mL of water.

Storage tanks in the Tarawa Terrace and Holcomb Boulevard water-distribution systems are categorized as either controlling or noncontrolling. Controlling elevated storage tanks are operated in the following manner. Finished water is supplied to the respective water-distribution system from the elevated controlling storage tank in response to system demand. When the water level in the controlling tank falls below a pre-set water-level mark, pumps turn on and fill the tank with finished water from a ground storage tank. When the water level in the controlling tank reaches a pre-set high water-level mark, the pumps are turned off. The water level in the tank then begins to drop based on demand until, once again, the water level reaches the pre-set low water level. The fill and drain process is then repeated. An example of water-level data collected by the Camp Lejeune supervisory control and data acquisition (SCADA) system for controlling storage tank STT-40 (Tarawa Terrace elevated, Figure A27) is shown in Figure A28. Two other elevated storage tanks are noncontrolling tanks. These elevated storage tanks show little water-level fluctuation because they are not exercised very often—they are primarily used for fire protection. The elevated storage tanks are S830 (Berkeley Manor) and LCH-4004 (Midway Park), both serving the Holcomb Boulevard water-distribution system (Figure A27).

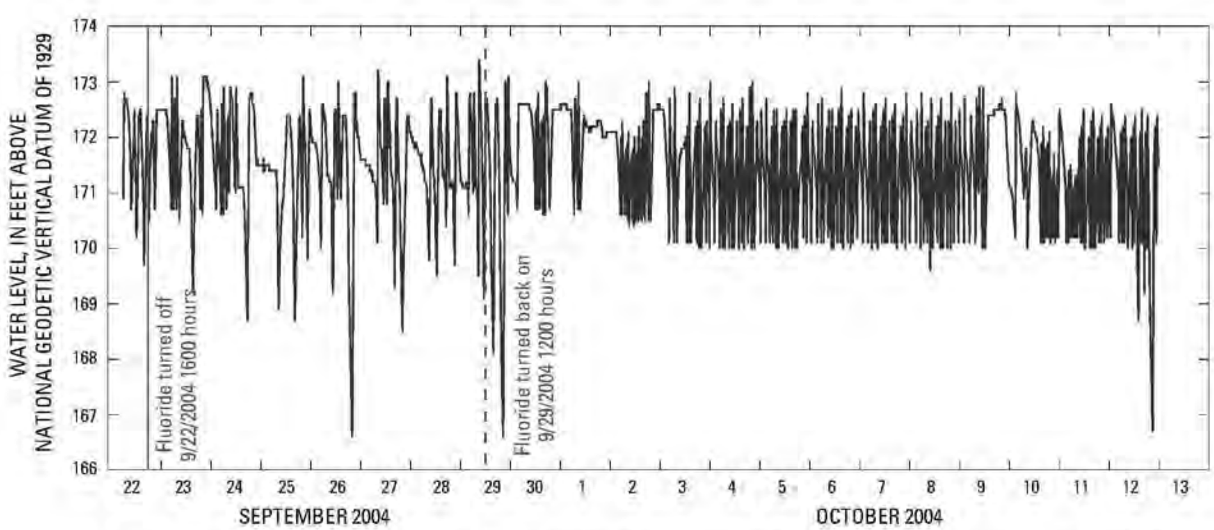


Figure A28. Measured water-level data from the Camp Lejeune SCADA system for controlling elevated storage tank STT-40, September 22–October 12, 2004, U.S. Marine Corps Base Camp Lejeune, North Carolina. [SCADA, supervisory control and data acquisition]

Using results from the fluoride tracer test described previously and the fire-flow test of August 2004, an all-pipes EPS model of the Tarawa Terrace water-distribution system was calibrated. To simplify and reduce the computational requirements, a skeletonized version of an all-pipes representation of the water-distribution system was used for all subsequent EPANET 2 simulations.[48] A 24-hour diurnal pattern based on measured flow data (delivered finished water) and calibrated demand factors is shown in Figure A29.[49] Flow data were measured using a venturi meter located in the Tarawa Terrace pump house (building adjacent to STT-39 in Figure A27).[50] Calibrated demand factors are in reasonable agreement with measured flow data. Details of the calibration procedure and calibration statistics are provided in the Chapter J report (Sautner et al. In press 2007).

[48] Skeletonization is the reduction or aggregation of a water-distribution system network so that only the major hydraulic characteristics need be represented by a model. Skeletonization often is used to reduce the computational requirements of modeling an all-pipes network.

[49] Data for measured delivered flow were previously presented and discussed in the section on Relation of Contamination to Water Supply, Production, and Distribution (Figure A8).

[50] A venturi meter is a device used to measure the flow rate or velocity of a fluid through a pipe. A photograph of the Tarawa Terrace pump house is shown on the front cover of this report.

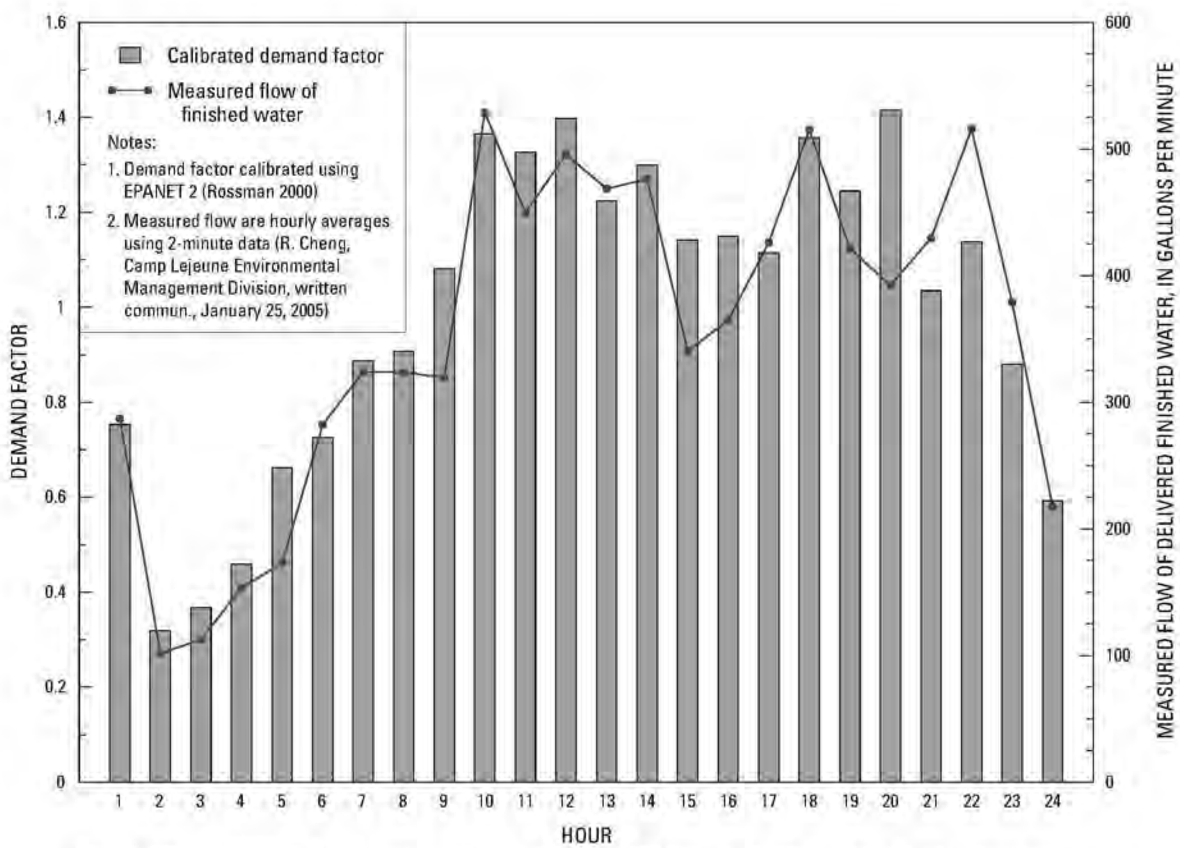
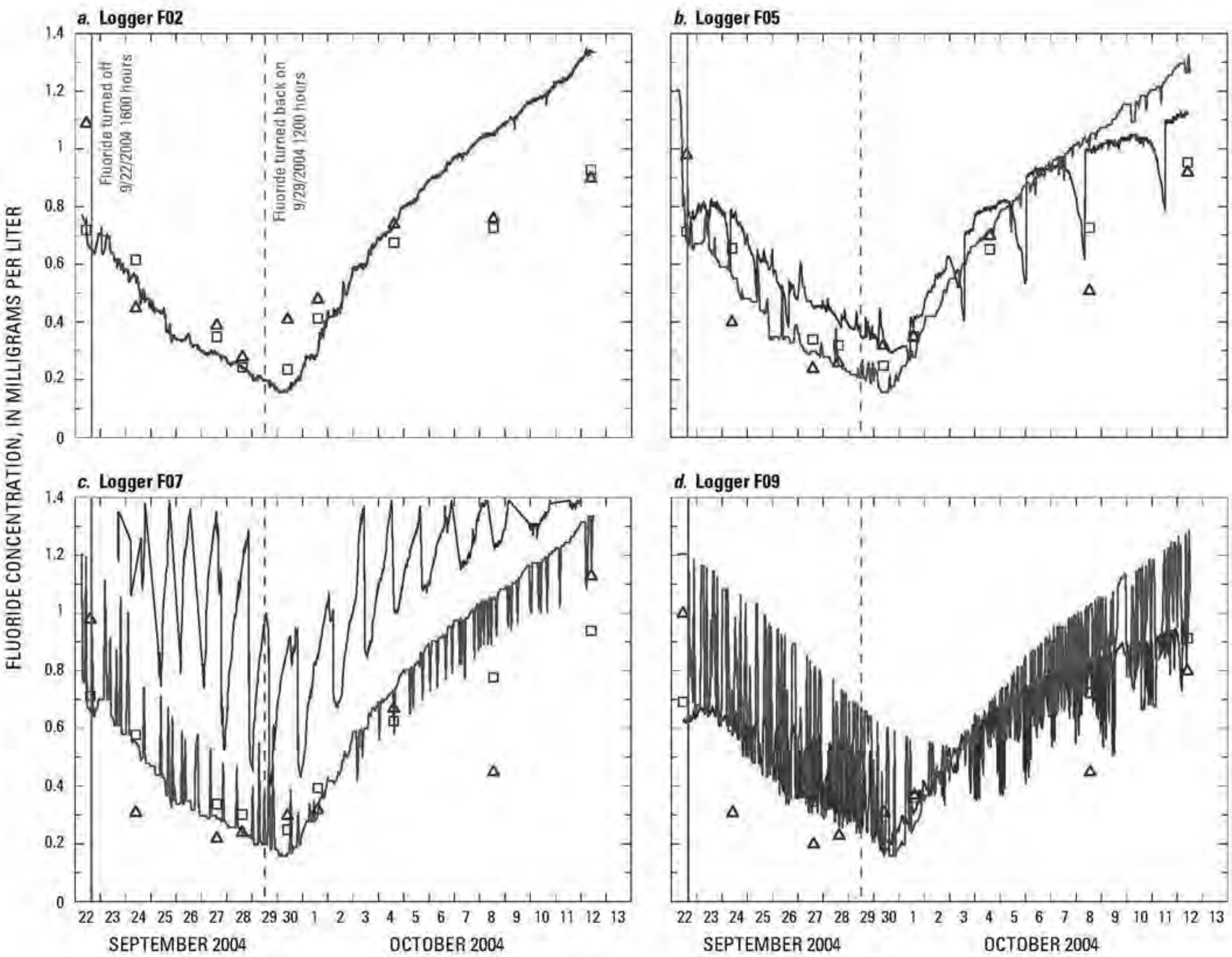


Figure A29. Calibrated and measured diurnal pattern (24 hours) of delivered finished water during field test, September 22–October 12, 2004, Tarawa Terrace water-distribution system, U.S. Marine Corps Base Camp Lejeune, North Carolina. [Flow data measured at venturi meter located in building STT-39A (Tarawa Terrace pump house)]

Simulated fluoride concentrations are compared with measured field data concentrations obtained from the CRWQME and with the grab sample measurements for the Tarawa Terrace water-distribution system at locations F02, F05, F07, and F09 (Figure A27). These comparisons are shown in the graphs of Figure A30. Note that monitoring location F02 is used as the source of fluoride for the Tarawa Terrace water-distribution system. Results shown in Figure A30 along with calibration statistics presented in the Chapter J report (Sautner et al. In press 2007) provide evidence that the EPS model of the Tarawa Terrace water-distribution system is reasonably calibrated and adequately characterizes the present-day (2004) Tarawa Terrace water-distribution system.



EXPLANATION

Fluoride concentration, in milligrams per liter

Measured

CRWQME

CL Lab

FOH Lab

Simulated

Notes: CRWQME = Continuous recording water-quality monitoring equipment

CL Lab = Holcomb Boulevard Water Treatment Plant onsite lab analysis, Camp Lejeune, North Carolina 25 milliliter sample

FOH Lab = Federal Occupational Health Lab, Chicago, Illinois 225 milliliter sample

Figure A30. Measured and simulated fluoride concentrations at four monitoring locations *(a)* F02, *(b)* F05, *(c)* F07, and *(d)* F09 in the Tarawa Terrace water-distribution system, September 22–October 12, 2004, U.S. Marine Corps Base Camp Lejeune, North Carolina. (See Figure A27 for monitoring locations and Table A16 for description of hydraulic device being monitored.)

Using the calibrated EPS model of the Tarawa Terrace water-distribution system, conditions representing December 1984 were simulated. This was a period of high water production and usage. The duration of the simulation was 744 hours (31 days). The purpose of the simulation was to test the concept that a mixing model, based on the principles of continuity and conservation of mass (Equations 2 and 3), could be used to estimate the street-by-street concentrations of a contaminant derived using a sophisticated numerical model of the water-distribution system, such as EPANET 2. The mixing model represents a condition of complete mixing and stationary water-quality dynamics in a water-distribution system like Tarawa Terrace where all source water (groundwater) is mixed at the treatment plant. Using the calibrated water-distribution system model, for a simulation period of 744 hours (31 days)—representing December 1984—and an initial source concentration of 173 μg/L at the Tarawa Terrace WTP (Figure A18, Appendix A2), the following results were obtained:

- 100% of the concentration of PCE in finished water at the Tarawa Terrace WTP (173 μg/L) reached locations F05 and F07 (Figure A27), located in the Tarawa Terrace housing area within 2 days,
- 100% of the concentration of PCE in finished water at the Tarawa Terrace WTP (173 μg/L) reached the Camp Johnson elevated storage tank within 3 days, and
- 100% of the simulated concentration of PCE in finished water at the Tarawa Terrace WTP (173 μg/L) reached the Montford Point area (farthest point from the Tarawa Terrace WTP) within 7 days.

These results demonstrate that on a monthly basis, the concentration of PCE at residential housing areas throughout Tarawa Terrace would be nearly the same as the concentration of PCE in finished water at the Tarawa Terrace WTP. Therefore, using a mixing model based on the principles of continuity and conservation of mass is appropriate for determining the concentration of PCE in finished water delivered from the Tarawa Terrace WTP.

Summary and Conclusions

Two of the three drinking-water systems that served family housing at U.S. Marine Corps Base Camp Lejeune were contaminated with VOCs. Groundwater was the sole source of drinking-water supply. One system, the Tarawa Terrace drinking-water system, was mostly contaminated with PCE when water-supply wells were contaminated by off-base dry-cleaning operations at ABC One-Hour Cleaners (Shiver 1985). The other system, the Hadnot Point drinking-water system, was contaminated mostly with TCE from on-base industrial operations. The contaminated wells were continuously used until 1985 and sporadically used until early 1987. ATSDR's health study will try to determine if an association exists between in utero and infant (up to 1 year of age) exposures to drinking-water contaminants and specific birth defects and childhood cancers. The study includes births occurring during 1968–1985 to mothers who lived in base family housing during their pregnancies. Historical exposure data needed for the epidemiological case-control study are limited. To obtain estimates of historical exposure, ATSDR is using water-modeling techniques and the process of historical reconstruction. These methods are used to quantify concentrations of particular contaminants in finished water and to compute the level and duration of human exposure to contaminated drinking water. The analyses and results presented and discussed in this Summary of Findings, and in reports described herein, refer solely to Tarawa Terrace and vicinity. Future analyses and reports will present information and data about contamination of the Hadnot Point water-distribution system.

Based on information, data, and simulation results, the onset of pumping at Tarawa Terrace is estimated to have begun during 1952. Water-supply well TT-26, located about 900 ft southeast of ABC One-Hour Cleaners, probably began operations during 1952 (Figure A1, Table A6). Additionally, the first occurrence of PCE contamination at a Tarawa Terrace water-supply well probably occurred at well TT-26, following the onset of dry-cleaning operations during 1953 (Faye In press 2007b).

Detailed analyses of PCE concentrations in groundwater monitor wells, hydrocone sample locations, and at Tarawa Terrace water-supply wells during the period 1991–1993 were sufficient to estimate the mass of PCE remaining in the Tarawa Terrace and Upper Castle Hayne aquifers. Similar methods were applied to compute the mass of PCE in the unsaturated zone (zone above the water table) at and in the vicinity of ABC One-Hour Cleaners using concentration-depth data determined from soil borings. The total mass of PCE computed in groundwater and within the unsaturated zone equals about 6,000 pounds and equates to a volume of about 430 gallons. This volume represents an average minimum loss rate of PCE to the subsurface at ABC One-Hour Cleaners of about 13 gallons per year (78,737 grams per year) for the period 1953–1985. Pankow and Cherry (1996) indicate that computations of contaminant mass similar to those summarized here represent only a small fraction of the total contaminant mass in the subsurface.

Calibration of the Tarawa Terrace models was accomplished in a hierarchical approach consisting of four successive stages or levels (Figure A9). Simulation results achieved for each calibration level were iteratively adjusted and compared to simulation results of previous levels until results at all levels satisfactorily conformed to pre-selected calibration targets (Table A8). In hierarchical order, calibration levels consisted of the simulation of (1) predevelopment groundwater-flow conditions (Figure A10*a*), (2) transient or pumping groundwater-flow conditions (Figure A10*b*), (3) the fate and transport of PCE from the source at ABC One-Hour Cleaners (Figure A11), and (4) the concentration of PCE in finished water at the Tarawa Terrace WTP (Figure A12).

Based on calibrated model simulations, water-supply well TT-26 had the highest concentration of PCE-contaminated groundwater and the longest duration of PCE-contaminated groundwater with respect to any other Tarawa Terrace water-supply well (Figure A18). The simulated PCE concentration in water-supply well TT-26 exceeded the current MCL of 5 μg/L during January 1957 (simulated value 5.2 μg/L) and reached a maximum simulated value of 851 μg/L during July 1984 (Table A12). The mean simulated PCE concentration during the period exceeding the current MCL of 5 μg/L—January 1957–January 1985—was 414 μg/L, a duration of 333 months.

The monthly concentrations of PCE assigned to finished water at the Tarawa Terrace WTP were determined using a materials mass balance model (simple mixing). The model is based on the principles of continuity and conservation of mass (Masters 1998) and is used to compute the flow-weighted average concentration of PCE. Finished water contaminated with PCE exceeded the current MCL of 5 μg/L during November 1957. Based on mixing model results, finished water exceeded the MCL for 346 months (29 years)—November 1957–February 1987 (Figure A18, Table A12).[51] The maximum simulated PCE concentration in finished water was 183 μg/L occurring during March 1984. The maximum observed PCE concentration was 215 μg/L measured on February 11, 1985 (Table A10). The average simulated PCE concentration for the period exceeding the current MCL of 5 μg/L—November 1957–February 1987—was 70 μg/L.

The calibrated fate and transport model simulated PCE as a single-specie contaminant dissolved in groundwater. However, evidence of the transformation of PCE to degradation by-products of TCE and 1,2-tDCE was found in water samples obtained from Tarawa Terrace water-supply wells TT-23 and TT-26. Thus, the simulation of PCE and its degradation by-products was necessary. For this simulation, a model code identified as TechFlowMP, developed by the Multimedia Environmental Simulations Laboratory (MESL) at the Georgia Institute of Technology, was used. TechFlowMP simulates three-dimensional multiphase, multispecies mass transport of PCE and its associated degradation by-products TCE, 1,2-tDCE, and VC in the unsaturated and saturated zones at Tarawa Terrace and vicinity (that is, the sequential biodegradation and transport of PCE). Simulation results for finished water at the Tarawa Terrace WTP (Figure A19*b*), contaminated with PCE degradation by-products TCE, 1,2-tDCE, and VC, show that: (1) TCE was below the current MCL value of 5 μg/L for nearly the entire historical period except during January 1984–January 1985 when it ranged between 5 and 6 μg/L; (2) 1,2-tDCE was below the current MCL value of 100 μg/L for the entire historical period; and (3) VC was at or above the current MCL value of 2 μg/L from May 1958 through February 1985 when water-supply well TT-26 was shut down. As part of the degradation by-product simulation using the TechFlowMP model, results also were obtained for VOCs in the vapor phase (above the water table in the unsaturated zone). Analyses of the distribution of vapor-phase PCE indicate there is

[51] This period does not include the months of July–August 1980 and January–February 1983, when water-supply well TT-26 was not operating.

potential for vapors from these plumes to enter buildings at Tarawa Terrace I, thereby providing a potential exposure pathway for inhalation of PCE vapor. At Tarawa Terrace I these buildings would include family housing and the elementary school (Figure A20).

To address issues of model uncertainty and parameter variability, three types of analyses were conducted: (1) water-supply well scheduling analysis, (2) sensitivity analysis, and (3) probabilistic analysis. All of the additional analyses were conducted using PCE as a single-specie contaminant dissolved in groundwater—the calibrated models described in Chapter C (Faye and Valenzuela In press 2007) and Chapter F (Faye In press 2007b) reports. The simulation tool, PSOpS, was used to investigate the effects of unknown and uncertain historical well operations and analyses of the variation in water-supply well scheduling. PSOpS simulations demonstrate that the current MCL for PCE (5 µg/L) would have been exceeded in finished drinking water from the Tarawa Terrace WTP as early as December 1956 and no later than June 1960 (points A and D, respectively, in Figure A21).

Sensitivity analyses were conducted using Tarawa Terrace models. Selected model parameters were varied one at a time from their respective calibrated values (Table A11). The effect of this variation on the change in the PCE concentration of finished drinking water at the Tarawa Terrace WTP was assessed. Four groundwater-flow and seven fate and transport model parameters were varied. Results of the sensitivity analyses showed that some parameters—specific yield, storage coefficient, and molecular diffusion—were insensitive to change, even when varied by factors of 10 and 20 (Table A14). Other parameters, for example, horizontal hydraulic conductivity for model layer 1 and infiltration (groundwater recharge), were extremely sensitive to values less than the calibrated values. Reducing the calibrated values for these parameters resulted in wells drying up during the simulation process. Generally, increasing or decreasing a calibrated parameter value by 10% (ratio of varied to calibrated parameter value of 0.9–1.1) resulted in changes of 6 months or less in terms of the date that finished drinking water first exceeded the current MCL of 5 µg/L for PCE. Results of parameter variations were used, in part, to assist in selecting parameters considered for a probabilistic analysis.

A probabilistic analysis approach was used to investigate model uncertainty and parameter variability using MCS and SGS. For the groundwater-flow and contaminant fate and transport models (Faye and Valenzuela In press 2007, Faye In press 2007b), eight parameters were assumed to be uncertain and variable: (1) horizontal hydraulic conductivity, (2) recharge rate, (3) effective porosity, (4) bulk density, (5) distribution coefficient, (6) dispersivity, (7) reaction rate, and (8) the PCE mass loading rate. With the exception of horizontal hydraulic conductivity, PDFs were generated for the remaining seven parameters of variation using Gaussian pseudo-random number generators. Horizontal hydraulic conductivity is a parameter for which there were spatially distributed field values. Therefore, an alternative method, SGS, was used to estimate the distribution of horizontal hydraulic conductivity for model layers 1, 3, and 5. The probabilistic analyses indicated that 95% of Monte Carlo simulations show the current MCL for PCE (5 µg/L) was first exceeded in finished water during October 1957–August 1958 (Figure A26); these solutions include November 1957, the date determined from the calibrated contaminant fate and transport model (Faye In press 2007b) that was based on a deterministic (single-value parameter input and output) approach. The PCE concentration in Tarawa Terrace WTP finished water during January 1985, simulated using the probabilistic analysis, ranges from 110 to 251 µg/L (95 percent of Monte Carlo simulations). This range includes the maximum calibrated value of 183 µg/L (derived without considering uncertainty and variability using MT3DMS) and the maximum measured value of 215 µg/L.

As part of this investigation, field tests were conducted on the present-day (2004) water-distribution system serving Tarawa Terrace. Data gathered from the investigation were used to construct a model of the water-distribution system using the EPANET 2 model code. Based on reviews of historical maps and information, the present-day (2004) water-distribution system is very similar to the historical water-distribution system. Thus, the operational and water-delivery patterns determined for the present-day (2004) water-distribution system from field investigations (Sautner et al. 2005, In press 2007) were used to characterize the historical water-distribution system. Using a calibrated water-distribution system model and an initial source concentration of 173 µg/L at the Tarawa Terrace WTP (Figure A18), an extended period simulation of 744 hours (31 days), representing December 1984, indicates:

- 100% of the concentration of PCE in finished water at the Tarawa Terrace WTP (173 μg/L) reached locations F05 and F07 (Figure A27), located in the Tarawa Terrace housing area within 2 days,
- 100% of the concentration of PCE in finished water at the Tarawa Terrace WTP (173 μg/L) reached the Camp Johnson elevated storage tank within 3 days, and
- 100% of the simulated concentration of PCE in finished water at the Tarawa Terrace WTP (173 μg/L) reached the Montford Point area (farthest point from the Tarawa Terrace WTP) within 7 days.

These results confirm the assumption that on a monthly basis, the concentration of PCE at residential housing areas throughout Tarawa Terrace would be the same as the concentration of PCE in finished water at the Tarawa Terrace WTP. Therefore, using a mixing model based on the principles of continuity and conservation of mass (Equations 2 and 3, respectively) was appropriate for reconstructing the historical concentrations of PCE in finished water delivered from the Tarawa Terrace WTP.

In summary, based on field data, modeling results, and the historical reconstruction process, the following conclusions are made with respect to drinking-water contamination at Tarawa Terrace:

1. Simulated PCE concentrations exceeded the current MCL of 5 μg/L at water-supply well TT-26 for 333 months—January 1957–January 1985; the maximum simulated PCE concentration was 851 μg/L; the maximum measured PCE concentration was 1,580 μg/L during January 1985.
2. Simulated PCE concentrations exceeded the current MCL of 5 μg/L in finished water at the Tarawa Terrace WTP for 346 months—November 1957–February 1987; the maximum simulated PCE concentration in finished water was 183 μg/L; the maximum measured PCE concentration in finished water was 215 μg/L during February 1985.
3. Simulation of PCE degradation by-products—TCE, *trans*-1,2-dichloroethylene (1,2-tDCE), and vinyl chloride—indicated that maximum concentrations of the degradation by-products generally were in the range of 10–100 μg/L at water-supply well TT-26; measured concentrations of TCE and 1,2-tDCE on January 16, 1985, were 57 and 92 μg/L, respectively.
4. Maximum concentrations of the degradation by-products in finished water at the Tarawa Terrace WTP generally were in the range of 2–15 μg/L; measured concentrations of TCE and 1,2-tDCE on February 11, 1985, were 8 and 12 μg/L, respectively.
5. PCE concentrations in finished water at the Tarawa Terrace WTP exceeding the current MCL of 5 μg/L could have been delivered as early as December 1956 and no later then December 1960. Based on probabilistic analyses, the most likely dates that finished water first exceeded the current MCL ranged from October 1957 to August 1958 (95 percent probability), with an average first exceedance date of November 1957.
6. Exposure to PCE and PCE degradation by-products from contaminated drinking water ceased after February 1987; the Tarawa Terrace WTP was closed March 1987.

Availability of Input Data Files, Models, and Simulation Results

Calibrated model input data files developed for simulating predevelopment groundwater flow, transient ground-water flow, the fate and transport of PCE as a single specie, and the distribution of water and contaminants in a water-distribution system are provided with this report in a DVD format. Public domain model codes used with these input files are available on the Internet at the following Web sites:

- Predevelopment and transient groundwater flow
  - Model code: MODFLOW-96
  - Web site: *http://water.usgs.gov/nrp/gwsoftware/modflow.html*

- Fate and transport of PCE as a single specie
  - Model code: MT3DMS
  - Web site: *http://hydro.geo.ua.edu/*
- Distribution of water and contaminants in a water-distribution system
  - Model code: EPANET 2
  - Web site: *http://www.epa.gov/nrmrl/wswrd/epanet.html*

Specialized model codes and model input data files were developed specifically for the Tarawa Terrace analyses by the MESL at the School of Civil and Environmental Engineering, Georgia Institute of Technology. These specialized codes and input data files were developed for simulating three-dimensional multispecies, multiphase, mass transport (TechFlowMP) and pumping schedule optimization (PSOpS) and are described in detail in the Chapter G (Jang and Aral In press 2007) and Chapter H (Wang and Aral In press 2007) reports, respectively. Contact information and questions related to these codes are provided on the Internet at the MESL Web site at: *http://mesl.ce.gatech.edu*.

Also included on the DVDs accompanying this report is a file that contains results for monthly simulated concentrations of PCE and PCE degradation by-products (TCE, 1,2-tDCE, and VC) in finished water at the Tarawa Terrace WTP for January 1951–March 1987. This file (also provided in Appendix A2) is prepared in Adobe® Portable Document Format (PDF).

Readers desiring information about the model input data files or the simulation results contained on the DVDs also may contact the Project Officer of ATSDR's Exposure-Dose Reconstruction Project at the following address:

Morris L. Maslia, MSCE, PE, D.WRE, DEE
Exposure-Dose Reconstruction Project
Division of Health Assessment and Consultation
Agency for Toxic Substances and Disease Registry
1600 Clifton Road, Mail Stop E-32
Atlanta, Georgia 30333
Telephone: (404) 498-0415
Fax: (404) 498-0069
E-mail: mmaslia@cdc.gov

Acknowledgments

A study of this complexity and magnitude is dependent upon the assistance, input, and suggestions of many colleagues. Thus, the authors of this report and all chapter reports acknowledge the managers and staff of the U.S. Geological Survey Water Science Centers in Raleigh, North Carolina, and Atlanta, Georgia. In particular, the contributions of Melinda J. Chapman, Douglas A. Harned, and Stephen S. Howe are acknowledged for providing the majority of well, water-level, and pumpage data used in this study. Keith W. McFadden is acknowledged for assistance with spatial analyses in preparing illustrations and with developing geodatabases, Web-based applications, and the querying system contained on the electronic media accompanying Chapters A and K. Gregory C. Mayer and Edward H. Martin also are acknowledged for their administrative assistance.

The authors acknowledge the staff of the Environmental Management Division, U.S. Marine Corps Base Camp Lejeune, North Carolina. In particular, Scott A. Brewer, Brynn Ashton, Scott R. Williams, and Rick Cheng for their assistance and cooperation during the course of this study, especially for providing a large number of technical reports, maps, and historical documents, which summarize the results of groundwater remedial investigations at and in the vicinity of Tarawa Terrace. The authors also acknowledge Joel Hartsoe and Danny E. Hill of the Camp Lejeune Public Works Department Utility Section.

The authors acknowledge the contributions of the USEPA, Region IV, Atlanta, Georgia, for providing reports and documents summarizing the results of investigations of groundwater contamination in the vicinity of ABC One-Hour Cleaners and in the northern part of Tarawa Terrace.

The authors acknowledge colleagues at ATSDR, Eastern Research Group, Inc., the Multimedia Environmental Simulations Laboratory at the Georgia Institute of Technology, and the Oak Ridge Institute for Science and Education for providing assistance and advice with all aspects of this study.

Thomas M. Plummer, Commander, U.S. Public Health Service, Indian Health Service, U.S. Department of Health and Human Services, assisted with planning, field instrumentation, and conducting tests of water-distribution systems serving Camp Lejeune, August 18–28, 2004.

Caryl J. Wipperfurth, Bonnie J. Turcott, Patricia L. Nobles, James E. Banton, and Kimberly A. Waltenbaugh, U.S. Geological Survey Enterprise Publishing Network, assisted with the preparation of text, illustrations, and electronic media.

References

Agency for Toxic Substances and Disease Registry. Preliminary Public Health Assessment for ABC One-Hour Cleaners, Jacksonville, Onslow County, North Carolina. Atlanta, GA: U.S. Department of Health and Human Services; 1990. Report No.: NCD024644494.

Agency for Toxic Substances and Disease Registry. Public Health Assessment for U.S. Marine Corps Base at Camp Lejeune, Military Reservation, Camp Lejeune, Onslow County, North Carolina. Atlanta, GA: U.S. Department of Health and Human Services; 1997. Report No.: NC6170022580.

Agency for Toxic Substances and Disease Registry. Volatile Organic Compounds in Drinking Water and Adverse Pregnancy Outcomes, United States Marine Corps Base, Camp Lejeune. Atlanta, GA: U.S. Department of Health and Human Services; 1998.

Agency for Toxic Substances and Disease Registry. Historical Reconstruction of the Water-Distribution System Serving the Dover Township Area, New Jersey: January 1962–December 1996—Summary of Findings. Atlanta, GA: Agency for Toxic Substances and Disease Registry; 2001 September.

AWWA Engineering Computer Applications Committee. Calibration Guidelines for Water Distribution System Modeling. Proceedings: 1999 AWWA Information Management and Technology Conference (IMTech); 1999 April; New Orleans, LA: New York: American Water Works Association; 1999.

Borowski EJ, and Borwein JM. The HarperCollins Dictionary of Mathematics. New York: HarperCollins Publishers; 1991.

Bove FJ, Fulcomer MC, Klotz JB, Esmart J, Dufficy EM, and Savrin JE. Public Drinking Water Contamination and Birth Outcomes. American Journal of Epidemiology. 1995;14:850–862.

Bove F, Shim Y, and Zeitz P. Drinking Water Contaminants and Adverse Pregnancy Outcomes: a Review. Environmental Health Perspectives. 2002;110(S):61–74.

Chiang W-H, and Kinzelbach W. 3D-Groundwater Modeling with PMWIN: A Simulation System for Modeling Groundwater Flow and Pollution. New York: Springer-Verlag Berlin Heidelberg; 2001.

CLW, Camp Lejeune Water Documents, 0001–8761 (not consecutively available), provided on DVD format, in Maslia ML, Sautner JB, Faye RE, Suárez-Soto RJ, Aral MM, Grayman WM, Jang W, Wang J, Bove FJ, Ruckart PZ, Valenzuela C, Green JW Jr, and Krueger AL. Analyses of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water at Tarawa Terrace and Vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina: Historical Reconstruction and Present-Day Conditions—Chapter A: Summary of Findings. Atlanta, GA: Agency for Toxic Substances and Disease Registry; 2007.

Cohn P, Klotz J, Bove F, Berkowitz M, and Fagliano J. Drinking Water Contamination and the Incidence of Leukemia and Non-Hodgkin's Lymphoma. Environmental Health Perspectives. 1994;102(6–7):556–561.

Costas K, Knorr RS, and Condon SK. A Case-Control Study of Childhood Leukemia in Woburn, Massachusetts: The Relationship Between Leukemia Incidence and Exposure to Public Drinking Water. The Science of the Total Environment. 2002;300:23–35.

Cullen AC, and Frey HC. Probabilistic Techniques in Exposure Assessment: A Handbook for Dealing with Variability and Uncertainty in Models and Inputs. New York: Plenum Press; 1999.

Deutsch CV, and Journel AG. GSLIB Geostatical Software Library and User's Guide. 2nd ed. New York, NY: Oxford University Press; 1998.

Doherty J. Groundwater Data Utilities/Part B: Program Descriptions. 2005 [cited 2007 January 3]; Available from *http://www.sspa.com/pest/utilities.shtml*

Doherty RE. A History of the Production and the Use of Carbon Tetrachloride, Tetrachloroethylene, Trichloroethylene and 1,1,1-Trichloroethane in the United States: Part 1—Historical Background; Carbon Tetrachloride and Tetrachloroethylene. Journal of Environmental Forensics. 2000a;1:69–81.

Doherty RE. A History of the Production and the Use of Carbon Tetrachloride, Tetrachloroethylene, Trichloroethylene and 1,1,1-Trichloroethane in the United States: Part 2—Trichloroethylene and 1,1,1-Trichloroethane. Journal of Environmental Forensics. 2000b;1:83–93.

Faye RE. Analyses of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water at Tarawa Terrace and Vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina: Historical Reconstruction and Present-Day Conditions—Chapter B: Geohydrologic Framework of the Castle Hayne Aquifer System. Atlanta, GA: Agency for Toxic Substances and Disease Registry; In press 2007a.

Faye RE. Analyses of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water at Tarawa Terrace and Vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina: Historical Reconstruction and Present-Day Conditions—Chapter F: Simulation of the Fate and Transport of Tetrachloroethylene (PCE). Atlanta, GA: Agency for Toxic Substances and Disease Registry; In press 2007b.

Faye RE, and Green JW Jr. Analyses of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water at Tarawa Terrace and Vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina: Historical Reconstruction and Present-Day Conditions—Chapter E: Occurrence of Contaminants in Groundwater. Atlanta, GA: Agency for Toxic Substances and Disease Registry; In press 2007.

Faye RE, and Valenzuela C. Analyses of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water at Tarawa Terrace and Vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina: Historical Reconstruction and Present-Day Conditions—Chapter C: Simulation of Groundwater Flow. Atlanta, GA: Agency for Toxic Substances and Disease Registry; In press 2007.

Goldberg SJ, Lebowitz MD, Graver EJ, and Hicks S. An Association of Human Congenital Cardiac Malformations and Drinking Water Contaminants. Journal of the American College of Cardiology. 1990;15:155–164.

Granger Laboratories. Analyses of Samples 206 and 207 from Site Coded "TT" and Samples 208 and 209 from Site Coded "HP." Letter from B.A. Babson to Commanding General, Marine Corp Base Camp Lejeune. August 10, 1982. (Camp Lejeune Water Document [CLW] 0592).

Grayman WM, Maslia ML, and Sautner JB. Calibrating Distribution System Models with Fire-Flow Tests. Opflow, American Water Works Association. 2006 April:10–12.

Haestad Methods, Walski TM, Chase DV, Savic DA, Grayman WM, Beckwith S, and Koelle E. Advanced Water Distribution Modeling and Management. 1st ed. Waterbury, CT: Haestad Press; 2003.

Harbaugh AW, Banta ER, Hill MC, and McDonald MG. MODFLOW-2000, The U.S. Geological Survey Modular Ground-Water Model: User Guide to Modularization Concepts and the Ground-Water Flow Process. Reston, VA: U.S. Geological Survey Open-File Report 00-92; 2000.

Harbaugh AW, and McDonald MG. User's Documentation of MODFLOW-96, an Update to the U.S. Geological Survey Modular Finite-Difference Ground-Water Flow Model. Reston, VA: U.S. Geological Survey Open-File Report 96-458; 1996.

Henry Von Oesen and Associates, Inc. Study of Two Water Plants, Tarawa Terrace-Montford Point, Camp Lejeune, North Carolina: Henry Von Oesen and Associates, Inc.; 1979.

Hill MC, and Tiedeman CR. Effective Groundwater Model Calibration. Hoboken: John Wiley & Sons, Inc.; 2007.

Huling SG, and Weaver JW. Dense Nonaqueous Phase Liquids. Washington, D.C.: U.S. Environmental Protection Agency, Office of Research and Development and Office of Solid Waste and Emergency Response; 1991 March. Report No.: EPA/540/4-91-002.

International Union of Pure and Applied Chemistry. Compendium of Chemical Terminology. 2006. [cited 2006 February 1]; Available from *http://www.iupac.org/publications/compendium/index.html*

Jang W, and Aral MM. Three-Dimensional Multiphase Flow and Multi-Species Transport Model, TechFlowMP. Atlanta, GA: Multimedia Environmental Simulations Laboratory (MESL), School of Civil and Environmental Engineering, Georgia Institute of Technology; 2005 September. Report No. MESL-02-05.

Jang W, and Aral MM. Simulation of Three-Dimensional Multi-Species, Multi-Phase Mass Transport of Tetrachloroethylene (PCE) and Associated Degradation By-Products. Atlanta, GA: Multimedia Environmental Simulation Laboratory (MESL), School of Civil and Environmental Engineering, Georgia Institute of Technology; 2007 March. Report No.: MESL-02-07.

Jang W, and Aral MM. Analyses of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water at Tarawa Terrace and Vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina: Historical Reconstruction and Present-Day Conditions—Chapter G: Simulation of Three-Dimensional Multispecies, Multiphase Mass Transport of Tetrachloroethylene (PCE) and Associated Degradation By-Products. Atlanta, GA: Agency for Toxic Substances and Disease Registry; In press 2007.

Kueper BH, Wealthall GP, Smith JWN, Leharne SA, and Lerner DN. 2003. An Illustrated Handbook of DNAPL Transport and Fate in the Subsurface. Environment Agency, R&D Publication 133, 2003 June, Bristol, United Kingdom.

Lawrence SJ. Description, Properties, and Degradation of Selected Volatile Organic Compounds Detected in Ground Water—A Review of Selected Literature. Atlanta, GA: U.S. Geological Survey Open-File Report 2006-1338; 2006. A Web-only publication at *http://pubs.usgs.gov/ofr/2006/1338/*.

Lawrence SJ. Analyses of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water at Tarawa Terrace and Vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina: Historical Reconstruction and Present-Day Conditions—Chapter D: Properties of Degradation Pathways of Common Organic Compounds in Groundwater. Atlanta, GA: Agency for Toxic Substances and Disease Registry; In press 2007.

Mackay DM, and Cherry JA. Groundwater Contamination: Pump-and-Treat Remediation. Environmental Science and Technology. 1989:23(6):630–636.

Maslia ML. Expert Peer Review Panel Evaluating ATSDR's Water-Modeling Activities in Support of the Current Study of Childhood Birth Defects and Cancer at U.S. Marine Corps Base Camp Lejeune, North Carolina: Atlanta, GA: Agency for Toxic Substances and Disease Registry; 2005.

Maslia ML, and Aral MM. Analytical Contaminant Transport Analysis System (ACTS)—Multimedia Environmental Fate and Transport. Practice Periodical of Hazardous, Toxic, and Radioactive Waste Management. 2004 July:181–198.

Maslia ML, Sautner JB, and Aral MM. Analysis of the 1998 Water-Distribution System Serving the Dover Township Area, New Jersey: Field-Data Collection Activities and Water-Distribution System Modeling. Atlanta, GA: Agency for Toxic Substances and Disease Registry; 2000.

References

Maslia ML, Sautner JB, Aral MM, Gillig RE, Reyes JJ, and Williams RC. Historical Reconstruction of the Water-Distribution System Serving the Dover Township Area, New Jersey: January 1962–December 1996. Atlanta, GA: Agency for Toxic Substances and Disease Registry; 2001 October.

Maslia ML, Sautner JB, Faye RE, Suárez-Soto RJ, Aral MM, Grayman WM, Jang W, Wang J, Bove FJ, Ruckart PZ, Valenzuela C, Green JW Jr, and Krueger AL. Analyses of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water at Tarawa Terrace and Vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina: Historical Reconstruction and Present-Day Conditions—Chapter A: Summary of Findings. Atlanta, GA: Agency for Toxic Substances and Disease Registry; 2007.

Maslia ML, Sautner JB, Faye RE, Suárez-Soto RJ, Aral MM, Grayman WM, Jang W, Wang J, Bove FJ, Ruckart PZ, Valenzuela C, Green JW Jr, and Krueger AL. Analyses of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water at Tarawa Terrace and Vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina: Historical Reconstruction and Present-Day Conditions—Chapter K: Supplemental Information. Atlanta, GA: Agency for Toxic Substances and Disease Registry; In press 2007a.

Maslia ML, Sautner JB, Valenzuela C, Grayman WM, Aral MM, and Green JW Jr. Use of Continuous Recording Water-Quality Monitoring Equipment for Conducting Water-Distribution System Tracer Tests: The Good, the Bad, and the Ugly. Proceedings: World Environmental and Water Resources Congress; 2005 May 15–19; Anchorage, AK; 2005.

Maslia ML, Suárez-Soto RJ, Wang J, Aral MM, Sautner JB, and Valenzuela C. Analyses of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water at Tarawa Terrace and Vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina: Historical Reconstruction and Present-Day Conditions—Chapter I: Parameter Sensitivity, Uncertainty, and Variability Associated with Model Simulations of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water. Atlanta, GA: Agency for Toxic Substances and Disease Registry; In press 2007b.

Massachusetts Department of Public Health, Centers for Disease Control and Prevention, and Massachusetts Health Research Institute. Final Report of the Woburn Environmental and Birth Study. Boston, MA: Massachusetts Department of Public Health; 1996.

Masters GM. Introduction to Environmental Engineering and Science. 2nd ed: Prentice Hall; 1998.

Melts VJ. Deposition, in the General Court of Justice, Superior Court Division; 2001 April 12. Report No.: 01-CVS-566.

New Jersey Department of Health and Senior Services. Case-Control Study of Childhood Cancers in Dover Township (Ocean County), New Jersey. Trenton, NJ: New Jersey Department of Health and Senior Services; 2003.

Pankow JF, and Cherry JA. Dense Chlorinated Solvents and Other DNAPLs in Groundwater: History, Behavior, and Remediation: Waterloo Press; 1996.

Rodenbeck SE, Sanderson LM, and Rene A. Maternal Exposure to Trichloroethylene in Drinking Water and Birth-Weight Outcomes. Archives of Environmental Health. 2000;55:188–194.

Rogers JF, Kilough GG, Thompson SJ, Addy CL, McKeown RE, and Cowen DJ. Estimating Environmental Exposures to Sulfur Dioxide from Multiple Industrial Sources for a Case-Control Study. Journal of Exposure Analysis and Environmental Epidemiology. 1999;9:535–545.

Rossman LA. EPANET 2 Users Manual. Cincinnati: U.S. Environmental Protection Agency, National Risk Management Research Laboratory; 2000 September. Report No.: EPA/600-R-00/057.

Roy F. Weston, Inc. Remedial Investigation Report, ABC One-Hour Cleaners, Jacksonville, North Carolina: Roy F. Weston, Inc.; 1992.

Roy F. Weston, Inc. Remedial Investigation, ABC One-Hour Cleaners, Operable Unit 2, Jacksonville, North Carolina: Roy F. Weston, Inc.; 1994.

Saltelli A, Chan K, and Scott EM, editors. Sensitivity Analysis. Chichester, England: John Wiley & Sons, Ltd; 2000.

Sautner JB, Maslia ML, and Grayman WM. Storage Tank Mixing Models: Comparison of Tracer Data with Model Simulations. World Environmental and Water Resources Congress; 2007 May 15–19; Tampa, FL; 2007.

Sautner JB, Maslia ML, Valenzuela C, Grayman WM, Aral MM, and Green JW Jr. Field Testing of Water-Distribution Systems at the U.S. Marine Corps Base, Camp Lejeune, North Carolina, in Support of an Epidemiologic Study. Proceedings: World Environmental and Water Resources Congress; 2005 May 15–19; Anchorage, AK; 2005.

Sautner JB, Valenzuela C, Maslia ML, and Grayman WM. Analyses of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water at Tarawa Terrace and Vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina: Historical Reconstruction and Present-Day Conditions—Chapter J: Field Tests, Data Analyses, and Simulation of the Distribution of Drinking Water. Atlanta, GA: Agency for Toxic Substances and Disease Registry; In press 2007.

Schwartz FW, and Zhang H. Fundamentals of Ground Water. New York: John Wiley & Sons, Inc.; 2003.

Schwille F. Dense Chlorinated Solvents in Porous and Fractured Media. Translated by Pankow, JF. Boca Raton: Lewis Publishers (CRC Press); 1988.

Shiver R. A Groundwater Investigation to Define the Source(s) of Tetrachloroethylene that Have Contaminated Three Community Water Supply Wells at Tarawa Terrace I, Camp Lejeune Marine Corps Base, Onslow County: North Carolina Department of Natural Resources and Community Development; 1985.

Sonnenfeld N, Hertz-Picciotto I, and Kaye WE. Tetrachloroethylene in Drinking Water and Birth Outcomes at the U.S. Marine Corps Base at Camp Lejeune, North Carolina. American Journal of Epidemiology. 2001;154(10):902–908.

Tung Y-K, and Yen B-C. Hydrosystems Engineering Uncertainty Analysis. New York: McGraw-Hill; 2005.

U.S. Environmental Protection Agency. Contaminant Specific Fact Sheets, Volatile Organic Chemicals—Technical Version. EPA 811-F-95-004-T. 1995. [cited 2006 January 11]; Available from *http://www.epa.gov/safewater/dwh/t-voc.html*

U.S. Environmental Protection Agency. Guiding Principles for Monte Carlo Analysis. Washington, DC: United States Environmental Protection Agency; 1997 March. Report No.: EPA 630-R-97-001.

U.S. Environmental Protection Agency. National Primary Drinking Water Standards. Report No.: EPA 816-F-03-016. 2003. [cited 2007 January 25]; Available from *http://www.epa.gov/water/*

U.S. Environmental Protection Agency. How to Evaluate Alternative Cleanup Technologies for Underground Storage Tank Sites—A Guide for Corrective Action Plan Reviewers. Washington, D.C.: U.S. Environmental Protection Agency; 2004. Report No.: EPA 510-B-95-007. Available from *http://www.epa.gov/swerust1/pubs/tums.htm*

Wang J, and Aral MM. Effect of Groundwater Pumping Schedule Variation on Arrival of Tetrachloroethylene (PCE) at Water-Supply Wells and the Water Treatment Plant. Atlanta, GA: Multimedia Environmental Simulation Laboratory (MESL), School of Civil and Environmental Engineering, Georgia Institute of Technology; 2007 January. Report No.: MESL-01-07.

Wang J, and Aral MM. Analyses of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water at Tarawa Terrace and Vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina: Historical Reconstruction and Present-Day Conditions—Chapter H: Effect of Groundwater Pumping Schedule Variation on Arrival of Tetrachloroethylene (PCE) at Water-Supply Wells and the Water Treatment Plant. Atlanta, GA: Agency for Toxic Substances and Disease Registry; In press 2007.

Zheng C, and Bennett GD. Applied Contaminant Transport Modeling. 2nd ed. New York: John Wiley & Sons, Inc.; 2002.

Zheng C, and Wang PP. MT3DMS: A Modular Three-Dimensional Multi-Species Model for Simulation of Advection, Dispersion, and Chemical Reactions of Contaminants in Groundwater Systems: Documentation and User's Guide. Vicksburg, MS: U.S. Army Engineer Research and Development Center; 1999. Report No.: SERDP-99.

Appendix A1. Summaries of Tarawa Terrace Chapter Reports

Summaries of Tarawa Terrace chapter reports are described below. Electronic versions of each chapter report and their supporting information and data will be made available on the ATSDR Camp Lejeune Web site at *http://www.atsdr.cdc.gov/sites/lejeune/index.html.*

Chapter A: Summary of Findings (Maslia et al. 2007—this report) provides a summary of detailed technical findings (described in Chapters B–K) focusing on the historical reconstruction analysis and present-day conditions of groundwater flow, contaminant fate and transport, and distribution of drinking water at Tarawa Terrace and vicinity. Among the topics that this report summarizes are: (1) methods of analyses, (2) data sources and requirements, (3) the four-stage hierarchical approach used for model calibration and estimating PCE concentrations in drinking water, (4) presentation, discussion, and implications of selected simulation results for PCE and its degradation by-products, and (5) quantifying confidence in simulation results by varying water-supply well historical pumping schedules and by using sensitivity and probabilistic analyses to address issues of uncertainty and variability in model parameters. In addition, this report provides a searchable electronic database—using digital video disc (DVD) format—of information and data sources used to conduct the historical reconstruction analysis. Data were obtained from a variety of sources, including ATSDR, USEPA, Environmental Management Division of U.S. Marine Corps Base Camp Lejeune, U.S. Geological Survey, private consulting organizations, published scientific literature, and community groups representing former marines and their families.

Chapter B: Geohydrologic Framework of the Castle Hayne Aquifer System (Faye In press 2007a) provides detailed analyses of well and geohydrologic data used to develop the geohydrologic framework of the Castle Hayne aquifer system at Tarawa Terrace and vicinity. Potentiometric levels, horizontal hydraulic conductivity, and the geohydrologic framework of the Castle Hayne aquifer system east of the New River are described and quantified. The geohydrologic framework is composed of 11 units, 7 of which correspond to the Upper, Middle, and Lower Castle Hayne aquifers and related confining units. Overlying the Upper Castle Hayne aquifer are the Brewster Boulevard and Tarawa Terrace aquifers and confining units. Much of the Castle Hayne aquifer system is composed of fine, fossiliferous sand, limestone, and shell limestone. The sands are frequently silty and contain beds and lenses of clay. Limestone units are probably discontinuous and occasionally cavernous. Confining units are characterized by clays and silty clays of significant thickness and are persistent across much of the study area. Maximum thickness of the Castle Hayne aquifer system within the study area is about 300 ft. In general, geohydrologic units thicken from northwest to the south and southeast. The limestones and sands of the Castle Hayne aquifer system readily yield water to wells. Aquifer-test analyses indicate that horizontal hydraulic conductivities of water-bearing units at supply wells commonly range from 10 to 30 feet per day. Estimated predevelopment potentiometric levels of the Upper and Middle Castle Hayne aquifers indicate that groundwater-flow directions are from highland areas north and east of the study area toward the major drainages of New River and Northeast Creek.

Chapter C: Simulation of Groundwater Flow (Faye and Valenzuela In press 2007) provides detailed analyses of groundwater flow at Tarawa Terrace and vicinity, including the development of a predevelopment (steady-state) and transient groundwater-flow model using the model code MODFLOW-96 (Harbaugh and McDonald 1996). Calibration and testing of the model are thoroughly described. The groundwater-flow model was designed with seven layers largely representing the Castle Hayne aquifer system. Comparison of 59 observed water levels representing estimated predevelopment conditions and corresponding simulated potentiometric levels indicated a high degree of similarity throughout most of the study area. The average absolute difference between simulated and observed predevelopment water levels was 1.9 ft, and the root-mean-square (RMS) of differences was 2.1 ft. Transient simulations represented pumping at Tarawa Terrace supply wells for 528 stress periods representing 528 months—January 1951–December 1994. Assigned pumpage at supply wells was estimated using reported well-capacity rates and annual rates of raw water treated at the Tarawa Terrace water treatment plant (WTP) during 1975–1986. Calibrated model results of 263 paired water levels representing observed and simulated water levels at monitor wells indicated an average absolute difference between simulated and observed water levels of 1.4 ft, a standard deviation of water-level difference of 0.9 ft, and a RMS of water-level difference of 1.7 ft. Calibrated model results of 526 paired water levels representing observed and simulated water levels at water-supply wells indicated an average absolute difference between simulated and observed water levels of 7.1 ft, a standard deviation of water-level difference of 4.6 ft, and a RMS of water-level difference of 8.5 ft.

Chapter D: Properties of Degradation Pathways of Common Organic Compounds in Groundwater (Lawrence In press 2007) describes and summarizes the properties, degradation pathways, and degradation by-products of VOCs (non-trihalomethane) commonly detected in groundwater contamination sites in the United States. This chapter also is published as U.S. Geological Survey Open-File Report 2006-1338 (Lawrence 2006) and provides abridged information describing the most salient properties and biodegradation of 27 VOCs. This report cross-references common names and synonyms associated with VOCs with the naming conventions supported by the IUPAC. In addition, the report describes basic physical characteristics of those compounds such as Henry's Law constant, water solubility, density, octanol-water partition (log K_{ow}), and organic carbon partition (log K_{oc}) coefficients. Descriptions and illustrations are provided for natural and laboratory biodegradation rates, chemical by-products, and degradation pathways.

Chapter E: Occurrence of Contaminants in Groundwater (Faye and Green In press 2007) describes the occurrence and distribution of PCE and related contaminants within the Tarawa Terrace aquifer and the Upper Castle Hayne aquifer system at and in the vicinity of the Tarawa Terrace housing area. The occurrence and distribution of benzene, toluene, ethylbenzene, and xylene (BTEX) and related compounds also are briefly described. This report describes details of historical investigations of VOC contamination of groundwater at Tarawa Terrace with emphasis on water-supply wells TT-23, TT-25, and TT-26 (Figure A1). Detailed analyses of concentrations of PCE at monitor wells, at hydrocone sample locations, and at Tarawa Terrace water-supply wells during the period 1991–1993 were sufficient to estimate the mass of PCE remaining in the Tarawa Terrace and Upper Castle Hayne aquifers. Similar methods were applied to compute the mass of PCE in the unsaturated zone (zone above the water table) at and in the vicinity of ABC One-Hour Cleaners using concentration-depth data determined from soil borings. The total mass of PCE computed in groundwater and within the unsaturated zone equals about 6,000 pounds and equates to a volume of about 430 gallons. This volume represents an average minimum loss rate of PCE to the subsurface at ABC One-Hour Cleaners of about 13 gallons per year for the period 1953–1985.

Chapter F: Simulation of the Fate and Transport of Tetrachloroethylene (PCE) in Groundwater (Faye In press 2007b) describes: (1) the fate and transport of PCE in groundwater from the vicinity of ABC One-Hour Cleaners to the intrusion of PCE into individual water-supply wells (for example, TT-23 and TT-26, Figure A1), and (2) the concentration of PCE in finished water at the Tarawa Terrace WTP computed using a materials mass balance model (simple mixing). The materials mass balance model was used to compute a flow-weighted average PCE concentration, which was assigned as the finished water concentration at the Tarawa Terrace WTP for a specified month. The contaminant fate and transport simulation was conducted using the code MT3DMS (Zheng and Wang 1999) integrated with the calibrated groundwater-flow model (Faye and Valenzuela In press 2007) based on the code MODFLOW-96. Simulated mass loading occurred at a constant rate of 1,200 grams per day using monthly stress periods representing the period January 1953–December 1984. The complete simulation time was represented by the period January 1951–December 1994. Until 1984, the vast majority of simulated PCE-contaminated groundwater was supplied to the Tarawa Terrace WTP by well TT-26. Simulated breakthrough of PCE at well TT-26 at the current MCL of 5 µg/L occurred during January 1957. Corresponding breakthrough at the location of well TT-23 occurred during December 1974; however, well TT-23 was not operational until about August 1984. Simulated maximum and average PCE concentrations at well TT-26 following breakthrough were 851 µg/L and 414 µg/L, respectively. Corresponding maximum and average concentrations at well TT-23 subsequent to the onset of operations were 274 µg/L and 252 µg/L, respectively. Simulated breakthrough of PCE in finished water at the Tarawa Terrace WTP occurred at the current MCL concentration of 5 µg/L during November 1957 and remained at or above a concentration of 40 µg/L from May 1960 until the termination of pumping at water-supply well TT-26 during February 1985. Computed maximum and average PCE concentrations at the WTP were 183 µg/L and 70 µg/L, respectively, during the period November 1957–February 1985, when well TT-26 was removed from service.

Chapter G: Simulation of Three-Dimensional Multispecies, Multiphase Mass Transport of Tetrachloroethylene (PCE) and Associated Degradation By-Products (Jang and Aral In press 2007) provides detailed descriptions and analyses of the development and application of a three-dimensional model (TechFlowMP) capable of simulating multispecies and multiphase (water and vapor) transport of PCE and associated degradation by-products—TCE, 1,2-tDCE, and VC. The development of the TechFLowMP model is described in Jang and Aral (2005) and its application to Tarawa Terrace and vicinity also is published as report MESL-02-07 by the Multimedia Environmental Simulations Laboratory in the School of Civil and Environmental Engineering, Georgia Institute of Technology (Jang and Aral 2007). Simulation results show that the maximum concentrations of PCE degradation by-products, TCE, 1,2-tDCE, and VC, generally ranged between 10 µg/L and 100 µg/L in Tarawa Terrace water-supply well TT-26 and between 2 µg/L and 15 µg/L in finished water delivered from the Tarawa Terrace WTP. As part of the degradation by-product simulation using the TechFlowMP model, results were obtained for PCE and PCE degradation by-products dissolved in groundwater and in the vapor phase (above the water table in the unsaturated zone). Analyses of the distribution of vapor-phase PCE and PCE degradation by-products indicate there is potential for vapors to enter buildings at Tarawa Terrace, thereby providing a potential exposure pathway from inhalation of PCE and PCE degradation by-product vapors. At Tarawa Terrace these buildings would include family housing and the elementary school.

Chapter H: Effect of Groundwater Pumping Schedule Variation on Arrival of Tetrachloroethylene (PCE) at Water-Supply Wells and the Water Treatment Plant (Wang and Aral In press 2007) describes a detailed analysis of the effect of groundwater pumping schedule variation on the arrival of PCE at water-supply wells and at the Tarawa Terrace WTP. Analyses contained in this chapter used the calibrated model parameters described in Chapter C (Faye and Valenzuela In press 2007) and Chapter F (Faye In press 2007b) reports in combination with the groundwater pumping schedule optimization system simulation tool (PSOpS) to assess the influence of unknown and uncertain historical well operations at Tarawa Terrace water-supply wells on PCE concentrations at water-supply wells and at the Tarawa Terrace WTP. This chapter also is published as report MESL-01-07 by the Multimedia Environmental Simulations Laboratory in the School of Civil and Environmental Engineering, Georgia Institute of Technology (Wang and Aral 2007). Variation in the optimal pumping schedules indicates that the arrival time of PCE exceeding the current MCL of 5 µg/L at water-supply well TT-26 varied between May 1956 and August 1959. The corresponding arrival time of PCE exceeding the current MCL of 5 µg/L at the Tarawa Terrace WTP varied between December 1956 and June 1960.

Chapter I: Parameter Sensitivity, Uncertainty, and Variability Associated with Model Simulations of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water (Maslia et al. In press 2007b) describes the development and application of a probabilistic analysis using Monte Carlo and sequential Gaussian simulation analysis to quantify uncertainty and variability of groundwater hydraulic and transport parameters. These analyses demonstrate quantitatively the high reliability and confidence in results determined using the calibrated parameters from the MODFLOW-96 and MT3DMS models. For example, 95% of Monte Carlo simulations indicated that the current MCL for PCE of 5 μg/L was exceeded in finished water at the Tarawa Terrace WTP between October 1957 and August 1958; the corresponding breakthrough simulated by the calibrated fate and transport model (Chapter F report, Faye [In press 2007b]) occurred during November 1957.

Chapter J: Field Tests, Data Analyses, and Simulation of the Distribution of Drinking Water (Sautner et al. In press 2007) describes field tests, data analyses, and the simulation of drinking-water supply at Tarawa Terrace and vicinity. Details of the development and calibration of a water-distribution system model for Tarawa Terrace and vicinity are described based on applying the model code EPANET 2 (Rossman 2000) to the study area. Comparisons are provided between the PCE concentrations computed by Faye (In press 2007b) using a simple mixing model and the more complex and detailed approach of Sautner et al. (In press 2007) that is based on a numerical water-distribution system model. Results of simulations conducted using extended period simulation confirm the assumption that, on a monthly basis, the concentrations of PCE in drinking water delivered to residential housing areas throughout Tarawa Terrace are the same as the concentrations of PCE in finished water at the Tarawa Terrace WTP. Therefore, a simple mixing model based on the principles of continuity and conservation of mass was an appropriate model to use for determining the concentration of PCE in finished water delivered from the Tarawa Terrace WTP.

Chapter K: Supplemental Information (Maslia et al. In press 2007a) presents additional information such as (1) a tabular listing of water-supply well pumpage by stress period (month and year); (2) synoptic maps showing groundwater levels, directions of groundwater flow, and the simulated distribution of PCE; (3) a tabular listing of simulated monthly concentrations of PCE dissolved in groundwater at Tarawa Terrace water-supply wells; (4) a tabular listing of simulated monthly concentrations of PCE and PCE degradation by-products—TCE, 1,2-tDCE, and VC at the Tarawa Terrace WTP; (5) a complete list of references used in conducting the water-modeling analyses and historical reconstruction process; and (6) other ancillary information and data that were used during the water-modeling analyses and historical reconstruction process.

Appendix A2. Simulated PCE and PCE Degradation By-Products in Finished Water, Tarawa Terrace Water Treatment Plant, January 1951–March 1987

Appendix A2. Simulated tetrachloroethylene and its degradation by-products in finished water, Tarawa Terrace water treatment plant, January 1951–March 1987.[1]

[PCE, tetrachloroethylene; µg/L, microgram per liter; 1,2-tDCE, *trans*-1,2-dichloroethylene; TCE, trichloroethylene; VC, vinyl chloride; WTP, water treatment plant]

Stress period	Month and year	Single specie using MT3DMS model[2]	Multispecies, multiphase using TechFlowMP model[3]			
		[4]PCE, in µg/L	[5]PCE, in µg/L	[5]1,2-tDCE, in µg/L	[5]TCE, in µg/L	[5]VC, in µg/L
1–12	Jan–Dec 1951	WTP not operating	WTP not operating	WTP not operating	WTP not operating	WTP not operating
13	Jan 1952	0.00	0.00	0.00	0.00	0.00
14	Feb 1952	0.00	0.00	0.00	0.00	0.00
15	Mar 1952	0.00	0.00	0.00	0.00	0.00
16	Apr 1952	0.00	0.00	0.00	0.00	0.00
17	May 1952	0.00	0.00	0.00	0.00	0.00
18	June 1952	0.00	0.00	0.00	0.00	0.00
19	July 1952	0.00	0.00	0.00	0.00	0.00
20	Aug 1952	0.00	0.00	0.00	0.00	0.00
21	Sept 1952	0.00	0.00	0.00	0.00	0.00
22	Oct 1952	0.00	0.00	0.00	0.00	0.00
23	Nov 1952	0.00	0.00	0.00	0.00	0.00
24	Dec 1952	0.00	0.00	0.00	0.00	0.00
25	Jan 1953	0.00	0.00	0.00	0.00	0.00
26	Feb 1953	0.00	0.00	0.00	0.00	0.00
27	Mar 1953	0.00	0.00	0.00	0.00	0.00
28	Apr 1953	0.00	0.00	0.00	0.00	0.00
29	May 1953	0.00	0.00	0.00	0.00	0.00
30	June 1953	0.00	0.00	0.00	0.00	0.00
31	July 1953	0.00	0.00	0.00	0.00	0.00
32	Aug 1953	0.00	0.00	0.00	0.00	0.00
33	Sept 1953	0.00	0.00	0.00	0.00	0.00
34	Oct 1953	0.00	0.00	0.00	0.00	0.00
35	Nov 1953	0.00	0.00	0.00	0.00	0.00
36	Dec 1953	0.00	0.00	0.00	0.00	0.00
37	Jan 1954	0.00	0.00	0.00	0.00	0.00
38	Feb 1954	0.00	0.00	0.00	0.00	0.00
39	Mar 1954	0.00	0.00	0.00	0.00	0.00
40	Apr 1954	0.00	0.00	0.00	0.00	0.00
41	May 1954	0.00	0.00	0.00	0.00	0.00
42	June 1954	0.00	0.00	0.00	0.00	0.00
43	July 1954	0.00	0.00	0.00	0.00	0.00
44	Aug 1954	0.00	0.00	0.00	0.00	0.00
45	Sept 1954	0.00	0.00	0.00	0.00	0.00
46	Oct 1954	0.00	0.00	0.00	0.00	0.00
47	Nov 1954	0.00	0.00	0.00	0.00	0.00
48	Dec 1954	0.00	0.00	0.00	0.00	0.00

Appendix A2. Simulated tetrachloroethylene and its degradation by-products in finished water, Tarawa Terrace water treatment plant, January 1951–March 1987[1].—Continued

[PCE, tetrachloroethylene; µg/L, microgram per liter; 1,2-tDCE, *trans*-1,2-dichloroethylene; TCE, trichloroethylene; VC, vinyl chloride; WTP, water treatment plant]

Stress-period	Month and year	Single specie using MT3DMS model[2]	Multispecies, multiphase using TechFlowMP model[3]			
		[4]PCE, in µg/L	[5]PCE, in µg/L	[5]1,2-tDCE, in µg/L	[5]TCE, in µg/L	[5]VC, in µg/L
49	Jan 1955	0.00	0.00	0.00	0.00	0.01
50	Feb 1955	0.00	0.00	0.01	0.00	0.01
51	Mar 1955	0.00	0.01	0.01	0.00	0.01
52	Apr 1955	0.00	0.01	0.01	0.00	0.02
53	May 1955	0.00	0.01	0.01	0.00	0.02
54	June 1955	0.01	0.01	0.02	0.00	0.03
55	July 1955	0.01	0.02	0.03	0.00	0.03
56	Aug 1955	0.01	0.03	0.03	0.00	0.04
57	Sept 1955	0.02	0.04	0.04	0.00	0.05
58	Oct 1955	0.03	0.05	0.05	0.00	0.07
59	Nov 1955	0.04	0.06	0.07	0.00	0.08
60	Dec 1955	0.06	0.08	0.08	0.01	0.10
61	Jan 1956	0.08	0.11	0.10	0.01	0.12
62	Feb 1956	0.10	0.14	0.12	0.01	0.14
63	Mar 1956	0.13	0.17	0.15	0.01	0.17
64	Apr 1956	0.17	0.22	0.18	0.01	0.20
65	May 1956	0.23	0.27	0.21	0.02	0.23
66	June 1956	0.29	0.33	0.25	0.02	0.26
67	July 1956	0.36	0.40	0.29	0.02	0.30
68	Aug 1956	0.46	0.49	0.33	0.03	0.34
69	Sept 1956	0.57	0.59	0.38	0.03	0.39
70	Oct 1956	0.70	0.70	0.44	0.04	0.44
71	Nov 1956	0.85	0.83	0.50	0.05	0.49
72	Dec 1956	1.04	0.97	0.57	0.06	0.55
73	Jan 1957	1.25	1.14	0.64	0.06	0.61
74	Feb 1957	1.47	1.33	0.72	0.07	0.68
75	Mar 1957	1.74	1.52	0.79	0.08	0.74
76	Apr 1957	2.04	1.75	0.88	0.10	0.81
77	May 1957	2.39	2.00	0.97	0.11	0.89
78	June 1957	2.77	2.28	1.08	0.12	0.97
79	July 1957	3.21	2.59	1.18	0.14	1.05
80	Aug 1957	3.69	2.93	1.29	0.16	1.13
81	Sept 1957	4.21	3.30	1.41	0.17	1.23
82	Oct 1957	4.79	3.69	1.53	0.19	1.32
83	Nov 1957	5.41	4.13	1.66	0.22	1.41
84	Dec 1957	6.10	4.59	1.80	0.24	1.51

Appendix A2. Simulated tetrachloroethylene and its degradation by-products in finished water, Tarawa Terrace water treatment plant, January 1951–March 1987[1].—Continued

[PCE, tetrachloroethylene; µg/L, microgram per liter; 1,2-tDCE, *trans*-1,2-dichloroethylene; TCE, trichloroethylene; VC, vinyl chloride; WTP, water treatment plant]

Stress period	Month and year	Single specie using MT3DMS model[2]	Multispecies, multiphase using TechFlowMP model[3]			
		[4]PCE, in µg/L	[5]PCE, in µg/L	[5]1,2 tDCE, in µg/L	[5]TCE, in µg/L	[5]VC, in µg/L
85	Jan 1958	6.86	5.11	1.94	0.26	1.62
86	Feb 1958	7.60	5.65	2.09	0.29	1.72
87	Mar 1958	8.47	6.17	2.22	0.31	1.81
88	Apr 1958	9.37	6.79	2.38	0.34	1.92
89	May 1958	10.37	7.41	2.53	0.37	2.02
90	June 1958	11.39	8.10	2.70	0.41	2.13
91	July 1958	12.91	9.09	2.96	0.45	2.32
92	Aug 1958	14.12	9.88	3.14	0.49	2.44
93	Sept 1958	15.35	10.73	3.33	0.53	2.56
94	Oct 1958	16.69	11.58	3.52	0.57	2.68
95	Nov 1958	18.03	12.52	3.72	0.61	2.81
96	Dec 1958	19.49	13.46	3.92	0.66	2.94
97	Jan 1959	20.97	14.48	4.13	0.71	3.07
98	Feb 1959	22.35	15.54	4.34	0.76	3.21
99	Mar 1959	23.92	16.54	4.54	0.80	3.33
100	Apr 1959	25.49	17.70	4.77	0.85	3.48
101	May 1959	27.15	18.84	4.99	0.91	3.61
102	June 1959	28.81	20.09	5.23	0.96	3.77
103	July 1959	30.56	21.34	5.46	1.02	3.91
104	Aug 1959	32.36	22.66	5.69	1.08	4.05
105	Sept 1959	34.14	24.01	5.93	1.14	4.19
106	Oct 1959	36.01	25.35	6.16	1.20	4.32
107	Nov 1959	37.85	26.77	6.40	1.27	4.46
108	Dec 1959	39.78	28.18	6.64	1.33	4.60
109	Jan 1960	41.86	29.67	6.88	1.40	4.74
110	Feb 1960	43.85	31.17	7.12	1.46	4.86
111	Mar 1960	46.03	32.58	7.33	1.52	4.97
112	Apr 1960	48.15	34.16	7.57	1.59	5.10
113	May 1960	50.37	35.67	7.79	1.66	5.21
114	June 1960	52.51	37.24	8.03	1.73	5.33
115	July 1960	54.74	38.79	8.26	1.80	5.45
116	Aug 1960	56.96	40.45	8.51	1.87	5.59
117	Sept 1960	59.09	42.13	8.76	1.94	5.73
118	Oct 1960	61.30	43.80	9.02	2.02	5.86
119	Nov 1960	63.42	45.57	9.28	2.09	6.01
120	Dec 1960	65.61	47.31	9.54	2.17	6.15

Appendix A2. Simulated tetrachloroethylene and its degradation by-products in finished water, Tarawa Terrace water treatment plant, January 1951–March 1987[1].—Continued

[PCE, tetrachloroethylene; µg/L, microgram per liter; 1,2-tDCE, *trans*-1,2-dichloroethylene; TCE, trichloroethylene; VC, vinyl chloride; WTP, water treatment plant]

Stress period	Month and year	Single specie using MT3DMS model[2]	Multispecies, multiphase using TechFlowMP model[3]			
		[4]PCE, in µg/L	[5]PCE, in µg/L	[5]1,2-tDCE, in µg/L	[5]TCE, in µg/L	[5]VC, in µg/L
121	Jan 1961	67.69	49.15	9.82	2.25	6.30
122	Feb 1961	69.54	51.03	10.10	2.33	6.46
123	Mar 1961	71.56	52.73	10.35	2.41	6.61
124	Apr 1961	73.49	54.69	10.64	2.49	6.77
125	May 1961	75.49	56.57	10.92	2.58	6.92
126	June 1961	77.39	58.53	11.20	2.66	7.07
127	July 1961	79.36	60.43	11.46	2.75	7.22
128	Aug 1961	81.32	62.42	11.74	2.83	7.36
129	Sept 1961	83.19	64.40	12.01	2.92	7.51
130	Oct 1961	85.11	66.32	12.27	3.00	7.64
131	Nov 1961	86.95	68.33	12.55	3.09	7.79
132	Dec 1961	88.84	70.28	12.80	3.17	7.92
133	Jan 1962	60.88	47.74	8.63	2.15	5.32
134	Feb 1962	62.10	49.86	9.00	2.25	5.56
135	Mar 1962	62.94	51.28	9.17	2.31	5.64
136	Apr 1962	63.59	52.37	9.25	2.36	5.67
137	May 1962	64.17	53.18	9.28	2.39	5.66
138	June 1962	64.70	53.88	9.28	2.41	5.63
139	July 1962	65.23	54.48	9.28	2.43	5.60
140	Aug 1962	65.74	55.06	9.26	2.45	5.56
141	Sept 1962	66.22	55.59	9.24	2.46	5.52
142	Oct 1962	66.71	56.07	9.22	2.48	5.47
143	Nov 1962	67.18	56.54	9.19	2.49	5.42
144	Dec 1962	67.65	56.97	9.16	2.50	5.38
145	Jan 1963	68.06	57.40	9.13	2.51	5.33
146	Feb 1963	68.39	57.78	9.09	2.52	5.28
147	Mar 1963	68.73	58.11	9.06	2.53	5.24
148	Apr 1963	69.03	58.49	9.02	2.54	5.20
149	May 1963	69.33	58.81	8.98	2.55	5.15
150	June 1963	69.62	59.14	8.94	2.56	5.11
151	July 1963	69.90	59.42	8.90	2.57	5.06
152	Aug 1963	70.17	59.70	8.86	2.57	5.02
153	Sept 1963	70.43	59.97	8.82	2.57	4.98
154	Oct 1963	70.69	60.21	8.78	2.58	4.94
155	Nov 1963	70.93	60.45	8.74	2.58	4.90
156	Dec 1963	71.17	60.67	8.70	2.59	4.86

Appendix A2. Simulated tetrachloroethylene and its degradation by-products in finished water, Tarawa Terrace water treatment plant, January 1951–March 1987[1].—Continued

[PCE, tetrachloroethylene; µg/L, microgram per liter; 1,2-tDCE, *trans*-1,2-dichloroethylene; TCE, trichloroethylene; VC, vinyl chloride; WTP, water treatment plant]

Stress period	Month and year	Single specie using MT3DMS model[2]	Multispecies, multiphase using TechFlowMP model[3]			
		[4]PCE, in µg/L	[5]PCE, in µg/L	[5]1,2 tDCE, in µg/L	[5]TCE, in µg/L	[5]VC, in µg/L
157	Jan 1964	71.40	60.89	8.67	2.59	4.83
158	Feb 1964	63.77	54.39	7.69	2.31	4.27
159	Mar 1964	63.95	54.42	7.58	2.30	4.17
160	Apr 1964	64.08	54.43	7.50	2.29	4.10
161	May 1964	64.19	54.36	7.42	2.29	4.04
162	June 1964	64.27	54.29	7.35	2.28	3.98
163	July 1964	64.34	54.21	7.28	2.27	3.93
164	Aug 1964	64.39	54.14	7.22	2.26	3.88
165	Sept 1964	64.43	54.06	7.16	2.26	3.84
166	Oct 1964	64.47	53.99	7.10	2.25	3.79
167	Nov 1964	64.49	53.92	7.05	2.24	3.75
168	Dec 1964	64.50	53.85	7.00	2.24	3.72
169	Jan 1965	64.50	53.78	6.95	2.23	3.68
170	Feb 1965	64.49	53.72	6.90	2.23	3.65
171	Mar 1965	64.47	53.64	6.86	2.22	3.61
172	Apr 1965	64.45	53.59	6.82	2.22	3.58
173	May 1965	64.42	53.52	6.78	2.21	3.55
174	June 1965	64.38	53.47	6.74	2.21	3.52
175	July 1965	64.33	53.40	6.70	2.20	3.50
176	Aug 1965	64.27	53.34	6.66	2.20	3.47
177	Sept 1965	64.20	53.27	6.63	2.19	3.44
178	Oct 1965	64.13	53.20	6.59	2.19	3.42
179	Nov 1965	64.05	53.14	6.56	2.18	3.40
180	Dec 1965	63.97	53.07	6.53	2.18	3.37
181	Jan 1966	63.88	53.00	6.50	2.17	3.35
182	Feb 1966	63.79	52.93	6.47	2.17	3.33
183	Mar 1966	63.68	52.84	6.44	2.16	3.31
184	Apr 1966	63.57	52.78	6.41	2.16	3.29
185	May 1966	63.46	52.70	6.38	2.15	3.27
186	June 1966	63.34	52.63	6.35	2.15	3.25
187	July 1966	63.21	52.54	6.33	2.14	3.23
188	Aug 1966	63.08	52.46	6.30	2.14	3.21
189	Sept 1966	62.94	52.38	6.27	2.13	3.20
190	Oct 1966	62.80	52.28	6.25	2.13	3.18
191	Nov 1966	62.65	52.20	6.22	2.12	3.16
192	Dec 1966	62.50	52.11	6.19	2.12	3.14

Appendix A2. Simulated tetrachloroethylene and its degradation by-products in finished water, Tarawa Terrace water treatment plant, January 1951–March 1987[1].—Continued

[PCE, tetrachloroethylene; µg/L, microgram per liter; 1,2-tDCE, *trans*-1,2-dichloroethylene; TCE, trichloroethylene; VC, vinyl chloride; WTP, water treatment plant]

Stress-period	Month and year	Single specie using MT3DMS model[2]	Multispecies, multiphase using TechFlowMP model[3]			
		[4]PCE, in µg/L	[5]PCE, in µg/L	[5]1,2-tDCE, in µg/L	[5]TCE, in µg/L	[5]VC, in µg/L
193	Jan 1967	62.25	52.02	6.17	2.11	3.13
194	Feb 1967	61.99	51.90	6.14	2.11	3.11
195	Mar 1967	61.67	51.76	6.11	2.10	3.09
196	Apr 1967	61.35	51.61	6.08	2.09	3.07
197	May 1967	61.02	51.43	6.04	2.08	3.05
198	June 1967	60.69	51.23	6.00	2.07	3.03
199	July 1967	60.37	51.02	5.96	2.06	3.00
200	Aug 1967	60.05	50.79	5.92	2.05	2.98
201	Sept 1967	59.74	50.57	5.87	2.04	2.95
202	Oct 1967	59.43	50.34	5.83	2.03	2.92
203	Nov 1967	59.13	50.11	5.79	2.02	2.90
204	Dec 1967	58.83	49.89	5.75	2.01	2.87
205	Jan 1968	58.41	49.66	5.70	2.00	2.85
206	Feb 1968	57.95	49.40	5.66	1.99	2.82
207	Mar 1968	57.43	49.10	5.60	1.97	2.79
208	Apr 1968	56.94	48.77	5.55	1.96	2.76
209	May 1968	56.45	48.43	5.49	1.94	2.73
210	June 1968	55.98	48.07	5.43	1.93	2.69
211	July 1968	55.49	47.67	5.36	1.91	2.65
212	Aug 1968	55.02	47.26	5.29	1.89	2.61
213	Sept 1968	54.58	46.84	5.23	1.87	2.57
214	Oct 1968	54.13	46.43	5.16	1.85	2.54
215	Nov 1968	53.71	46.03	5.10	1.84	2.50
216	Dec 1968	53.28	45.63	5.04	1.82	2.46
217	Jan 1969	53.07	45.24	4.98	1.80	2.43
218	Feb 1969	52.97	44.91	4.93	1.79	2.40
219	Mar 1969	52.94	44.64	4.88	1.78	2.37
220	Apr 1969	52.93	44.47	4.86	1.77	2.35
221	May 1969	52.93	44.32	4.83	1.76	2.34
222	June 1969	52.92	44.20	4.81	1.76	2.32
223	July 1969	52.90	44.09	4.79	1.75	2.31
224	Aug 1969	52.86	44.01	4.78	1.75	2.30
225	Sept 1969	52.81	43.92	4.77	1.75	2.29
226	Oct 1969	52.75	43.83	4.76	1.74	2.29
227	Nov 1969	55.19	45.75	4.97	1.82	2.38
228	Dec 1969	55.19	45.96	5.01	1.83	2.42

Appendix A2. Simulated tetrachloroethylene and its degradation by-products in finished water, Tarawa Terrace water treatment plant, January 1951–March 1987[1].—Continued

[PCE, tetrachloroethylene; µg/L, microgram per liter; 1,2-tDCE, *trans*-1,2-dichloroethylene; TCE, trichloroethylene; VC, vinyl chloride; WTP, water treatment plant]

Stress period	Month and year	Single specie using MT3DMS model[2]	Multispecies, multiphase using TechFlowMP model[3]			
		[4]PCE, in µg/L	[5]PCE, in µg/L	[5]1,2 tDCE, in µg/L	[5]TCE, in µg/L	[5]VC, in µg/L
229	Jan 1970	55.01	46.05	5.03	1.84	2.43
230	Feb 1970	54.79	46.03	5.03	1.84	2.43
231	Mar 1970	54.49	45.94	5.03	1.83	2.43
232	Apr 1970	54.20	45.84	5.03	1.83	2.44
233	May 1970	53.90	45.70	5.01	1.82	2.44
234	June 1970	53.61	45.54	5.00	1.82	2.43
235	July 1970	53.32	45.37	4.98	1.81	2.43
236	Aug 1970	53.04	45.20	4.96	1.80	2.42
237	Sept 1970	52.78	45.00	4.94	1.79	2.41
238	Oct 1970	52.53	44.79	4.91	1.78	2.40
239	Nov 1970	52.29	44.58	4.89	1.78	2.39
240	Dec 1970	52.05	44.37	4.87	1.77	2.38
241	Jan 1971	51.96	44.17	4.84	1.76	2.37
242	Feb 1971	51.93	43.99	4.82	1.75	2.35
243	Mar 1971	51.95	43.86	4.80	1.74	2.34
244	Apr 1971	51.99	43.76	4.79	1.74	2.34
245	May 1971	52.03	43.66	4.78	1.74	2.33
246	June 1971	52.08	43.60	4.78	1.73	2.33
247	July 1971	52.12	43.53	4.77	1.73	2.33
248	Aug 1971	52.16	43.47	4.77	1.73	2.33
249	Sept 1971	52.20	43.41	4.77	1.73	2.33
250	Oct 1971	52.23	43.35	4.77	1.72	2.33
251	Nov 1971	52.26	43.31	4.77	1.72	2.33
252	Dec 1971	52.29	43.26	4.77	1.72	2.34
253	Jan 1972	49.34	41.02	4.53	1.63	2.22
254	Feb 1972	49.01	40.49	4.44	1.61	2.17
255	Mar 1972	48.68	40.01	4.37	1.58	2.13
256	Apr 1972	48.40	39.51	4.30	1.56	2.09
257	May 1972	48.14	39.03	4.24	1.54	2.06
258	June 1972	47.90	38.55	4.17	1.52	2.02
259	July 1972	47.67	38.11	4.11	1.50	1.98
260	Aug 1972	47.45	37.68	4.05	1.48	1.95
261	Sept 1972	47.25	37.26	3.99	1.46	1.92
262	Oct 1972	47.05	36.88	3.94	1.45	1.89
263	Nov 1972	46.87	36.51	3.89	1.43	1.86
264	Dec 1972	46.69	36.15	3.85	1.42	1.84

Appendix A2. Simulated tetrachloroethylene and its degradation by-products in finished water, Tarawa Terrace water treatment plant, January 1951–March 1987[1].—Continued

[PCE, tetrachloroethylene; µg/L, microgram per liter; 1,2-tDCE, *trans*-1,2-dichloroethylene; TCE, trichloroethylene; VC, vinyl chloride; WTP, water treatment plant]

Stress-period	Month and year	Single specie using MT3DMS model[2]	Multispecies, multiphase using TechFlowMP model[3]			
		[4]PCE, in µg/L	[5]PCE, in µg/L	[5]1,2-tDCE, in µg/L	[5]TCE, in µg/L	[5]VC, in µg/L
265	Jan 1973	54.28	41.48	4.40	1.62	2.10
266	Feb 1973	54.19	42.32	4.57	1.67	2.21
267	Mar 1973	53.98	42.49	4.60	1.68	2.23
268	Apr 1973	53.76	42.42	4.60	1.68	2.24
269	May 1973	53.52	42.25	4.59	1.67	2.24
270	June 1973	53.30	42.05	4.58	1.66	2.25
271	July 1973	53.08	41.78	4.56	1.65	2.24
272	Aug 1973	52.87	41.53	4.53	1.64	2.23
273	Sept 1973	52.68	41.27	4.51	1.63	2.22
274	Oct 1973	52.51	41.01	4.48	1.62	2.21
275	Nov 1973	52.35	40.75	4.45	1.61	2.20
276	Dec 1973	52.20	40.48	4.42	1.60	2.19
277	Jan 1974	52.43	40.22	4.40	1.59	2.17
278	Feb 1974	52.82	40.13	4.39	1.59	2.17
279	Mar 1974	53.39	40.10	4.38	1.58	2.16
280	Apr 1974	53.99	40.20	4.40	1.59	2.17
281	May 1974	54.63	40.35	4.43	1.60	2.18
282	June 1974	55.25	40.59	4.48	1.61	2.21
283	July 1974	55.90	40.82	4.52	1.62	2.24
284	Aug 1974	56.53	41.08	4.57	1.63	2.27
285	Sept 1974	57.10	41.35	4.62	1.64	2.31
286	Oct 1974	57.70	41.61	4.68	1.65	2.34
287	Nov 1974	58.30	41.91	4.74	1.67	2.39
288	Dec 1974	58.92	42.19	4.81	1.68	2.43
289	Jan 1975	61.00	43.76	5.02	1.74	2.55
290	Feb 1975	61.24	43.90	5.06	1.75	2.59
291	Mar 1975	61.41	44.03	5.11	1.75	2.63
292	Apr 1975	61.57	44.18	5.16	1.76	2.68
293	May 1975	61.72	44.29	5.20	1.77	2.71
294	June 1975	61.88	44.38	5.24	1.77	2.75
295	July 1975	62.05	44.45	5.28	1.77	2.78
296	Aug 1975	62.25	44.52	5.31	1.78	2.81
297	Sept 1975	62.46	44.57	5.34	1.78	2.83
298	Oct 1975	62.69	44.62	5.36	1.78	2.85
299	Nov 1975	62.92	44.69	5.39	1.78	2.87
300	Dec 1975	63.18	44.74	5.41	1.78	2.89

Appendix A2. Simulated tetrachloroethylene and its degradation by-products in finished water, Tarawa Terrace water treatment plant, January 1951–March 1987[1].—Continued

[PCE, tetrachloroethylene; μg/L, microgram per liter; 1,2-tDCE, *trans*-1,2-dichloroethylene; TCE, trichloroethylene; VC, vinyl chloride; WTP, water treatment plant]

Stress period	Month and year	Single specie using MT3DMS model[2]	Multispecies, multiphase using TechFlowMP model[3]			
		[4]PCE, in μg/L	[5]PCE, in μg/L	[5]1,2 tDCE, in μg/L	[5]TCE, in μg/L	[5]VC, in μg/L
301	Jan 1976	73.96	51.53	6.24	2.06	3.34
302	Feb 1976	74.94	53.43	6.62	2.15	3.60
303	Mar 1976	75.97	54.44	6.80	2.20	3.72
304	Apr 1976	76.97	55.38	6.99	2.24	3.85
305	May 1976	78.00	56.21	7.16	2.28	3.98
306	June 1976	79.02	57.07	7.34	2.32	4.10
307	July 1976	80.07	57.86	7.51	2.35	4.22
308	Aug 1976	81.13	58.73	7.69	2.39	4.34
309	Sept 1976	82.17	59.58	7.86	2.43	4.46
310	Oct 1976	83.25	60.41	8.02	2.46	4.57
311	Nov 1976	84.31	61.28	8.19	2.50	4.68
312	Dec 1976	85.41	62.10	8.35	2.53	4.79
313	Jan 1977	86.61	62.97	8.52	2.57	4.89
314	Feb 1977	87.70	63.98	8.71	2.62	5.01
315	Mar 1977	88.91	64.81	8.86	2.65	5.11
316	Apr 1977	90.10	65.83	9.05	2.70	5.22
317	May 1977	91.32	66.76	9.21	2.74	5.32
318	June 1977	92.53	67.76	9.38	2.78	5.43
319	July 1977	93.75	68.70	9.55	2.82	5.53
320	Aug 1977	94.99	69.70	9.72	2.86	5.63
321	Sept 1977	96.20	70.70	9.88	2.90	5.72
322	Oct 1977	97.42	71.65	10.04	2.94	5.82
323	Nov 1977	98.62	72.71	10.21	2.99	5.92
324	Dec 1977	99.84	73.68	10.36	3.03	6.00
325	Jan 1978	101.18	74.73	10.53	3.07	6.10
326	Feb 1978	102.77	76.25	10.80	3.14	6.26
327	Mar 1978	103.04	78.73	11.26	3.26	6.56
328	Apr 1978	104.31	77.97	11.02	3.21	6.37
329	May 1978	105.18	79.28	11.27	3.27	6.53
330	June 1978	106.88	79.72	11.29	3.28	6.51
331	July 1978	107.95	82.31	11.78	3.41	6.83
332	Aug 1978	108.69	83.81	12.00	3.47	6.96
333	Sept 1978	109.61	84.16	12.00	3.48	6.93
334	Oct 1978	111.18	84.92	12.09	3.51	6.97
335	Nov 1978	111.08	87.48	12.55	3.63	7.25
336	Dec 1978	111.93	85.67	12.04	3.52	6.87

Appendix A2. Simulated tetrachloroethylene and its degradation by-products in finished water, Tarawa Terrace water treatment plant, January 1951–March 1987[1].—Continued

[PCE, tetrachloroethylene; µg/L, microgram per liter; 1,2-tDCE, *trans*-1,2-dichloroethylene; TCE, trichloroethylene; VC, vinyl chloride; WTP, water treatment plant]

Stress period	Month and year	Single specie using MT3DMS model[2]	Multispecies, multiphase using TechFlowMP model[3]			
		[4]PCE, in µg/L	[5]PCE, in µg/L	[5]1,2-tDCE, in µg/L	[5]TCE, in µg/L	[5]VC, in µg/L
337	Jan 1979	113.14	85.41	11.95	3.50	6.79
338	Feb 1979	114.05	86.75	12.16	3.56	6.91
339	Mar 1979	114.98	87.55	12.23	3.60	6.93
340	Apr 1979	115.82	88.43	12.32	3.63	6.97
341	May 1979	116.68	89.21	12.40	3.66	7.00
342	June 1979	117.47	90.09	12.49	3.70	7.05
343	July 1979	118.29	90.82	12.56	3.73	7.07
344	Aug 1979	119.08	91.67	12.65	3.76	7.11
345	Sept 1979	119.82	92.44	12.72	3.79	7.14
346	Oct 1979	120.59	93.22	12.81	3.82	7.18
347	Nov 1979	121.31	94.00	12.88	3.85	7.21
348	Dec 1979	122.04	94.78	12.96	3.89	7.24
349	Jan 1980	123.28	95.56	13.03	3.92	7.27
350	Feb 1980	122.98	98.20	13.49	4.04	7.56
351	Mar 1980	124.03	96.35	12.98	3.94	7.19
352	Apr 1980	123.90	97.86	13.28	4.01	7.39
353	May 1980	124.69	96.00	12.78	3.90	7.03
354	June 1980	125.83	96.23	12.80	3.91	7.03
355	July 1980	0.72	0.00	0.00	0.00	0.00
356	Aug 1980	0.75	0.00	0.00	0.00	0.00
357	Sept 1980	121.36	95.07	12.43	3.92	6.83
358	Oct 1980	121.72	91.40	11.24	3.63	5.84
359	Nov 1980	122.14	91.00	11.17	3.63	5.82
360	Dec 1980	122.95	90.64	11.14	3.62	5.81
361	Jan 1981	114.05	84.14	10.41	3.37	5.46
362	Feb 1981	114.39	84.80	10.53	3.41	5.55
363	Mar 1981	115.60	84.13	10.37	3.37	5.44
364	Apr 1981	116.55	85.90	10.74	3.46	5.69
365	May 1981	117.30	87.53	11.02	3.54	5.87
366	June 1981	118.36	88.90	11.26	3.60	6.03
367	July 1981	133.29	102.10	13.12	4.17	7.09
368	Aug 1981	134.31	105.46	13.75	4.33	7.50
369	Sept 1981	120.72	96.34	12.64	3.96	6.93
370	Oct 1981	121.04	96.29	12.60	3.95	6.90
371	Nov 1981	121.41	96.69	12.67	3.96	6.93
372	Dec 1981	121.81	97.27	12.74	3.98	6.97

Appendix A2. Simulated tetrachloroethylene and its degradation by-products in finished water, Tarawa Terrace water treatment plant, January 1951–March 1987[1].—Continued

[PCE, tetrachloroethylene; µg/L, microgram per liter; 1,2-tDCE, *trans*-1,2-dichloroethylene; TCE, trichloroethylene; VC, vinyl chloride; WTP, water treatment plant]

Stress-period	Month and year	Single specie using MT3DMS model[2]	Multispecies, multiphase using TechFlowMP model[3]			
		[4]PCE, in µg/L	[5]PCE, in µg/L	[5]1,2 tDCE, in µg/L	[5]TCE, in µg/L	[5]VC, in µg/L
373	Jan 1982	103.95	81.28	10.65	3.33	5.81
374	Feb 1982	105.86	83.47	11.06	3.43	6.09
375	Mar 1982	107.52	85.42	11.40	3.51	6.31
376	Apr 1982	108.83	87.32	11.75	3.60	6.55
377	May 1982	148.50	120.45	16.30	4.98	9.13
378	June 1982	110.78	92.65	12.81	3.86	7.26
379	July 1982	111.98	92.98	12.77	3.86	7.21
380	Aug 1982	113.07	94.09	12.97	3.91	7.34
381	Sept 1982	114.04	95.33	13.18	3.96	7.46
382	Oct 1982	114.60	96.51	13.37	4.01	7.57
383	Nov 1982	113.87	96.63	13.31	4.00	7.51
384	Dec 1982	115.16	93.14	12.43	3.80	6.88
385	Jan 1983	1.25	0.10	0.04	0.00	0.05
386	Feb 1983	1.29	0.12	0.05	0.01	0.07
387	Mar 1983	111.76	88.43	11.55	3.65	6.37
388	Apr 1983	112.66	86.39	10.85	3.43	5.77
389	May 1983	113.97	87.67	11.04	3.52	5.88
390	June 1983	106.10	82.26	10.54	3.33	5.70
391	July 1983	116.70	92.03	11.95	3.75	6.52
392	Aug 1983	117.72	94.46	12.45	3.87	6.87
393	Sept 1983	117.83	96.92	12.94	3.99	7.21
394	Oct 1983	117.97	96.60	12.82	3.96	7.12
395	Nov 1983	118.63	95.49	12.58	3.89	6.95
396	Dec 1983	120.78	95.52	12.60	3.89	6.96
397	Jan 1984	132.87	111.52	15.09	4.61	8.43
398	Feb 1984	180.39	145.48	19.20	5.94	10.56
399	Mar 1984	183.02	155.54	21.34	6.47	11.97
400	Apr 1984	151.46	132.07	18.23	5.52	10.26
401	May 1984	153.42	132.19	18.09	5.49	10.13
402	June 1984	182.13	158.14	21.85	6.60	12.28
403	July 1984	156.39	140.96	19.72	5.92	11.14
404	Aug 1984	170.47	118.88	16.05	4.81	8.94
405	Sept 1984	181.22	149.36	19.60	6.17	11.20
406	Oct 1984	173.73	136.04	17.33	5.56	9.39
407	Nov 1984	173.77	131.63	16.46	5.34	8.87
408	Dec 1984	173.18	128.47	15.83	5.18	8.46

Appendix A2. Simulated tetrachloroethylene and its degradation by-products in finished water, Tarawa Terrace water treatment plant, January 1951–March 1987[1].—Continued

[PCE, tetrachloroethylene; µg/L, microgram per liter; 1,2-tDCE, *trans*-1,2-dichloroethylene; TCE, trichloroethylene; VC, vinyl chloride; WTP, water treatment plant]

Stress period	Month and year	Single specie using MT3DMS model[2]	Multispecies, multiphase using TechFlowMP model[3]			
		[4]PCE, in µg/L	[5]PCE, in µg/L	[5]1,2-tDCE, in µg/L	[5]TCE, in µg/L	[5]VC, in µg/L
409	Jan 1985	176.12	127.80	15.48	5.13	8.20
410	Feb 1985	3.64	1.10	0.29	0.05	0.22
411	Mar 1985	8.71	3.88	0.68	0.17	0.47
412	Apr 1985	8.09	3.70	0.68	0.16	0.49
413	May 1985	4.76	1.65	0.44	0.07	0.35
414	June 1985	5.14	1.88	0.50	0.08	0.41
415	July 1985	5.54	2.10	0.56	0.09	0.47
416	Aug 1985	6.01	2.34	0.63	0.10	0.52
417	Sept 1985	6.50	2.62	0.71	0.12	0.59
418	Oct 1985	7.06	2.91	0.79	0.13	0.65
419	Nov 1985	7.64	3.24	0.87	0.15	0.71
420	Dec 1985	8.27	3.58	0.95	0.16	0.76
421	Jan 1986	8.85	3.95	1.04	0.18	0.82
422	Feb 1986	9.42	4.24	1.08	0.19	0.83
423	Mar 1986	12.14	5.40	1.34	0.24	1.01
424	Apr 1986	10.83	4.93	1.20	0.22	0.89
425	May 1986	11.56	5.25	1.25	0.23	0.91
426	June 1986	12.28	5.61	1.30	0.25	0.92
427	July 1986	13.06	5.97	1.35	0.26	0.94
428	Aug 1986	13.84	6.36	1.39	0.28	0.96
429	Sept 1986	14.61	6.75	1.44	0.30	0.97
430	Oct 1986	15.42	7.12	1.48	0.31	0.99
431	Nov 1986	16.21	7.52	1.52	0.33	1.00
432	Dec 1986	17.03	7.89	1.56	0.34	1.01
433	Jan 1987	17.85	8.28	1.59	0.36	1.01
434	Feb 1987	18.49	8.71	1.64	0.38	1.03
435	Mar 1987	**WTP closed**	**WTP closed**	**WTP closed**	**WTP closed**	**WTP closed**

[1]Current maximum contaminant levels (MCLs) are: tetrachloroethylene (PCE) and trichloroethylene (TCE), 5 µg/L; *trans*-1,2-dichloroethylene (1,2-tDCE), 100 µg/L; and vinyl chloride (VC), 2 µg/L (USEPA, 2003); effective dates for MCLs are as follows: TCE and VC, January 9, 1989; PCE and 1,2-tDCE, July 6, 1992 (40 CFR, Section 141.60, Effective Dates, July 1, 2002, ed.)

[2]MT3DMS: A three-dimensional mass transport, multispecies model developed by C. Zheng and P. Wang (1999) on behalf of the U.S. Army Engineer Research and Development Center in Vicksburg, Mississippi (*http://hydro.geo.ua.edu/mt3d/*)

[3]TechFlowMP: A three-dimensional multispecies, multiphase mass transport model developed by the Multimedia Environmental Simulations Laboratory (Jang and Aral 2007) at the Georgia Institute of Technology, Atlanta, Georgia (*http://mesl.ce.gatech.edu*)

[4]Results from Chapter F report (Faye In press 2007b)

[5]Results from Chapter G report (Jang and Aral In press 2007)

Appendix A3. Questions and Answers

What is the purpose of the ATSDR health study?

Two of the three drinking-water systems that served family housing at U.S. Marine Corps Base Camp Lejeune were contaminated. One system, the Tarawa Terrace drinking-water system, was mostly contaminated with tetrachloroethylene (or perchloroethylene, PCE) from off-base dry-cleaning operations. The other system, the Hadnot Point drinking-water system, was contaminated mostly with trichloroethylene (TCE) from on-base industrial operations. The contaminated wells were continuously used until 1985 and sporadically used until early 1987. ATSDR's health study will try to determine if there was a link between in utero and infant (up to 1 year of age) exposures to drinking-water contaminants and specific birth defects and childhood cancers. The study includes births occurring during 1968–1985 to mothers who lived in base family housing during their pregnancy. The birth defects and childhood cancers that will be studied are:

- neural tube defects (spina bifida and anencephaly),
- cleft lip and cleft palate, and
- leukemia and non-Hodgkin's lymphoma.

Why is ATSDR studying exposure to VOC-contaminated drinking water since other studies have already done this?

Only a few studies have looked at the risk of birth defects and childhood cancers among children born to women exposed during pregnancy to volatile organic compounds (VOCs) such as TCE and PCE in drinking water. This study is unique because it will estimate monthly levels of drinking-water contaminants to determine exposures.

What is in the ATSDR reports about the Tarawa Terrace drinking-water system?

Chapter A provides a summary of detailed technical findings (found in Chapters B–K) for Tarawa Terrace and vicinity. The findings focus on modeling techniques used to reconstruct historical and present-day conditions of groundwater flow, contaminant fate and transport, and distribution of drinking water. Information from the water-modeling analyses will be given to researchers conducting the health study. (Future analyses and reports will present information and data about the Hadnot Point drinking-water system.)

Why is ATSDR using water modeling to estimate exposure rather than real data?

Data on the levels of VOC contaminants in drinking water are not available before 1982. To determine levels before 1982, ATSDR is using a process called "historical reconstruction." This process uses data on the amount of the chemicals dumped on the ground. It also uses the properties of the soil, the groundwater, and the water-distribution system. These data are then used in computer models. The models estimate when contaminants first reached drinking-water wells. The models also estimate monthly levels of contaminants in drinking water at family housing units. This information is important for the health study. It can also be used by those who lived in base family housing to estimate their exposures.

What is a water model?

A water model is a general term that describes a computer program used to solve a set of mathematical equations that describe the:

- flow of groundwater in aquifers,
- movement of a contaminant mixed with groundwater,
- mixing of water from contaminated and uncontaminated water-supply wells at a water treatment plant, or
- flow of water and contaminants from reservoirs, wells, and storage tanks through a network of pipelines.

What information did ATSDR use to develop the water models and what were the sources of the information?

The historical reconstruction process required information and data describing physical characteristics of the groundwater-flow system, conservation principles that describe the flow system, the specific data on the contaminant (PCE) and its degradation by-products, and the water-distribution system. The following specific data needs were required:

- aquifer characteristics: geohydrologic, hydraulic, water production, fate, transformation, and transport;
- chemical properties characteristics: physical, fate, transformation, and transport; and
- water-distribution system characteristics: pipeline characteristics, storage-tank geometry, pumps, water-production data, and water-quality parameters.

Information and data used to conduct the historical reconstruction analysis were obtained from a variety of sources. These sources included ATSDR, U.S. Environmental Protection Agency, Environmental Management Division of U.S. Marine Corps Base Camp Lejeune, U.S. Geological Survey, private consulting organizations, published scientific literature, and community groups representing former marines and their families. Chapters A and K of the Tarawa Terrace report provide searchable electronic databases—on DVD format—of information and data sources used to conduct the historical reconstruction analysis.

How can ATSDR be sure that water-modeling results represent historical "real-world" conditions?

A water model requires information on the specific properties or "parameters" of the soil, groundwater, and water system at the base. Often assumptions are needed because complete and accurate data are not available for all the parameters that must be modeled. In particular, historical data are often lacking. To be sure that water-modeling results are accurate and represent historical "real-world" conditions, a model needs to be calibrated. A calibration process compares model results with available "real-world" data to see if the model's results accurately reflect "real-world" conditions. This is done in the following way. Models are constructed using different combinations of values for the parameters. Each model makes a prediction about the groundwater-flow rate, the amount of water produced by each well, and the contamination level in the drinking-water system at a particular point in time. These predictions are then compared to "real-world" data. When the combination of parameter values that best predicts the actual "real-world" conditions are selected, the model is "calibrated." The model is now ready to make predictions about historical conditions.

Why did ATSDR develop and calibrate two models for simulating the migration of PCE from ABC One-Hour Cleaners to Tarawa Terrace water-supply wells?

At first, ATSDR developed a model that simulated the fate and transport (migration) of PCE that was completely mixed in groundwater in the saturated zone (zone below the water table). The model code used is known as MT3DMS. ATSDR developed a second model because of suggestions from a panel of experts and requests from former marines and their technical advisers. The second model is capable of simulating the fate and transport of PCE and its degradation by-products of TCE, *trans*-1,2-dichloroethylene (1,2-tDCE), and vinyl chloride (VC) in the unsaturated zone (area above the water table) and the saturated zone. This model, known as TechFlowMP, is based on significantly more complex mathematical equations and formulations. This highly complex model also can simulate PCE and its degradation by-products in both the vapor and water phases. Values of simulated PCE concentrations in the saturated zone obtained using the two different models (MT3DMS and TechFlowMP) are very close.

Why is ATSDR providing simulated PCE concentrations in finished water at the Tarawa Terrace water treatment plant (WTP) rather than at locations of specific family housing units?

ATSDR did in-depth reviews of historical data, including water-supply well and WTP operational data when available. ATSDR concluded that the Tarawa Terrace water-distribution system—including the WTP—was *not* interconnected with other water-distribution systems at Camp Lejeune for any time longer than 2 weeks. All water arriving at the WTP was obtained solely from Tarawa Terrace water-supply wells. Also it was assumed to be completely and uniformly mixed prior to delivery to residents of Tarawa Terrace. On a monthly basis, the concentration of PCE delivered to specific family housing units at Tarawa Terrace was assumed to be the same as the simulated concentration of PCE in finished water at the WTP.

Can ATSDR water modeling results be used to determine the concentration of PCE that my family and I were exposed to on a daily basis?

No. The available data are not specific enough to accurately estimate daily levels of PCE in the Tarawa Terrace water system. The modeling approach used by ATSDR provides a high level of detail and accuracy to estimate monthly PCE exposure concentrations in finished water at the Tarawa Terrace WTP. It is assumed that simulated monthly concentrations of PCE represent a typical day during a month.

Were my family and I more exposed to contaminated drinking water than other families because we lived near one of the contaminated Tarawa Terrace water-supply wells?

No. Water from all Tarawa Terrace water-supply wells (uncontaminated and contaminated) was mixed at the WTP prior to being distributed through a network of pipelines to storage tanks and family housing areas. On a monthly basis, the concentration of PCE delivered to specific family housing units at Tarawa Terrace has been shown to be the same as the concentration of PCE in finished water at the WTP.

Were my family and I exposed to other contaminants besides PCE in finished drinking water while living in family housing at Tarawa Terrace?

Yes. A small amount of PCE degrades in the groundwater to other VOCs. These include TCE, 1,2-tDCE, and VC. Degradation by-products of PCE were found in water samples obtained on January 16, 1985, from Tarawa Terrace water-supply wells TT-23 and TT-26. Historical reconstruction analyses conducted by ATSDR and its partners provide simulated monthly concentrations of PCE and its degradation by-products in finished water at the Tarawa Terrace WTP.

How can I get a list of the monthly PCE (and PCE degradation by-product) concentrations in finished water that my family and I were exposed to at Tarawa Terrace?

ATSDR and its partners have developed a Web site where former Camp Lejeune residents can enter the dates they lived on base and receive information on whether they were exposed to VOCs and to what levels. The Web site will list the simulated monthly concentrations of PCE and its degradation by-products in finished water at the Tarawa Terrace WTP. The Web site can be accessed at *http://www.atsdr.cdc.gov/sites/lejeune/index.html.*

ATSDR's historical reconstruction analysis documents that Tarawa Terrace drinking water was contaminated with PCE that exceeded the current maximum contaminant level (MCL) of 5 micrograms per liter (μg/L) during 1957 and reached a maximum value of 183 μg/L. What does this mean in terms of my family's health?

ATSDR's exposure assessment cannot be used to determine whether you, or your family, suffered any health effects as a result of past exposure to PCE-contaminated drinking water at Camp Lejeune. The study will help determine if there is an association between certain birth defects and childhood cancers among children whose mothers used this water during pregnancy. Epidemiological studies such as this help improve scientific knowledge of the health effects of these chemicals.

The National Toxicology Program of the U.S. Department of Health and Human Services has stated that PCE "is reasonably anticipated to be a human carcinogen." However, the lowest level of PCE in drinking water at which health effects begin to occur is unknown. The MCL for PCE was set at 5 μg/L (or 5 parts per billion) in 1992 because, given the technology at that time, 5 μg/L was the lowest level that water systems could be required to achieve.

Many factors determine whether people will suffer adverse health effects because of chemical exposures. These factors include:

- dose (how much),
- duration (how long the contact period is),
- when in the course of life the exposures occurred (for example, while in utero, during early childhood, or in later years of life),
- genetic traits that might make a person more vulnerable to the chemical exposure, and
- other factors such as occupational exposures, exposures to other chemicals in the environment, gender, diet, lifestyle, and overall state of health.

What is soil vapor?

Soil vapor or soil gas is the air found in the open or pore spaces between soil particles in the soil above the water table (also called the "unsaturated zone"). The source of the soil vapor is the contaminated groundwater. PCE and its degradation by-products are VOCs; therefore, some amounts of these chemicals volatilize (or vaporize) off the groundwater plume and enter the soil in the unsaturated zone as gases. The soil vapor plume (also known as the "vapor-phase" plume) is the area where the gases or vapors have entered the soil in the unsaturated zone above the water table.

Could the soil vapor enter buildings at Tarawa Terrace?

Soil at Camp Lejeune is sandy, so the vapors can readily vaporize up to the surface. The buildings are on concrete slabs, so soil vapor can enter these buildings through cracks or perforations in slabs or through openings for pipes or wiring. In addition, because the vapor enters the building due to pressure differences, the operation of heating or air-conditioning systems can create a negative pressure in the building that draws the vapors from the soil into the building. This is similar to the situation with radon gas.

Could historical exposure to soil vapors contaminated with PCE and PCE degradation by-products affect the current ATSDR epidemiological study?

The results of the PCE and PCE degradation by-product soil vapor modeling will not have a major impact on the current epidemiological study of specific birth defects (neural tube defects, cleft lip, and cleft palate) and childhood cancers (leukemia and non-Hodgkin's lymphoma—also known as childhood hematopoietic cancers). The focus of the study is on drinking-water exposures to the fetus up to the child's first year of life. The drinking-water exposure is considerably greater than any exposure that might occur due to soil vapor infiltration into a home. However, the analysis may incorporate the soil vapor results to determine if these exposures significantly change the results obtained from the analysis of drinking-water exposures.

How certain is ATSDR that finished water exceeding the current MCL for PCE of 5 μg/L was delivered from the Tarawa Terrace WTP beginning in November 1957?

Historical data on the levels of contaminants in the drinking water is very limited. That is why there is uncertainty and variability concerning when the MCL of 5 μg/L was reached at the Tarawa Terrace WTP. Therefore, ATSDR and its partners conducted exhaustive sets of simulations to quantify this uncertainty and variability. Based on these analyses, finished water contaminated with PCE exceeding the MCL of 5 μg/L could have been delivered from the Tarawa Terrace WTP as early as December 1956 but most likely during November 1957.

How does ATSDR know where all of the Tarawa Terrace water-supply wells were located if they have been destroyed? What is the accuracy of this information?

ATSDR relied on a variety of sources to obtain information on the location of Tarawa Terrace water-supply wells. These included historical water utility maps, well construction and location maps, aerial photographs, use of geographic information system technology, and assistance from Environmental Management Division staff at U.S. Marine Corps Base Camp Lejeune. The accuracy of this information is believed to be within ± 50 feet of the actual well location.

What did ATSDR do to be sure that water-modeling analyses are scientifically credible?

Throughout this investigation, ATSDR has sought external expert input and review. Activities included convening an expert peer review panel and submitting individual chapter reports to outside national and international experts for technical reviews. For example, on March 28–29, 2005, ATSDR convened an external expert panel to review the approach used in conducting the historical reconstruction analysis. The panel also provided input and recommendations on preliminary analyses and modeling. ATSDR used a number of recommendations made by the panel members. ATSDR also used technical comments from outside expert reviewers when finalizing reports on Tarawa Terrace water-modeling analyses.

Where and how can I get a copy of this ATSDR report and the information and data that were used in the Tarawa Terrace water-modeling analyses?

A small number of printed copies of this report and subsequent chapter reports (A–K) will be available to interested parties and placed in public repositories. Electronic versions of all chapter reports will be available on the ATSDR Camp Lejeune Web site at *http://www.atsdr.cdc.gov/sites/lejeune/index.html*. Chapters A and K provide a searchable electronic database—on DVD format—of information and data sources used to conduct the historical reconstruction analysis for Tarawa Terrace and vicinity.

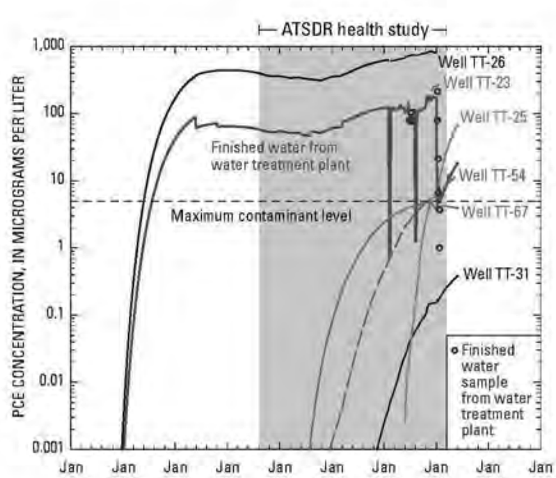
Analyses of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water at Tarawa Terrace and Vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina: Historical Reconstruction and Present-Day Conditions—Chapter A: Summary of Findings

Printed on recycled paper

EXHIBIT 11

Analyses of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water at Tarawa Terrace and Vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina: Historical Reconstruction and Present-Day Conditions

Chapter C: Simulation of Groundwater Flow



ATSDR
AGENCY FOR TOXIC SUBSTANCES AND DISEASE REGISTRY

Atlanta, Georgia–November 2007

Front cover: Historical reconstruction process using data, information sources, and water-modeling techniques to estimate historical exposures

Maps: U.S. Marine Corps Base Camp Lejeune, North Carolina; Tarawa Terrace area showing historical water-supply wells and site of ABC One-Hour Cleaners

Photographs on left: Ground storage tank STT-39 and four high-lift pumps used to deliver finished water from tank STT-39 to Tarawa Terrace water-distribution system

Photograph on right: Equipment used to measure flow and pressure at a hydrant during field test of the present-day (2004) water-distribution system

Graph: Reconstructed historical concentrations of tetrachloroethylene (PCE) at selected water-supply wells and in finished water at Tarawa Terrace water treatment plant

Analyses of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water at Tarawa Terrace and Vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina: Historical Reconstruction and Present-Day Conditions

Chapter C: Simulation of Groundwater Flow

By Robert E. Faye and Claudia Valenzuela

Agency for Toxic Substances and Disease Registry
U.S. Department of Health and Human Services
Atlanta, Georgia

November 2007

Authors

Robert E. Faye, MSCE, PE
Civil Engineer/Hydrologist
Robert E. Faye and Associates, Inc.
Consultant to Eastern Research Group, Inc.
Lexington, Massachusetts

Claudia Valenzuela, MSCE
Post Graduate Research Fellow
Oak Ridge Institute for Science and Education
Agency for Toxic Substances and Disease Registry
Atlanta, Georgia

For additional information write to:

Project Officer
Exposure-Dose Reconstruction Project
Division of Health Assessment and Consultation
Agency for Toxic Substances and Disease Registry
1600 Clifton Road, Mail Stop E-32
Atlanta, Georgia 30333

Suggested citation: Faye RE, and Valenzuela C. Analyses of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water at Tarawa Terrace and Vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina: Historical Reconstruction and Present-Day Conditions—Chapter C: Simulation of Groundwater Flow. Atlanta, GA: Agency for Toxic Substances and Disease Registry; 2007.

Foreword

The Agency for Toxic Substances and Disease Registry (ATSDR), an agency of the U.S. Department of Health and Human Services, is conducting an epidemiological study to evaluate whether in utero and infant (up to 1 year of age) exposures to volatile organic compounds in contaminated drinking water at U.S. Marine Corps Base Camp Lejeune, North Carolina, were associated with specific birth defects and childhood cancers. The study includes births occurring during the period 1968–1985 to women who were pregnant while they resided in family housing at the base. During 2004, the study protocol received approval from the Centers for Disease Control and Prevention Institutional Review Board and the U.S. Office of Management and Budget.

Historical exposure data needed for the epidemiological case-control study are limited. To obtain estimates of historical exposure, ATSDR is using water-modeling techniques and the process of historical reconstruction. These methods are used to quantify concentrations of particular contaminants in finished water and to compute the level and duration of human exposure to contaminated drinking water.

Final interpretive results for Tarawa Terrace and vicinity—based on information gathering, data interpretations, and water-modeling analyses—are presented as a series of ATSDR reports. These reports provide comprehensive descriptions of information, data analyses and interpretations, and modeling results used to reconstruct historical contaminant levels in drinking water at Tarawa Terrace and vicinity. Each topical subject within the water-modeling analysis and historical reconstruction process is assigned a chapter letter. Specific topics for each chapter report are listed below:

- **Chapter A:** Summary of Findings
- **Chapter B:** Geohydrologic Framework of the Castle Hayne Aquifer System
- **Chapter C:** Simulation of Groundwater Flow
- **Chapter D:** Properties and Degradation Pathways of Common Organic Compounds in Groundwater
- **Chapter E:** Occurrence of Contaminants in Groundwater
- **Chapter F:** Simulation of the Fate and Transport of Tetrachloroethylene (PCE) in Groundwater
- **Chapter G:** Simulation of Three-Dimensional Multispecies, Multiphase Mass Transport of Tetrachloroethylene (PCE) and Associated Degradation By-Products
- **Chapter H:** Effect of Groundwater Pumping Schedule Variation on Arrival of Tetrachloroethylene (PCE) at Water-Supply Wells and the Water Treatment Plant
- **Chapter I:** Parameter Sensitivity, Uncertainty, and Variability Associated with Model Simulations of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water
- **Chapter J:** Field Tests, Data Analyses, and Simulation of the Distribution of Drinking Water
- **Chapter K:** Supplemental Information

An electronic version of this report, *Chapter C: Simulation of Groundwater Flow*, will be made available on the ATSDR Camp Lejeune Web site at *http://www.atsdr.cdc.gov/sites/lejeune/index.html*. Readers interested solely in a summary of this report or any of the other reports should refer to *Chapter A: Summary of Findings* that also is available at the ATSDR Web site.

Contents

Figures

Tables

Conversion Factors

Multiply	By	To obtain
	Length	
inch	2.54	centimeter (cm)
foot (ft)	0.3048	meter (m)
mile (mi)	1.609	kilometer (km)
	Area	
square foot (ft^2)	0.09290	square meter (m^2)
square mile (mi^2)	259.0	hectare (ha)
square mile (mi^2)	2.590	square kilometer (km^2)
	Volume	
gallon (gal)	3.785	liter (L)
gallon (gal)	0.003785	cubic meter (m^3)
million gallons (MG)	3,785	cubic meter (m^3)
	Flow rate	
foot per day (ft/d)	0.3048	meter per day (m/d)
cubic foot per day (ft^3/d)	0.02832	cubic meter per day (m^3/d)
gallon per minute (gal/min)	0.06309	liter per second (L/s)
million gallons per day (MGD)	0.04381	cubic meter per second (m^3/s)
inch per year (in/yr)	25.4	millimeter per year (mm/yr)
	Mass	
pound, avoirdupois (lb)	4.535×10^{-4}	gram (g)
pound, avoirdupois (lb)	0.4536	kilogram (kg)
	Hydraulic conductivity	
foot per day (ft/d)	0.3048	meter per day (m/d)
	Transmissivity	
foot squared per day (ft^2/d)	0.09290	meter squared per day (m^2/d)

Concentration Conversion Factors

Unit	To convert to	Multiply by
microgram per liter (µg/L)	milligram per liter (mg/L)	0.001
microgram per liter (µg/L)	milligram per cubic meter (mg/m^3)	1
microgram per liter (µg/L)	microgram per cubic meter ($µg/m^3$)	1,000
parts per billion by volume (ppbv)	parts per million by volume (ppmv)	1,000

Vertical coordinate information is referenced to the National Geodetic Vertical Datum of 1929 (NGVD 29).

Horizontal coordinate information is referenced to the North American Datum of 1983 (NAD 83).

Altitude, as used in this report, refers to distance above the vertical datum.

Glossary and Abbreviations

1,1,1-TCA	1,1,1-trichloroethane
1,1- and 1,2-DCA	1,1- and 1,2-dichloroethane
AKA	also known as
ATSDR	Agency for Toxic Substances and Disease Registry
BTEX	benzene, toluene, ethylbenzene, and xylene
cfs	cubic foot per second
CEE	School of Civil and Environmental Engineering
CLP	Clinical Laboratory Program
DCE	1,1-DCE 1,1-dichloroethylene or 1,1-dichloroethene 1,2-DCE 1,2-dichloroethylene or 1,2-dichloroethene 1,2-cDCE *cis*-1,2-dichloroethylene or *cis*-1,2-dichloroethene 1,2-tDCE *trans*-1,2-dichloroethylene or *trans*-1,2-dichloroethene
GC/MS	chromatograph/mass spectrometer
MGD	million gallons per day
MODFLOW	original version of the numerical code for a three-dimensional groundwater-flow model, developed by the U.S. Geological Survey
MODFLOW-96	a three-dimensional groundwater-flow model, 1996 version, developed by the U.S. Geological Survey
NCDNRCD	North Carolina Department of Natural Resources and Community Development
PCE	tetrachloroethene, tetrachloroethylene, 1,1,2,2-tetrachloroethylene, or perchloroethylene; also know as PERC® or PERK®
PMWINPro™	Processing MODFLOW Pro, version 7.017
psi	pound per square inch
RASA	Regional Aquifer-System Analysis
TCE	1,1,2-trichloroethene, 1,1,2-trichloroethylene, or trichloroethylene
TCLP	Toxicity Characteristic Leaching Procedure
USEPA	U.S. Environmental Protection Agency
USGS	U.S. Geological Survey
UST	underground storage tank
VOC	volatile organic compound
WTP	water treatment plant

Use of trade names and commercial sources is for identification only and does not imply endorsement by the Agency for Toxic Substances and Disease Registry or the U.S. Department of Health and Human Services.

x

Analyses of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water at Tarawa Terrace and Vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina: Historical Reconstruction and Present-Day Conditions

Chapter C: Simulation of Groundwater Flow

By Robert E. Faye[1] and Claudia Valenzuela[2]

Abstract

Two of three water-distribution systems that have historically supplied drinking water to family housing at U.S. Marine Corps Base Camp Lejeune, North Carolina, were contaminated with volatile organic compounds (VOCs). Tarawa Terrace was contaminated mostly with tetrachloroethylene (PCE), and Hadnot Point was contaminated mostly with trichloroethylene (TCE). Because scientific data relating to the harmful effects of VOCs on a child or fetus are limited, the Agency for Toxic Substances and Disease Registry (ATSDR), an agency of the U.S. Department of Health and Human Services, is conducting an epidemiological study to evaluate potential associations between in utero and infant (up to 1 year of age) exposures to VOCs in contaminated drinking water at Camp Lejeune and specific birth defects and childhood cancers. The study includes births occurring during the period 1968–1985 to women who were pregnant while they resided in family housing at Camp Lejeune. Because limited measurements of contaminant and exposure data are available to support the epidemiological study, ATSDR is using modeling techniques to reconstruct historical conditions of groundwater flow, contaminant fate and transport, and the distribution of drinking water contaminated with VOCs delivered to family housing areas. This report, Chapter C, describes the development and calibration of a digital model applied to the simulation of groundwater flow within the Tarawa Terrace aquifer and Upper Castle Hayne aquifer system at and in the vicinity of the Tarawa Terrace housing areas.

[1] Consultant to Eastern Research Group, Inc., Lexington, Massachusetts.

[2] Oak Ridge Institute of Science and Education, Agency for Toxic Substances and Disease Registry, Atlanta, Georgia.

Background

U.S. Marine Corps Base Camp Lejeune is located in the Coastal Plain of North Carolina, in Onslow County, south of the City of Jacksonville and about 70 miles northeast of the City of Wilmington, North Carolina. The major cultural and geographic features of Camp Lejeune are shown in Figure C1 and on Plate 1. A major focus of this investigation is the water-supply and distribution network at Tarawa Terrace, a noncommissioned officers' housing area located near the northwest corner of the base (Plate 1). Tarawa Terrace was constructed during 1951 and was subdivided into housing areas I and II. Areas I and II originally contained a total of 1,846 housing units described as single, duplex, and multiplex, and accommodated a resident population of about 6,000 persons (Sheet 3 of 18, U.S. Marine Corps Base Camp Lejeune, Map of Tarawa Terrace II Quarters, June 30, 1961; Sheet 7 of 34, U.S. Marine Corps Base Camp Lejeune, Tarawa Terrace I Quarters, July 31, 1984). The general area of Tarawa Terrace is bordered on the east by Northeast Creek, to the south by New River and Northeast Creek, and generally to the west and north by drainage boundaries of these streams (Plate 1).

Groundwater is the source of contaminants that occurred in the water-distribution networks at Tarawa Terrace and was supplied to the distribution networks via water-supply wells open to one or several water-bearing zones of the Castle Hayne aquifer system. Faye (2007) provides a complete description of the geohydrologic framework at and in the vicinity of Tarawa Terrace, including data and maps that summarize the geometry of individual aquifers and confining units.

Contamination of groundwater by a halogenated hydrocarbon—tetrachloroethylene (PCE)—was first detected in water supplies at Tarawa Terrace during 1982 (Grainger Laboratories, written communication, August 10, 1982). The source

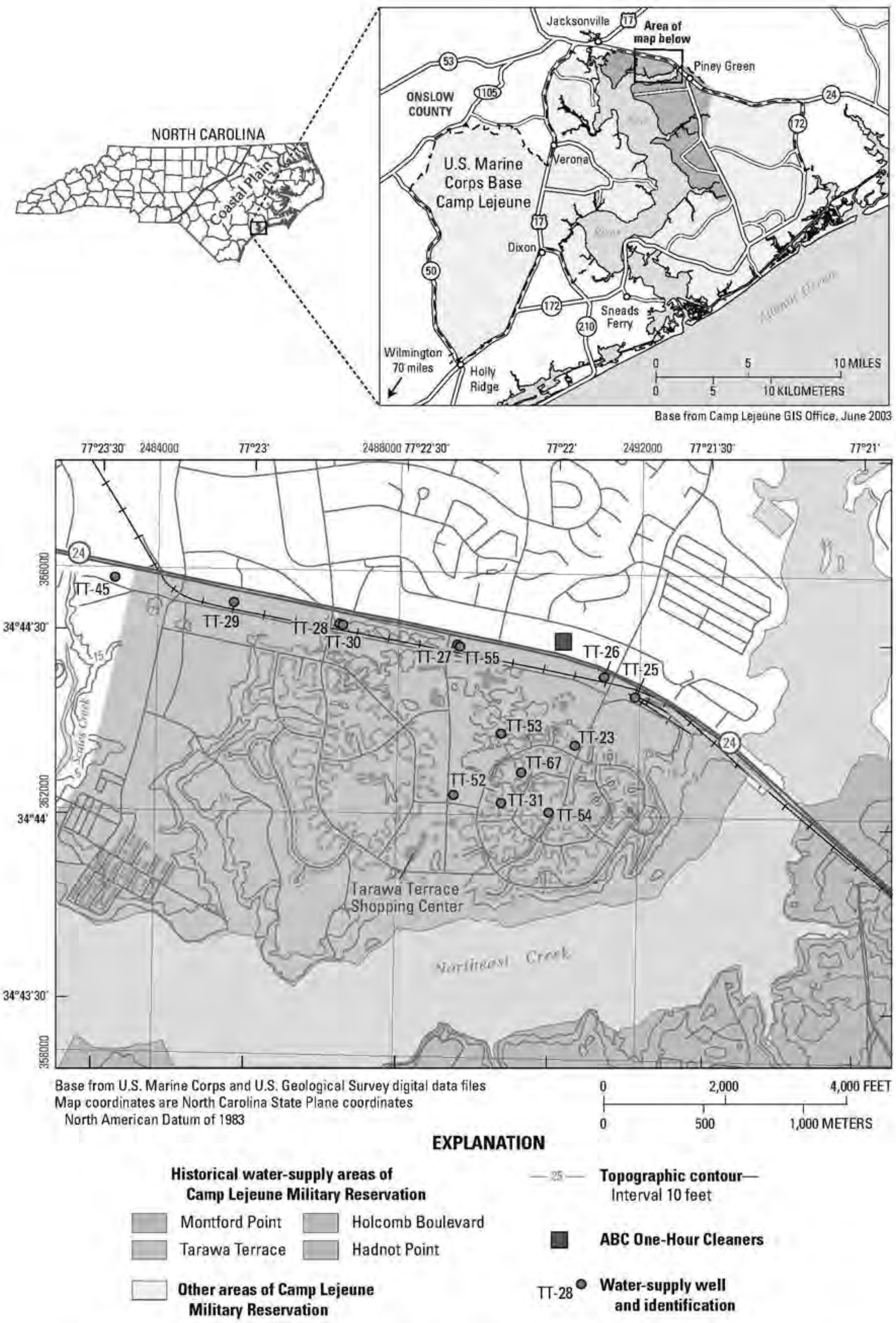


Figure C1. U.S. Marine Corps Base Camp Lejeune, Tarawa Terrace water-supply wells, Tarawa Terrace Shopping Center, and ABC One-Hour Cleaners, Onslow County, North Carolina.

of contamination was later determined to be ABC One-Hour Cleaners, located on North Carolina Highway 24 (SR 24) and less than a half-mile west and slightly north of several Tarawa Terrace water-supply wells (Shiver 1985, Figure 4). Production at supply wells TT-26 and TT-23 (Figure C1) was terminated during February 1985 because of contamination by PCE and related degradation products—trichloroethylene (TCE) and dichloroethylene (DCE).

Historical reconstruction characteristically includes the application of simulation tools, such as models, to re-create or represent past conditions. At Camp Lejeune, historical reconstruction methods include linking materials mass balance (mixing) and water-distribution system models to groundwater fate and transport models. Groundwater fate and transport models are based to a large degree on groundwater-flow velocities or specific discharges simulated by a calibrated groundwater-flow model. The unified assemblage of hydraulic characteristics and the related geologic, hydraulic, and hydrologic elements that characterize vertically contiguous aquifers and confining units is termed in this report a geohydrologic framework. An aquifer system is defined herein as composed of two or more water-bearing units separated at least locally by confining units that impede the vertical movement of groundwater but do not greatly affect the hydraulic continuity of the system (Poland et al. 1972). The Castle Hayne aquifer system described in this report generally comprises the "Castle Hayne aquifer" of Harned et al. (1989) and Cardinell et al. (1993) and the Castle Hayne Formation and so-called "limestone unit" of LeGrand (1959).

Purpose of Study

This study seeks to construct and calibrate a groundwater-flow model that represents the geohydrologic framework (Faye, 2007) and related groundwater-flow conditions at and in the vicinity of Tarawa Terrace, U.S. Marine Corps Base Camp Lejeune. A groundwater-flow model is characterized by the vertical and spatial distribution of aquifers and confining units, their respective boundaries, and their hydraulic characteristics, such as hydraulic conductivity and specific storage. The assemblage of these and related geologic, hydraulic, and hydrologic elements into a multilayer, calibrated model that reasonably simulates groundwater flow in vertically contiguous aquifers and confining units at Tarawa Terrace and vicinity is the focus of studies summarized in this report.

Geologic Framework

Geologic units of interest to this study are those that occur at or near land surface and extend to a depth generally recognized as the base of the Castle Hayne Formation. The lithostratigraphic top of the Castle Hayne Formation has not been definitively identified. In the northern part of Tarawa Terrace, borehole logs collected in conjunction with the drilling of monitor wells by Roy F. Weston, Inc. (1992, 1994) variously identify the top of the Castle Hayne Formation, "Castle Hayne Limestone," or the " Castle Hayne aquifer" at or near the top of the first occurrence of limestone or shell limestone, at depths ranging from about 60 to 70 feet (ft) at most sites but ranging in depth to about 90 ft at one location. Borehole and other drillers' and geophysical logs in the remainder of the study area do not indicate the top of the Castle Hayne Formation. Overlying the limestone or fossiliferous rock in the Roy F. Weston, Inc. logs is a dark gray silty clay, silt, or sandy silt that ranges in thickness from about 5 to 15 ft. This clay is also identified as a "lean" and sandy clay. For this study, the top of this clay or sandy silt is assigned as the top of the Castle Hayne Formation and is part of a well-recognized, somewhat to highly persistent geohydrologic unit that occurs throughout most of Camp Lejeune east of Northeast Creek (Harned et al. 1989, Sections A–A' and B–B', and C–C'; Cardinell et al. 1993, Sections A–A' and B–B'). This unit is designated herein the Local confining unit. Consequently, contours of equal altitude at the top of the Local confining unit are considered to also approximate the top of the Castle Hayne Formation (Figure C2). As shown, the top of the Castle Hayne Formation occurs near land surface in the northern part of and west of Tarawa Terrace, at altitudes ranging from about –20 to –30 ft, and dips to the east-southeast at a generally uniform rate to the vicinity of Northeast Creek, where the altitude at the top of the formation is less than –50 ft. Harned et al. (1989) and Cardinell et al. (1993) report that the base of the Castle Hayne Formation occurs at the top of the Beaufort Formation, which is capped by a relatively thick unit of clay, silt, and sandy clay. This clay is named in this report the Beaufort confining unit, following similar usage by Harned et al. (1989) and Cardinell et al. (1993), and is a recognizable unit in logs of deep wells at Camp Lejeune. The top of the Beaufort confining unit occurs at about altitude –215 ft in the northern and western parts of the study area and dips gradually to the south and southeast to a minimum altitude of about –250 ft in the vicinity of Northeast Creek (Figure C3). Comparing the maps that show the approximate top and base of the Castle Hayne Formation (Figures C2 and C3), the thickness of the Castle Hayne Formation is shown to range from about 180 ft west of Tarawa Terrace to a maximum thickness of about 200 ft near Northeast Creek (Figure C4). Irregularities of contours shown in Figures C2–C4 are caused by interpolation of the small set of point data used to define the unit altitude or thickness. The base of the Castle Hayne Formation or the top of the Beaufort confining unit is considered the base of groundwater flow of interest to this study.

In general, the Castle Hayne Formation at Camp Lejeune consists primarily of silty and clayey sand and sandy limestone with interbedded deposits of clay and sandy clay. LeGrand (1959) indicates a "tendency toward layering" with respect to the alternating (with depth) beds of predominantly sandy or clayey sediments. LeGrand (1959) also points out that at Tarawa Terrace, Montford Point, and Hadnot Point (Plate 1) the "shellrock is subordinate in quantity to sand" within the Castle Hayne Formation. The sand is fine, often gray in color, and frequently fossiliferous. Much of the limestone is shell limestone, also called "shell hash," "shellrock," or coquina in drillers' logs. Several of the clay deposits, such as the Local confining unit, appear to be continuous and areally extensive (Harned et al. 1989, Sections A–A', B–B', and C–C'; Cardinell et al. 1993, Sections A–A' and B–B') and range in thickness from about 10 ft to more than 30 ft. Lensoidal and discontinuous clay units probably occur frequently. The occurrence of limestone is probably also discontinuous, particularly in the vicinity of Tarawa Terrace. Limestone units of the Castle Hayne Formation at Camp Lejeune are marine and likely were deposited in near shore environments. Clastic units are probably beach deposits or were formed in deltaic or other near shore transitional environments.

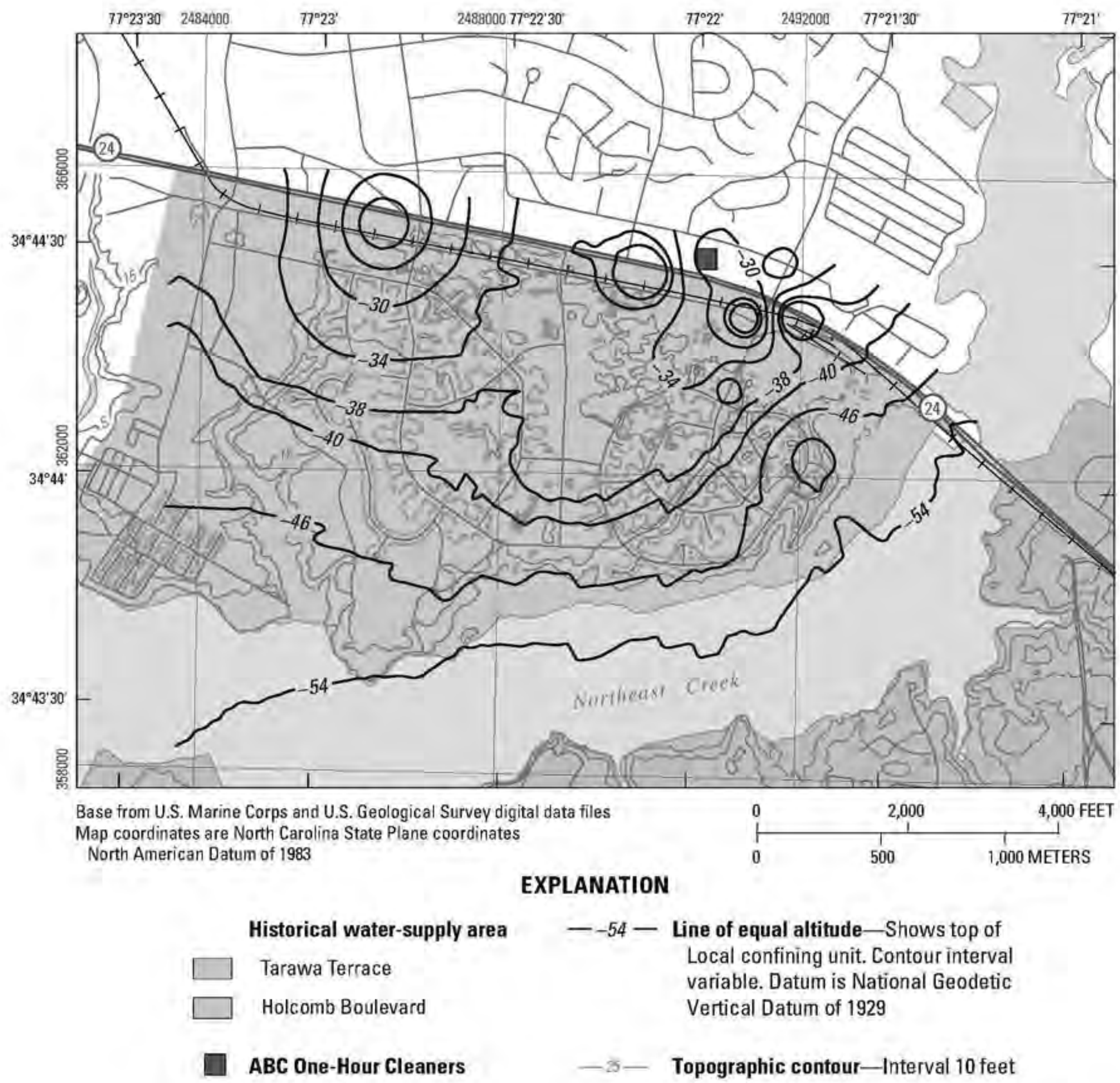


Figure C2. Altitude at the top of the Local confining unit, approximates the lithostratographic top of the Castle Hayne Formation, Tarawa Terrace and vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina.

Harned et al. (1989) and Cardinell et al. (1993) assigned an Eocene undifferentiated age to the Castle Hayne Formation, and this age is assigned as well in this report. Similarly, they assigned a Paleocene age to the Beaufort Formation at Camp Lejeune, and this age is adopted as well for this study.

Sediments that occur between land surface and the top of the Castle Hayne Formation are variously referred to as the River Bend Formation of Oligocene age and Belgrade Formation of early Miocene age (Harned et al. 1989; Cardinell et al. 1993). These sediments consist mainly of fine to medium, silty, gray and white sand interbedded with clay and sandy clay. Clays and sands are generally unfossiliferous at Tarawa Terrace but are fossiliferous southeast of Tarawa Terrace in the vicinities of Holcomb Boulevard and Hadnot Point (Plate 1), particularly at depths greater than 30 ft. The base of these units conforms to the top of the Castle Hayne Formation (Figure C2) and dips uniformly to the south and southeast. Unit thickness is zero at land surface and ranges from about 50 to 75 ft within the study area.

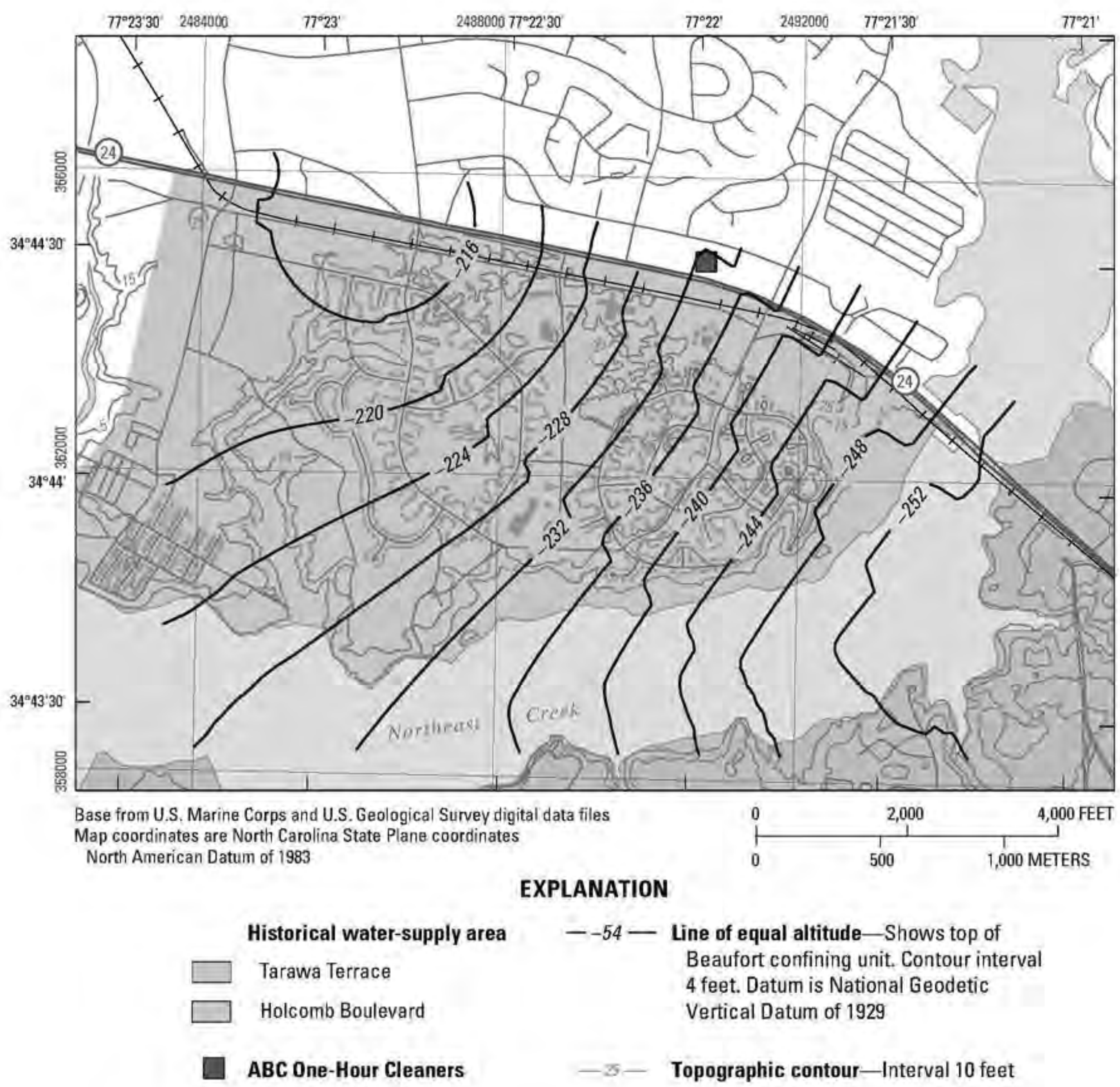


Figure C3. Altitude at the top of the Beaufort confining unit, Tarawa Terrace and vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina.

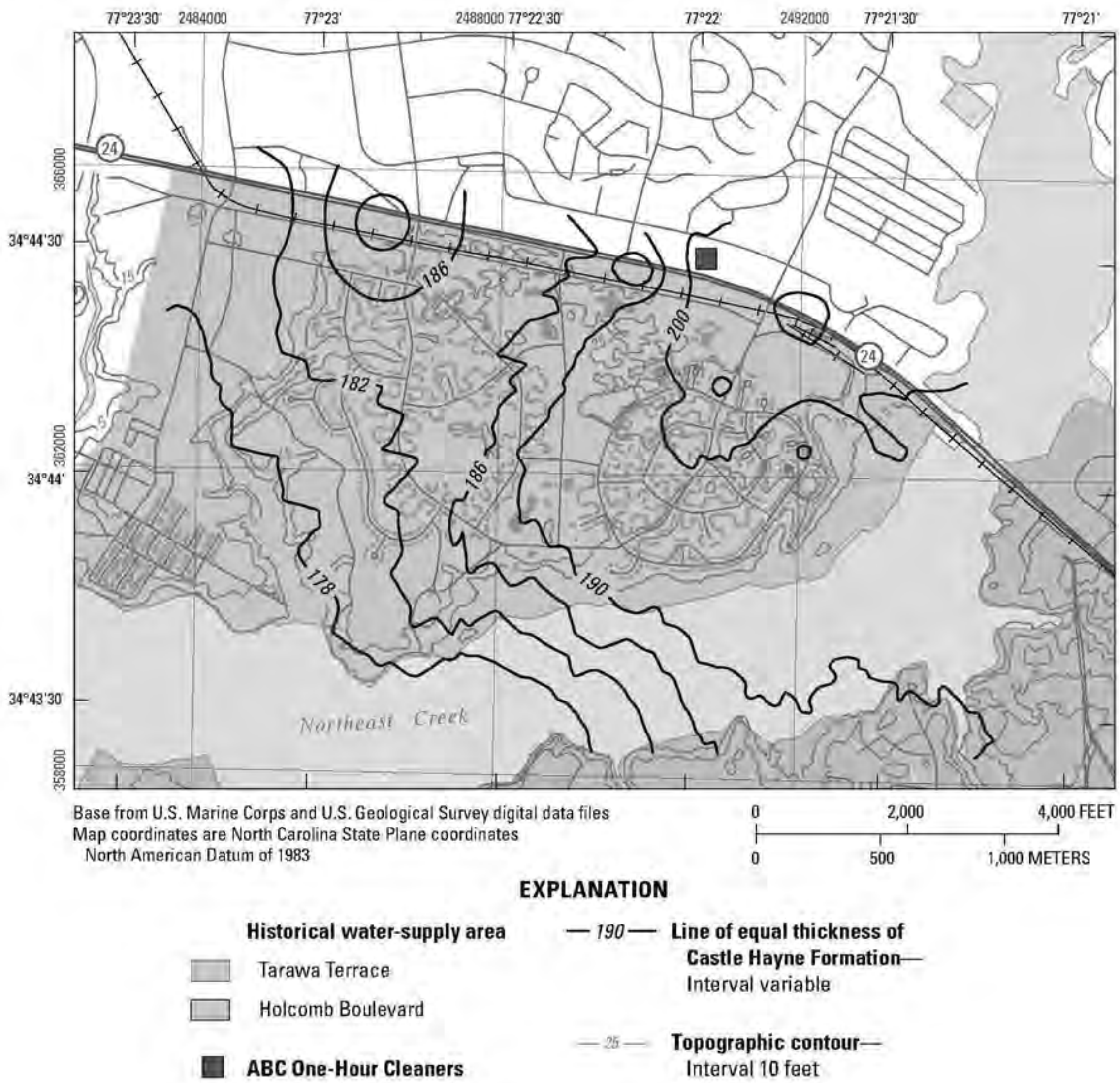


Figure C4. Thickness of the Castle Hayne Formation, Tarawa Terrace and vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina.

Geohydrologic Framework

A total of nine aquifers and confining units that occur between land surface and the top of the Beaufort Formation in the vicinity of Tarawa Terrace were identified and named after local cultural features where the units were first identified or as subdivisions of the Castle Hayne Formation. From shallowest to deepest these units are the Tarawa Terrace aquifer, Tarawa Terrace confining unit, Upper Castle Hayne aquifer–River Bend unit, Local confining unit, Upper Castle Hayne aquifer–Lower unit, Middle Castle Hayne confining unit, Middle Castle Hayne aquifer, Lower Castle Hayne confining unit, Lower Castle Hayne aquifer, and Beaufort confining unit (Table C1). The River Bend unit of the Upper Castle Hayne aquifer is so named to conform to the upper part of the "Castle Hayne aquifer" as described by Cardinell et al. (1993). As defined in this study, the River Bend unit probably includes sediments of the Castle Hayne Formation only at the base, if at all. The Local confining unit separates the River Bend and Lower units of the Upper Castle Hayne aquifer and conforms in areal extent and thickness to the silty or sandy clay described previously at the top of the Castle Hayne Formation (Figure C2). The aquifers and confining units, ranging from the top of the Upper Castle Hayne aquifer–River Bend unit to the top of the Beaufort confining unit, are inclusive of the Castle Hayne aquifer system, as defined in this study. The water table in the northern part of the study area generally occurs near the base of the Tarawa Terrace confining unit or near the top of the Upper Castle Hayne aquifer–River Bend unit. During periods of significant and prolonged rainfall, the water table possibly resides temporarily near the base of the Tarawa Terrace aquifer; however, sediments equivalent to the Tarawa Terrace

Table C1. Geohydrologic units, unit thickness, and corresponding model layer, Tarawa Terrace and vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina.

[Units are listed shallowest to deepest and youngest to oldest; N/A, not applicable]

Geohydrologic unit	Thickness range, in feet	Model layer
Tarawa Terrace aquifer	8 to 30	1
Tarawa Terrace confining unit	8 to 20	1
Castle Hayne aquifer system		
Upper Castle Hayne aquifer–River Bend unit	16 to 56	1
Local confining unit	7 to 17	2
Upper Castle Hayne aquifer–Lower unit	8 to 30	3
Middle Castle Hayne confining unit	12 to 28	4
Middle Castle Hayne aquifer	32 to 90	5
Lower Castle Hayne confining unit	18 to 30	6
Lower Castle Hayne aquifer	41 to 64	7
Beaufort confining unit	N/A	Base of model

aquifer are generally unsaturated. Available water-level data from paired wells individually open to the Upper Castle Hayne aquifer–River Bend and Lower units indicate little or no head difference between the aquifers or a slightly downward gradient from the River Bend unit to the Lower unit (Roy F. Weston, Inc. 1992, 1994). In the southern part of the study area, in the vicinity of the Tarawa Terrace Shopping Center, the Tarawa Terrace confining unit is mainly absent and the Tarawa Terrace aquifer and the Upper Castle Hayne aquifer–River Bend unit are undifferentiated. The water table in this area probably occurs consistently within the middle or base of sediments equivalent to the Tarawa Terrace aquifer.

Altitudes at the top of the Local confining unit and the Beaufort confining unit were shown previously in Figures C2 and C3. Point data used for interpolation control when plotting unit tops and thicknesses generally decrease in number and density with unit depth, increasing the subjectivity of interpolated results. Nevertheless, such maps are considered integral elements of the groundwater-flow model necessary for historical reconstruction and were used to assign layers and layer geometry during flow-model construction. Contour maps showing altitude at the unit top and unit thickness for all flow-model layers (Table C1) and lists of related point data are included in Faye (2007). Most unit surfaces trend to the south and southeast and increase in thickness in the same directions, similar to contours shown in Figures C2 and C3. The tops of most units exhibit a moderate to high degree of irregularity at one or several locations and probably at one or several times since their deposition were erosional surfaces, exposed to the effects of rain, ice, runoff, weathering, dissolution, and similar agents. Accordingly, surface irregularities may represent relict stream channels or hilltops. Where a unit is mainly limestone in composition, surface irregularities possibly represent the remnants of a karst terrain such as sinkholes or related solution or fracture features.

Previous Investigations

Reports and documents that describe or refer to the geology, hydrology, groundwater quality, and water supply at Tarawa Terrace and vicinity can be classified into two general categories—geohydrology and groundwater contamination. Previous investigations discussed herein are grouped into these two categories according to their dominant subject matter. Many reports and documents also contain ancillary information related to both geohydrology and groundwater contamination, as well as other topics of interest.

Geohydrology

Investigations of groundwater supplies in the area that would later become U.S. Marine Corps Base Camp Lejeune were conducted by David G. Thompson of the U.S. Geological Survey (USGS) during April 1941 and reported to the Navy Department by memorandum (Thompson 1941). Thompson's report briefly described the results of test well drilling in the vicinities of Paradise Point and Hadnot Point (Plate 1) and concluded that the best sources of groundwater were the limestone rocks and related coquina rocks of the "Castle Hayne Formation."

LeGrand (1959) evaluated the contemporary water supply at Camp Lejeune east of New River and constructed 22 test wells, ranging in depth from about 200 to 500 ft. Detailed construction and lithologic data were collected at each test site along with geophysical logs, water-level, and water-quality data. Test wells T-9–T-14 (Plate 1) were constructed at or nearby Tarawa Terrace and provided the first detailed description of the Castle Hayne aquifer system in that part of Camp Lejeune. Downward leakage as recharge was estimated to be about 19 inches per year (in/yr) in the vicinity of most well fields operating at Camp Lejeune during the period of investigation.

Harned et al. (1989) conducted a comprehensive and detailed review of groundwater data and conditions throughout Camp Lejeune for the period 1986–1987. Water-level measurements were obtained at almost all supply and other observation wells. Continuous water-level data at several supply and observation wells were published in the form of hydrographs for several months during 1986–1987. Construction and well-capacity test data also were reported for numerous wells. Annual water use as an average in million gallons per day (MGD) were reported for seven Camp Lejeune water treatment plants (WTPs), including Tarawa Terrace, for the period 1975–1987. Existing borehole geophysical logs and drillers' logs were assembled, and additional geophysical logs were collected at test wells and where existing wells were accessible. Published well data refer to the period 1941–1986, when the majority of supply wells were constructed at Camp Lejeune. Significantly, three "hydrogeologic" sections were constructed, located generally east to west and north to south across Camp Lejeune east of the New River. These sections subdivide the "Castle Hayne aquifer" into several distinct aquifers and confining units based on the correlation of generally continuous clays. The vertical sequence of sediments represented on each section extends generally from land surface to the base of the Castle Hayne aquifer system (Faye 2007). Correlation of units from site to site was mainly based on borehole electric log signatures. Well locations, well-capacity tests, well construction, pumpage, and water-level data reported by Harned et al. (1989) were essential and necessary elements of flow-model construction and calibration described in this report.

Cardinell et al. (1993) used much of the borehole data collected previously by Harned et al. (1989), slightly modified the geohydrologic interpretations of Harned et al. (1989), and extended their "hydrogeologic" sections west of the New River and south to the coastal margin of Camp Lejeune. Highly generalized maps showing the altitude at the top and base of the "Castle Hayne aquifer" also were constructed for the entire Camp Lejeune area.

Giese and Mason (1991, Plate 1) subdivided the North Carolina Coastal Plain into three "hydrologic areas," mainly based on soil type and topography. These areas were classified as clay soils, sandy soils, and sand hills. Low streamflow characteristics were computed for each unique hydrologic area. The area classification assigned to U.S. Marine Corps Base Camp Lejeune, including the Tarawa Terrace area, was HA2 or "sandy soils." Using generally the same hydrologic area classifications and respective area boundaries of Giese and Mason (1991), Heath (1994) assigned groundwater recharge rates ranging from about 4 to 13 in/yr to North Carolina Coastal Plain "hydrogeologic units," with the highest rates assigned to "sand hills and sandy soils" (Heath 1994, Figure 21, Table 6). The recharge rates of Heath (1994) probably represent effective recharge; that is, net recharge to the water table after accounting for evapotranspiration and surface runoff.

Giese et al. (1997) developed and calibrated a groundwater-flow model of the entire North Carolina Coastal Plain as a part of the USGS Regional Aquifer-System Analysis (RASA) program. The "Castle Hayne aquifer" was modeled as a single aquifer for the RASA study. Simulated information specific to Tarawa Terrace or the Camp Lejeune area is highly generalized as a result. For example, the Tarawa Terrace area of interest to this study is located entirely within a single cell of the RASA flow model.

Baker Environmental, Inc. (1998) constructed a groundwater-flow model of the entire Camp Lejeune area to evaluate water-level changes and related effects of groundwater pumping at various groundwater remediation sites. The model was vertically subdivided into five layers corresponding to a "surficial unit," a "Castle Hayne confining unit," an "Upper Castle Hayne aquifer," a "Castle Hayne Fractured Limestone unit," and a "Lower Castle Hayne aquifer." These framework components generally correspond to the subdivisions described in sections published in Harned et al. (1989) and Cardinell et al. (1993). Maps were not provided that illustrate the spatial distribution or thickness of aquifers and confining units. Horizontal hydraulic conductivity assigned to the model aquifer units was 5, 7, and 10 feet per day (ft/d) for the "surficial," "Upper Castle Hayne," and "Lower Castle Hayne" aquifers, respectively, and was applied uniformly throughout the model layers. Horizontal hydraulic conductivity assigned to the "Castle Hayne confining unit" was 0.1 ft/d throughout most of the model domain but was selectively assigned as 0.00073 and 5 ft/d, depending on conditions observed during field investigations. A horizontal hydraulic conductivity of 100 ft/d was assigned uniformly to the "Fractured Limestone unit." All wells assigned to the model pumped only from the "Fractured Limestone unit." Vertical hydraulic conductivities assigned to each model layer equaled one-tenth the horizontal hydraulic conductivity. Recharge to the water table was simulated at a rate of 11 in/yr. Model cells were square with dimensions of 1,000 ft per side. The total model grid consisted of 101 rows and 80 columns. Model run conditions were steady state. Model calibration was based on 142 water-level measurements at wells open to the four designated aquifers. These wells were located mostly north and east of New River (Plate 1). Water-level data represented conditions during 1992–1993. Simulated water levels matched observed water levels within 10 ft at all but one site.

Groundwater Contamination

During August 1982, routine chromatograph/mass-spectrometer (GC/MS) analyses for trihalomethane in water samples collected from the Tarawa Terrace and Hadnot Point WTPs at U.S. Marine Corps Base Camp Lejeune were interrupted by interference from constituents in the water samples thought to be halogenated hydrocarbons (Grainger Laboratories, written communication, August 10, 1982; Elizabeth A. Betz, written communication, August 19, 1982; AH Environmental Consultants, Inc., written communication, June 18, 2004; Camp Lejeune water documents CLW 592–595 and CLW 606–607). Subsequent analyses confirmed the presence of PCE in samples of finished water supplies from both locations ranging in concentration from 76 to 104 micrograms per liter (μg/L) at Tarawa Terrace and from 15 μg/L to below detectable limits at Hadnot Point. Concentrations of TCE determined in samples from the Hadnot Point WTP ranged from 19 to 1,400 μg/L. Samples analyzed were collected during May and July 1982 (Faye and Green 2007, Table E12).

During July 1984, routine sampling and analyses of community water-supply wells at Camp Lejeune, as a part of the Base Naval Assessment and Control of Installation Pollutants Program, indicated the occurrence of TCE in samples obtained from wells TT-23 (37 μg/L), TT-25 (trace), and TT-26 (3.9 μg/L) (Maslia et al. 2007). Well TT-26 was open only to the Upper Castle Hayne aquifer; whereas, wells TT-23 and TT-25 were open to both the Upper and Middle Castle Hayne aquifers (Faye and Green 2007, Table E2).

Beginning during January 1985 and continuing into September 1985, the North Carolina Department of Natural

Resources and Community Development (NCDNRCD) periodically sampled wells TT-23, TT-25, and TT-26 and water treated at the Tarawa Terrace WTP for PCE and its degradation products, TCE, DCE, and vinyl chloride (McMorris 1987). On occasion, duplicate samples were analyzed by NCDNRCD and by JTC Environmental Consultants Inc. (Shiver 1985; R.A. Tiebout, Memorandum for the Commanding General, Chief of Staff, written communication, November 6, 1985; J.R. Bailey to U.S. Environmental Protection Agency, written communication, April 25, 1986; Camp Lejeune water documents CLW 1338–1339, 1475–1483). Concentrations of PCE in samples from water-supply well TT-26 ranged from 3.8 to 1,580 μg/L in seven samples collected during this period. Concentrations in 10 samples from water-supply well TT-23 ranged from "not detected" to 132 μg/L. Concentrations also were detected of TCE, *trans*-1,2-dichloroethylene (1,2-tDCE), and vinyl chloride. Tarawa Terrace water-supply wells TT-30, TT-31, TT-52, TT-54, and TT-67 also were sampled during this period, and subsequent analyses detected no concentrations of PCE or related degradation products above detection limits at these wells (JTC Environmental Consultants Report 85-047, Report 19, written communication, February 5–6, 1985). However, JTC Environmental Consultants detected benzene at a concentration of 6.3 μg/L in a sample collected at well TT-23 on February 19, 1985 (JTC Environmental Consultants Report 85-072, Report 37, written communication, March 1, 1985). An estimated concentration of 0.43 μg/L PCE was determined in a sample from well TT-25 during September 1985. The sampling and analyses for volatile organic compounds (VOCs) during January and February 1985 caused wells TT-23 and TT-26 to be removed from service during February 1985. Well TT-26 was permanently closed at this time; however, well TT-23 was used to deliver water to the Tarawa Terrace WTP for several days during March and April 1985 (Camp Lejeune water document CLW 1182; Camp Lejeune water document CLW 1193, "Direction to Operators at Tarawa Terrace," April 30, 1985; Camp Lejeune water document CLW 1194, "Procedures for operating the 'New Well' at Tarawa Terrace," date unknown). At the time of discovery of PCE and related contaminants at Tarawa Terrace supply wells, the Tarawa Terrace WTP provided drinking water to about 6,200 people in the service area (McMorris 1987).

During April 1985, the NCDNRCD began a field investigation to determine the source or sources of PCE and related constituents occurring at wells TT-23 and TT-26. Samples were collected at these wells and at well TT-25 for analyses of VOCs. Three monitor wells were installed in the "Water Table aquifer" northwest of well TT-26 parallel to SR 24 to collect additional samples and water-level data (Shiver, 1985; wells X24B4, X24B5, X24B6 [shown on Plate 1 as B4, B5, and B6, respectively]). Results of analyses of samples collected at supply and monitor wells were sufficient to delineate a highly generalized plume of PCE in groundwater of the aquifer. The northwest apex of the plume was located at monitor well X24B6, immediately opposite the entrance of ABC One-Hour Cleaners at 2127 Lejeune Boulevard (SR 24). The PCE concentration determined in the sample from this well was 12,000 μg/L. These and ancillary water-level data, indicating the direction of groundwater flow to the southeast toward supply well TT-26, pinpointed ABC One-Hour Cleaners as the source of PCE in Tarawa Terrace water-supply wells (Shiver 1985, Figure 4).

ABC One-Hour Cleaners always used PCE in its dry-cleaning operations, beginning during 1953 when the business opened (Hopf & Higley, P.A., "Deposition of Victor John Melts," written communication, April 12, 2001). A primary pathway of contaminants from the dry-cleaning operations at ABC One-Hour Cleaners to the soil and subsequently to groundwater was apparently through a septic tank-soil absorption system to which ABC One-Hour Cleaners discharged waste and wastewater. Shiver (1985) reports that an inspection of the PCE storage area at ABC One-Hour Cleaners indicated that PCE releases could and did enter the septic system through a floor drain, probably as a result of spillage in the storage area (Roy F. Weston, Inc. 1994). In addition, spent PCE was routinely reclaimed using a filtration-distillation process that produced dry "still bottoms," which until about 1982 (Hopf & Higley, P.A., "Deposition of Victor John Melts," written communication, April 12, 2001) or 1984/1985 (McMorris 1987), were disposed of onsite, generally by filling potholes in a nearby alleyway. When ABC One-Hour Cleaners totally discontinued the use of the floor drain and the onsite disposal of still bottoms is not known exactly, but such practices probably terminated completely during 1985.

The disposal of dry-cleaning solvents to the septic system and subsequently to groundwater placed ABC One-Hour Cleaners in violation of various State laws and statutes. During January 1986, the owners were ordered by the State of North Carolina to cease such disposal and propose a plan to restore the quality of affected groundwater to an acceptable level as determined by the State (Roy F. Weston, Inc. 1994). Pursuant to this plan, ABC One-Hour Cleaners hired Law Engineering and Testing Company, Inc., to investigate the septic tank and the surrounding soil for contaminant content. Samples collected and analyzed by Law Engineering and Testing Company, Inc., indicated PCE concentrations of the septic tank sludge were as high as 1,400 milligrams per liter (mg/L) and that soil 4 ft below the tank contained PCE concentrations as high as 400 milligrams per kilogram (mg/kg) (Law Engineering and Testing Company, Inc. 1986a; Roy F. Weston, Inc. 1992). Subsequently Law Engineering and Testing Company, Inc., conducted additional investigations to determine the vertical and horizontal extent of contamination within the soil profile. These investigations were completed by December 1986 and indicated the depth of PCE contamination in the vicinity of the septic tank to be in excess of 16 ft. A PCE concentration at a depth of 8 ft was 860 mg/kg (Law Engineering and Testing Company, Inc. 1986b; Roy F. Weston, Inc. 1992; Faye and Green 2007, Table E4).

By March 1987, all water-supply wells at Tarawa Terrace were removed from service. During March 1989, the ABC One-Hour Cleaners site was placed on the U.S.

Environmental Protection Agency's (USEPA) National Priority List (Final List); and during June 1990, USEPA hired Roy F. Weston, Inc., to conduct a remedial investigation at the site aimed at determining the areal and vertical extent of contaminant plumes (Operable Unit 1) and characterizing the source of contaminants in the unsaturated soils beneath and in the vicinity of the septic disposal system at ABC One-Hour Cleaners (Operable Unit 2) (Roy F. Weston, Inc. 1994; event chronology, no author, written communication, "as of October 1998").

Operable Unit 1 of the remedial investigation included the installation of eight soil borings to depths ranging from 16 to 20 ft surrounding and in the immediate vicinity of ABC One-Hour Cleaners (SB-1–SB-6, SB-10, and SB-12; Faye and Green 2007, Table E4). These borings occurred entirely within the unsaturated zone. Ten shallow and five deep monitor wells also were installed during Operable Unit 1, not only in the immediate vicinity of ABC One-Hour Cleaners, but northwest of the site as well as proximate to wells TT-26 and TT-25. Several monitor wells also were located between SR 24 (Lejeune Boulevard) and the Tarawa Terrace housing area. The shallow wells, S1–S10, were constructed to depths ranging from 28 to 40 ft and were open at the base of the well to the Upper Castle Hayne aquifer–River Bend unit (Table C1.10). Four of the deep wells—C1, C2, C3, and C5—ranged in depth from about 90 to 100 ft and were open at the base to the Upper Castle Hayne aquifer–Lower unit. Well C4 was constructed to a depth of about 200 ft and was open to the Middle Castle Hayne aquifer.

Operable Unit 2 included the construction of an additional shallow well (S11) about 1,000 ft northwest of ABC One-Hour Cleaners. Two additional deep wells, C9 and C10, were constructed east and south of the cleaners. Additional well C11 was located in the northeast part of the Tarawa Terrace housing area. Depths of the additional deep wells ranged from about 75 to 175 ft. Wells C9 and C11 were open to the Upper Castle Hayne aquifer–Lower unit. Well C10 was open to the Middle Castle Hayne aquifer. Also installed as part of Operable Unit 2 were six piezometers, three shallow (PZ-02, -04, -06) and three deep (PZ-01, -03, -05), in the immediate vicinity of ABC One-Hour Cleaners and open to the Upper Castle Hayne aquifer–River Bend and Lower units, respectively. The depths of PZ-02, -03, and -04 ranged from 29.5 to 34.5 ft. Depths of PZ-01, -03, and -05 ranged from 74.5 to 79.5 ft.

Results of analyses of periodic water samples collected from the monitor wells during Operable Units 1 and 2 indicated that concentrations of PCE ranged from below detectable limits at several wells to 5,400 μg/L at well S3. Samples from monitor wells also were analyzed for various metals and semivolatile compounds.

During Operable Unit 2, similar constituent-analysis schedules were used during analyses of effluent from the septic tank at ABC One-Hour Cleaners and of soil samples obtained from the unsaturated zone in the vicinity of the tank. PCE concentration in the tank effluent was 6,800 μg/L during June 1991. Concentrations of PCE in soil borings at various depths in the immediate vicinity of ABC One-Hour Cleaners ranged from not detected to more than 2,000,000 micrograms per kilogram (μg/kg) (Faye and Green 2007, Table E4).

Deep monitor wells C1–C5 were paired with their respective shallow well counterparts S1–S5. Piezometers with odd and even numbers were likewise paired, in an effort to determine vertical hydraulic gradients. Water levels at paired wells and piezometers were measured to hundredths of a foot periodically during 1992–1993 (Appendix C1, Table C1.10). Vertical-head gradients were downward at all paired wells at all times, with the exception of slightly upward gradients at PZ-01/02 and PZ-03/04 during November 1993. A maximum head difference of 2.23 ft occurred at paired wells S1/C1 during April 1992. Head differences between the Upper Castle Hayne aquifer–River Bend unit and the Middle Castle Hayne aquifer were always less than 2 ft. These and similar water-level measurements at all monitor wells were used to map local potentiometric surfaces in the vicinity and downgradient of ABC One-Hour Cleaners (Roy F. Weston, Inc. 1992, Figures 4-6 and 4-9). Potentiometric levels in the Upper Castle Hayne aquifer–River Bend and Lower units were similar and ranged from about 23 to 10 ft, National Geodetic Vertical Datum of 1929 (NGVD 29). Potentiometric levels trended from northwest to southeast, greater to lesser, and generally corresponded to groundwater-flow directions. The potentiometric gradient of the Upper Castle Hayne aquifer–River Bend unit ranged from about 0.006 to 0.007 foot per foot (ft/ft) (Roy F. Weston, Inc. 1992). Corresponding gradients for the Upper Castle Hayne aquifer–Lower unit were from 0.005 to 0.006 ft/ft. Aquifer-tests were conducted in conjunction with several monitor wells. Test results indicated that values of horizontal hydraulic conductivity ranged from about 10 to 30 ft/d for the "surficial aquifer" (Upper Castle Hayne aquifer–River Bend unit). Corresponding storativity ranged from magnitude 10^{-4} to 10^{-3}. Water-levels at supply and monitor wells at and in the vicinity of Tarawa Terrace are listed in Appendix C1, Tables C1.1–C1.11. Corresponding well-construction data are listed in Appendix C2, Tables C2.1–C2.3.

In order to characterize the depth, areal extent, and water quality of the contaminant plumes emanating from the vicinity of ABC One-Hour Cleaners, hydrocone penetrations using direct-push technology were accomplished at 47 sites, near, east, and south of the cleaners. Two levels of samples were collected at each site, generally from about 20 and 40 ft, respectively. The constituent-analysis schedule used for hydrocone sample analyses included PCE, TCE, 1,2-tDCE and vinyl chloride, as well as 1,1,1-trichloroethane (1,1,1-TCA), 1,1- and 1,2-dichloroethane (1,1-, 1,2-DCA), and carbon tetrachloride. Samples were analyzed in the field using a mobile laboratory. Several duplicate samples were submitted to "CLP" laboratories for quality assurance of results. Although not defined in the respective Operable Unit reports, CLP probably refers to "Clinical Laboratory Program," a process that inspects State and Federal public health laboratories for purposes of certification. The CLP laboratories also determined concentrations of carbon disulfide, benzene, ethylbenzene, and total xylenes, in addition to the constituents discussed previously. Benzene and related toluene, ethylbenzene, and total xylenes (BTEX) were detected infrequently in the hydrocone samples. Benzene concentrations ranged from below detectable limits to 12 µg/L (Faye and Green 2007, Table E9). Results of mobile and CLP laboratory analyses were not highly consistent (Roy F. Weston, Inc. 1992, Table 5-12). Most constituents were noted in one or more samples. PCE was detected most frequently and was found in 75 samples at concentrations ranging from 1 to 30,000 µg/L. The maximum depth of PCE occurrence determined by hydrocone penetration was 64 ft (sample HC-6-64), which is near the base or slightly below the Upper Castle Hayne aquifer–River Bend unit (Faye and Green 2007, Table E7).

During 1990, the Agency for Toxic Substances and Disease Registry (ATSDR) completed an assessment of public health effects related to groundwater contamination at ABC One-Hour Cleaners and expressed a public health concern that offsite (namely Tarawa Terrace) exposure of contaminants to humans had occurred through the groundwater pathway. During 1997, ATSDR conducted a comprehensive Public Health Assessment of U.S. Marine Corps Base Camp Lejeune, which included an assessment of human exposure to contaminated groundwater at Tarawa Terrace. Maximum contaminant concentrations for PCE (215 µg/L), TCE (8 µg/L), and DCE (12 µg/L) determined from samples obtained within the Tarawa Terrace water-distribution system were listed, and a definitive exposure timeframe was identified for the period 1982–1985. The period 1954–1982 was identified as an unknown exposure timeframe (ATSDR 1997).

Investigations of groundwater contamination at and near Tarawa Terrace not related to ABC One-Hour Cleaners also have occurred since 1990, mainly in conjunction with known or suspected releases to groundwater of refined-petroleum products from underground and above-ground storage tanks. Six large (30,000 gallons [gal]) above-ground petroleum storage tanks (STT61–STT66) were located just west of Tarawa Terrace in the narrow strip between the railroad tracks and SR 24 (Plate 1). Tarawa Terrace water-supply wells TT-27 and TT-55 were located just south and slightly west of these tanks. The tanks were constructed during 1942; and until about 1980, petroleum product deliveries were offloaded from railcars. About 1980, the tanks were converted to waste oil storage (O'Brien & Gere Engineers, Inc. 1992, 1993). Well TT-27 was installed during 1951 and was mostly out of service by 1962. Well TT-55 was installed during 1961 and was out of service by 1971. At least one spill is documented at the tank site—a spill from tank STT66 occurred about 1986 or 1987 (O'Brien & Gere Engineers, Inc. 1992, 1993).

Field investigations of groundwater conditions at and in the vicinity of the tanks included the installation of 20 monitor wells during 1991–1992. Half the wells were installed to a depth of about 15 ft and half to a depth of about 30 ft (Appendix C2, Table C2.3). Ten-foot slotted screens were installed at the base of all wells. The shallow wells were open to the base of the Tarawa Terrace aquifer. The deep wells were open to the Upper Castle Hayne aquifer–River Bend unit. Water-level data collected in monitor wells indicated potentiometric levels ranged from about 20 to 27 ft during January 1992 (Appendix C1, Table C1.10). Groundwater was shown to flow in a generally southerly direction away from the tanks. Hydrocone samples obtained using direct-push techniques were collected at 10 additional sites about 4 ft below the water table. Samples obtained from each well and hydrocone site were analyzed for a great variety of constituents. Most constituents are included in the Toxicity Characteristic Leaching Procedure (TCLP) protocols. Of major interest to this study were concentrations of benzene, which ranged from not detected to 23 µg/L. All occurrences of benzene were in four of the deep wells. Benzene also was detected in three hydrocone samples and ranged in concentration from 7 to 22 µg/L (Faye and Green 2007, Table E9). A highly generalized boundary of a benzene plume was constructed using these data representing conditions during 1993. The elongated part of the plume is pointed almost directly south, corresponding to groundwater-flow directions (O'Brien and Gere Engineers Inc. 1992, 1993). An aquifer test conducted during December 1992, using several monitor wells as observation wells, indicated a transmissivity of water-bearing sands open to the wells of about 500 feet squared per day (ft^2/d) and a storativity of about 0.05. Discharge at the pumped well during the test was 5.5 gallons per minute (gal/min).

A "strong gasoline-type odor" was noted at supply well TT-53 (Figure C1) during October 1986 while USGS personnel performed a routine well reconnaissance (U.S. Geological Survey well inventory, written communication, October 21, 1986). The well at the time was out of service, and the pump had been removed. This well is located about 1,500 ft southeast of the benzene plume located in the vicinity of the STT storage tanks and is the nearest most recently active Tarawa Terrace supply well to the plume.

The Tarawa Terrace Shopping Center is located in the southern part of Tarawa Terrace north of the shoreline of Northeast Creek (Figure C1). Eleven buildings associated with the shopping center are numbered beginning at TT-2455 and ending at TT-2475. The construction date of the shopping center is unknown, but the major buildings and the name "Shopping Center" are shown on maps of Tarawa Terrace dated June 1961 (Sheet 3 of 18, U.S. Marine Corps Base Camp Lejeune, Map of Tarawa Terrace II Quarters, June 30, 1961). Twelve underground storage tanks (USTs) ranging in capacity from 300 to 500 gal and several above-ground storage tanks were associated with various buildings at the shopping center. The installation and release history of these tanks is unknown; however, releases from two tanks were confirmed during 1994. Many of these tanks were abandoned by 1995 or possibly earlier (Richard Catlin & Associates, Inc. 1994a,b, 1995a,b).

Adjacent to or nearby the shopping center are Buildings TT-2477, TT-2478, and TT-2453. Building TT-2477 was constructed during the 1950s as a full-service gasoline station. This building originally contained one 10,000-gal gasoline UST and one 550-gal UST for hydraulic/gear fluids. These tanks were probably installed at the time of the construction of Building TT-2477. The 550-gal tank was removed during 1992, and the 10,000-gal tank was abandoned in place at that time (Law Engineering, Inc. 1995a). The release history of both tanks is unknown.

Building TT-2478 is located about 250 ft north of Building TT-2477 and was constructed during 1986. Three 10,000-gal gasoline USTs were installed at the time of construction. By 1992, at least two of the tanks were determined to be leaking (Law Engineering, Inc. 1994a,b).

Building TT-2453, located slightly southeast of Building TT-2455 of the shopping center and about 450 ft south of Building TT-2477, was also a gasoline station at one time. The installation and release history of tanks at Building TT-2453 is unknown, but this building also is shown on maps of Tarawa Terrace dated June 1961 and is identified on same as a "filling station" (Sheet 3 of 18, U.S. Marine Corps Base Camp Lejeune, Map of Tarawa Terrace II Quarters, June 30, 1961). DiGiano et al. (1988) summarized the results of gasoline plume discovery and delineation at Building TT-2453 (Industrial Marine Services, Inc. 1985). The presence of gasoline in the subsurface at Building TT-2453 apparently originated from two sources: (1) a catastrophic tank failure on September 21, 1985, with a subsequent loss of 4,400 gal of unleaded gasoline to the subsurface; and (2) a 3,000-gal tank of leaded gasoline discovered leaking on July 23, 1986. A release history by DiGiano et al. (1988, Table 3) indicates that small leaks of product probably occurred at this site beginning during the 1950s. As of May 4, 1987, more than 2 ft of "free product" was identified above the water table in the vicinity of Building TT-2453. The contamination associated with Building TT-2453 was undergoing active remediation as of May 1987 (DiGiano et al. 1988).

About 1995, Buildings TT-2455, TT-2463, TT-2465, TT-2467, TT-2469, and TT-2471 of the shopping center were subjects of active investigations of groundwater contamination as were UST sites associated with Buildings TT-2477 and TT-2478 (Richard Catlin & Associates, Inc. 1994a,b, 1995a,b, 1996, 1998; Law Engineering, Inc. 1994a,b, 1995a,b; Law Engineering and Environmental Services, Inc. 1996; OHM Remediation Services, Corp. 2001). Numerous monitor wells were installed during these investigations and were the locations of periodic collections of water levels and water-quality samples (Appendix C1, Table C1.11; Faye and Green 2007, Tables E9 and E10). All wells were installed in the Tarawa Terrace aquifer or the Upper Castle Hayne aquifer–River Bend unit.

Water-level measurements, accurate to a hundredth of a foot, were collected at paired wells collected in conjunction with investigations at Buildings TT-2477 and TT-2478 and indicated that vertical-head gradients between depths of 15 and 50 ft were generally downward and ranged from zero to order of magnitude 10^{-4} ft/ft (Law Engineering, Inc. 1994a). Water-level data also indicated the direction of groundwater flow in the shopping center area to be almost directly south toward Northeast Creek. Water-table altitudes ranged from about 8 to 11 ft, NGVD 29 (Law Engineering, Inc. 1995a, drawing 5.1).

Water-quality samples collected at monitor wells and at several hydrocone sampling sites were analyzed for all BTEX constituents. The approximate extent of a benzene plume delineated during 1994 in front of the shopping center extended about 600 ft from north to south (Law Engineering, Inc. 1995a, drawing 5.3). This plume possibly represents the merger of older plumes originally emanating from near Buildings TT-2477 and TT-2453. Benzene concentrations at the northern apex of the plume were in excess of 6,000 µg/L. This northern apex is located about 700 ft almost directly south of Tarawa Terrace water-supply well TT-52, which was placed in service during 1961 and removed from service during March 1987. Tarawa Terrace water-supply well TT-31 is located about 1,300 ft northeast of the plume's northern apex. Well TT-31 was placed in service during 1973 and also was removed from service during March 1987.

In addition to active remedial investigations at buildings of and in the vicinity of the Tarawa Terrace Shopping Center and at storage tanks, several other sites within the Tarawa Terrace housing areas were the subject of UST removal and related soil and groundwater investigations. The site designators at these locations also correspond to Tarawa Terrace building addresses and include: TT-44, TT-48, TT-779, TT-2254/2256, TT-2258/2260, TT-2302/2304, TT-2634, TT-3140/3142, TT-3165/3167, TT-3233/3235, TT-3524/3526, and TT-3546/3548 (Law Engineering and Environmental Services, Inc. 1998; Catlin Engineers and Scientists 2002a,b; Mid-Atlantic Associates, P.A. 2002a,b,c,d,e,f,g; Mid-Atlantic Associates, Inc. 2003a,b). Monitor wells were installed at most of these sites in conjunction with the collection of soil borings and boring logs. Water levels were measured at least once, and concentrations of BTEX constituents were determined at most monitor wells. Concentrations of benzene ranged from 290 µg/L at monitor well 14 near Building TT-2478 in the vicinity of the shopping center to "not detected." A concentration of benzene at the vast majority of sites was "not detected" (Faye and Green 2007, Table E9).

During 1991, Haliburton NUS Environmental Corporation (1992) conducted soil borings and installed several monitor wells at the Tarawa Terrace Dump (TT-Dump) located immediately south of the shopping center and between it and Northeast Creek (Figure C1). Concentrations of constituents of interest to this study were determined in soil samples from several locations and were generally low or below detectable limits. Water-level data collected during this investigation indicated groundwater flow was entirely from the dump site toward Northeast Creek. Water-level altitudes at monitor wells ranged from about 2 to 6 ft.

Periodic water levels measured at Camp Lejeune supply wells, at monitor wells installed during ABC One-Hour Cleaners Operable Units 1 and 2, and at monitor wells installed during investigations of USTs and petroleum-product spills are listed in Appendix C1, Tables C1.1–C1.11. Construction data for these wells are listed in Appendix C2, Tables C2.1–C2.3 (U.S. Geological Survey well inventory, written communication, October 21, 1986; DiGiano et al. 1988; Haliburton NUS Environmental Corporation 1992; O'Brien & Gere Engineers, Inc. 1992, 1993; Law Engineering, Inc. 1994a,b, 1995a,b; Richard Catlin & Associates, Inc. 1994a,b, 1995a,b, 1996, 1998; Law Engineering and Environmental Services, Inc. 1996, 1998; OHM Remediation Services, Corp. 2001; Catlin Engineers and Scientists 2002a,b; Mid-Atlantic Associates, P.A. 2002a,b,c,d,e,f,g; Mid-Atlantic Associates, Inc. 2003a,b). Results of aquifer tests at Camp Lejeune water-supply wells and at monitor wells installed during various investigations of groundwater contamination at and in the vicinity of Tarawa Terrace are listed in Tables C2–C4. Faye and Green (In press 2007) provide a detailed history of groundwater contamination at Tarawa Terrace supply wells and compute an approximate mass of PCE remaining in the Upper Castle Hayne aquifer during 1991.

Conceptual Model of Groundwater Flow

A conceptual model of groundwater-flow directions and budget quantities is a necessary element of model development and calibration. The source of water to the Tarawa Terrace and underlying aquifers in the study area is recharge from precipitation. Recharge to the Castle Hayne aquifer system occurs originally as infiltration of precipitation to the water table. Average annual effective recharge, defined herein as recharge to the water table remaining after discharge to evapotranspiration, is described in previous investigations as ranging from about 11 to about 19 in/yr in the study area (LeGrand 1959; Heath 1994; Giese et al. 1997; Baker Environmental, Inc. 1998). These rates conform to maps of average annual rainfall and annual potential evaporation by Heath (1994, Figures 9 and 12), which indicate rates of about 56 to 60 in/yr and 42 in/yr, respectively, for Onslow County. Within the study area, surface soils are generally sands or silty sands and the land surface is mainly undissected by streams, indicating little or minimal runoff. Thus long-term, average annual effective recharge rates in the study area could be as much as 18 in/yr, the maximum difference between rates of average annual rainfall and annual potential evaporation (Heath 1994, Figures 9 and 12).

The spatial configuration of the water table prior to development of local aquifers by wells probably resembled to a large degree a subdued replica of surface topography (Plate 1). Consequently, precipitation recharged to the water table flowed laterally from highland to lowland areas and eventually discharged to surface-water bodies. Northeast Creek and New River are partially or completely incised within the Tarawa Terrace aquifer and the Upper Castle Hayne aquifer–River Bend unit and receive water directly from these aquifers. Frenchmans Creek, near the western limit of the study area, is apparently a perennial stream through most of its reach and also probably derives baseflow directly from the Tarawa Terrace aquifer and the Upper Castle Hayne aquifer–River Bend unit.

Lateral flow directions within the Middle and Lower Castle Hayne aquifers probably mimic, to a large degree, corresponding directions within the Upper Castle Hayne aquifer–River Bend unit, except in the immediate vicinity of discharge areas such as Northeast Creek and New River, where flow directions within the deeper confined aquifers are vertically upward. Diffuse vertical leakage across confining units and between aquifers is probably pronounced in the vicinity of pumping wells where vertical-head gradients are relatively large but is limited elsewhere by small vertical-head gradients and the thickness and vertical hydraulic conductivity of confining units. Groundwater probably flows vertically downward through the Upper and Middle Castle Hayne aquifers in the northern part of the study area near and somewhat south of Lejeune Boulevard (SR 24) and is probably vertically upward within these same aquifers in the vicinity of New River and Northeast Creek. Paired observations that measure water levels in individual aquifers of the Upper Castle Hayne aquifer system are not available for the study area; however, long-term measurements are available for the Upper and Lower Castle Hayne aquifers at site X24S located just north of Wallace Creek. These data are possibly influenced by local pumping but indicate less than a 3-ft head difference occurred between the Upper and Lower Castle Hayne aquifers during 1987–2004. The head gradient was vertically upward (North Carolina Division of Water Resources, written communication, August 30, 2005). Similar flow conditions probably occurred within the study area during the period of interest to this investigation in the vicinities of Northeast Creek and New River.

Following the onset of pumping at water-supply wells, groundwater flow that under predevelopment conditions was entirely directed toward Northeast Creek, New River, and Frenchmans Creek was partially diverted to pumping wells. Consequently, (1) predevelopment potentiometric levels near and in the vicinity of pumping wells declined in the aquifers open to the wells, (2) predevelopment flow directions changed preferentially toward wells from natural points of discharge such as Northeast Creek, and (3) potentiometric levels possibly declined near groundwater/topographic divides resulting in the migration of boundaries farther west or north of predevelopment locations. Water-level declines near or in the vicinity of Northeast Creek or New River possibly caused a complete reversal in the direction of groundwater flow such that saltwater or brackish water from these surface-water bodies intruded landward into the Tarawa Terrace or Upper Castle Hayne aquifers.

Horizontal Hydraulic Conductivity

Results of 36 aquifer-test analyses at Tarawa Terrace and adjacent areas of Montford Point and Paradise Point are summarized in Tables C2–C4. Test data are summarized, respectively, for the combined Tarawa Terrace aquifer and Upper Castle Hayne aquifer–River Bend unit, Upper Castle Hayne aquifer–Lower unit, and Middle Castle Hayne aquifer. Most well locations are shown on Plate 1. Site names prefaced with "C," "PZ," and "S" indicate wells constructed during ABC One-Hour Cleaners Operable Units 1 and 2, which are located in the immediate vicinity of ABC One-Hour Cleaners and in the northern part of Tarawa Terrace. Well names prefaced with "TTSC" are located at or in the vicinity of the shopping center, in the southernmost part of Tarawa Terrace, just north of the shoreline of Northeast Creek. A site name prefaced with "TTUST" indicates monitor wells constructed during investigations of possible groundwater contamination caused by the leakage of refined-petroleum products from USTs and are located somewhat randomly throughout the Tarawa Terrace housing areas. Site names prefaced with "LCH," "M," and "HP" refer to wells located in the vicinity of Montford Point and between Northeast Creek and Wallace Creek, respectively, and were used to provide lateral control to interpolated flow model arrays of horizontal hydraulic conductivity at Tarawa Terrace and vicinity. Well S190A is an irrigation well at a golf course at Paradise Point. Coordinate locations of Hadnot Point (HP- and LCH-) water-supply wells used in this series of reports were current at the time of analysis and may differ slightly from updated coordinate locations published in subsequent reports.

Calculated horizontal hydraulic conductivity at all sites ranged from about 5 to 50 ft/d and averaged about 19 ft/d. Standard deviation was about 10 ft/d. With the exception of two tests, at least one open interval at tested wells was open to the Upper Castle Hayne aquifer. Horizontal hydraulic conductivity at these sites ranged from about 5 to 40 ft/d. Several tests included wells open to the Upper and Middle Castle Hayne aquifers. Horizontal hydraulic conductivity at these sites ranged from 5 to 30 ft/d. Horizontal-hydraulic-conductivity data unique to the Tarawa Terrace aquifer are located, with one exception, only in the immediate vicinity of Tarawa Terrace and ranged from 20 to 50 ft/d. Horizontal hydraulic conductivity at a test well open to the Tarawa Terrace aquifer and confining unit at the STT site was 2 ft/d. These data were not included in Table C2.

The horizontal hydraulic conductivity of the Lower Castle Hayne aquifer was not uniquely determined at any site. Descriptions of the lithology of this aquifer, however, indicate a preponderance of fine sands and clayey sands, when compared to lithologies reported for the Upper and Middle Castle Hayne aquifers (Faye 2007). Accordingly, the average horizontal hydraulic conductivity of the Lower Castle Hayne aquifer is estimated to be half or less of the average computed for all analyses (Tables C2–C4).

Table C2. Horizontal hydraulic-conductivity data used to create a cell-by-cell distributed array for the combined Tarawa Terrace aquifer and Upper Castle Hayne aquifer–River Bend unit (model layer 1), Tarawa Terrace and vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina.

[Contributing aquifers: UCH, Upper Castle Hayne aquifer-undifferentiated; TT, Tarawa Terrace aquifer; UCHRBU, Upper Castle Hayne aquifer–River Bend unit; karst, a zone of relatively high hydraulic conductivity indicated on drillers' logs by the loss of drilling fluids at a certain depth or a sudden drop of the drill stem during drilling]

Site name[1]	Location coordinates[2]		Horizontal hydraulic conductivity, in feet per day	Contributing aquifers
	East	North		
HP-710	2507781	351490	20	UCH
HP-711	2509200	352130	10	TT, UCH
LCH-4009	2499585	358589	20	UCHRBU
M-142	2478313	360422	30	UCHRBU, karst
M-628	2479434	362735	10	UCH
PZ-06	2490707	364926	20	UCHRBU
S190A	2487640	353870	30	UCHRBU
S2	2490787	364883	20	UCHRBU
S6	2490617	364938	10	TT, UCHRBU
STT61to66-MW03	2489186	364740	50	TT
[3]TTUST-2477-MW01	2488759	361550	20	TT
[3]TTUST-2477-MW06	2488738	361521	20	TT, UCHRBU
[3]TTUST-2478-PW01	2488879	361898	10	TT(?), UCHRBU

[1]See Plate 1 for location

[2]Location coordinates are North Carolina State Plane coordinates, North American Datum of 1983

[3]Because of scale, not shown on Plate 1

Table C3. Horizontal hydraulic-conductivity data used to create a cell-by-cell distributed array for the Upper Castle Hayne aquifer–Lower unit (model layer 3), Tarawa Terrace and vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina.

[Contributing aquifers: UCHLU, Upper Castle Hayne aquifer–Lower unit; UCHRBU&LU, Upper Castle Hayne aquifer–River Bend and Lower units; UCH, Upper Castle Hayne aquifer–undifferentiated; karst, a zone of relatively high hydraulic conductivity indicated on drillers' logs by the loss of drilling fluids at a certain depth or a sudden drop of the drill stem during drilling]

Site name[1]	Location coordinates[2]		Horizontal hydraulic conductivity, in feet per day	Contributing aquifers
	East	North		
C2	2490793	364902	30	UCHLU
HP-650	2510615	354320	40	UCHRBU&LU
HP-663	2510881	352712	10	UCHRBU&LU
HP-700	2488520	355270	8	UCH
HP-705	2501260	356200	30	UCH
HP-707	2492300	353850	20	UCH
M-243	2476839	359734	10	UCHLU
M-267	2476609	359232	10	UCHRBU&LU
M-630	2475763	361256	20	UCHLU
PZ-03	2490812	364858	20	UCHLU
TT-26	2491461	364356	20	UCHLU, karst(?)
TT-52	2489060	362321	10	UCH
TT-55	2489070	364767	10	UCHLU (?)
TT-67	2490160	362730	20	UCHLU

[1]See Plate 1 for location

[2]Location coordinates are North Carolina State Plane coordinates, North American Datum of 1983

Table C4. Horizontal hydraulic-conductivity data used to create a cell-by-cell distributed array for the Middle Castle Hayne aquifer (model layer 5), Tarawa Terrace and vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina.

[Contributing aquifers: UCHRBU, Upper Castle Hayne aquifer–River Bend unit; MCH, Middle Castle Hayne aquifer; TT, Tarawa Terrace aquifer; UCH, Upper Castle Hayne aquifer–undifferentiated; UCHRBU&LU, Upper Castle Hayne aquifer–River Bend and –Lower units]

Site name[1]	Location coordinates[2]		Horizontal hydraulic conductivity, in feet per day	Contributing aquifers
	East	North		
HP-622	2494248	353323	20	UCHRBU, MCH
HP-623	2495617	350860	20	TT, UCH, MCH
HP-644	2485841	356243	10	UCHRBU, MCH
HP-645	2497333	356430	20	UCHRBU, MCH
HP-646	2497870	357826	10	UCHRBU, MCH
HP-647	2499461	356343	30	UCHRBU, MCH
M-197	2477521	361501	5	UCH, MCH
TT-23	2491024	363208	10	UCHRBU&LU, MCH
TT-25	2491984	364042	9	UCHRBU&LU, MCH

[1]See Plate 1 for location

[2]Location coordinates are North Carolina State Plane coordinates, North American Datum of 1983

Potentiometric Surfaces

The oldest and/or highest water-level measurements out of a total data set of several hundred measurements were selected at 59 locations in the study area to estimate the predevelopment potentiometric surface of the Tarawa Terrace aquifer and the Castle Hayne aquifer system (Table C5). Potentiometric levels are predominantly from wells open only to the Tarawa Terrace and Upper Castle Hayne aquifers. Detailed water-level measurements obtained at paired monitor wells in conjunction with investigations of groundwater contamination at various locations throughout Tarawa Terrace and vicinity indicate that little or no head difference exists between the River Bend and Lower units of the Upper Castle Hayne aquifer (Roy F. Weston, Inc. 1992, 1994; O'Brien & Gere Engineers, Inc. 1992, 1993; Law Engineering, Inc. 1994a,b, 1995a,b; Richard Catlin & Associates, Inc. 1994a,b, 1995a,b, 1996; Law Engineering and Environmental Testing, Inc. 1996). In addition, water-level data collected at a well cluster representing the Tarawa Terrace and Upper and Lower Castle Hayne aquifers at site X24S1-S7, north of Wallace Creek (Plate 1), indicate only about 3 ft of head difference occurred between the Upper and Lower Castle Hayne aquifers between 1987 and 2004 (Harned and others, 1989; North Carolina Division of Water Resources, written communication, August 30, 2005). Head gradients were generally vertically upward at this site. Although the water level measured in the Lower Castle Hayne aquifer was possibly influenced by pumping, a head difference slightly greater than 3 ft probably also is representative of head differences within the Castle Hayne aquifer system in the vicinity of Northeast Creek and New River at Tarawa Terrace. The small differences in head measured between the Tarawa Terrace and Upper Castle Hayne aquifers in the study area, as well as at site X24S, indicate that potentiometric surfaces of the individual Upper, Middle, and Lower Castle Hayne aquifers are highly similar.

Contours of equal potentiometric level based on all measurements listed in Table C5 and selected measurements from Appendix C1, Table C1.10 are shown in Figure C5. The spatial distribution of potentiometric levels conforms to the conceptual model discussed previously. Assuming that lines orthogonal to the potentiometric level contours approximate directions of groundwater flow, groundwater flows west to east from highland areas toward Northeast Creek and south toward Northeast Creek and New River. As noted previously, the potentiometric surface shown in Figure C5 probably closely resembles corresponding potentiometric surfaces within the Middle and Lower Castle Hayne aquifers.

Table C5. Estimated predevelopment water levels at Tarawa Terrace and vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina.

[NGVD 29, National Geodetic Vertical Datum of 1929; contributing aquifers: UCHLU, Upper Castle Hayne aquifer–Lower unit; MCH, Middle Castle Hayne aquifer; UCHRBU, Upper Castle Hayne aquifer–River Bend unit; TT, Tarawa Terrace aquifer; UCHRBU&LU, Upper Castle Hayne aquifer–River Bend and Lower units; UCH, Upper Castle Hayne aquifer–undifferentiated]

Site name[1]	Measuring date	Water-level altitude, in feet above NGVD 29	Contributing aquifers
C1	4/22/1992	21.5	UCHLU
C2	4/22/1992	19.6	UCHLU
C3	4/22/1992	15.8	UCHLU
C4	4/22/1992	11.9	MCH
C5	4/22/1992	15.7	UCHLU
C9	11/18/1993	13.0	UCHLU
C10	11/18/1993	12.6	MCH
C11	10/1/1993	6.3	UCHLU
CCC-1	9/17/1941	3.3	UCHRBU
CCC-2	6/19/1942	5.2	UCHRBU
PZ-01	11/18/1993	16.7	UCHLU
PZ-02	11/18/1993	16.7	UCHRBU
PZ-03	11/18/1993	16.6	UCHLU
PZ-04	11/18/1993	16.4	UCHRBU
PZ-05	10/1/1993	15.7	UCHLU
PZ-06	10/1/1993	16.1	UCHRBU
S1	4/22/1992	23.7	TT, UCHRBU(?)
S2	4/22/1992	19.9	UCHRBU
S3	4/22/1992	16.0	TT, UCHRBU
S4	4/22/1992	13.6	TT, UCHRBU(?)

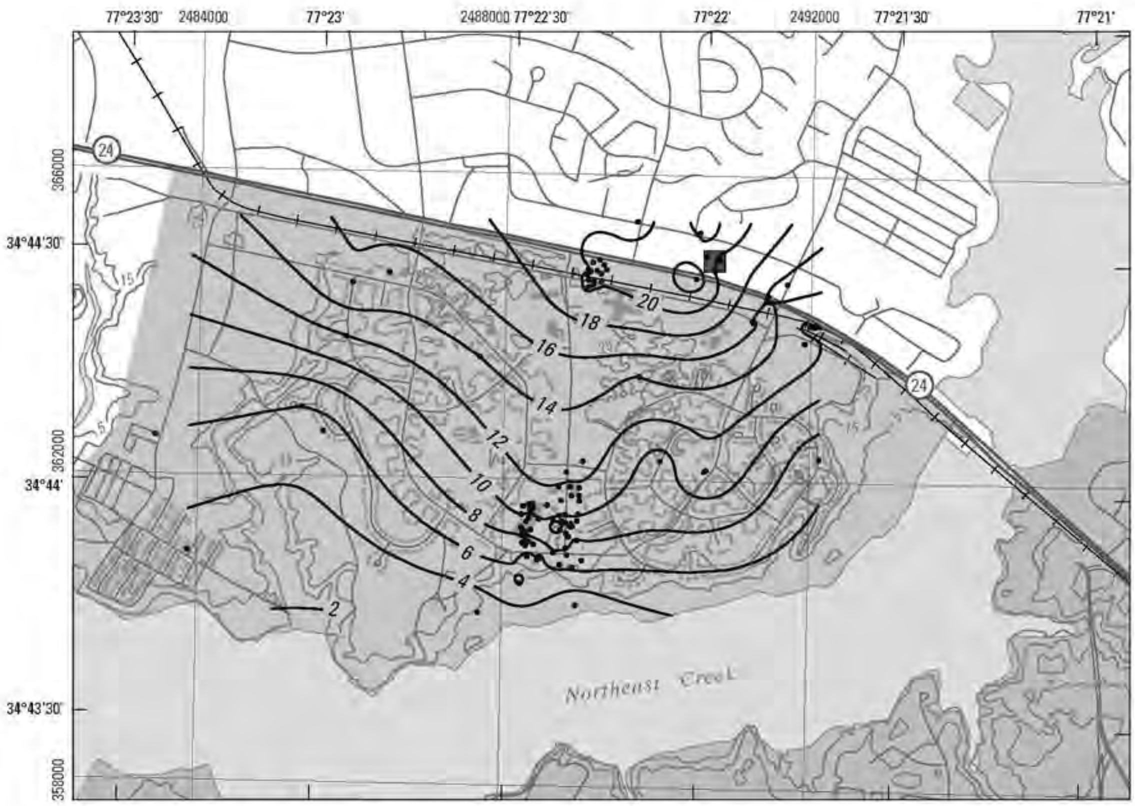
Table C5. Estimated predevelopment water levels at Tarawa Terrace and vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina.—Continued

[NGVD 29, National Geodetic Vertical Datum of 1929; contributing aquifers: UCHLU, Upper Castle Hayne aquifer–Lower unit; MCH, Middle Castle Hayne aquifer; UCHRBU, Upper Castle Hayne aquifer–River Bend unit; TT, Tarawa Terrace aquifer; UCHRBU&LU, Upper Castle Hayne aquifer–River Bend and Lower units; UCH, Upper Castle Hayne aquifer–undifferentiated]

Site name[1]	Measuring date	Water-level altitude, in feet above NGVD 29	Contributing aquifers
S5	4/22/1992	16.4	TT, UCHRBU(?)
S6	4/22/1992	20.6	TT, UCHRBU
S7	4/22/1992	19.8	TT, UCHRBU
S8	4/22/1992	20.9	TT, UCHRBU
S9	4/22/1992	15.4	TT, UCHRBU
S10	6/25/1992	13.3	TT, UCHRBU
S11	11/18/1993	19.0	TT, UCHRBU
STT61to66-MW01	1/29/1992	21.6	TT
STT61to66-MW20	12/17/1992	20.1	TT, UCHRBU
T-9	4/10/1987	23.4	TT, UCHRBU
TT-25	4/7/1987	10.9	UCHRBU&LU, MCH
TT-26	5/16/1951	14.0	UCHLU
TT-52	10/17/1961	12.9	UCH
TT-53	7/22/1961	14	UCHRBU&LU
TT-54	6/30/1961	12.1	UCH
TT-55	11/1/1961	18.9	UCHLU(?)
TTDump MW01	6/26/1991	2.4	TT
TTDump MW02	6/26/1991	6.2	TT
TTDump MW03	6/26/1991	2.2	TT
[2]TTUST-44-MW01	11/15/2001	6.0	TT, UCHRBU
[2]TTUST-48-MW01	9/1/1998	19	TT, UCHRBU
[2]TTUST-779-MW01	7/25/2002	9	TT
[2]TTUST-2254-MW01	7/24/2002	13	TT
[2]TTUST-2258-MW01	7/24/2002	12	TT
[2]TTUST-2302-MW01	7/24/2002	12	TT
[2]TTUST-2455-MW13	10/28/1993	9.2	TT, UCHRBU
[2]TTUST-2455-MW15	10/28/1993	5.6	TT, UCHRBU
[2]TTUST-2477-MW11	11/4/1994	11.6	UCHRBU
[2]TTUST-2477-MW14	11/9/1994	7.9	TT
[2]TTUST-2478-MW08	11/22/1993	12.6	TT
[2]TTUST-2478-MW23	9/28/2000	6.2	TT, UCHRBU
[2]TTUST-2634-MW01	11/1/2001	14	TT, UCHRBU(?)
[2]TTUST-3140-MW01	7/24/2002	15	TT, UCHRBU(?)
[2]TTUST-3165-MW01	7/24/2002	16	TT, UCHRBU(?)
[2]TTUST-3233-MW01	7/24/2002	12	TT, UCHRBU(?)
[2]TTUST-3524-MW01	7/25/2002	6	TT
[2]TTUST-3546-MW01	7/25/2002	5	TT
[2]TTUST-TTSC-09	12/28/1994	8.8	TT
[2]TTUST-TTSC-15	12/28/1994	11.2	UCHRBU

[1]See Plate 1 for location

[2]Because of scale, not shown on Plate 1



Base from U.S. Marine Corps and U.S. Geological Survey digital data files
Map coordinates are North Carolina State Plane coordinates
North American Datum of 1983

0 2,000 4,000 FEET
0 500 1,000 METERS

EXPLANATION

Historical water-supply area

Tarawa Terrace

Holcomb Boulevard

ABC One-Hour Cleaners

— *10* — **Line of equal potentiometric level**—Combined Tarawa Terrace aquifer and Upper Castle Hayne aquifer–River Bend Unit. Contour interval 2 feet. Datum is National Geodetic Vertical Datum of 1929

— *25* — **Topographic contour**—Interval 10 feet

• **Control point**

Figure C5. Estimated predevelopment potentiometric levels of the combined Tarawa Terrace aquifer and Upper Castle Hayne aquifer–River Bend unit, Tarawa Terrace and vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina.

Tarawa Terrace Groundwater-Flow Model

The original version of the numerical code used in this study to simulate groundwater flow was written by McDonald and Harbaugh (1984) and was designated a modular finite-difference groundwater-flow model (MODFLOW). The code simulates groundwater flow in a three-dimensional heterogeneous and anisotropic porous medium. Updates to the original MODFLOW code were developed periodically along with various modules to expand simulation capability and computational performance. The MODFLOW version used in this study is known as MODFLOW-96 (Harbaugh and McDonald, 1996) and is part of a highly integrated simulation system called PMWINPro™ (Processing MODFLOW Pro, version 7.017), which also includes codes that support and augment groundwater-flow simulation using techniques such as particle tracking and inverse modeling (Chiang and Kinzelbach 2001). The capability to simulate advective transport also is integrated within PMWINPro™ and is based on techniques and codes first published by Pollock (1989, 1994). Two flow models were calibrated: a predevelopment model representing long-term, average groundwater-flow conditions prior to the development of the Castle Hayne aquifer system, and a transient model representing pumping of the Castle Hayne aquifer system as a water supply for Tarawa Terrace. The transient model is temporally subdivided into 528 stress periods, representing monthly conditions beginning January 1951 and ending December 1994. The active model domain, the model grid, model boundary conditions, model geometry, hydraulic characteristic arrays, and all other model elements common to the calibrated predevelopment and transient models are identical.

Model Domain and Boundary Conditions

The total domain of the Tarawa Terrace flow model comprises most of the area north and west of the mid-channel line of Northeast Creek shown in Figure C6. Approximate State Plane coordinates (North American Datum of 1983) of the four corners of the model domain are listed in Table C6. The total area shown in Figure C6 is the model domain, which, for modeling purposes, is subdivided into active and inactive domains. The active domain, which corresponds to the area pertinent to the simulation of groundwater flow, is the blue gridded area and also includes the dark blue area that extends to the mid-channel of Northeast Creek. The remaining area within the total model domain, but outside the gridded area, is the inactive domain. The total model domain was subdivided into 270 columns and 200 rows of square cells representing a length of 50 ft per side. The model was subdivided vertically into seven layers. Model layer 1 corresponds to the combined Tarawa Terrace aquifer, the Tarawa Terrace confining unit, and the Upper Castle Hayne aquifer–River Bend unit (Table C1). The remaining six layers correspond, respectively, to the Local confining unit, the Upper Castle Hayne aquifer–Lower unit, the Middle Castle Hayne confining unit, the Middle Castle Hayne aquifer, the Lower Castle Hayne confining unit, and the Lower Castle Hayne aquifer. The area represented by the total model domain is about 135,000,000 square feet (ft^2) or about 4.8 square miles (mi^2). The active model domain corresponds to an area of about 59,400,000 ft^2, about 2.1 mi^2 or about 1,360 acres. Model layer 1 is specified as an unconfined aquifer and contains the water table. All other model layers are specified as confined.

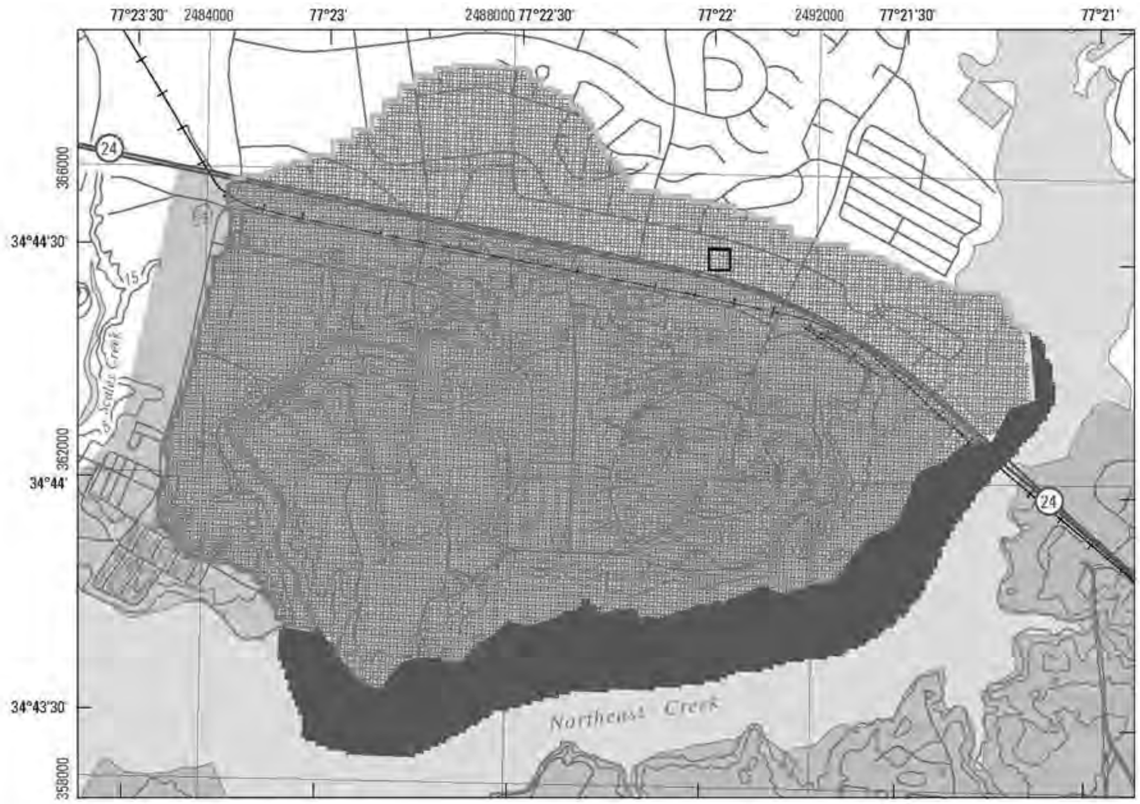
The base of simulated groundwater flow corresponds to the top of the Beaufort confining unit and is implicitly a no-flow boundary. Boundaries assigned to the eastern, western, and southern perimeters of the active model domain were all no-flow and are equal in location and condition for each layer. The southern and most of the eastern boundary conform to the mid-channel line of Northeast Creek. The western boundary conforms to the topographic divide that separates the drainage areas of Scales and Frenchmans Creeks (Figure C6). The northern boundary also generally conforms to a topographic divide but was assigned as a general-head (head-dependent) boundary in all model layers because of the proximity of water-supply wells to the boundary in the northwestern and north-central parts of the active model domain. Conductance values applied to general-head boundary cells were computed using the equation:

$$C = (K_h bW)/L, \tag{1}$$

where

- K_h equals the cell horizontal hydraulic conductivity, in ft/d;
- b equals the cell thickness, in ft;
- W equals the width of the cell face perpendicular to the direction of flow, in ft; and
- L equals the distance between the source-head boundary and the model general-head boundary, in ft.

To compute cell conductances, values of K_h for each layer at each boundary cell were determined from the calibrated predevelopment flow model. Cell widths (W) were assigned a constant value of 50 ft. The layer thickness at each cell was determined by subtracting the assigned value of the altitude at the top of each layer at each boundary cell from the assigned altitude at the bottom of each corresponding boundary cell. The distance L from each boundary cell to the source-head boundary was arbitrarily assigned as the length of 10 grid cells or 500 ft and was constant for the entire boundary for each layer. The assigned potentiometric level at each source-head boundary cell was estimated using as guidelines potentiometric levels simulated at respective cells by the calibrated predevelopment flow model. Source heads closely resemble or equal the respective simulated predevelopment water levels with the possible exception of source heads at several cells in the central part of the active model domain in model layer 1. Potentiometric levels at these cells were assigned 1–3 ft higher than calibrated predevelopment water levels, conforming to slightly higher land-surface altitudes at the source-head boundary compared to those at the northern boundary of the active model domain (Figure C6).



Base from U.S. Marine Corps and U.S. Geological Survey digital data files
Map coordinates are North Carolina State Plane coordinates
North American Datum of 1983

0 2,000 4,000 FEET
0 500 1,000 METERS

EXPLANATION

Historical water-supply area
- Tarawa Terrace
- Holcomb Boulevard

Topographic contour— Interval 10 feet

ABC One-Hour Cleaners

Groundwater-flow and fate and transport model boundary
- Domain

Boundary conditions for groundwater-flow model
- General head
- No flow
- Specified head
- Drain (Frenchmans Creek)

Model grid—Active model domain

Figure C6. Groundwater-flow model grid and model boundaries, Tarawa Terrace and vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina.

Table C6. Approximate location coordinates of the corners of the Tarawa Terrace groundwater-flow model domain, U.S. Marine Corps Base Camp Lejeune, North Carolina.

Position	Location coordinates[1]	
	North	East
Northeastern corner	367370	2495790
Northwestern corner	367370	2482290
Southeastern corner	357370	2495790
Southwestern corner	357370	2482290

[1]Location coordinates are North Carolina State Plane coordinates, North American Datum of 1983

The surface of Northeast Creek within the active domain was assigned a specified head of zero in model layer 1, corresponding to sea level. A drain also was assigned to model layer 1 along the channel of Frenchmans Creek in the western part of the model area. An initial hydraulic conductance of 50 ft^2/d was assigned to every drain cell. The final calibrated conductance of 200 ft^2/d was determined by trial-and-error calibration. Drain altitudes were interpolated to the center of drain cells using detailed topographic maps and ranged from zero to about 16 ft.

Effective recharge was assigned to the uppermost active cells regardless of layer at a rate that varied by stress period and annual rainfall. Precipitation data used for this study are daily values recorded at the Maysville–Hoffman Forest station located about 8.5 miles northeast of Jacksonville, North Carolina, along U.S. Highway 17, and about midway between Jacksonville and Maysville, North Carolina. The Maysville–Hoffman Forest record is the most complete of 10 precipitation station records local to the general vicinity of Camp Lejeune and pertinent to the period of interest of this study (1951–1994). Daily precipitation values are substantially complete beginning January 1951 and were used to compute total monthly precipitation for the period January 1951–December 1994. Incomplete data prevented the reasonable computation of a monthly total for 23 months during 12 years of this period (Table C7). Average monthly precipitation computed using these records was 4.72 inches or 56.64 in/yr. Long-term average annual effective recharge was estimated at 13.31 in/yr during calibration of the predevelopment-flow model. The ratio of the rates of long-term, average effective groundwater recharge computed using the calibrated predevelopment-flow model (13.31 in/yr) and average annual precipitation for the period 1951–1994 (56.64 in/yr) equals 0.235. The product of this ratio and total annual rainfall measured at the Maysville–Hoffman Forest station was considered the average rate of effective groundwater recharge for the respective year and was assigned, as such, to the groundwater-flow model at a constant rate in feet per day for each stress period (month of the year). The long-term average rate of effective groundwater recharge (13.31 in/yr) was assigned to each month of 1951, in order to establish a predevelopment distribution of potentiometric levels and flow prior to the onset of simulated pumping during January 1952.

Table C7. Summary of annual rainfall and effective recharge rates assigned during flow model calibration, U.S. Marine Corps Base Camp Lejeune, North Carolina.

Year	Rainfall,[1] inches per year	Effective groundwater recharge, inches per year	Effective groundwater recharge, in feet per day
1952	56.37	13.2	0.0030
1953	63.81	15.0	0.0034
1954	58.30	13.7	0.0031
1955	[2]57.59	13.5	0.0031
1956	[2]48.44	11.4	0.0026
1957	[2]44.63	10.5	0.0024
1958	[2]58.18	13.7	0.0031
1959	42.47	10.0	0.0023
1960	69.94	16.4	0.0038
1961	61.32	14.4	0.0033
1962	53.37	12.5	0.0029
1963	58.65	13.8	0.0031
1964	[2]50.38	11.8	0.0027
1965	[2]50.93	12.0	0.0027
1966	50.65	11.9	0.0027
1967	[2]41.06	9.6	0.0022
1968	[2]28.72	6.7	0.0015
1969	53.66	12.6	0.0029
1970	37.99	8.9	0.0020
1971	54.61	12.8	0.0029
1972	51.02	12.0	0.0027
1973	[2]34.28	8.1	0.0018
1974	81.86	19.2	0.0044
1975	49.46	11.6	0.0027
1976	57.33	13.5	0.0031
1977	61.81	14.5	0.0033
1978	57.79	13.6	0.0031
1979	53.95	12.7	0.0029
1980	54.49	12.8	0.0029
1981	64.48	15.2	0.0035
1982	50.24	11.8	0.0027
1983	[2]52.71	12.4	0.0028
1984	51.75	12.2	0.0028
1985	61.25	14.4	0.0033
1986	51.18	12.0	0.0027
1987	[2]38.92	9.1	0.0021
1988	52.92	12.4	0.0028
1989	55.84	13.1	0.0030
1990	71.88	16.9	0.0039
1991	[2]55.90	13.1	0.0030
1992	55.28	13.0	0.0030
1993	60.54	14.2	0.0032
1994	67.64	15.9	0.0036

[1]Rainfall data from the Maysville–Hoffman Forest station

[2]Incomplete record

Model Geometry and Initial Conditions

Model-layer geometry was assigned as distributed arrays of altitude at the top of each layer (geohydrologic unit; Table C1). Representations of distributed arrays are similar to contour maps shown herein in Figures C2 and C3 and were based on appropriate site (point) data interpolated to the entire active model domain using the Shepard's Inverse Distance method. The PMWINPro™ flow model automatically checks each cell to verify that assigned altitudes do not overlap vertically adjacent layers. Site data for each geohydrologic unit component of the Tarawa Terrace flow models are listed in Faye (2007, Tables B3–B14).

Hydraulic characteristic data assigned to each model layer are horizontal and vertical hydraulic conductivity and specific storage. Horizontal hydraulic conductivities at selected locations within and adjacent to the model domain were selected from Tables C2–C4 as representative of model layers 1, 3, and 5, respectively. These point data were interpolated by the Shepard's Inverse Distance method to the entire model domain to provide an initial distributed array of horizontal hydraulic conductivity for the specified model layers. The interpolated array originally assigned to model layer 1 was uniformly increased by a factor of 1.35 during model calibration. Horizontal hydraulic conductivity of model layer 7 (Lower Castle Hayne aquifer) was assigned uniformly at 5 ft/d. Initially, horizontal hydraulic conductivity of each confining unit was assigned uniformly at 1.0 ft/d.

Initial cell-by-cell vertical hydraulic conductivities assigned to each layer equaled one-tenth the respective cell horizontal hydraulic conductivity. During model calibration, the ratio of vertical to horizontal hydraulic conductivity for model layers 1 and 3 was increased from 1:10 to 1:7.3 and 1:8.3, respectively. At model cells that correspond to the location of water-supply wells, the vertical hydraulic conductivity of confining units penetrated by the well was increased to 100 ft/d to duplicate the effect of gravel and sand packs used to complete well construction. At several supply wells (TT-23, TT-26, and TT-67), the well bore was drilled to a depth substantially greater than the completed well. The unused well bore was then typically backfilled with gravel or sand. At these sites, the assigned vertical hydraulic conductivity of confining layers penetrated by the unused well bore was also 100 ft/d.

Specific storage for model layers 2 through 7 was assigned based on an assumed storativity of 0.0004 for each layer divided by respective cell-by-cell thickness. The distributed thickness array for each layer was computed as the difference between cell-by-cell altitudes at the top of vertically adjacent layers. A specific yield of 0.05 was assigned uniformly to model layer 1. The same array of initial potentiometric levels was assigned to each model layer and corresponds to the potentiometric surface shown in Figure C5.

Pumpage Data

Data indicating pumpage at individual Tarawa Terrace water-supply wells were unavailable for the period of interest to this study. Accordingly, pumping rates at supply wells were estimated and were assigned to monthly stress periods based on: (1) reported well-capacity data, (2) average annual and monthly rates of water-supply demand reported for the Tarawa Terrace WTP, and (3) records of supply well operations. Annualized daily rates of raw water treated by the Tarawa Terrace WTP for the years 1975–1987 are listed in Table C8 and were obtained from the USGS (U.S. Geological Survey, Raleigh, North Carolina, "Water Use for Camp Lejeune Military Base Water Systems," written communications, March 2004). Monthly operation records of Tarawa Terrace water-supply wells during 1978–1985 included notes regarding equipment replacement and periods when individual wells were out of service (Camp Lejeune water documents CLW 3559–4053; monthly well operation reports, written communications, September 22, 2004).

Well-capacity records are available for most Tarawa Terrace water-supply wells, many from the onset of well operation. These records are summarized in Appendix C3, Tables C3.1–C3.10, and were used to estimate well capacity for monthly pumping rates assigned to stress periods of the groundwater-flow model. The actual date (month and year) when a supply well began service is unknown. With the exception of well TT-23, all supply wells were placed in service, for purposes of model simulation, during January

Table C8. Annualized daily average flow rate of raw water treated at the Tarawa Terrace water treatment plant, 1975–1987, U.S. Marine Corps Base Camp Lejeune, North Carolina.

Year	Raw water treated,[1] in million gallons per day
1975	0.83
1976	0.85
1977	0.86
1978	0.90
1979	0.83
1980	0.78
1981	0.88
1982	0.98
1983	0.94
1984	0.85
1985	0.83
1986	0.90
1987	0.12

[1]U.S. Geological Survey, Raleigh, North Carolina, "Water Use for Camp Lejeune Military Base Water Systems," written communications, March 2004

following the year of construction. Simulation of pumpage from well TT-23 began during August 1984. Construction of well TT-23 was completed during March 1983.

Annualized daily average flow rates of total water treated at the Tarawa Terrace WTP for the period 1975–1987 are listed in Table C8. The average rate for the period 1975–1986 was 0.87 MGD or about 116,200 cubic feet per day (ft^3/d) and ranged from 0.78 to 0.98 MGD. The Tarawa Terrace WTP was closed during March 1987; hence, the partial rate of 0.12 MGD was reported for 1987. These annual average rates are considered for this study to equal average annual total pumpage from all active Tarawa Terrace water-supply wells for the respective years. Pumpage data and surrogate pumpage information pertinent to Tarawa Terrace prior to 1975 are not available. Accordingly, the average rate of 116,200 ft^3/d determined for the period 1975–1986 also was considered the average rate of total pumpage cumulative to all active Tarawa Terrace water-supply wells for the period January 1952–December 1974.

Total monthly pumpage cumulative to all active Tarawa Terrace water-supply wells was reported by Camp Lejeune for all of 1984 and February, March, April, and July 1985 (Camp Lejeune water documents CLW 1056, 1118, 1125, 1197, and 1290, written communications, no date). Additional total monthly pumpage and treated water rates during 1978 at Tarawa Terrace are included in Henry Von Oesen and Associates, Inc. (1979), who reported that the average daily rate of water delivered to the Tarawa Terrace WTP during 1978 was 0.90 MGD, the identical rate reported by the USGS (Table C8). Monthly cumulative pumpage rates at Tarawa Terrace for the period January 1980–December 1984 were provided by Camp Lejeune (Steven Whited, U.S. Marine Corps Base Camp Lejeune, written communication, March 18, 2005). These data are incomplete for several months during 1981 and most of 1982. The USGS provided cumulative pumpage rates for active Tarawa Terrace water-supply wells for January–March 1987 (U.S. Geological Survey, "Water Treatment Plants-Water Flow," written communication, January–March 1987). These documents probably were originally obtained from U.S. Marine Corps Base Camp Lejeune.

Pumping rates assigned to individual Tarawa Terrace water-supply wells were applied to the transient model for 528 stress periods. Each stress period represents a single month beginning January 1951 and ending December 1994. Stress periods were not subdivided into time steps. Accordingly, each stress period equaled 28, 29, 30, or 31 days. Assigned pumpage for stress periods 1–12 (January–December 1951) was zero. Pumping at Tarawa Terrace water-supply wells is assumed to have commenced during January 1952 at all wells located within the active model domain at that time; that is, wells TT-26 (#1), TT-27 (#2), TT-28 (#3), and TT-29 (#4) (Figure C1). Three additional water-supply wells—#6, #7, and TT-45—also delivered water to the Tarawa Terrace WTP at this time but were located outside the active model domain (Tarawa Terrace well capacity list, written communication, June 24, 1958; LeGrand 1959; North Carolina State Plane coordinates: #6 [highly approximate] North 369730, East 2481720; #7 [highly approximate] North 370500, East 2481530; and TT-45 North 365688, East 2483352).

The month and year when a particular water-supply well was placed in service, for simulation purposes, are indicated in Appendix C3, Tables C3.1–C3.10, along with the corresponding date that service was terminated. Other operational conditions such as dates when the well was out of service or tested also are listed. The dates and operational conditions listed in these tables are honored explicitly in the groundwater-flow model by changing pumping rates, adding or deleting pumping for a particular stress period (month), or removing a well entirely or adding a well to the model at a given month and year. Well capacities listed in Appendix C3, Tables C3.1–C3.10, were used to assign pumping rates to individual water-supply wells for each stress period and were changed periodically over time as indicated. Well capacities, as listed, were originally intended as guidelines but also were honored explicitly for most stress periods.

Pumping rates at individual water-supply wells for each stress period were estimated based on a percentage of total well capacity available at Tarawa Terrace at the given time. An example allocation is shown in Table C9 for stress period 408, December 1984. Active water-supply wells at that time were TT-23, TT-25, TT-26, TT-30, TT-31, TT-52, TT-54, and TT-67. Total raw water delivered to the Tarawa Terrace WTP during December 1984 was 25,092,000 gal or about 108,211 ft^3/d. Total well capacity was estimated to be 1,083 gal/min. Pumping rates assigned to individual Tarawa Terrace wells during each stress period, using the method of allocation shown in Table C9, are listed in Maslia et al (In press 2008).

Table C9. Example allocation of pumping rates to Tarawa Terrace water-supply wells, stress period 408 (December 1984), U.S. Marine Corps Base Camp Lejeune, North Carolina.

[gpm, gallon per minute; ft^3/d, cubic foot per day]

Site name[1]	Well capacity, in gpm	Percentage of total capacity, decimal	Estimated pumping rate, in ft^3/d
TT-23	254	0.2345	25,379
TT-25	130	0.1200	12,989
TT-26	150	0.1385	14,988
TT-30	50	0.0462	4,996
TT-31	119	0.1099	11,890
TT-52	130	0.1200	12,989
TT-54	150	0.1385	14,988
TT-67	100	0.0923	9,992
Total	**1,083**	**1.0000**	**108,211**

[1]See Figure C1 for location

Model Calibration

Calibration of the Tarawa Terrace flow model was accomplished in a hierarchical process consisting of four successive stages or levels. Simulation results achieved for each calibration level were iteratively adjusted and compared to simulation results of previous levels until results at all levels satisfactorily conformed to calibration standards. Hydraulic characteristic arrays and model boundary conditions were equivalent at all calibration levels. All flow model calibrations also were required to conform to the conceptual flow model described previously. In hierarchical order, calibration levels consisted of the simulation of (1) predevelopment conditions, (2) transient or pumping conditions, (3) the fate and transport of a PCE source at ABC One-Hour Cleaners, and (4) the concentration of PCE at the Tarawa Terrace WTP and within the Tarawa Terrace water-distribution network. Calibration levels 1 and 2 are described in detail in this report. Calibration levels 3 and 4 are similarly described in Faye (In press 2007).

Calibration standards for the predevelopment flow model calibration (level 1) required that simulated water levels at water-supply and monitor well locations match estimated observed predevelopment water levels within an absolute difference of 3 ft. This standard is derived from the least accurate water levels used for predevelopment calibration, which were obtained by estimating land-surface altitude at the well site from a topographic map and subtracting a reported depth to water. The contour interval of the topographic maps was 5 ft, and land-surface altitudes were estimated at an accuracy of ±2.5 ft or one-half contour interval. The half-contour interval level of accuracy was rounded upward to 3 ft to provide a predevelopment calibration standard. Most of the water levels listed in Table C5 were used to evaluate predevelopment simulation results (Table C10).

Water-level data listed in Appendix C1, Tables C1.1–C1.11, were used to evaluate the quality of the level 2 or transient model calibration. The bulk of these data represent water levels at Tarawa Terrace water-supply wells. Data listed in Appendix C1, Tables C1.10 and C1.11, are water levels observed at various monitor wells installed during ABC One-Hour Cleaners Operable Units 1 and 2 at and in the vicinity of ABC One-Hour Cleaners and during remedial investigations of petroleum product spills and leaks from surface and underground storage tanks at Tarawa Terrace.

Monthly logs of operational information at Tarawa Terrace water-supply wells were obtained from USGS and Camp Lejeune records (Camp Lejeune water documents CLW 3559–4053, monthly well operation reports, written communication, September 22, 2004). Monthly logs were obtained for the period January 1978–April 1986. "Static" water levels were reported per month and were obtained by airline measurements. The actual date of measurement was not reported and, for this study, each measurement is assumed to have occurred on the last day of the designated month. Typically, reported water levels vary in excess of 20 ft during the period of measurement, and frequently 10 ft or more from month to month. Large changes in water levels from month to month may be indicative of water-level measurements obtained shortly after the termination of pumping and may not represent a static or near static measurement. Such variability also may indicate leaking or damaged airlines or pressure gages. LeGrand (1959) describes various problems associated with the use of airlines to measure water levels at Camp Lejeune including airline obstructions, leaks, and poor gage resolution. Similar problems probably occurred, as well, relative to airline measurements used for this study. For example, such problems possibly occurred at water-supply well TT-23 during its brief period of operation (August 1984–April 1985). The earliest static water-level measurement at a supply well is typically obtained immediately following well construction and is the highest measurement until routine operation is terminated for an extended period of time (Appendix C1, Tables C1.1–C1.3, C1.6–C1.8). However, at well TT-23, the earliest static water level, obtained prior to a well capacity test (March 1983), is substantially lower than subsequent airline measurements obtained during well operation (Appendix C1, Table C1.1), but is similar to water levels obtained by tape measurements reported by Shiver (September 1985) and the USGS (October 1986). A possible explanation for these differences is an improperly calibrated airline gage.

Pressure gages attached to airlines at Tarawa Terrace water-supply wells were not available for inspection but probably were accurate only to within ±5 pounds per square inch (psi) or greater or within an estimated range of about ±12 ft. Accordingly, for transient model calibration, the calibration standard applied to water-level data obtained from airline measurements was an absolute difference of 12 ft between simulated and observed water levels.

Highly accurate water-level measurements, obtained using tapes or similar devices, were available for the period 1992–1994 at monitor wells installed during investigations of groundwater contamination in the northern and southern parts of Tarawa Terrace (Appendix C1, Tables C1.10 and C1.11). The USGS also measured water levels periodically at Tarawa Terrace water-supply wells during 1986–1987 using similar methods. The calibration standard applied to these measurements and miscellaneous measurements of water levels obtained at supply wells by drillers immediately following well construction was an absolute difference of 3 ft between simulated and observed levels. A standard of 3 ft again refers to the least accurate estimates of water-level altitude, which were obtained by estimating land-surface altitude from topographic maps.

Final calibration results for levels 1 and 2 are described in the following text and are the result of several trial-and-error iterations at each calibration level and feedback of results to previous calibration levels.

Table C10. Simulated and observed predevelopment water levels in wells and related statistics, Tarawa Terrace and vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina.

[NGVD 29, National Geodetic Vertical Datum of 1929]

Site name[1]	Simulated water level, in feet above NGVD 29	Observed water level, in feet above NGVD 29	Absolute water-level difference, in feet
C1	18.4	21.5	3.1
C2	17.2	19.6	2.4
C3	14.6	15.8	1.2
C4	11.7	11.9	0.2
C5	14.2	15.9	1.7
C9	14.9	13.0	1.9
C10	14.3	12.6	1.7
C11	6.7	6.3	0.4
CCC-1	6.2	3.3	2.9
PZ-01	17.3	16.7	0.6
PZ-02	17.5	16.7	0.8
PZ-03	17.1	16.6	0.5
PZ-04	17.2	16.4	0.8
PZ-05	17.4	15.7	1.7
PZ-06	17.6	16.1	1.5
S1	18.7	23.7	5.0
S2	17.3	19.9	2.6
S3	14.6	16.0	1.4
S4	12.3	13.6	1.3
S5	14.3	16.4	2.1
S6	17.8	20.6	2.8
S7	17.1	19.8	2.7
S8	16.3	21.1	4.8
S9	14.5	15.4	0.9
S10	12.0	13.3	1.3
S11	20.1	19.0	1.1
STT61to66-MW01	19.4	21.6	2.2
STT61to66-MW20	18.6	20.1	1.5
T-9	17.0	23.4	6.4
TT-25	12.0	10.9	1.1
TT-26	14.4	14.0	0.4
TT-52	11.1	12.9	1.8
TT-53	14.7	14.0	0.7
TT-54	9.2	12.1	2.9
TT-55	19.1	18.9	0.2
TTDump MW02	4.3	6.2	1.9
TTDump MW03	2.9	2.2	0.7
[2]TTUST-44-MW01	5.6	6.0	0.4
[2]TTUST-48-MW01	11.7	19	7.3
[2]TTUST-779-MW01	10.6	9	1.6
[2]TTUST-2254-MW01	9.7	13	3.3
[2]TTUST-2258-MW01	9.6	12	2.4
[2]TTUST-2302-MW01	8.3	12	3.7
[2]TTUST-2453-A1	7.1	8.4	1.3
[2]TTUST-2453-OB8	5.7	6.5	0.8
[2]TTUST-2455-MW13	8.2	9.2	1.0
[2]TTUST-2455-MW15	6.0	5.6	0.4
[2]TTUST-TTSC-MW09	7.6	8.8	1.2
[2]TTUST-TTSC-MW15	8.8	11.2	2.4
[2]TTUST-2477-MW11	7.3	11.6	4.3
[2]TTUST-2477-MW14	6.5	7.9	1.4
[2]TTUST-2478-MW08	10.7	12.6	1.9
[2]TTUST-2478-MW23	4.7	6.2	1.5
[2]TTUST-2634-MW01	15.0	14	1.0
[2]TTUST-3140-MW01	17.4	15	2.4
[2]TTUST-3165-MW01	16.3	16	0.3
[2]TTUST-3233-MW01	12.3	12	0.3
[2]TTUST-3524-MW01	8.6	6	2.6
[2]TTUST-3546-MW01	8.8	5	3.8

[1]See Plate 1 for location

[2]Because of scale, not shown on Plate 1

Statistics:

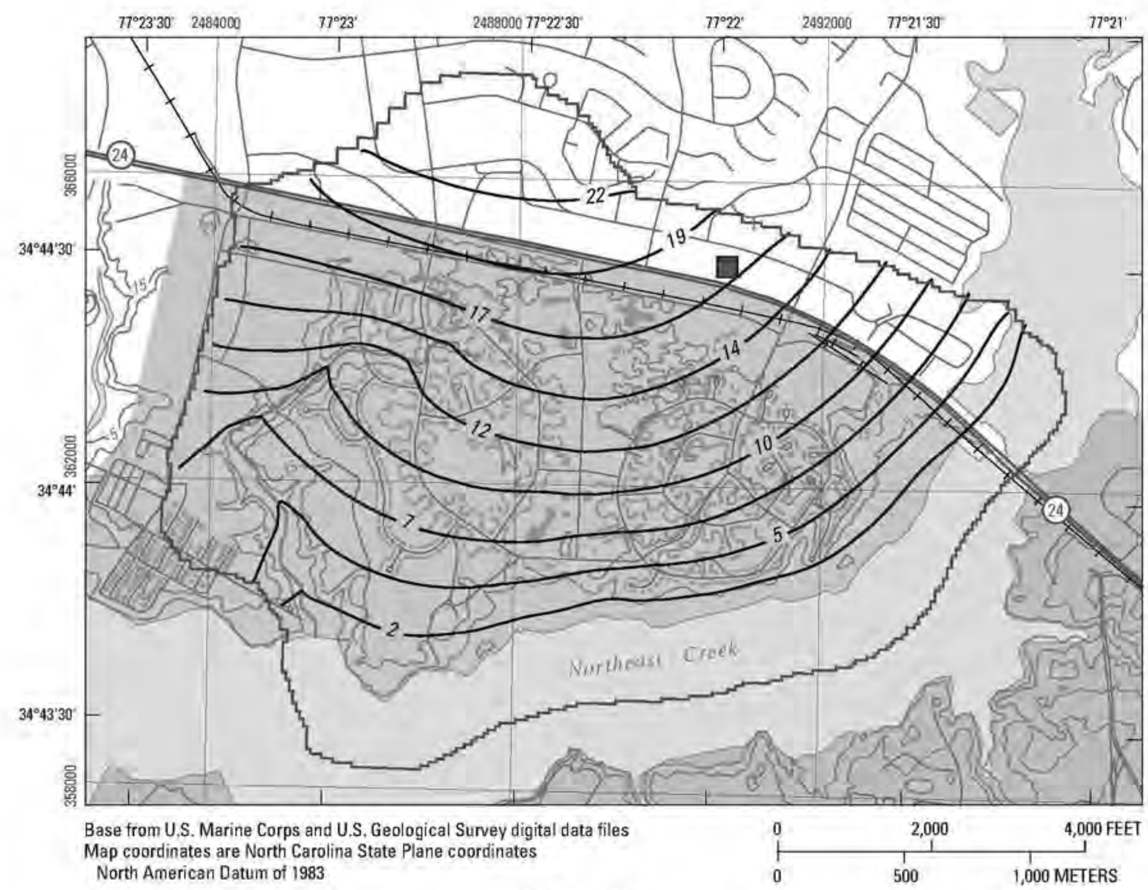
Average water-level difference = 1.9 feet

Standard deviation of water-level difference = 1.5 feet

Root-mean square error of water-level difference = 2.1 feet

Level 1 Calibration (Predevelopment Conditions)

Level 1 calibration of the Tarawa Terrace groundwater-flow model was accomplished by successfully simulating estimated predevelopment conditions; that is, flow and water-level conditions prior to development of the various aquifers by wells. Predevelopment conditions are considered representative of long-term, average annual flow and water-level conditions within the Tarawa Terrace aquifer and the Upper Castle Hayne aquifer system at Tarawa Terrace and vicinity. Criteria used to determine a satisfactory predevelopment calibration were (1) conformance of simulated conditions to the conceptual model and (2) a satisfactory comparison of simulated and observed water levels within the active model



EXPLANATION

Historical water-supply area

Tarawa Terrace

Holcomb Boulevard

ABC One-Hour Cleaners

Model boundary—Active domain

— 10 — **Simulated line of equal potentiometric level**—Combined Tarawa Terrace aquifer and Upper Castle Hayne aquifer–River Bend unit. Contour interval in feet is variable. Datum is National Geodetic Vertical Datum of 1929

— 25 — **Topographic contour**—Interval 10 feet

Figure C7. Simulated predevelopment potentiometric levels of the combined Tarawa Terrace aquifer and Upper Castle Hayne aquifer–River Bend unit (model layer 1), Tarawa Terrace and vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina.

domain. Observed water levels included most of the water levels listed in Table C5. Model runs representing predevelopment conditions were steady state. Simulated predevelopment potentiometric levels in the combined Tarawa Terrace aquifer and Upper Castle Hayne aquifer–River Bend unit (model layer 1) and the Lower Castle Hayne aquifer (model layer 7) are shown in Figures C7 and C8, respectively. Note that potentiometric-level distributions in both layers are highly similar with simulated potentiometric levels in highland areas in the northern part of the study area slightly higher in model layer 1 than in model layer 7. Conversely, simulated levels in the vicinity of Northeast and Frenchmans Creeks are slightly higher in model layer 7 than in model layer 1; both conditions conform explicitly to the conceptual model.

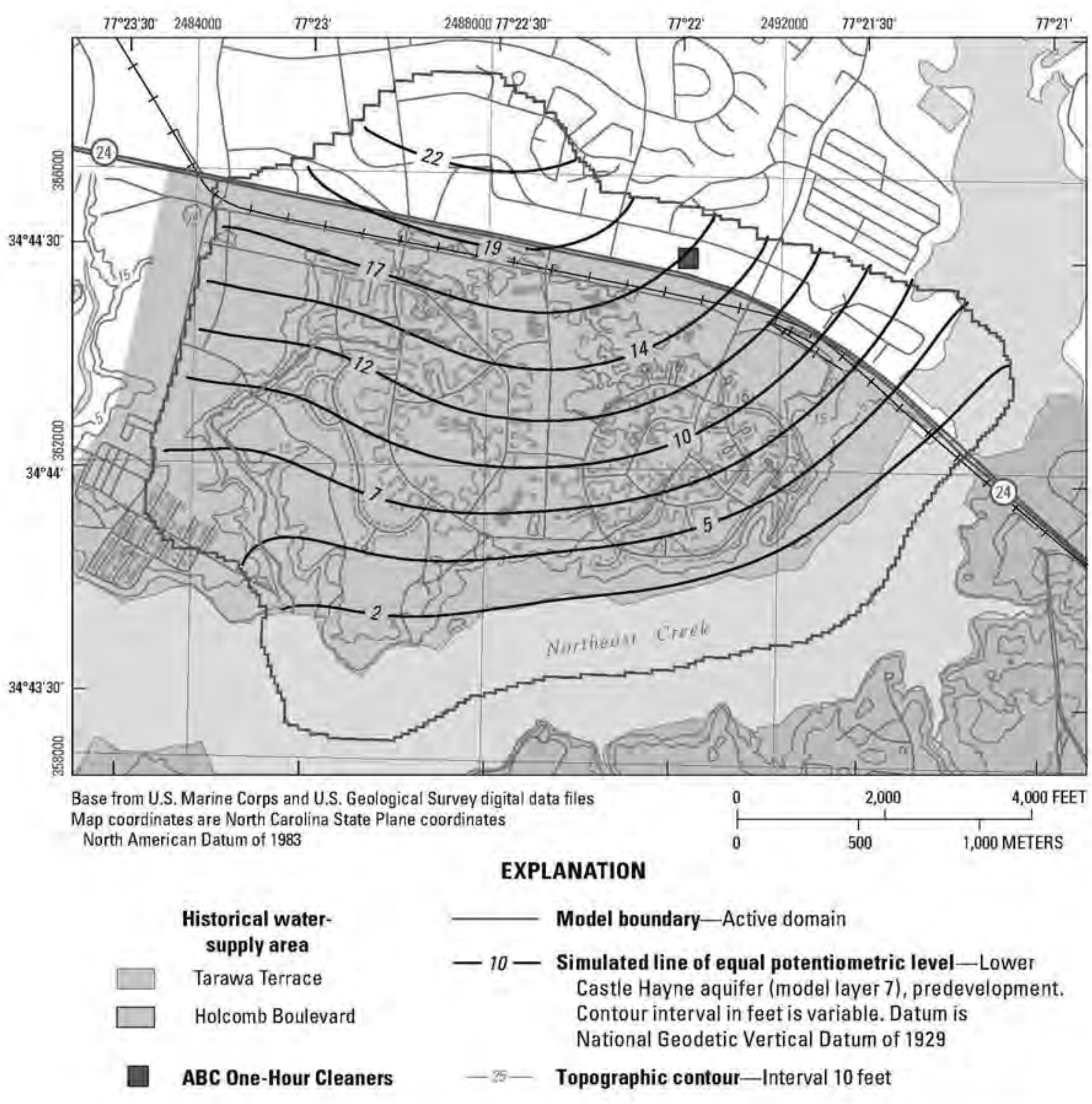


Figure C8. Simulated predevelopment potentiometric levels of the Lower Castle Hayne aquifer (model layer 7), Tarawa Terrace and vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina.

A scatter diagram showing the agreement between simulated and observed water levels for simulated predevelopment conditions is shown in Figure C9. The flow model spatially interpolates simulated results from cell centers to the location coordinates assigned to various observation points, such as well locations, in order to facilitate direct comparisons of simulated and observed conditions. All Tarawa Terrace water-supply wells and several monitor wells are open to multiple aquifers. At these sites, simulated water levels were processed post calibration by proportioning simulated water levels in several aquifers at multiaquifer wells to compute a composite water level. This composite water level was then compared to the observed water level to evaluate calibration "goodness." Proportions were based on the percentage of interval open to individual aquifers (model layers) compared to the total open interval at the well (Hill et al. 2000).

Simulated and observed predevelopment water levels are listed in Table C10. Of the 59 paired data, the absolute difference between simulated and observed water levels at only nine sites exceeded the calibration standard of 3 ft or less. Of these nine sites, the absolute water-level difference at four sites was between 3 and 4 ft, and the largest difference was 7.3 ft. Absolute water-level differences at 17 sites were 1.0 ft or less. The average of all absolute differences between observed and simulated water levels was 1.9 ft, and the root-mean-square error of all absolute water-level differences was 2.4 ft.

Total simulated flow to the active model domain occurred at a rate of about 2.09 cubic feet per second (cfs) from effective recharge and about 0.26 cfs from the general-head boundaries. Of this, about 1.62 cfs was discharged to Northeast Creek and about 0.73 cfs was discharged to Frenchmans Creek. The mass balance error between simulated rates of recharge and discharge was 0.00 percent.

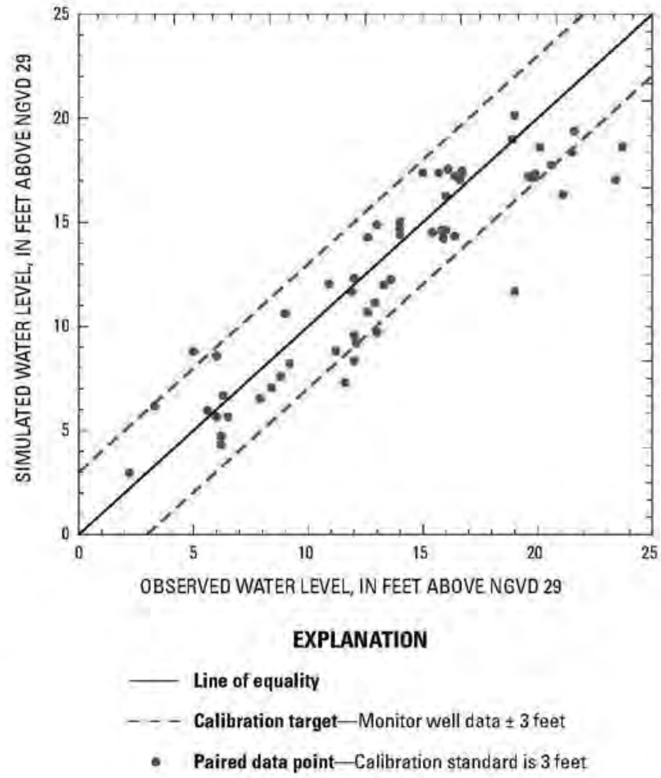


Figure C9. Simulated and observed predevelopment water levels, Tarawa Terrace and vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina.

Level 2 Calibration (Transient Conditions)

Calibration of the transient flow model was achieved using pumpage (Tables C8 and C9), water-level (Appendix C1, Tables C1.1–C1.11), and well capacity (Appendix C3, Tables C3.1–C3.10) data collected at Tarawa Terrace and vicinity. Effective recharge was assigned uniformly to the highest active model cell and was varied annually according to annual rainfall (Table C7). The hydraulic characteristic, drain, and general-head and specified-head arrays assigned to the calibrated predevelopment-flow model were applied exactly to the transient-flow model. A storativity of 0.0004 was assigned uniformly to model layers 2–7. A specific yield of 0.05 was assigned uniformly to model layer 1. Transient flow was simulated for a total of 528 stress periods (Appendix C4). Each stress period represented a single month beginning January 1951 and ending December 1994. A single month corresponded to a single stress period, and each stress period represented a single time step. The unit of time was days. Thus, the appropriate number of days representing a particular month was assigned as the time interval of the stress period. Pumpage was assigned to the transient model at Tarawa Terrace water-supply wells based on flow, capacity, construction, and operational data described previously. Calibration was based on comparisons of simulated and observed water levels at supply and monitor wells and conformance of simulated results to predetermined calibration standards and the conceptual model.

Available construction data for Tarawa Terrace water-supply wells are incomplete (Appendix C2, Tables C2.1–C2.3) but indicate that most of the wells probably were open to the Upper Castle Hayne aquifer–River Bend unit and the Upper Castle Hayne aquifer–Lower unit either directly by open interval or indirectly by gravel or sand packing within the annular space of the well bore. In addition, supply wells TT-23 and TT-25 were directly open, as well, to the Middle Castle Hayne aquifer. Total estimated pumpage at wells TT-23, TT-25, TT-26, TT-27, TT-28, TT-29, TT-30, and TT-67 was assigned to model layer 3. Total estimated pumpage at wells TT-53 and TT-55 was assigned to model layer 1. Total estimated pumpage at wells TT-31, TT-52, and TT-54 was subdivided equally between model layers 1 and 3.

Simulated and observed transient water levels at discrete time intervals are listed in Appendix C5, Tables C5.1–C5.11. Hydrographs of simulated and observed monthly water levels are shown at most Tarawa Terrace water-supply wells in Figures C10–C17. Most plots generally represent conditions occurring between January 1978 and April 1987. Simulated water levels represent an average condition for the respective stress period (month and year). Observed water levels represent conditions during a single measurement day. With few exceptions, observed data plotted in Figures C10–C17 were determined by airline measurements. Accordingly, the absolute differences between observed and simulated water levels are subject to a calibration standard of 12 ft. A similar standard applies to most of the data listed in Appendix C5, Tables C5.1–C5.8. Observed water-level data listed in Appendix C5, Tables C5.9–C5.11, were determined by tape or similar measurement. The absolute difference between simulated and observed water levels listed on these tables is, thus, subject to a calibration standard of 3 ft. These data at a single site are few in number and are compressed in time to 1 or 2 years, and observed water levels were not plotted against simulated water levels.

Based on these standards, calibration of the transient-flow model is generally good and ranges from fair to excellent, depending on comparisons at specific water-supply or monitor wells. For example, the average absolute difference between simulated and observed water levels at wells TT-25 and TT-67 is 5.7 and 4.0 ft, respectively (Appendix C5, Tables C5.1 and C5.8), and simulated and observed water-level trends are similar (Appendix C1, Tables C1.2 and C1.9). The root-mean-square error of absolute water-level differences at these sites is 6.6 and 5.0 ft; whereas, the calibration standard applied to these data was 12 ft. On the other hand, the average absolute difference between simulated and observed water levels at wells TT-31 and TT-53 is 8.7 and 8.6 ft, respectively, and simulated and observed water levels are, at best, somewhat similar (Appendix C5, Tables C5.4 and C5.6). Of the 509 paired water levels listed in Appendix C5, Tables C5.1–C5.8, 83 absolute differences, or about 16 percent, exceed the 12-ft calibration standard. Of the 280 paired water levels listed in Appendix C5, Tables C5.9–C5.11, only 26 absolute differences, or about 9 percent, exceed the 3-ft calibration standard. Two hundred and sixty-three measurements are at monitor wells installed during investigations of groundwater contamination at Tarawa Terrace and vicinity (Appendix C5, Tables C5.10 and C5.11). The average and root-mean-square error of absolute water-level differences at these sites ranges from about 1.2 to 1.8 ft and from 1.4 to 2.1 ft, respectively.

Absolute differences between simulated and observed water levels at well TT-30 exceeded 12 ft on 18 occasions (Appendix C5, Table C5.3). Observed water levels began to decline sharply at this site beginning about August 1978 and continued downward until about March 1982, when a sharp recovery occurred (Appendix C1, Table C1.4). Such trends are typically caused by pumping from a nearby well. Well TT-30 was located just south of SR 24, an area of considerable commercial development, and far to the west of any active Tarawa Terrace water-supply wells during 1978–1982. A likely cause of the declining water levels at TT-30 was the use of an unknown supply well in the nearby commercial area north of SR 24, a use that was terminated about March 1982. This well and the related pumpage were not accounted for during transient simulations. Following termination of the presumed commercial pumping, simulated and observed water levels at well TT-30 were highly similar (Appendix C1, Table C1.4).

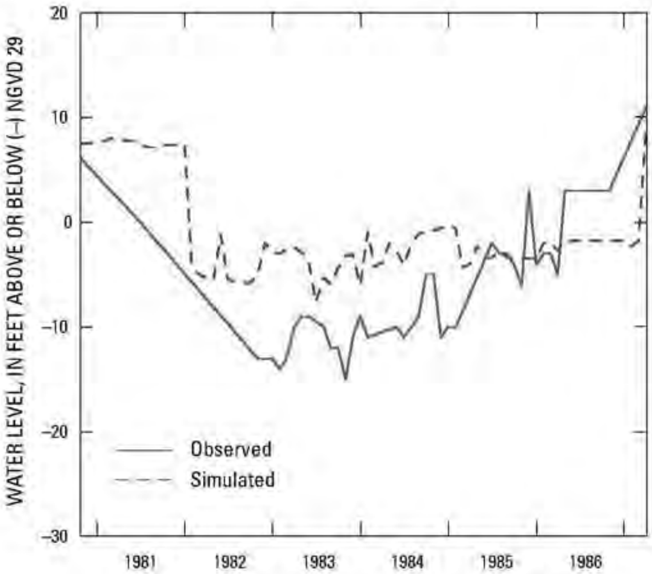


Figure C10. Simulated and observed water levels in supply well TT–25, November 1980–April 1987, Tarawa Terrace, U.S. Marine Corps Base Camp Lejeune, North Carolina.

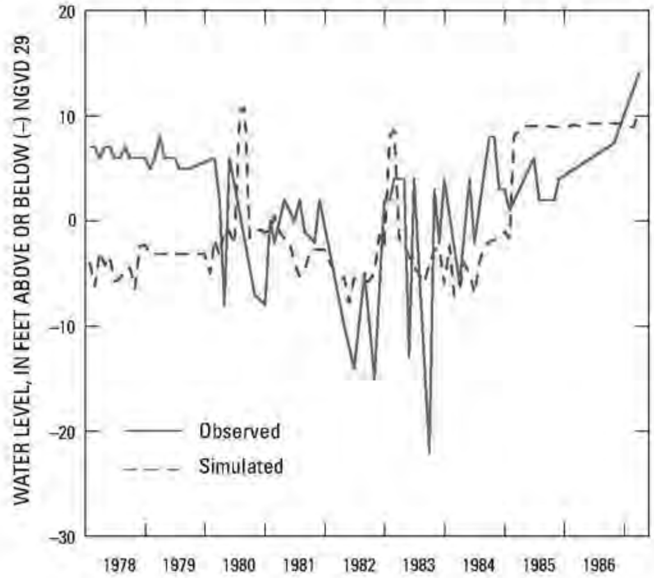


Figure C11. Simulated and observed water levels in supply well TT–26, January 1978–April 1987, Tarawa Terrace, U.S. Marine Corps Base Camp Lejeune, North Carolina.

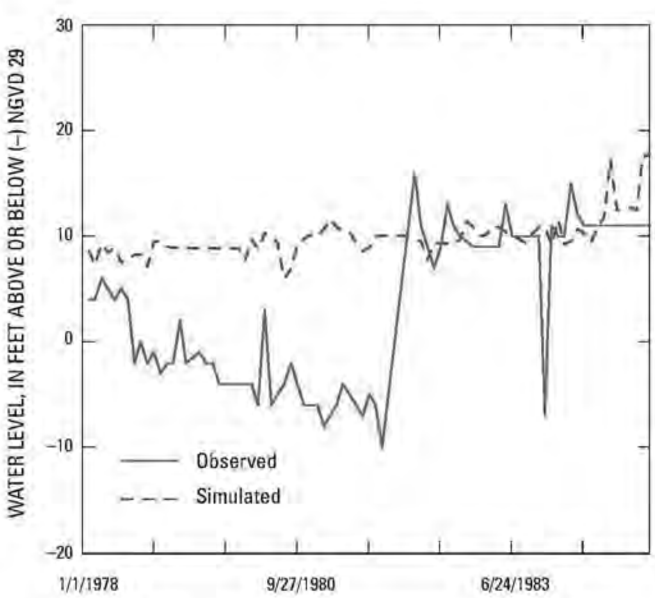


Figure C12. Simulated and observed water levels in supply well TT–30, January 1978–April 1985, Tarawa Terrace, U.S. Marine Corps Base Camp Lejeune, North Carolina.

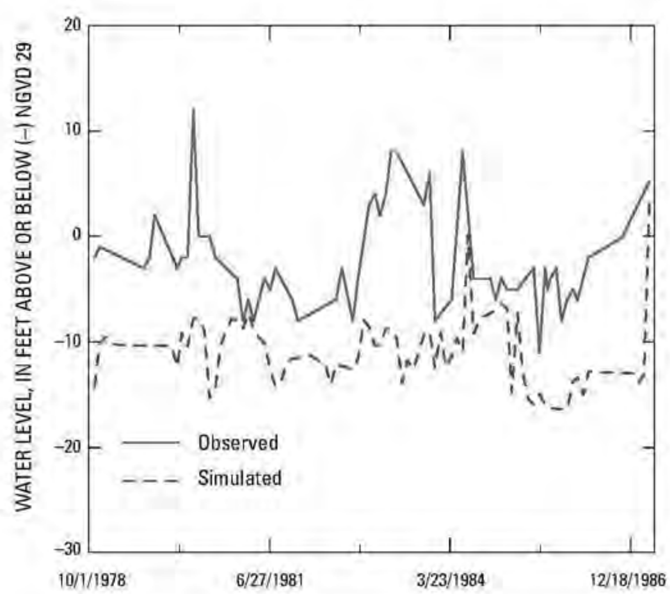


Figure C13. Simulated and observed water levels in supply well TT–31, October 1978–April 1987, Tarawa Terrace, U.S. Marine Corps Base Camp Lejeune, North Carolina.

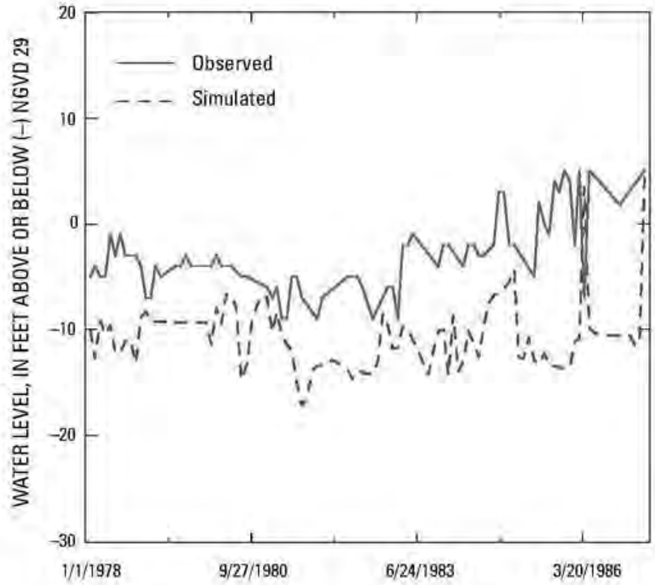


Figure C14. Simulated and observed water levels in supply well TT–52, January 1978–April 1987, Tarawa Terrace, U.S. Marine Corps Base Camp Lejeune, North Carolina.

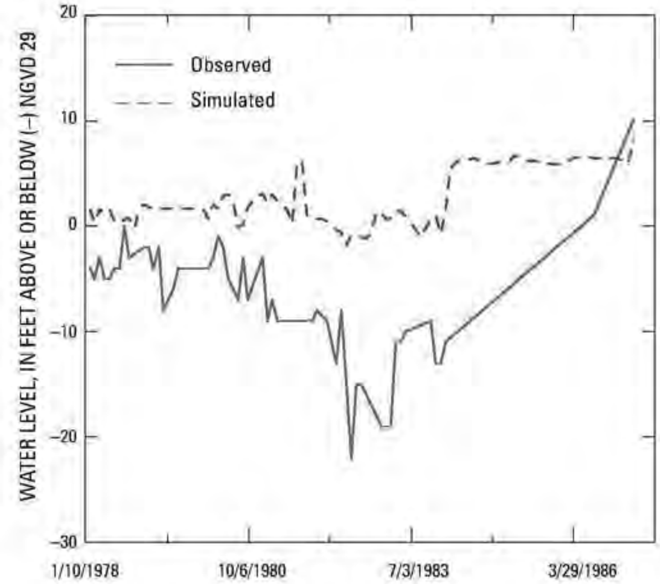


Figure C15. Simulated and observed water levels in supply well TT–53, January 1978–January 1984, Tarawa Terrace, U.S. Marine Corps Base Camp Lejeune, North Carolina.

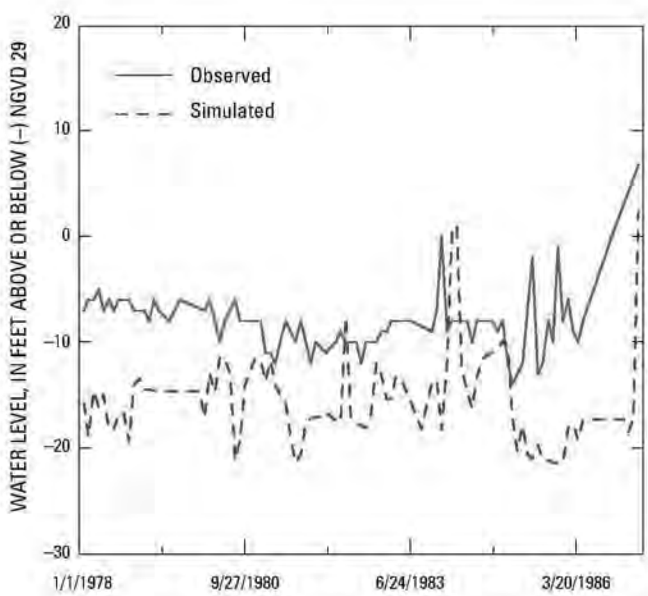


Figure C16. Simulated and observed water levels in supply well TT–54, January 1978–April 1987, Tarawa Terrace, U.S. Marine Corps Base Camp Lejeune, North Carolina.

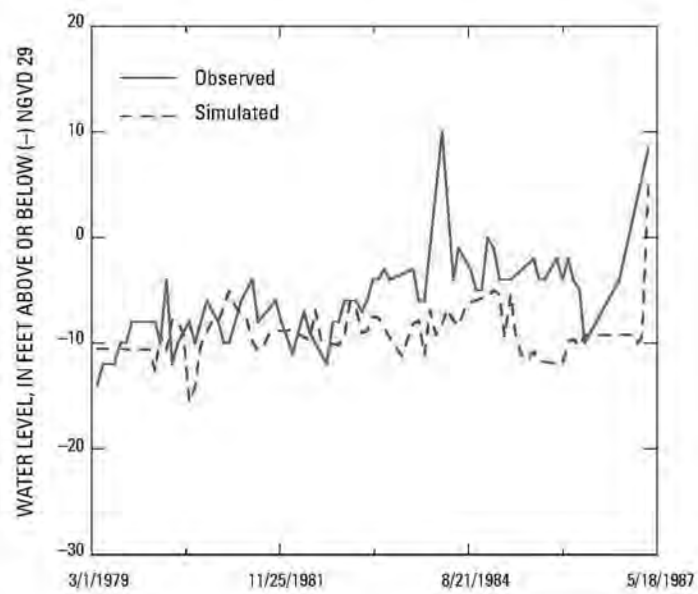


Figure C17. Simulated and observed water levels in supply well TT–67, March 1979–April 1987, Tarawa Terrace, U.S. Marine Corps Base Camp Lejeune, North Carolina.

Simulated layer-by-layer groundwater flow to and from the Tarawa Terrace flow model for stress period 408 (December 1984) is summarized in Tables C11 and C12, respectively. With the exception of well TT-23, pumping at active Tarawa Terrace water-supply wells at this time had been ongoing for several years and, at several wells, for several decades. Accordingly, changes in storage are insignificant, even in model layers 1 and 3, where all of the assigned pumpage occurs. Discharge to Northeast Creek occurs at a rate of about 0.9 cfs, considerably less than the corresponding rate noted during predevelopment simulations (1.6 cfs). Similar reductions from predevelopment conditions were noted in the discharge to Frenchmans Creek (from 0.73 to 0.56 cfs). Such reductions are the result of disruptions in the predevelopment flow gradients away from natural lines of discharge and toward pumping wells. Conversely, flow from general-head

Table C11. Simulated layer-by-layer groundwater flow *into* the Tarawa Terrace model, stress period 408 (December 1984), U.S. Marine Corps Base Camp Lejeune, North Carolina.

[N/A, not applicable]

Model layer	Layer to layer	Budget components (rates in cubic foot per second)				
		Storage	Recharge	Constant head	General head	Totals
1		0.00	1.92	0.00	0.49	
2 to 1	0.34					2.74
2		0.00	0.00	N/A	0.00	
1 to 2	1.02					
3 to 2	0.33					1.35
3		0.00	0.00	N/A	0.07	
2 to 3	1.02					
4 to 3	0.59					1.68
4		0.00	0.00	N/A	0.00	
3 to 4	0.33					
5 to 4	0.57					0.90
5		0.00	0.00	N/A	0.18	
4 to 5	0.32					
6 to 5	0.16					0.66
6		0.00	0.00	N/A	0.00	
5 to 6	0.09					
7 to 6	0.14					0.23
7		0.00	0.00	N/A	0.06	
6 to 7	0.08					0.15
Total	**4.99**		**1.92**		**0.80**	**7.71/7.71**

boundaries to the active model domain increased during transient conditions compared to predevelopment conditions from 0.26 to 0.80 cfs, also as a result of pumping at water-supply wells, particularly at wells TT-25 and TT-26, which were located relatively close to the boundary. Differences between total inflow and outflow rates listed in Tables C11 and C12 are caused by rounding errors at the second decimal place. Simulated flow conditions conform explicitly to the conceptual model of groundwater flow described previously.

Simulated potentiometric surfaces of model layers 1 and 3 for stress period 408 are illustrated in Figures C18 and C19, respectively. A substantial cone of depression occurs in the immediate vicinity of the Tarawa Terrace housing area where the majority of active water-supply wells are located and reflects a coalescing of several cones developed at individual wells. A comparatively small coalesced cone of depression is evident in model layer 3 north of Tarawa Terrace near SR 24 and is caused by pumping at wells TT-25 and TT-26.

Table C12. Simulated layer-by-layer groundwater flow *out of* the Tarawa Terrace model, stress period 408 (December 1984), U.S. Marine Corps Base Camp Lejeune, North Carolina.

[N/A, not applicable]

Model layer	Layer to layer	Budget components (rates in cubic foot per second)					
		Storage	Wells	Constant head	General head	Drains	Totals
1		0.06	0.23	0.88	0.00	0.56	0.06
1 to 2	1.02						2.75
2		0.00	0.00	N/A	0.00	N/A	
2 to 1	0.34						
2 to 3	1.02						1.36
3		0.00	1.02	N/A	0.00	N/A	
3 to 2	0.33						
3 to 4	0.33						1.68
4		0.00	0.00	N/A	0.00	N/A	
4 to 3	0.59						
4 to 5	0.32						0.91
5		0.00	0.00	N/A	0.00	N/A	
5 to 4	0.57						
5 to 6	0.09						0.66
6		0.00	0.00	N/A	0.00	N/A	
6 to 5	0.16						
6 to 7	0.08						0.24
7							
7 to 6	0.14	0.00	0.00	N/A	0.00	N/A	0.15
Total	**4.99**	**0.06**	**1.25**	**0.88**	**0.00**	**0.56**	**7.74/7.75**

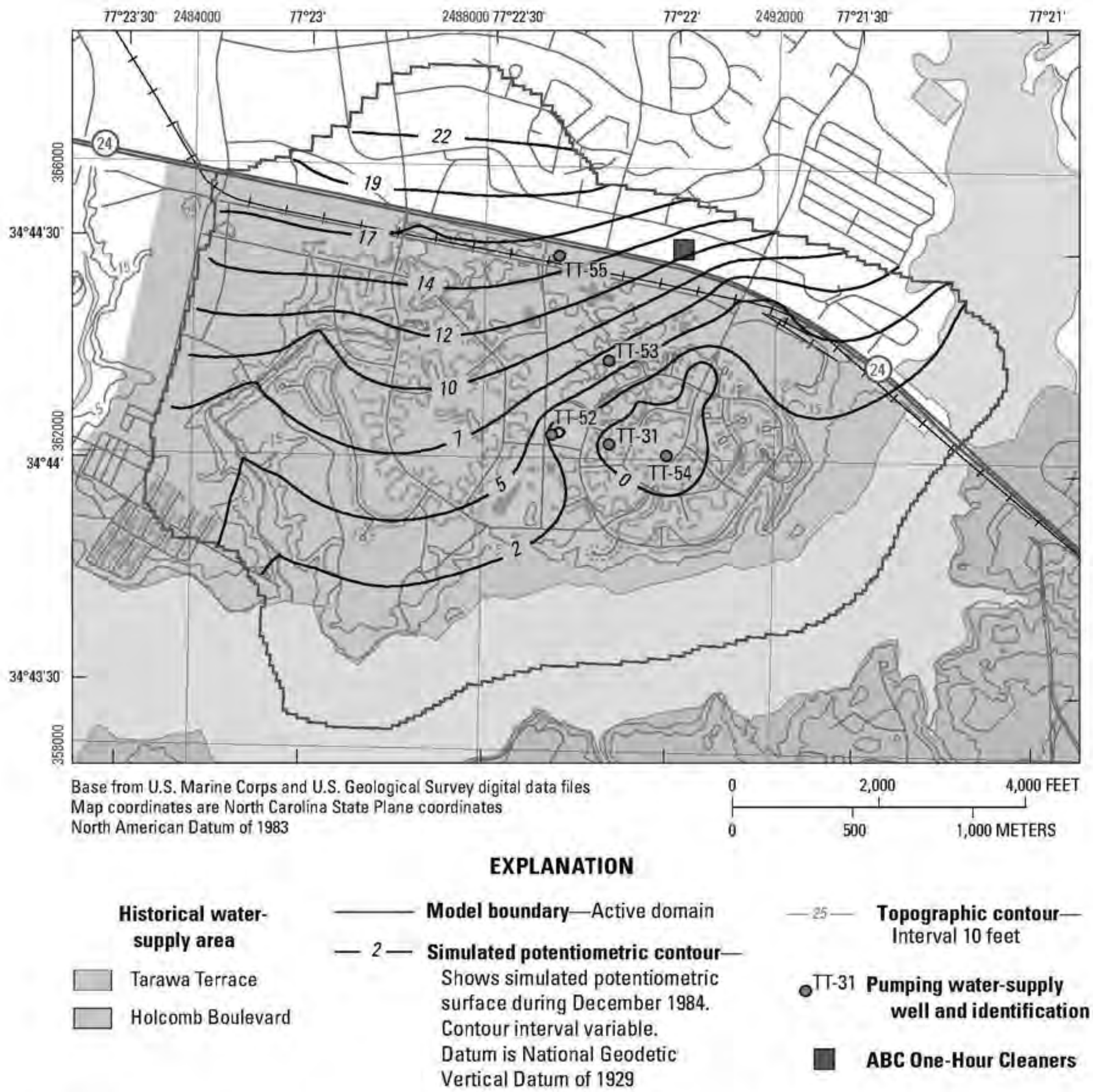


Figure C18. Simulated potentiometric levels, combined Tarawa Terrace aquifer and Upper Castle Hayne aquifer–River Bend unit (model layer 1), stress period 408 (December 1984), Tarawa Terrace and vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina.

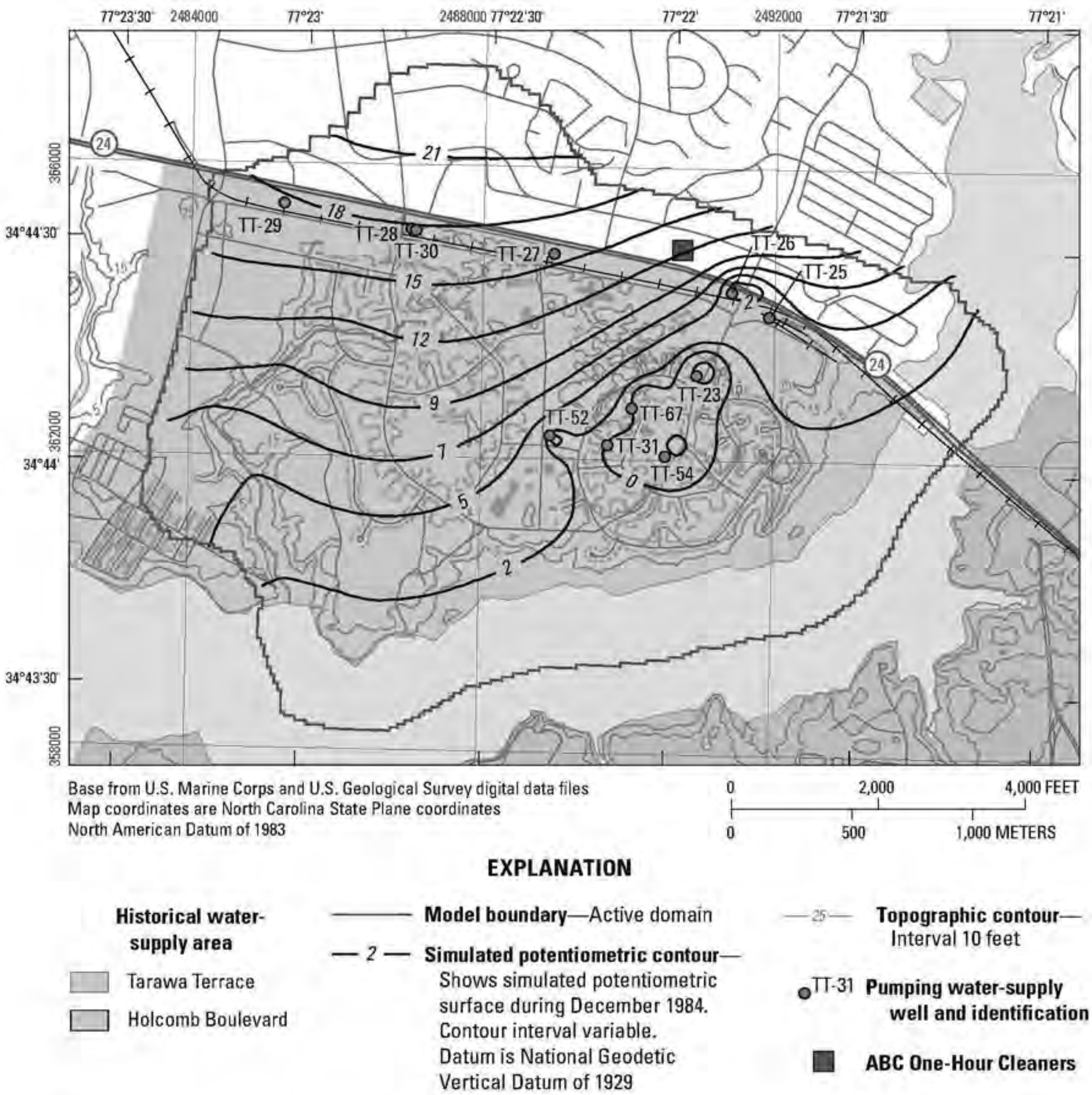


Figure C19. Simulated potentiometric levels, Upper Castle Hayne aquifer–Lower unit (model layer 3), stress period 408 (December 1984), Tarawa Terrace and vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina.

An indication of gross model calibration is shown in the scatter diagram of Figure C20. Paired data shown within the bottom half of the diagram generally correspond to water-supply well data listed in Appendix C5, Tables C5.1–C5.8. Paired data within the upper part of the diagram generally correspond to data listed in Appendix C5, Tables C5.9–C5.11. The average absolute difference between simulated and observed water levels for the 789 paired water levels shown in Figure C20 is 5.2 ft. The root-mean-square error of the absolute differences is 7.0 ft.

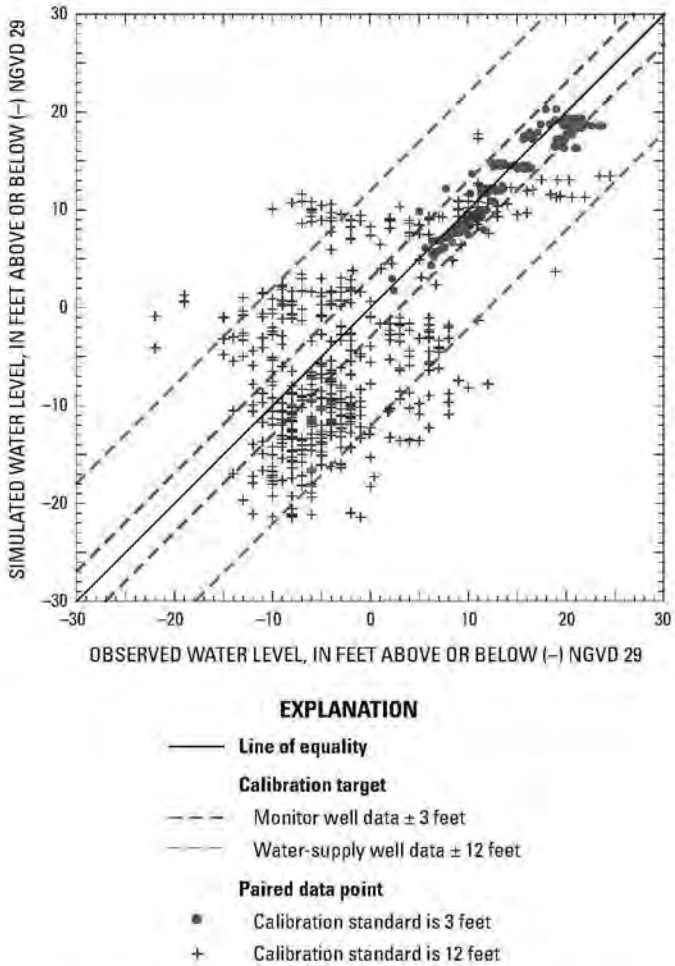


Figure C20. Simulated and observed transient water levels, Tarawa Terrace and vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina.

Sensitivity Analysis

Sensitivity analyses determine the relative importance of hydraulic characteristic and model input parameters, such as recharge, to simulated results. Sensitivity analysis quantitatively evaluates the effects of changes in calibrated model parameters by individually adjusting these parameters and comparing the simulated results to a predetermined measure of calibration quality. Two measures of calibration quality were used for this study: (1) variance and (2) root-mean-square error. Variance is a measure of the absolute water-level difference between simulated and observed water levels around the mean difference. The square root of the variance is the standard deviation around the mean. Root-mean-square error is a direct measure of the absolute difference between simulated and observed water levels. Variance and root-mean-square error were computed using the simulated and observed water levels listed in Appendix C5, Tables C5.1–C5.11. Sensitivity of simulation results to changes in parameter values is substantially affected by model boundary conditions. Assigned potentiometric levels that occur in every layer along the northern perimeter of the active model domain as part of general-head boundaries and specified heads assigned to model layer 1 along the southern and eastern perimeters where active cell locations coincide with Northeast Creek tend to dampen sensitivity.

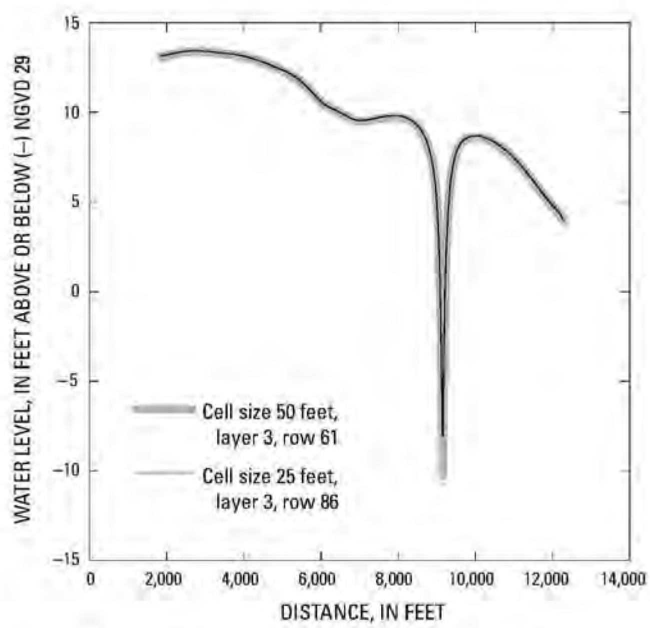


Figure C21. Simulated water levels for stress period 157 in supply well TT-26 along designated rows using model cell dimensions of 50 feet per side and 25 feet per side, Tarawa Terrace, U.S. Marine Corps Base Camp Lejeune, North Carolina.

Implementation of sensitivity analyses was accomplished by globally increasing or decreasing the calibrated value of a specified parameter within a range of values considered reasonable for the study area. Model parameters tested for sensitivity were recharge, horizontal and vertical hydraulic conductivity, drain conductance, specific storage, and assigned potentiometric levels at general-head boundaries. Results of the sensitivity analyses are listed in Table C13. Changes in horizontal hydraulic conductivity most significantly affected simulation results. Variance and root-mean-square error were degraded by about 57 and 29 percent, respectively, when horizontal hydraulic conductivity was increased globally by a factor of 2.5 compared to calibrated arrays. A global increase in vertical hydraulic conductivity by a factor of 2.5 resulted in the lowest variance and root-mean-square error values, an improvement of about 3 and 2 percent, respectively, compared to calibrated arrays. Sensitivity of simulation results to increased recharge and decreased water levels within the general-head boundary arrays was not significant. Sensitivity of simulation results to changes in drain conductance and specific storage was minimal.

Sensitivity of simulation results to model cell dimensions also was tested. Cell dimensions were uniformly changed from 50 ft per side to 25 ft per side throughout the model domain. Simulated water levels were compared along model rows that included the location of water-supply well TT-26 for stress periods 60, 133, 157, and 253. Simulated water levels were nearly identical for all stress periods regardless of cell size and are shown for stress period 157 in Figure C21.

Table C13. Summary of sensitivity analyses of the Tarawa Terrace transient flow model, U.S. Marine Corps Base Camp Lejeune, North Carolina.

[$(ft/d)^2$, feet per day squared; N/A, not applicable; +, plus; –, minus; $feet^{-1}$, 1/foot]

Model parameter	Global change	Variance, in $(ft/d)^2$	Root-mean-square error, in feet	Remarks
Horizontal hydraulic conductivity, in feet per day	Multiplied by			
	0.25	N/A	N/A	Wells pumped dry
	0.5	N/A	N/A	Wells pumped dry
	1.0	53.3	7.3	
	1.5	61.2	7.82	
	2.5	83.7	9.15	
Vertical hydraulic conductivity, in feet per day	Multiplied by			
	0.25	N/A	N/A	Wells pumped dry
	0.5	N/A	N/A	Wells pumped dry
	1.0	53.3	7.3	
	1.5	52.4	7.24	
	2.5	51.5	7.17	
Recharge, in inches per year	Annual rate			
	10	N/A	N/A	Wells pumped dry
	12	N/A	N/A	Wells pumped dry
	Calibrated rate	53.3	7.30	
	14.5	53.5	7.31	
	16	54.6	7.39	
Assigned head at general head boundaries	Increased +5 feet	61.4	7.84	
	Calibrated head	53.3	7.30	
	Decreased –5 feet	N/A	N/A	Wells pumped dry
Specific storage, in $feet^{-1}$	Multiplied by			
	1	53.3	7.30	
	5	53.2	7.29	
	10	53.0	7.28	
	20	52.9	7.27	
Drain conductance, in feet per day	Multiplied by			
	0.25	52.8	7.26	
	0.5	53.0	7.28	
	1	53.3	7.30	
	2.5	53.7	7.33	

Discussion

Results and interpretations described in this report are substantially dependent on the accuracy of water-level and site-location data. The accuracy of water-level data used for model calibration was discussed previously and qualified in terms of methods of measurement. Highly accurate water levels were classified as those probably or possibly measured with tapes or similar methods and are listed in Table C5 and Appendix C5, Tables C5.9–C5.11. Less accurate water levels, probably measured using airlines, are listed in Appendix C5, Tables C5.1–C5.8; observed water levels listed in these tables reported only to the nearest foot are indicative of altitudes computed using land-surface altitude estimated from topographic maps or obtained from airline measurements. Absolute water-level differences and related statistics, however, are reported to the nearest tenth of a foot in order to maintain consistent bases of comparison with corresponding data listed in Table C5 and Appendix C5, Tables C5.9–C5.11. According to accepted rules of reporting significant figures, the statistics reported in Appendix C5, Tables C5.1–C5.8, are accurate only to the nearest unit value.

Location Coordinates

Locations of Tarawa Terrace water-supply wells are probably highly accurate and are based, for the most part, on large-scale site maps of individual wells developed prior to well and well house construction (NAVFAC drawings 4049523, 1244002, 4001327, and 1244061, written communication, various dates; Y & D drawing 765472, written communication, various dates; P.W. drawing 13060, written communication, various dates) and U.S. Marine Corps Base Camp Lejeune Quarters Maps (U.S. Marine Corps Base Camp Lejeune, Map of Tarawa Terrace II Quarters Map, written communication, June 30, 1961; U.S. Marine Corps Base Camp Lejeune, Tarawa Terrace I Quarters Map, written communication, July 31, 1984). Accordingly, location coordinates of Tarawa Terrace water-supply wells listed in various tables are considered accurate within a radius of about 50 ft.

Many reports that describe the investigation and removal of USTs within the Tarawa Terrace housing areas also contained detailed maps showing monitor well and soil boring locations as well as a single latitude and longitude site locator. For this study, the latitude and longitude location was considered the location of the tank or the number one monitor well, and all other site locations were georeferenced to that point using the various site plans and maps provided in the report. Monitor well locations at these sites are considered accurate to within a radius of 100 ft (Appendix C1, Table C1.11). Location coordinates at monitor wells installed during ABC One-Hour Cleaners Operable Unit 1 (Appendix C1, Table C1.10) were based on the mapped location of well sites and coordinates of a local grid established during the operable unit (Roy F. Weston, Inc. 1992). Unfortunately, the origin of the local grid was not referenced to any typical map coordinate system, such as North Carolina State Plane coordinates. In addition, comparison of mapped well locations to the local coordinates indicated that the north and east local coordinates were possibly reversed at several sites. Not even local coordinates were provided for the several monitor wells constructed during ABC One-Hour Cleaners Operable Unit 2. Location coordinates at these sites were determined by referencing the mapped location to an obvious cultural feature, such as intersecting roads, that was easily recognized on USGS 1:24,000-scale maps. Operable Unit 1 local site coordinates also were cross-referenced with their mapped locations in a similar manner. Accordingly, the accuracy of location coordinates of monitor wells installed during Operable Units 1 and 2 varies by location and proximity to cultural features as well as the accuracy of the original well-location maps, which is unknown. Locations of wells constructed during Operable Unit 1 with assigned local coordinates and in the immediate vicinity of ABC One-Hour Cleaners and Tarawa Terrace water-supply wells are considered accurate within a radius of about 50 ft. Other wells constructed during Operable Unit 1 and all wells and piezometers constructed during Operable Unit 2 are located within unknown accuracy limits but probably within distances ranging from several dozen to several hundred feet. The locations of monitor wells installed during the investigations of refined-petroleum products in the subsurface at storage tanks STT61–66 were georeferenced using the published well-location map and the estimated State Plane coordinates of the southeast corner of Building TT-47, which was included on the well-location map and also could be located on a 1:24,000-scale topographic map. Locations are considered accurate to within a radius of about 50 ft. Locations of monitor wells installed during remedial investigations at and in the vicinity of the Tarawa Terrace Shopping Center were determined using published maps and easily identified cultural features as described previously and also are considered accurate to within a radius of about 50 ft (Appendix C1, Table C1.11).

Flow Model

Numerical models of groundwater flow, such as MODFLOW, even when supported by excessive quantities of high-quality data and excellent ancillary analytical tools, represent, at best, a gross approximation of real-world conditions. Accordingly, simulation results must be evaluated and qualified within the context of the quality and density of data used for model construction and calibration and within the context of the completeness and validity of the conceptual model. The quality and completeness of water-level and pumpage data were discussed previously. Historical water-level data were mainly unavailable prior to 1978, with the exception of one or two measurements at the time of construction of several wells. Thus, for the most part, simulation results are unqualified for the years 1951–1977, based on comparisons of observed and simulated water levels. In addition, an inherent disparity between simulated and observed water levels must be kept in mind when such data are compared, regardless of the origin or date of the water-level measurement; that is, simulated levels always represent average monthly conditions, whereas observed data may represent short-term hourly or daily conditions. This disparity is at least partly addressed for comparative purposes by using static or recovered water levels, as reported, at water-supply wells.

Pumpage data were unavailable prior to 1975 and much of the data used for years 1975–1986 were limited to average annual or monthly rates for all wells, rather than known rates that could be assigned to individual wells. Accordingly, an average annual pumping rate representing 1975–1986 conditions was applied to the model for all stress periods representing the years 1952–1974 (Table C9). This assumption is partly justified because the number of housing units and population of Tarawa Terrace was probably constant, or nearly so, during these years, as was the corresponding average household water use. The use of well capacity as a surrogate for the computation of pumpage at individual wells also was necessary, given the total lack of pumpage data pertinent to individual water-supply wells. Pumpage computation errors caused by this approach and introduced into model simulations may partially explain the relatively poor comparisons between observed and simulated water levels at several supply wells (Figures C10–C17). Water-supply well operations as simulated and as actually occurred were also somewhat different. Changes in simulated operations could occur only at a stress period (monthly) interval. However, actual changes in well operation, such as cycling pumps on and off, probably occurred on an hourly or daily basis. Whether or not disparities between actual and simulated well operations introduced substantial error into simulated average monthly water levels and groundwater-flow rates is unknown. Operations, such as removing wells from service for repair or equipment replacement for weeks or several months, were noted in operation logs beginning during 1978. Such intervals are represented in the flow model pumpage array.

Well construction data also were somewhat limited and possibly affected the assignment of pumpage to model layers (Appendix C2, Tables C2.1–C2.3). Pumping intervals at water-supply wells were assigned to either model layer 1 or 3 in conformance with known construction information. Construction data were incomplete at supply wells TT-28 and TT-29, which were completed during 1951 (LeGrand 1959), as were wells TT-26 and TT-27. Based on construction information at wells TT-26 and TT-27, the completed depths of wells TT-28 and TT-29 probably ranged between 50 and 100 ft (LeGrand 1959). Accordingly, pumpage at these wells was assigned to model layer 3. The depth of well TT-55 is reported to be greater than 50 ft. Additional construction information for this well is not available and pumpage from this well was assigned to model layer 1. Several or all of these wells may have been, and probably were, open to water-bearing units that correspond to layer 3 of the flow model. Only the depth of the finished well is known at supply wells TT-31, TT-52, and TT-54; these depths range between 94 and 104 ft. However, these wells were all constructed during 1961, as was well TT-53 where construction is known. Well TT-53 was constructed with screens open to model layers 1 and 3. Accordingly, one-half of total estimated pumpage at wells TT-31, TT-52, and TT-54 was assigned equally to model layers 1 and 3.

Water-supply-well boreholes were typically drilled to depths substantially greater than the depth of the finished wells and unused borehole volume was backfilled with coarse sand or pea gravel. Such construction techniques created a substantial, if not direct, hydraulic connection between the backfilled volume and the gravel pack placed opposite the well screens of the open well interval. To account for multiaquifer construction of supply wells, vertical hydraulic conductivities of cells in layers representing confining units penetrated by the supply well boreholes were increased from 0.1 to 100 ft/d. Borehole continuity across confining units was, thus, at least partially accounted for by modifying the vertical hydraulic conductivity of appropriate model cells, and increased multiaquifer flow was simulated at supply wells regardless of the model layer to which pumpage was assigned. Regardless of these modifications, however, a substantial disparity probably occurs between actual (real-world) multiaquifer flow in a pumping supply well and the model's ability to simulate such flow. Much, if not most, of this disparity occurs as a result of model cell resolution where, for example, pumpage at a 10-inch diameter supply well is assigned within a 50-ft by 50-ft cell area. Accordingly, a composite potentiometric level was computed at each supply well for each stress period based on the percentage of total open interval known or estimated to occur at discrete model layers (aquifers). The methodology described by Hill et al. (2000) was used to proportion the discrete layer-by-layer simulated water levels.

Horizontal hydraulic conductivity data based on aquifer tests are limited geographically to the eastern half of the model domain and stratigraphically to the Tarawa Terrace aquifer and Upper Castle Hayne aquifer–River Bend unit (Table C2). To partially compensate for the limited number of point data, horizontal hydraulic conductivity at well sites at Montford Point ("M" sites) and in the vicinity of Brewster Boulevard ("HP" and "LCH" sites) was used to establish east-west trends for interpolating arrays throughout the model domain (Tables C2–C4). No hydraulic-conductivity data unique to the Middle and Lower Castle Hayne aquifers are available. Data assigned exclusively to the Middle Castle Hayne aquifer (model layer 5; Table C4) were segregated from other hydraulic characteristic data based on borehole geophysical logs, which generally indicated that the Middle Castle Hayne aquifer is composed of higher percentages of clays and fine sands than sediments of the Upper Castle Hayne aquifer–River Bend unit and Tarawa Terrace aquifer. A horizontal hydraulic conductivity of 5 ft/d was assigned uniformly to the Lower Castle Hayne aquifer (model layer 7), also partly based on interpretations of borehole geophysical logs. Bias or selective distribution from east to west within model horizontal hydraulic conductivity arrays possibly occurs because of the geographically restricted point data used to create the arrays. The degree of bias, if it occurs, is unknown. The influence of such bias on simulation results also is unknown; however, sensitivity analyses indicate that substantial global increases and decreases in horizontal hydraulic conductivity substantially degrade simulated results compared to results based on calibrated arrays.

Only four aquifer tests in the vicinity of Tarawa Terrace used observation wells, and these tests were conducted using wells completed either in the Tarawa Terrace aquifer or Upper Castle Hayne aquifer–River Bend unit. Aquifer storativity computed as a result of these tests ranged from 0.05 to 0.009. The largest of these values, 0.05, was assigned uniformly to model layer 1 as specific yield. The majority of aquifer tests conducted at Tarawa Terrace and vicinity were single-well, step-drawdown tests. Resulting test data were analyzed using methods published by Halford and Kuniansky (2002). The default storativity used in these analyses to compute head losses caused by skin effects is 0.0004, a reasonable value of storativity for confined Southeastern Coastal Plain aquifers (Faye and McFadden 1986; Newcome 1993; Giese et al. 1997). An equivalent storativity was assigned uniformly to model layers 2–7 and then divided by cell-by-cell thickness to compute cell-by-cell specific storage. The resulting specific storage arrays were used to simulate transient-flow conditions. Sensitivity analyses indicate that order-of-magnitude changes in specific storage from calibrated values are insignificant with respect to simulated results.

Other uncertainties that potentially influence simulation results are the no-flow boundaries assigned to the western, southern, and eastern boundaries of the active model domain. These boundaries and the general-head boundary to the north generally conform to topographic boundaries. An additional constant-head boundary of zero potentiometric level was assigned to those cells in model layer 1 that correspond to the location of Northeast Creek. Northeast Creek is an estuary of the Atlantic Ocean and long-term, average water levels probably closely approximate sea level or zero potentiometric level.

Mainly based on regional flow concepts articulated by Hubbard (1940) and quantified by Toth (1962, 1963) and Freeze and Witherspoon (1966, 1967), topographic boundaries were considered to approximate the respective limits of the water table as groundwater divides. The water table and, by extension, potentiometric surfaces of underlying confined aquifers, were considered subdued replicas of surface topography. Accordingly, the no-flow and general-head boundaries defined for model layer 1 also were assigned to the same locations in model layers 2–7. These boundaries are probably entirely appropriate for predevelopment conditions, as indicated by the simulated predevelopment budget wherein only about 12 percent of total discharge originated at general-head boundaries, and almost all of that was contributed to model layer 1. Simulated predevelopment discharge was entirely to model cells representing Northeast Creek and Frenchmans Creek, either directly or by diffuse upward leakage. Such conditions exactly conform to the conceptual model as well as to regional flow concepts. The high degree of similarity between the predevelopment water table simulated for model layer 1 and the potentiometric surface simulated for model layer 7 also conforms to regional flow concepts and the conceptual model (Figures C7 and C8).

During simulation of transient conditions, however, groundwater pumping at water-supply wells lowered water table and potentiometric surfaces and possibly significantly disrupted water-level and flow conditions at model boundaries, especially where supply wells were located in close proximity to model boundaries. Wells TT-25 and TT-26 were located about 1,000 ft from the general-head boundary. In addition, the coalescing of drawdown caused by pumping at supply wells in the vicinity of the Tarawa Terrace housing area possibly lowered water levels and altered flow directions in the vicinity of Northeast Creek (Figure C18). A test of the reasonableness of the assigned no-flow boundaries was accomplished by (1) comparing simulated predevelopment and transient water-levels at assigned no-flow boundaries to determine water-level changes and (2) comparing simulated predevelopment and transient flow to or from constant-head cells that represent Northeast Creek. Substantial changes in water levels at layer-by-layer model boundaries west of Frenchmans Creek, along the western part of the northern boundary, and at the no-flow boundary assigned along the mid-channel of Northeast Creek or a reversal of flow from constant-head cells to model layer 1 could indicate an inappropriate assignment of boundary conditions. Although contour values are not exactly comparable, the simulated potentiometric surfaces of model layer 1 during predevelopment conditions and for stress period 408 (December 1984) are everywhere nearly identical within the western half of the active model domain (Figures C7 and C18). In addition, budget components simulated for stress period 408 indicate that no reverse flow occurred from constant-head cells to model layer 1 anywhere along the shoreline boundary with Northeast Creek (Table C11). Within the eastern part of the model domain, which is most significantly affected by pumping from supply wells, simulated potentiometric levels in model layers 2–7 in the vicinity of Northeast Creek for stress period 408 were lower than simulated predevelopment water levels by about a foot. Simulated potentiometric levels immediately at the no-flow boundary near the mid-channel of Northeast Creek were lower than corresponding predevelopment water levels by about 0.5 ft or less in model layers 4–7. Corresponding differences within model layers 1–3 were about 0.2 ft or less. Simulated potentiometric levels within all layers along the general-head boundary in the vicinity of pumping wells were lower by a maximum of about 3 ft, and this change is reflected in increased flow across the boundary in model layers 1, 3, and 5, as expected (Table C11). These tests and the overall conformance of simulated predevelopment and transient conditions to the conceptual model indicate that boundaries and boundary conditions assigned to the active model domain are appropriate and that assigned no-flow and constant-head boundary conditions exerted only minimal influence on simulated transient results.

Monthly rates of effective recharge could not be computed because corresponding rates of surface runoff and evapotranspiration were not available from literature sources and could not be calculated with any reasonable accuracy, given available streamflow and meteorological data. To test the sensitivity of simulated results to monthly rather than annual variations in assigned recharge rates, a partial hydrologic budget for each month of the transient simulation was computed using total monthly precipitation and pan evaporation. The difference between monthly rates of precipitation and pan evaporation was assigned as effective recharge. Negative differences were assigned as zero recharge. These simulated results could not be directly compared to calibrated model results because surface runoff was not accounted for; also, pan evaporation does not equal evapotranspiration. However, simulated water-level changes from month to month and from year to year using the partial hydrologic budget were compared at model cells in the western part of the active model domain, far removed from areas of active pumping. Simulated month-to-month and year-to-year water-level changes were shown to be small, equaling only plus or minus several tenths of feet for any given year. Year-to-year changes were highly comparable to calibrated model results. This test indicates that varying annual, rather than monthly, rates of assigned effective recharge does not materially affect simulated water levels or water budgets from month to month or from year to year.

Summary

The MODFLOW code was used to simulate predevelopment and transient groundwater flow at Tarawa Terrace and vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina. Seven layers were assigned to the flow model mainly representing the Castle Hayne aquifer system. No-flow, constant-head, and general-head boundaries were assigned to define the active model domain. No-flow boundaries were assigned to the mid-channel of Northeast Creek, to the east and south, and to a topographic divide to the west. The general-head boundary was assigned along the northern perimeter of the active model domain and also approximately conformed to a topographic boundary. No-flow boundaries were equal in condition and location for each model layer. A constant head of zero was assigned in model layer 1 to the cells representing Northeast Creek. The base of simulated groundwater flow corresponds to the top of the Beaufort confining unit and is implicitly a no-flow boundary. Simulated predevelopment potentiometric levels indicated groundwater flows from highland areas toward Northeast and Frenchmans Creeks. Simulated potentiometric levels and flow directions were highly similar in all model layers. Simulated predevelopment recharge to the active model domain equaled about 2.1 cubic feet per second (cfs) from rainfall infiltration and 0.3 cfs from the general-head boundary and was discharged at rates of 1.6 cfs to Northeast Creek and 0.7 cfs to Frenchmans Creek. A difference in mass balance of 0.1 cfs is due to rounding error. Comparison of 59 observed water levels representing estimated predevelopment conditions and corresponding simulated potentiometric levels indicated a high degree of similarity throughout most of the study area. The average absolute difference between simulated and observed predevelopment water levels was 1.9 feet (ft), and the root-mean-square error of differences was 2.1 ft.

Transient simulations represented pumping at Tarawa Terrace water-supply wells for the period January 1951–December 1994. Groundwater flow was simulated for 528 stress periods representing 528 months. Assigned pumpage at supply wells was estimated using reported well capacity rates and annual rates of raw water treated at the Tarawa Terrace water treatment plant during 1975–1986. A total pumpage rate of 116,200 cubic feet per day was applied to the model for the period January 1952–December 1974 and represented the average rate reported during 1975–1986. Assigned pumpage at individual supply wells also conformed to known operational conditions, such as periods when a well was reportedly out of production for equipment repair or maintenance. Transient calibration was mainly based on comparisons of simulated and observed water levels. Several hundred measurements of water levels at Tarawa Terrace water-supply wells and at monitor wells installed during investigations of groundwater contamination were available for the period 1978–1994. Calibrated model results based on 789 paired water levels representing observed and simulated water levels at monitor wells and water-supply wells indicated an average absolute difference between simulated and observed water levels of 5.2 ft. The root-mean-square error of the absolute differences was 7.0 ft. Similar statistics varied considerably from supply well to supply well. The average absolute difference between simulated water levels at well TT-67 for the period 1979–1987 was 4.0 ft. The corresponding statistic at well TT-31 was 8.7 ft for about the same period of time.

Sensitivity analyses using transient calibration criteria indicated that simulation results were most sensitive to changes in horizontal hydraulic conductivity and assigned potentiometric levels along the general-head boundary. Simulation results were insensitive to changes in model arrays representing effective recharge, drain conductance, and specific storage.

Availability of Input Data Files, Models, and Simulation Results

Calibrated model input data files developed for simulating predevelopment groundwater flow, transient groundwater flow, the fate and transport of PCE as a single specie, and the distribution of water and contaminants in a water-distribution system are provided with Chapter A (Morris et al. 2007) of this report in a digital video disc (DVD) format. Public domain model codes used with these input files are available on the Internet at the following Web sites:

- Predevelopment and transient groundwater flow
  - Model code: MODFLOW-96
  - Web site: *http://water.usgs.gov/nrp/gwsoftware/modflow.html*
- Fate and transport of PCE as a single specie
  - Model code: MT3DMS
  - Web site: *http://hydro.geo.ua.edu/*
- Distribution of water and contaminants in a water-distribution system
  - Model code: EPANET 2
  - Web site: *http://www.epa.gov/nrmrl/wswrd/epanet.html*

Readers desiring information about the model input data files or the simulation results contained on the DVDs also may contact the Project Officer of ATSDR's Exposure-Dose Reconstruction Project at the following address:

Morris L. Maslia, MSCE, PE, D.WRE, DEE
Exposure-Dose Reconstruction Project
Division of Health Assessment and Consultation
Agency for Toxic Substances and Disease Registry
1600 Clifton Road, Mail Stop E-32
Atlanta, Georgia 30333
Telephone: (404) 498-0415
Fax: (404) 498-0069
E-mail: mmaslia@cdc.gov

Acknowledgments

A study of this complexity and magnitude is dependent upon the assistance, input, and suggestions of many colleagues. Thus, the authors of this report and all chapter reports acknowledge the managers and staff of the U.S. Geological Survey Water Science Centers in Raleigh, North Carolina, and Atlanta, Georgia. In particular, the contributions of Melinda J. Chapman, Douglas A. Harned, and Stephen S. Howe are acknowledged for providing the majority of well, water-level, and pumpage data used in this study. Keith W. McFadden is acknowledged for assistance with spatial analyses in preparing illustrations and with developing geodatabases, Web-based applications, and the querying system contained on the electronic media accompanying Chapters A and K. Gregory C. Mayer and Edward H. Martin also are acknowledged for their administrative assistance.

The authors acknowledge the staff of the Environmental Management Division, U.S. Marine Corps Base Camp Lejeune, North Carolina. In particular, Scott A. Brewer, Brynn Ashton, Scott R. Williams, and Rick Cheng for their assistance and cooperation during the course of this study, especially for providing a large number of technical reports, maps, and historical documents, which summarize the results of groundwater remedial investigations at and in the vicinity of Tarawa Terrace. The authors also acknowledge Joel Hartsoe and Danny E. Hill of the Camp Lejeune Public Works Department Utility Section.

The authors acknowledge the contributions of the USEPA, Region IV, Atlanta, Georgia, for providing reports and documents summarizing the results of investigations of groundwater contamination in the vicinity of ABC One-Hour Cleaners and in the northern part of Tarawa Terrace.

The authors acknowledge colleagues at ATSDR, Eastern Research Group Inc., the Multimedia Environmental Simulations Laboratory at the Georgia Institute of Technology, and the Oak Ridge Institute for Science and Education for providing assistance and advice with all aspects of this study.

Thomas M. Plummer, Commander, U.S. Public Health Service, Indian Health Service, U.S. Department of Health and Human Services, assisted with planning, field instrumentation, and conducting tests of water-distribution systems serving Camp Lejeune, August 18–28, 2004.

Caryl J. Wipperfurth, Bonnie J. Turcott, Patricia L. Nobles, James E. Banton, and Kimberly A. Waltenbaugh, U.S. Geological Survey Enterprise Publishing Network, assisted with the preparation of text, illustrations, and electronic media.

References

Baker Environmental, Inc. Basewide Remediation Assessment, Groundwater Study (BRAGS), U.S. Marine Corps Base, Camp Lejeune, North Carolina; 1998.

Cardinell AP, Berg SA, and Lloyd OB Jr. Hydrogeologic Framework of U.S. Marine Corps Base at Camp Lejeune, North Carolina. U.S. Geological Survey Water-Resources Investigations Report 93-4049; 1993.

Catlin Engineers and Scientists. Leaking Underground Storage Tank (LUST) Phase I, Limited Site Assessment Report for TT-44, Marine Corps Base Camp Lejeune, North Carolina. Raleigh, NC: Catlin Engineers and Scientists; 2002a. Report No.: N62470-95-D-6009.

Catlin Engineers and Scientists. Leaking Underground Storage Tank (LUST) Phase I, Limited Site Assessment Report for TT-2634, Marine Corps Base Camp Lejeune, North Carolina. Raleigh, NC: Catlin Engineers and Scientists; 2002b. Report No.: N62470-95-D-6009.

Chiang W-H and Kinzelbach W. 3D-Groundwater Modeling with PMWIN: Springer-Verlag; 2001.

CLW, Camp Lejeune Water Documents, 0001–8761 (not consecutively available), provided on DVD format, in Maslia ML, Sautner JB, Faye RE, Suárez-Soto RJ, Aral MM, Grayman WM, Jang W, Wang J, Bove FJ, Ruckart PZ, Valenzuela C, Green JW Jr, and Krueger AL. Analyses of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water at Tarawa Terrace and Vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina: Historical Reconstruction and Present-Day Conditions—Chapter A: Summary of Findings. Atlanta, GA: Agency for Toxic Substances and Disease Registry; 2007.

DiGiano FA, Miller CT, Roche AC, and Wallingford ED. Methodology for Assessment of Contamination of the Unsaturated Zone by Leaking Underground Storage Tanks: Water Resources Research Institute of the University of North Carolina; 1988.

Faye RE. Analyses of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water at Tarawa Terrace and Vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina: Historical Reconstruction and Present-Day Conditions—Chapter B: Geohydrologic Framework of the Castle Hayne Aquifer System. Atlanta, GA: Agency for Toxic Substances and Disease Registry; 2007.

Faye RE. Analyses of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water at Tarawa Terrace and Vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina: Historical Reconstruction and Present-Day Conditions—Chapter F: Simulation of the Fate and Transport of Tetrachloroethylene (PCE) Atlanta, GA: Agency for Toxic Substances and Disease Registry; In press 2007.

Faye RE, and Green JW Jr. Analyses of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Potable Water at Tarawa Terrace and Vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina: Historical Reconstruction and Present-Day Conditions—Chapter E: Occurrence of Contaminants in Groundwater. Atlanta, GA: Agency for Toxic Substances and Disease Registry; 2007.

Faye RE, and McFadden KW. Hydraulic Characteristics of Upper Cretaceous and Lower Tertiary Clastic Aquifers—Eastern Alabama, Georgia, and Western South Carolina: U.S. Geological Survey Water-Resources Investigations Report 86-4210; 1986.

Freeze RA, and Witherspoon PA. Theoretical Analysis of Regional Groundwater Flow: 1. Analytical and Numerical Solutions to the Mathematical Model: Water Resources Research, v. 2, no. 4; 1966.

Freeze RA, and Witherspoon PA. Theoretical Analysis of Regional Groundwater Flow: 2. Effect of Water-Table Configuration and Subsurface Permeability Variation: Water Resources Research, v. 3, no. 2; 1967.

Giese GL, and Mason RR Jr. Low-Flow Characteristics of Streams in North Carolina: U.S. Geological Survey Open-File Report 90-399; 1991.

Giese GL, Eimers JL, and Coble RW. Simulation of Groundwater Flow in the Coastal Plain Aquifer System of North Carolina: U.S. Geological Survey Professional Paper 1404-M; 1997.

Halford KJ, and Kuniansky EL. Documentation of Spreadsheets for the Analysis of Aquifer-Test and Slug-Test Data: U.S. Geological Survey Open-File Report 02-197; 2002.

Haliburton NUS Environmental Corporation. Draft Site Inspection Report, Site 07: Tarawa Terrace Dumps; 1992. Report No.: N62470-90-B-7629.

Harbaugh AW, and McDonald MG. User's Documentation for MODFLOW-96, and Update to the U.S. Geological Survey Modular Finite-Difference Groundwater-Flow Model: U.S. Geological Survey Open-File Report 96-458; 1996.

Harbaugh AW, Banta ER, Hill MC, and McDonald MG. MODFLOW-2000, The U.S. Geological Survey Modular Groundwater Model, User Guide to Modularization Concepts and the Groundwater Flow Process: U.S. Geological Survey Open-File Report 00-92; 2000.

Harned DA, Lloyd OB Jr, and Treece MW Jr. Assessment of Hydrologic and Hydrogeologic Data at Camp Lejeune Marine Corps Base, North Carolina. Raleigh, NC: U.S. Geological Survey Water-Resources Investigations Report 89-4096; 1989.

Heath RC. Groundwater Recharge in North Carolina: Groundwater Section, Division of Environmental Management, North Carolina Department of Environment, Health, and Natural Resources; 1994.

Henry Von Oesen and Associates, Inc. Study of Two Water Plants, Tarawa Terrace–Montford Point, Camp Lejeune, North Carolina; 1979.

Hill MC, Banta ER, Harbaugh AW, and Anderman ER. MODFLOW-2000, The U.S. Geological Survey Modular Ground-Water Model—User Guide to the Observation, Sensitivity, and Parameter-Estimation Processes and Three Post-Processing Programs: U.S. Geological Survey Open-File Report 00-184; 2000.

Hubbard MK. The Theory of Groundwater Motion, Part 1, Part 2: The Journal of Geology, v. XLVIII; 1940.

Industrial Marine Services, Inc. Delineation and Proposed Recovery of a Subsurface Fuel Plume, Camp Lejeune. Norfolk, VA: IMS Inc.; 1985.

Law Engineering, Inc. Leaking Underground Storage Tank Site Assessment Report, Building TT2478, Marine Corps Base, Camp Lejeune, North Carolina, vol. I & II; 1994a,b.

Law Engineering, Inc. Leaking Underground Storage Tank Site Assessment Report, Building TT2477, Marine Corps Base, Camp Lejeune, North Carolina, vol. I & II; 1995a,b.

Law Engineering and Environmental Services, Inc. Corrective Action Plan for the Recovery of Free Product and the Restoration of Petroleum Contaminated Soil and Groundwater, Building TT-2477/2478, Marine Corps Base, Camp Lejeune, Onslow County, North Carolina; 1996. Report No.: 7176.

Law Engineering and Environmental Services, Inc. Leaking Underground Storage Tank Limited Site Assessment Addendum, UST TT-48-2, Tarawa Terrace II Elementary School, Marine Corps Base Camp Lejeune, North Carolina; 1998. Report No.: 30740-6-06009.

Law Engineering and Testing Company, Inc. On-Site Sampling—Septic Tank and Outlying Area, ABC One-Hour Cleaners Inc., Jacksonville, North Carolina LETCO Job; 1986a. Report No.: J-473-86-1623.

Law Engineering and Testing Company, Inc. On-Site Sampling ABC One-Hour Cleaners Inc., Jacksonville, North Carolina; 1986b.

LeGrand HE. Evaluation of Well-Water Supply, Marine Corps Base, Camp Lejeune, North Carolina: Project Report, Contract NBy-7595; 1959.

Maslia ML, Sautner JB, Faye RE, Suárez-Soto RJ, Aral MM, Grayman WM, Jang W, Wang J, Bove FJ, Ruckart PZ, Valenzuela C, Green JW Jr, and Krueger AL. Analyses of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water at Tarawa Terrace and Vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina: Historical Reconstruction and Present-Day Conditions—Chapter K: Supplemental Information. Atlanta, GA: Agency for Toxic Substances and Disease Registry; In press 2008.

McDonald MG, and Harbaugh AW. A Modular Three-Dimensional Finite-Difference Groundwater-Flow Model: U.S. Geological Survey Open-File Report 83-875; 1984.

McMorris CA. Site Inspection Report—ABC One Hour Cleaners, NC DO24644494, 2127 Lejeune Boulevard, Jacksonville, NC, 28340: North Carolina Solid and Hazardous Waste Branch, Environmental Health Section; 1987.

Mid-Atlantic Associates, Inc. Leaking Underground Storage Tank, Phase I Limited Site Assessment, UST TT-2302/2304, Tarawa Terrace II Housing Area, Marine Corps Base Camp Lejeune, North Carolina: Mid-Atlantic Associates, Inc.; 2003a. Report No.: N62470-90-R-7626.

Mid-Atlantic Associates, Inc. Leaking Underground Storage Tank, Phase I Limited Site Assessment, UST TT-3546/3548 Site, Tarawa Terrace II Housing Area, Marine Corps Base Camp Lejeune, North Carolina: Mid-Atlantic Associates, Inc.; 2003b. Report No.: N62740-95-D-6009.

Mid-Atlantic Associates, P.A. Leaking Underground Storage Tank (LUST), Phase I Limited Site Assessment Report for UST TT-779 Site, Tarawa Terrace I Housing Area, Marine Corps Base Camp Lejeune, North Carolina: Mid-Atlantic Associates, P.A.; 2002a. Report No.: N62470-01-D-3009.

Mid-Atlantic Associates, P.A. Leaking Underground Storage Tank (LUST), Phase I Limited Site Assessment Report for UST TT-2254/2256 Site, Tarawa Terrace II Housing Area, Marine Corps Base Camp Lejeune, North Carolina: Mid-Atlantic Associates, P.A.; 2002b. Report No.: N62470-01-D-3009.

Mid-Atlantic Associates, P.A. Leaking Underground Storage Tank (LUST), Phase I Limited Site Assessment Report for UST TT-2258/2260 Site, Tarawa Terrace II Housing Area, Marine Corps Base Camp Lejeune, North Carolina: Mid-Atlantic Associates, P.A.; 2002c. Report No.: N62470-01-D-3009.

Mid-Atlantic Associates, P.A. Leaking Underground Storage Tank (LUST), Phase I Limited Site Assessment Report for UST TT-3140/3142 Site, Tarawa Terrace II Housing Area, Marine Corps Base Camp Lejeune, North Carolina: Mid-Atlantic Associates, P.A.; 2002d. Report No.: N62470-01-D-3009.

Mid-Atlantic Associates, P.A. Leaking Underground Storage Tank, Phase I Limited Site Assessment, UST TT-3165/3167, Marine Corps Base Camp Lejeune, North Carolina: Mid-Atlantic Associates, P.A.; 2002e. Report No.: N62470-01-D-3009.

Mid-Atlantic Associates, P.A. Leaking Underground Storage Tank, Phase I Limited Site Assessment, UST TT-3233/3235, Marine Corps Base Camp Lejeune, North Carolina: Mid-Atlantic Associates P.A.; 2002f. Report No.: N62470-01-D-3009.

Mid-Atlantic Associates, P.A. Leaking Underground Storage Tank (LUST), Phase I Limited Site Assessment Report for UST TT-3524/3526 Site, Tarawa Terrace II Housing Area, Marine Corps Base Camp Lejeune, North Carolina: Mid-Atlantic Associates, P.A.; 2002g. Report No.: N62470-01-D-3009.

Newcome R Jr. Pumping Tests of the Coastal Plain Aquifers in South Carolina: South Carolina Water Resources Commission Report 174; 1993.

O'Brien & Gere Engineers, Inc. Site Assessment, Tank STT61–STT66, Tarawa Terrace, Marine Corps Base, Camp Lejeune, North Carolina; 1992.

O'Brien & Gere Engineers, Inc. Addendum Site Assessment, Tanks STT61–STT66, Tarawa Terrace, Marine Corps Base Camp Lejeune; 1993.

OHM Remediation Services Corp. Final Additional Investigation Report, Buildings TT-2477/78, Marine Corps Base Camp Lejeune, North Carolina, Contract No. N62470-97-D-9000; 2001.

Poland JF, Lofgren BF, and Riley FS. Glossary of Selected Terms Useful in Studies of the Mechanics of Aquifer System and Land Subsidence Due to Fluid Withdrawal: U.S. Geological Survey Water-Supply Paper 2025; 1972.

Pollock DW. Documentation of Computer Programs to Compute and Display Pathlines Using Results from the U.S. Geological Survey Modular Three-Dimensional Finite-Difference Groundwater Model: U.S. Geological Survey Open-File Report 89-381; 1989.

Pollock DW. User's Guide for MODPATH/MODPATH-PLOT, Version 3: A Particle Tracking Post-Processing Package for MODFLOW, the U.S. Geological Survey Finite-Difference Groundwater-Flow Model: U.S. Geological Survey Open-File Report 94-464; 1994.

Richard Catlin & Associates, Inc. Leaking Underground Storage Tank Comprehensive Site Assessment, Building TT-2455, Marine Corps Air Station New River, Jacksonville, North Carolina, Volume I: Richard Catlin & Associates, Inc.; 1994a. Contract No.: N62470-93-D-4020.

Richard Catlin & Associates, Inc. Leaking Underground Storage Tank Comprehensive Site Assessment, Building TT-2455, Marine Corps Air Station New River, Jacksonville, North Carolina, Volume II: Richard Catlin & Associates, Inc.; 1994b. Contract No.: N62470-93-D-4020.

Richard Catlin & Associates, Inc. Leaking Underground Storage Tank Comprehensive Site Assessment Buildings TT-2465, TT-2465, TT-2467 and TT-2471, Marine Corps Base, Camp Lejeune, North Carolina, Volume I: Richard Catlin & Associates, Inc.; 1995a. Contract No.: N62470-93-D-4020.

Richard Catlin & Associates, Inc. Leaking Underground Storage Tank Comprehensive Site Assessment, Buildings TT-2463, TT-2465, TT-2467 and TT-2471, Marine Corps Base Camp Lejeune, North Carolina. Volume II: Richard Catlin & Associates, Inc.; 1995b. Contract No.: N62470-93-D-4020.

Richard Catlin & Associates, Inc. Leaking Underground Storage Tanks Corrective Action Plan, UST TT-2463-2473, Marine Corps Base, Camp Lejeune, North Carolina: Richard Catlin & Associates, Inc.; 1996. Contract No.: N62470-93-D-4020.

Richard Catlin & Associates, Inc. Leaking Underground Storage Tanks Corrective Action Plan Building TT-2455, Marine Corps Base Camp Lejeune, North Carolina: Richard Catlin & Associates, Inc.; 1998. Contract No.: N62470-93-D-4020.

Roy F. Weston, Inc. Remedial Investigation Report, ABC One-Hour Cleaners, Jacksonville, North Carolina: Roy F. Weston, Inc.; 1992.

Roy F. Weston, Inc. Remedial Investigation Report, ABC One-Hour Cleaners, Operable Unit 2, Jacksonville, North Carolina: Roy F. Weston, Inc.; 1994.

Shiver RA. Groundwater Investigation to Define the Source(s) of Tetrachloroethylene that Have Contaminated Three Community Water Supply Wells at Tarawa Terrace I, Camp Lejeune Marine Corps Base, Onslow County: North Carolina Department of Natural Resources and Community Development; 1985.

Thompson DG. Groundwater Supplies in the Vicinity of Jacksonville, North Carolina: U.S. Geological Survey Memorandum to the Record, May 20, 1941, to Rear Admiral, Ben Moreell, Chief, Bureau of Yards and Docks, Navy Department; 1941.

Toth JA. Theoretical Analysis of Groundwater Motion in Small Drainage Basins in Central Alberta, Canada: Journal of Geophysical Research, v. 67, no. 11; 1962.

Toth JA. Theoretical Analysis of Groundwater Flow in Small Drainage Basins: Journal of Geophysical Research, v. 68, no. 16; 1963.

Appendix C1. Water-Level Measurements in Selected Wells, Tarawa Terrace and Vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina

Tables

Sources:

Catlin Engineers and Scientists 2002a,b
DiGiano et al. 1988
Haliburton NUS Environmental Corporation 1992
Law Engineering and Environmental Services, Inc. 1996, 1998
Law Engineering, Inc. 1994a,b, 1995a,b
Mid-Atlantic Associates, Inc. 2003a,b
Mid-Atlantic Associates, P.A. 2002a,b,c,d,e,f,g
O'Brien & Gere Engineers, Inc. 1992, 1993
OHM Remediation Services Corp, 2001
Richard Catlin & Associates, Inc. 1994a,b, 1995a,b, 1996, 1998
U.S. Geological Survey well inventory, written communication, October 21, 1986

Appendix C1. Water-Level Measurements in Selected Wells, Tarawa Terrace and Vicinity

Table C1.1. Water-level measurements in Tarawa Terrace supply wells TT-23, TT-27, and TT-55, test well T-9, and Civilian Conservation Corps well CCC-1 used during model calibration, Tarawa Terrace, U.S. Marine Corps Base Camp Lejeune, North Carolina.

[NGVD, National Geodetic Vertical Datum of 1929; –, below NGVD 29; contributing aquifers: UCHRBU&LU, Upper Castle Hayne aquifer–River Bend and Lower units; MCH, Middle Castle Hayne aquifer; UCH, Upper Castle Hayne aquifer–undifferentiated; UCHRBU, Upper Castle Hayne aquifer–River Bend unit]

Site name[1]	Location coordinates[2]		Land-surface altitude, in feet above NGVD 29	Contributing aquifers	Measurement date	Water-level altitude, in feet above or below NGVD 29
	North	East				
TT-23	363208	2491024	23.9	UCHRBU&LU, MCH	3/14/1983	–1.8
					9/25/1985	1.1
					10/21/1986	2.2
					4/7/1987	9.3
					9/4/1984	[3]19
					9/31/1984	[3]12
					10/14/1984	[3]16
					10/31/1984	[3]16
					11/30/1984	[3]16
					1/31/1985	[3]16
TT-27	364794	2489026	26.4	UCH	1/10/1963	16.6
					4/17/1963	18.4
					1/16/1964	19.4
					7/14/1964	19.0
					9/17/1964	20.6
					10/14/1964	21.9
TT-55	364767	2489069	26.4	UCH	11/1/1961	18.9
T-9	364648	2490489	28.7	UCHRBU&LU	9/24/1986	17.5
					10/21/1986	19.1
					4/10/1987	23.4
CCC-1	360997	2483873	24.3	UCHRBU	9/17/1941	3.3

[1]See Plate 1 for location
[2]Location coordinates are North Carolina State Plane coordinates, North American Datum of 1983
[3]Airline measurements. Not used for model calibration

Table C1.2. Water-level measurements in supply well TT-25[1] used during model calibration, Tarawa Terrace, U.S. Marine Corps Base Camp Lejeune, North Carolina.

[NGVD 29, National Geodetic Vertical Datum of 1929; –, below NGVD 29]

Contributing aquifer— Middle Castle Hayne aquifer, Upper Castle Hayne aquifer–River Bend unit and –Lower unit

Location coordinates[2], 364042 North, 2491984 East

Land-surface altitude, 32.0 feet above NGVD 29

Measurement date	Water-level altitude, in feet above or below NGVD 29	Measurement date	Water-level altitude, in feet above or below NGVD 29
11/14/1980	6.0	11/30/1984	–11
7/9/1981	0.0	12/31/1984	–10
10/31/1982	–13	1/31/1985	–10
12/31/1982	–13	6/30/1985	–2
1/31/1983	–14	7/31/1985	–3
2/28/1983	–13	8/31/1985	–3
3/31/1983	–10	9/11/1985	–6
4/30/1983	–9	9/25/1985	–26.2
5/31/1983	–9	9/30/1985	–4
7/31/1983	–10	10/31/1985	–6
8/31/1983	–12	11/30/1985	3
9/30/1983	–12	12/31/1985	–6
10/31/1983	–15	1/31/1986	–3
11/30/1983	–11	2/28/1986	–3
12/31/1983	–9	3/31/1986	–5
1/31/1984	–11	4/30/1986	3
5/31/1984	–10	10/21/1986	3
6/30/1984	–11	4/7/1987	10.9
7/31/1984	–10		
8/31/1984	–9		
9/30/1984	–5		
10/31/1984	–5		

[1]See Figure C1 for location
[2]Location coordinates are North Carolina State Plane coordinates, North American Datum of 1983

Table C1.3. Water-level measurements in supply well TT-26[1] used during model calibration, Tarawa Terrace, U.S. Marine Corps Base Camp Lejeune, North Carolina.

[NGVD 29, National Geodetic Vertical Datum of 1929; –, below NGVD 29]

Contributing aquifer—Upper Castle Hayne aquifer–Lower unit

Location coordinates[2], 364356 North, 2491461 East

Land-surface altitude, 34.0 feet above NGVD 29

Measurement date	Water-level altitude, in feet above or below NGVD 29
5/16/1951	14.0
1/31/1978	7
2/28/1978	7
3/31/1978	6
4/30/1978	7
5/31/1978	7
6/30/1978	6
7/31/1978	6
8/31/1978	7
9/30/1978	6
10/31/1978	6
11/30/1978	6
12/31/1978	6
1/31/1979	5
2/28/1979	6
3/31/1979	8
4/30/1979	6
6/30/1979	6
7/31/1979	5
9/30/1979	5
2/29/1980	6
3/31/1980	2
4/30/1980	–8
5/31/1980	6
10/31/1980	–7
12/31/1980	–8
1/31/1981	0
2/28/1981	–2
3/31/1981	0
4/30/1981	2
6/30/1981	0
7/31/1981	2
8/31/1981	–1
10/31/1981	–2
11/30/1981	2
4/30/1982	–10
6/30/1982	–14
9/14/1982	–5
10/31/1982	–15
12/31/1982	2
1/31/1983	2
2/28/1983	4
3/31/1983	4
4/30/1983	4
5/31/1983	–13
6/30/1983	4
9/30/1983	–22
10/31/1983	3
11/30/1983	–2
12/31/1983	4
3/31/1984	–6
5/31/1984	4
6/30/1984	–2
9/30/1984	8
10/31/1984	8
11/30/1984	3
12/31/1984	3
1/31/1985	1
6/30/1985	6
7/31/1985	2
9/30/1985	2
10/31/1985	2
11/30/1985	4
10/21/1986	7.4
4/7/1987	14.0

[1]See Figure C1 for location

[2]Location coordinates are North Carolina State Plane coordinates, North American Datum of 1983

Table C1.4. Water-level measurements in supply well TT-30[1] used during model calibration, Tarawa Terrace, U.S. Marine Corps Base Camp Lejeune, North Carolina.

[NGVD 29, National Geodetic Vertical Datum of 1929; –, below NGVD 29]

Contributing aquifers—Upper Castle Hayne aquifer–River Bend unit and –Lower unit

Location coordinates[2], 365044 North, 2487130 East

Land-surface altitude, 26 feet above NGVD 29

Measurement date	Water-level altitude, in feet above or below NGVD 29
1/31/1978	4
2/28/1978	4
3/31/1978	6
4/30/1978	5
5/31/1978	4
6/30/1978	5
7/31/1978	4
8/31/1978	–2
9/30/1978	0
10/31/1978	–2
11/30/1978	–1
12/31/1978	–3
1/31/1979	–2
2/28/1979	–2
3/31/1979	2
4/30/1979	–2
6/30/1979	–1
7/31/1979	–2
8/31/1979	–2
9/30/1979	–4
1/31/1980	–4
2/29/1980	–4
3/31/1980	–6
4/30/1980	3
5/31/1980	–6
7/31/1980	–4
8/31/1980	–2
9/30/1980	–4
10/31/1980	–6
12/31/1980	–6
1/31/1981	–8
2/28/1981	–7
3/31/1981	–6
4/30/1981	–4
5/31/1981	–5
6/30/1981	–6
7/31/1981	–7
8/31/1981	–5
9/30/1981	–6
10/31/1981	–10
3/31/1982	16
4/30/1982	11
6/30/1982	7
7/31/1982	9
8/31/1982	13
9/30/1982	11
10/31/1982	10
12/31/1982	9
1/31/1983	9
2/28/1983	9
3/31/1983	9
4/30/1983	9
5/31/1983	13
6/30/1983	10
7/31/1983	10
8/31/1983	10
9/30/1983	10
10/31/1983	10
11/30/1983	–7
12/31/1983	11
1/31/1984	10
2/29/1984	10
3/31/1984	15
4/30/1984	12
5/31/1984	11
6/30/1984	11
7/31/1984	11
9/30/1984	11
10/31/1984	11
11/30/1984	11
12/31/1984	11
1/31/1985	11
4/30/1985	11

[1]See Figure C1 for location

[2]Location coordinates are North Carolina State Plane coordinates, North American Datum of 1983

Table C1.5. Water-level measurements in supply well TT-31[1] used during model calibration, Tarawa Terrace, U.S. Marine Corps Base Camp Lejeune, North Carolina.

[NGVD 29, National Geodetic Vertical Datum of 1929; –, below NGVD 29]

Contributing aquifer—Upper Castle Hayne aquifer–undifferentiated

Location coordinates[2], 362224 North, 2489843 East

Land-surface altitude, 25.8 feet above NGVD 29

Measurement date	Water-level altitude, in feet above or below NGVD 29
10/31/1978	–2
11/30/1978	–1
7/31/1979	–3
8/31/1979	–2
9/30/1979	2
1/31/1980	–3
2/29/1980	–2
3/31/1980	–2
4/30/1980	12
5/31/1980	0
7/31/1980	0
8/31/1980	–2
12/31/1980	–4
1/31/1981	–8
2/28/1981	–6
3/31/1981	–8
5/31/1981	–4
6/30/1981	–5
7/31/1981	–3
10/31/1981	–6
11/30/1981	–8
6/30/1982	–6
7/31/1982	–3
9/14/1982	–8
10/31/1982	–4
12/31/1982	3
1/31/1983	4
2/28/1983	2
3/31/1983	4
4/30/1983	8
5/31/1983	8
10/31/1983	3
11/30/1983	6
12/31/1983	–8
3/31/1984	–6
5/31/1984	8
7/6/1984	–4
9/30/1984	–4
10/31/1984	–4
11/30/1984	–6
12/31/1984	–4
1/31/1985	–5
3/31/1985	–5
6/30/1985	–3
7/31/1985	–11
8/31/1985	–3
9/30/1985	–4
9/13/1985	–5
9/30/1985	–3
10/31/1985	–3
11/30/1985	–8
12/31/1985	–6
1/31/1986	–5
2/29/1986	–6
4/30/1986	–2
10/21/1986	–0.1
4/7/1987	5.2

[1]See Figure C1 for location

[2]Location coordinates are North Carolina State Plane coordinates, North American Datum of 1983

Table C1.6. Water-level measurements in supply well TT-52[1] used during model calibration, Tarawa Terrace, U.S. Marine Corps Base Camp Lejeune, North Carolina.

[NGVD 29, National Geodetic Vertical Datum of 1929; –, below NGVD 29]

Contributing aquifer—Upper Castle Hayne aquifer–undifferentiated

Location coordinates[2], 362321 North, 2489060 East

Land-surface altitude, 24.9 feet above NGVD 29

Measurement date	Water-level altitude, in feet above or below NGVD 29	Measurement date	Water-level altitude, in feet above or below NGVD 29
10/17/1961	12.9	7/31/1982	–6
3/28/1962	9	9/14/1982	–9
1/31/1978	–5	12/31/1982	–6
2/28/1978	–4	1/31/1983	–6
3/31/1978	–5	2/28/1983	–9
4/30/1978	–5	3/31/1983	–2
5/31/1978	–1	4/30/1983	–2
6/30/1978	–3	5/31/1983	–1
7/31/1978	–1	10/31/1983	–4
8/31/1978	–3	11/30/1983	–2
9/30/1978	–3	12/31/1983	–2
10/31/1978	–3	3/31/1984	–4
11/30/1978	–4	4/30/1984	–2
12/31/1978	–7	5/31/1984	–2
1/31/1979	–7	6/30/1984	–3
2/28/1979	–4	7/31/1984	–3
3/31/1979	–5	9/30/1984	–2
6/30/1979	–4	10/31/1984	3
7/31/1979	–4	11/30/1984	3
8/31/1979	–3	12/31/1984	–2
9/30/1979	–4	1/31/1985	–2
1/31/1980	–4	5/31/1985	–5
2/29/1980	–3	6/30/1985	2
3/31/1980	–4	7/31/1985	0
4/30/1980	–4	8/31/1985	–1
5/31/1980	–4	9/11/1985	5
7/31/1980	–5	9/30/1985	4
8/31/1980	–5	10/31/1985	3
12/31/1980	–6	11/30/1985	5
1/31/1981	–7	12/31/1985	4
2/28/1981	–6	1/31/1986	–2
3/31/1981	–9	2/28/1986	5
4/30/1981	–9	3/31/1986	–7
5/31/1981	–5	4/30/1986	5
6/30/1981	–5	10/21/1986	1.8
7/31/1981	–7	4/7/1987	5.0
10/31/1981	–9		
11/30/1981	–7		
4/30/1982	–5		
6/30/1982	–5		

[1]See Figure C1 for location

[2]Location coordinates are North Carolina State Plane coordinates, North American Datum of 1983

Table C1.7. Water-level measurements in supply well TT-53[1] used during model calibration, Tarawa Terrace, U.S. Marine Corps Base Camp Lejeune, North Carolina.

[NGVD 29, National Geodetic Vertical Datum of 1929; –, below NGVD 29]

Contribution aquifer—Upper Castle Hayne aquifer–River Bend and –Lower units

Location coordinates[2], 363360 North, 2489800 East

Land-surface altitude, 25 feet above NGVD 29

Measurement date	Water-level altitude, in feet above or below NGVD 29
7/22/1961	14
3/28/1962	11
1/31/1978	–4
2/28/1978	–5
3/31/1978	–3
4/30/1978	–5
5/31/1978	–5
6/30/1978	–4
7/31/1978	–4
8/31/1978	0
9/30/1978	–3
12/31/1978	–2
1/31/1979	–2
2/28/1979	–4
3/31/1979	–2
4/30/1979	–8
6/30/1979	–6
7/31/1979	–4
1/31/1980	–4
2/29/1980	–5
3/31/1980	–1
4/30/1980	–2
5/31/1980	–5
7/31/1980	–7
8/31/1980	–3
9/30/1980	–7
12/31/1980	–3
1/31/1981	–9
2/28/1981	–7
3/31/1981	–9
4/30/1981	–9
6/30/1981	–9
10/31/1981	–9
11/30/1981	–8
1/31/1982	–9
3/31/1982	–13
4/30/1982	–8
6/30/1982	–22
7/31/1982	–15
8/31/1982	–15
12/31/1982	–19
1/31/1983	–19
2/28/1983	–19
3/31/1983	–11
4/30/1983	–11
5/31/1983	–10
10/31/1983	–9
11/30/1983	–13
12/31/1983	–13
1/31/1984	–11
8/6/1986	1
4/7/1987	10

[1]See Figure C1 for location

[2]Location coordinates are North Carolina State Plane coordinates, North American Datum of 1983

Table C1.8. Water-level measurements in supply well TT-54[1] used during model calibration, Tarawa Terrace, U.S. Marine Corps Base Camp Lejeune, North Carolina.

[NGVD 29, National Geodetic Vertical Datum of 1929; –, below NGVD 29]

Contribution aquifer—Upper Castle Hayne aquifer–undifferentiated

Location coordinates[2], 362090 North, 2490630 East

Land-surface altitude, 22.1 feet above NGVD 29

Measurement date	Water-level altitude, in feet above or below NGVD 29	Measurement date	Water-level altitude, in feet above or below NGVD 29
6/30/1961	12.1	7/31/1982	–10
3/28/1962	6	9/30/1982	–10
1/31/1978	–7	9/14/1982	–12
2/28/1978	–6	10/31/1982	–10
3/31/1978	–6	11/30/1982	–10
4/30/1978	–5	12/31/1982	–9
5/31/1978	–7	1/31/1983	–9
6/30/1978	–6	2/28/1983	–8
7/31/1978	–7	3/31/1983	–8
8/31/1978	–6	4/30/1983	–8
9/30/1978	–6	5/31/1983	–8
10/31/1978	–6	6/30/1983	–8
11/30/1978	–7	10/31/1983	–9
12/31/1978	–7	11/30/1983	–7
1/31/1979	–7	12/31/1983	0
2/28/1979	–8	1/31/1984	–9
3/31/1979	–6	2/29/1984	–8
4/30/1979	–7	5/31/1984	–8
6/30/1979	–8	6/30/1984	–10
8/31/1979	–6	7/31/1984	–8
1/31/1980	–7	9/30/1984	–8
2/29/1980	–6	10/31/1984	–8
3/31/1980	–8	11/30/1984	–9
4/30/1980	–10	12/1/1984	–8
5/31/1980	–8	1/31/1985	–12
7/31/1980	–6	2/28/1985	–14
8/31/1980	–8	4/30/1985	–12
12/31/1980	–8	6/30/1985	–2
1/31/1981	–11	7/31/1985	–13
2/28/1981	–11	8/31/1985	–12
3/31/1981	–12	9/30/1985	–8
4/30/1981	–10	9/13/1985	–8
5/31/1981	–8	10/31/1985	–10
7/31/1981	–10	11/30/1985	–1
8/31/1981	–8	12/31/1985	–8
10/31/1981	–12	1/31/1986	–6
11/30/1981	–10	2/30/1986	–9
1/31/1982	–11	3/31/1986	–10
3/31/1982	–10	4/30/1986	–8
4/30/1982	–9	10/21/1986	0.4
5/31/1982	–10	4/7/1987	6.7
6/30/1982	–10		

[1]See Figure C1 for location

[2]Location coordinates are North Carolina State Plane coordinates, North American Datum of 1983

Table C1.9. Water-level measurements in supply well TT-67[1] used during model calibration, Tarawa Terrace, U.S. Marine Corps Base Camp Lejeune, North Carolina.

[NGVD 29, National Geodetic Vertical Datum of 1929; –, below NGVD 29]

Contribution aquifer—Upper Castle Hayne aquifer–Lower unit

Location coordinates[2], 362730 North, 2490160 East

Land-surface altitude, 27.5 feet above NGVD 29

Measurement date	Water-level altitude, in feet above or below NGVD 29
3/31/1979	–14
4/30/1979	–12
6/30/1979	–12
7/31/1979	–10
8/31/1979	–10
9/30/1979	–8
1/31/1980	–8
2/29/1980	–10
3/31/1980	–4
4/30/1980	–12
5/31/1980	–10
7/31/1980	–8
8/31/1980	–10
10/31/1980	–6
12/31/1980	–8
1/31/1981	–10
2/28/1981	–10
3/31/1981	–8
4/30/1981	–6
6/30/1981	–4
7/31/1981	–8
10/31/1981	–6
11/30/1981	–8
1/31/1982	–11
3/31/1982	–7
4/30/1982	–9
6/30/1982	–11
7/31/1982	–12
9/14/1982	–8
10/31/1982	–6
12/31/1982	–6
1/31/1983	–7
2/28/1983	–6
3/31/1983	–4
4/30/1983	–4
5/18/1983	–5
5/31/1983	–5
6/30/1983	–4
10/31/1983	–3
11/30/1983	–6
12/31/1983	–6
3/31/1984	10
5/31/1984	–4
6/30/1984	–1
8/21/1984	–3
9/30/1984	–5
10/31/1984	–5
11/30/1984	0
12/31/1984	–1
1/31/1985	–4
3/31/1985	–4
7/31/1985	–2
8/31/1985	–4
9/13/1985	–2
9/30/1985	–4
10/31/1985	–3
11/30/1985	–2
12/31/1985	–4
1/31/1986	–2
2/29/1986	–4
3/31/1986	–5
4/30/1986	–10
4/7/1987	8.4

[1]See Figure C1 for location

[2]Location coordinates are North Carolina State Plane coordinates, North American Datum of 1983

Table C1.10. Water-level measurements in ABC One-Hour Cleaners Operable Units 1 and 2 monitor wells and North Carolina Department of Natural Resources and Community Development monitor wells used during model calibration, Tarawa Terrace and vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina.

[NGVD 29, National Geodetic Vertical Datum of 1929; contributing aquifers: UCHLU, Upper Castle Hayne aquifer–Lower unit; MCH, Middle Castle Hayne aquifer; UCHRBU, Upper Castle Hayne aquifer–River Bend unit; TT, Tarawa Terrace aquifer]

Site name[1]	Location coordinates[2]		Land-surface altitude, in feet above NGVD 29	Contributing aquifers	Measurement date	Water-level altitude, in feet above NGVD 29
	North	East				
C1	365232	2490503	30.6	UCHLU	4/22/1992	21.5
					6/2/1992	20.8
					6/25/1992	21.2
C2	364902	2490793	32.0	UCHLU	4/22/1992	19.6
					6/2/1992	19.0
					6/25/1992	19.6
C3	364437	2491433	33.4	UCHLU	4/22/1992	15.8
					6/2/1992	14.7
					6/25/1992	15.6
C4	364045	2492080	32.2	MCH	4/22/1992	11.9
					6/2/1992	11.3
					6/25/1992	10.2
C5	364107	2491233	32.0	UCHLU	4/22/1992	15.7
					6/2/1992	15.0
					6/25/1992	15.9
C9	364800	2491730	32.1	UCHLU	10/1/1993	12.4
					11/18/1993	13.0
C10	364360	2491380	32.5	MCH	11/18/1993	12.6
C11	362300	2492130	31.0	UCHLU	10/1/1993	6.3
PZ-01	364860	2490667	31.9	UCHLU	10/1/1993	15.9
					11/18/1993	16.7
PZ-02	364860	2490677	31.9	UCHRBU	10/1/1993	16.0
					11/18/1993	16.7
PZ-03	364858	2490812	32.5	UCHLU	10/1/1993	15.6
					11/18/1993	16.6
PZ-04	364858	2490812	32.5	UCHRBU	10/1/1993	15.8
					11/18/1993	16.4
PZ-05	364926	2490707	32.0	UCHLU	10/1/1993	15.7
PZ-06	364926	2490707	32.0	UCHRBU	10/1/1993	16.1
S1	365251	2490534	30.6	TT, UCHRBU(?)	4/22/1992	23.7
					6/2/1992	23.3
					6/25/1992	22.6
					10/1/1993	17.4
					11/18/1993	18.3
S2	364883	2490787	32.5	UCHRBU	4/22/1992	19.9
					6/2/1992	19.2
					6/25/1992	19.8
					10/1/1993	16.4
					11/18/1993	16.6
S3	364357	2491413	33.4	TT, UCHRBU	4/22/1992	16.0
					6/2/1992	14.8
					6/25/1992	15.8
					10/1/1993	13.1
					11/18/1993	13.6

Table C1.10. Water-level measurements in ABC One-Hour Cleaners Operable Units 1 and 2 monitor wells and North Carolina Department of Natural Resources and Community Development monitor wells used during model calibration, Tarawa Terrace and vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina.—Continued

[NGVD 29, National Geodetic Vertical Datum of 1929; contributing aquifers: UCHLU, Upper Castle Hayne aquifer–Lower unit; MCH, Middle Castle Hayne aquifer; UCHRBU, Upper Castle Hayne aquifer–River Bend unit; TT, Tarawa Terrace aquifer]

Site name[1]	Location coordinates[2] North	Location coordinates[2] East	Land-surface altitude, in feet above NGVD 29	Contributing aquifers	Measurement date	Water-level altitude, in feet above NGVD 29
S4	364065	2492060	32.2	TT, UCHRBU(?)	4/22/1992	13.6
					6/2/1992	12.4
					6/25/1992	11.9
					10/1/1993	11.2
					11/18/1993	13.5
S5	364081	2491244	31.9	TT, UCHRBU(?)	4/22/1992	16.4
					6/2/1992	15.2
					6/25/1992	16.2
					10/1/1993	13.5
					11/18/1993	13.7
S6	364938	2490617	31.1	TT, UCHRBU	4/22/1992	20.6
					6/2/1992	20.0
					6/25/1992	20.5
					10/1/1993	16.3
					11/18/1993	17.1
S7	364753	2490732	31.3	TT, UCHRBU	4/22/1992	19.8
					6/2/1992	19.0
					6/25/1992	19.4
					10/1/1993	15.8
					11/18/1993	16.6
S8	364938	2491312	30.8	TT, UCHRBU	4/22/1992	20.9
					6/2/1992	19.8
					6/25/1991	21.1
					10/1/1993	18.8
					11/18/1993	19.0
S9	364593	2491682	32.7	TT, UCHRBU	4/22/1992	15.4
					6/2/1992	14.2
					6/25/1992	13.3
					10/1/1993	12.5
					11/18/1993	13.0
S10	363818	2491922	31.6	TT, UCHRBU	4/22/1992	12.2
					6/2/1992	12.8
					6/25/1992	13.3
					10/1/1993	12.4
					11/18/1993	12.7
S11	365390	2489710	30.8	TT, UCHRBU	10/1/1993	17.9
					11/18/1993	19.0
[3]X24B4	364530	2491570	32.3	UCHRBU	9/25/1985	5.0
[3]X24B5	364640	2491050	31.0	UCHRBU	9/25/1985	7.7
[3]X24B6	364810	2490710	33.2	UCHRBU	9/25/1985	10.4

[1]See Plate 1 for location

[2]Location coordinates are North Carolina State Plane coordinates, North American Datum of 1983

[3]On Plate 1 shown as B4, B5, and B6, respectively

Table C1.11. Water-level measurements in monitor wells installed during investigations of releases of refined petroleum products to groundwater and used during model calibration, Tarawa Terrace and vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina.

[NGVD 29, National Geodetic Vertical Datum of 1929; contributing aquifers: TT, Tarawa Terrace aquifer; UCHRBU, Upper Castle Hayne aquifer–River Bend unit]

Site name[1]	Location coordinates[2]		Land-surface altitude, in feet above NGVD 29	Contributing aquifers	Measurement date	Water-level altitude, in feet above NGVD 29
	North	East				
STT61to66-MW01	364847	2489130	26.9	TT	1/8/1992	20.6
					1/11/1992	20.7
					1/29/1992	21.6
					12/17/1992	21.1
STT61to66-MW02	364847	2489130	26.8	TT, UCHRBU	1/8/1992	20.2
					1/11/1992	20.1
					1/29/1992	21.6
					12/17/1992	20.4
STT61to66-MW03	364740	2489186	27.1	TT	1/9/1992	20.4
					1/11/1992	20.3
					1/29/1992	21.3
					12/17/1992	21.0
STT61to66-MW04	364740	2489186	27	TT, UCHRBU	1/9/1992	20.1
					1/11/1992	20.9
					1/29/1992	20.7
					12/17/1992	20.4
STT61to66-MW05	364818	2489276	27.5	TT	1/9/1992	20.9
					1/11/1992	18.9
					1/29/1992	19.6
					12/17/1992	21.3
STT61to66-MW06	364816	2489276	27.6	TT, UCHRBU	1/9/1992	20.4
					1/11/1992	20.1
					1/29/1992	20.8
					12/17/1992	20.5
STT61to66-MW07	364885	2489219	27.7	TT	1/9/1992	20.9
					1/11/1992	20.9
					1/29/1992	21.5
					12/17/1992	21.1
STT61to66-MW08	364885	2489219	27.7	TT, UCHRBU	1/9/1992	19.8
					1/11/1992	19.9
					1/29/1992	20.8
					12/17/1992	20.5
STT61to66-MW09	364732	2489102	27.1	TT	1/9/1992	20.9
					1/11/1992	20.8
					1/29/1992	21.6
					12/17/1992	21.4
STT61to66-MW10	364732	2489102	27	TT, UCHRBU	1/9/1992	20.7
					1/11/1992	20.0
					1/29/1992	20.7
					12/17/1992	20.4
STT61to66-MW11	364700	2489241	27.6	TT	1/10/1992	20.1
					1/11/1992	20.9
					1/29/1992	21.9
					12/17/1992	21.5

Table C1.11. Water-level measurements in monitor wells installed during investigations of releases of refined petroleum products to groundwater and used during model calibration, Tarawa Terrace and vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina.—Continued

[NGVD 29, National Geodetic Vertical Datum of 1929; contributing aquifers: TT, Tarawa Terrace aquifer; UCHRBU, Upper Castle Hayne aquifer–River Bend unit]

Site name[1]	Location coordinates[2] North	Location coordinates[2] East	Land-surface altitude, in feet above NGVD 29	Contributing aquifers	Measurement date	Water-level altitude, in feet above NGVD 29
STT61to66-MW12	364700	2489241	27.5	TT, UCHRBU	1/10/1992	19.7
					1/11/1992	19.8
					1/29/1992	20.6
					12/17/1992	20.3
STT61to66-MW13	364612	2489148	26.2	TT	1/11/1992	20.4
					1/11/1992	20.2
					1/29/1992	21.8
					12/17/1992	21.2
STT61to66-MW14	364612	2489148	26.2	TT, UCHRBU	1/11/1992	19.8
					1/11/1992	19.7
					1/29/1992	20.5
					12/17/1992	20.3
STT61to66-MW15	364754	2489310	26.3	TT	12/17/1992	21.0
STT61to66-MW16	364603	2489247	25.6	TT, UCHRBU	12/17/1992	20.2
STT61to66-MW17	364693	2489062	24.7	TT	12/17/1992	21.3
STT61to66-MW18	364616	2489072	25.7	TT, UCHRBU	12/17/1992	20.2
STT61to66-MW19	364525	2489072	26.4	TT	12/17/1992	20.5
STT61to66-MW20	364554	2489135	26.5	TT, UCHRBU	12/17/1992	20.1
TTDump MW01	360343	2488970	2.6	TT	6/26/1991	2.4
TTDump MW02	360623	2488230	6.4	TT	6/26/1991	6.2
TTDump MW03	360230	2487690	2.9	TT	6/26/1991	2.2
[3]TTUST-44-MW01	360936	2488458	24.4	TT, UCHRBU	11/15/2001	6.0
[3]TTUST-44-MW02	360962	2488506	24.4	TT, UCHRBU	11/15/2001	5.7
[3]TTUST-44-MW03	360978	2488487	23.8	TT, UCHRBU	11/15/2001	5.9
[3]TTUST-48-MW01	362540	2487640	25	TT	9/1/1998	19
[3]TTUST-779-MW01	362251	2490046	25	TT	7/25/2002	9
[3]TTUST-2254-MW01	362204	2486721	24	TT	7/24/2002	13
[3]TTUST-2258-MW01	362175	2486658	24	TT	7/24/2002	12
[3]TTUST-2302-MW01	361702	2486831	24	TT	7/24/2002	12
[3]TTUST-2453-A1	361286	2488830	26.9	TT	6/7/1989	8.4
[3]TTUST-2453-A2	361090	2488716	25.7	TT	6/7/1989	6.6
[3]TTUST-2453-A3	361092	2488773	26.5	TT	6/7/1989	6.6
[3]TTUST-2453-A4	361187	2488760	26.8	TT	6/7/1989	7.6
[3]TTUST-2453-A5	361160	2488901	25.2	TT	6/7/1989	7.4
[3]TTUST-2453-A6	361102	2488864	26.8	TT	6/7/1989	6.4
[3]TTUST-2453-A7	361109	2488874	26.6	TT	6/7/1989	6.7
[3]TTUST-2453-A8	361092	2488868	26.2	TT	6/7/1989	6.5
[3]TTUST-2453-A9	361109	2488881	26.4	TT	6/7/1989	6.7
[3]TTUST-2453-OB1	361111	2488903	25.2	TT(?)	6/7/1989	6.8
[3]TTUST-2453-OB2	361104	2488812	27.1	TT(?)	6/7/1989	6.6

Table C1.11. Water-level measurements in monitor wells installed during investigations of releases of refined petroleum products to groundwater and used during model calibration, Tarawa Terrace and vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina.—Continued

[NGVD 29, National Geodetic Vertical Datum of 1929; contributing aquifers: TT, Tarawa Terrace aquifer; UCHRBU, Upper Castle Hayne aquifer–River Bend unit]

Site name[1]	Location coordinates[2]		Land-surface altitude, in feet above NGVD 29	Contributing aquifers	Measurement date	Water-level altitude, in feet above NGVD 29
	North	East				
[3]TTUST-2453-OB3	361061	2488867	24.8	TT(?)	6/7/1989	6.4
[3]TTUST-2453-OB4	361166	2488864	26.6	TT(?)	6/7/1989	7.3
[3]TTUST-2453-OB7	361228	2488907	25.4	TT(?)	6/7/1989	1.9
[3]TTUST-2453-OB8	361002	2488849	23.8	TT(?)	6/7/1989	6.5
[3]TTUST-2453-OB9	361099	2488852	24.9	TT(?)	6/7/1989	6.6
[3]TTUST-2453-OB10	361067	2488814	24.9	TT(?)	6/7/1989	6.3
[3]TTUST-2453-OB11	361181	2488817	27.8	TT(?)	6/7/1989	7.4
[3]TTUST-2453-RW	361111	2488874	26.8	TT	6/7/1989	6.8
[3]TTUST-2455-MW01	361322	2488307	24.4	TT	10/7/1993	9.0
[3]TTUST-2455-4	361356	2488245	[4]22.1	TT, UCHRBU	10/28/1993	8.6
[3]TTUST-2455-5	361436	2488312	[4]22.9	TT, UCHRBU	10/28/1993	9.0
[3]TTUST-2455-6	361255	2488250	[4]22.7	TT, UCHRBU	10/28/1993	8.0
[3]TTUST-2455-7	361120	2488302	[4]24.2	TT, UCHRBU	10/28/1993	6.8
[3]TTUST-2455-8	361203	2488302	[4]21.5	TT, UCHRBU	10/28/1993	7.6
[3]TTUST-2455-9	361255	2488321	[4]21.9	TT, UCHRBU	10/28/1993	7.9
[3]TTUST-2455-10	361171	2488350	[4]22.6	TT, UCHRBU	10/28/1993	7.4
[3]TTUST-2455-11	361155	2488259	[4]22.8	TT, UCHRBU	10/28/1993	7.3
[3]TTUST-2455-12	361292	2488261	[4]21.2	TT, UCHRBU	10/28/1993	8.2
[3]TTUST-2455-13	361484	2488341	[4]23.1	TT, UCHRBU	10/28/1993	9.2
					12/14/1993	9.2
[3]TTUST-2455-14	361136	2488407	[4]25.5	TT, UCHRBU	10/28/1993	7.0
[3]TTUST-2455-15	360972	2488327	[4]17.2	TT, UCHRBU	10/28/1993	5.6
[3]TTUST-2455-16	361310	2488291	[4]25.5	TT, UCHRBU	10/28/1993	8.3
[3]TTUST-2455-18	361196	2488312	[4]22.0	TT, UCHRBU	10/28/1993	7.6
[3]TTUST-2477-MW01	361550	2488738	25.2	TT	12/6/1994	10.0
[3]TTUST-2477-MW02	361562	2488738	25.1	TT	12/6/1994	10.1
[3]TTUST-2477-MW06	361521	2488738	24.5	TT, UCHRBU	10/28/1994	10.0
					12/6/1994	9.8
[3]TTUST-2477-MW07	361519	2488745	24.8	UCHRBU	12/6/1994	9.8
[3]TTUST-2477-MW08	361459	2488658	24.6	TT	11/3/1994	9.8
					12/6/1994	9.5
[3]TTUST-2477-MW09	361447	2488774	25.4	TT	11/3/1994	9.5
					12/6/1994	9.3
[3]TTUST-2477-MW10	361324	2488759	26.3	TT	11/3/1994	8.8
					12/6/1994	8.6
[3]TTUST-2477-MW11	361329	2488754	26.3	UCHRBU	11/4/1994	11.6
					12/6/1994	8.6
[3]TTUST-2477-MW12	361243	2488858	26.2	UCHRBU	11/8/1994	10.0
					12/6/1994	8.1

Table C1.11. Water-level measurements in monitor wells installed during investigations of releases of refined petroleum products to groundwater and used during model calibration, Tarawa Terrace and vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina.—Continued

[NGVD 29, National Geodetic Vertical Datum of 1929; contributing aquifers: TT, Tarawa Terrace aquifer; UCHRBU, Upper Castle Hayne aquifer–River Bend unit]

Site name[1]	Location coordinates[2]		Land-surface altitude, in feet above NGVD 29	Contributing aquifers	Measurement date	Water-level altitude, in feet above NGVD 29
	North	East				
[3]TTUST-2477-MW13	361240	2488865	26.2	TT	11/9/1994	8.1
					12/6/1994	8.1
[3]TTUST-2477-MW14	361197	2488975	22.9	TT	11/9/1994	7.9
					12/6/1994	7.8
[3]TTUST-2478-MW08	362092	2488829	24.4	TT	11/22/1993	12.6
					1/9/1994	12.3
[3]TTUST-2478-MW09	361888	2488997	22	TT	11/23/1993	11.8
					1/9/1994	11.4
[3]TTUST-2478-MW10	361785	2488999	21.8	TT	11/23/1993	11.4
					1/9/1994	11.0
					12/6/1994	11.2
[3]TTUST-2478-MW11	361716	2489004	21.9	TT	11/29/1993	9.9
					1/9/1994	10.6
					12/6/1994	10.9
					9/28/2000	10.4
[3]TTUST-2478-MW11D	361716	2489004	22.0	UCHRBU	12/15/1993	11.0
					1/9/1994	10.6
					12/6/1994	10.8
[3]TTUST-2478-MW12	361540	2488990	22.6	TT	12/2/1993	10.2
					1/9/1994	9.7
					12/6/1994	9.9
[3]TTUST-2478-MW13	361718	2488764	24.9	TT	11/30/1993	11.1
					1/9/1994	10.7
					12/6/1994	11.0
[3]TTUST-2478-MW14	361780	2488898	24.2	TT	11/30/1993	11.3
					1/9/1994	10.9
					12/6/1994	11.2
					9/28/2000	8.1
[3]TTUST-2478-MW14D	361780	2488898	24.3	UCHRBU	12/16/1993	11.4
					1/9/1994	10.9
					12/6/1994	11.2
[3]TTUST-2478-MW15	361900	2488730	24.6	TT	11/30/1993	11.9
					1/9/1994	11.6
[3]TTUST-2478-MW16	361452	2488973	23.2	TT	12/6/1993	9.5
					1/9/1994	9.1
					12/6/1994	9.3
[3]TTUST-2478-MW17	361377	2488896	25.6	TT	12/7/1993	9.1
					1/9/1994	8.6
					12/6/1994	8.8
					9/28/2000	10.6

Table C1.11. Water-level measurements in monitor wells installed during investigations of releases of refined petroleum products to groundwater and used during model calibration, Tarawa Terrace and vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina.—Continued

[NGVD 29, National Geodetic Vertical Datum of 1929; contributing aquifers: TT, Tarawa Terrace aquifer; UCHRBU, Upper Castle Hayne aquifer–River Bend unit]

Site name[1]	Location coordinates[2]		Land-surface altitude, in feet above NGVD 29	Contributing aquifers	Measurement date	Water-level altitude, in feet above NGVD 29
	North	East				
[3]TTUST-2478-MW17D	361377	2488896	25.7	UCHRBU	12/14/1993	9.1
					1/9/1994	8.7
					12/6/1994	8.9
					9/28/2000	10.5
[3]TTUST-2478-MW18	361425	2488824	26.1	TT	12/7/1993	9.4
					1/9/1994	8.9
					1/6/1994	9.2
[3]TTUST-2478-MW19	361528	2488819	25.4	TT	1/9/1994	10.0
					1/9/1994	9.6
					12/6/1994	9.9
[3]TTUST-2478-MW20	361093	2488831	26.5	TT, UCHRBU(?)	9/28/2000	8.3
[3]TTUST-2478-MW21D	361087	2488826	27.2	UCHRBU	9/28/2000	8.4
[3]TTUST-2478-MW22	360933	2489041	20.5	TT, UCHRBU(?)	9/28/2000	7.1
[3]TTUST-2478-MW23	360836	2488918	19.3	TT, UCHRBU	9/28/2000	6.2
[3]TTUST-2478-MW24	360877	2488755	23.6	TT, UCHRBU	9/28/2000	6.5
[3]TTUST-2478-MW25	361031	2488668	25.8	TT, UCHRBU(?)	9/28/2000	7.8
[3]TTUST-2478-PW01	361898	2488879	24.7	TT(?), UCHRBU	1/9/1994	11.6
[3]TTUST-2634-MW01	363587	2487670	22	TT, UCHRBU(?)	11/1/2001	14
[3]TTUST-3140-MW01	364679	2486468	26	TT, UCHRBU(?)	7/24/2002	15
[3]TTUST-3165-MW01	364540	2485990	26	TT, UCHRBU(?)	7/24/2002	16
[3]TTUST-3233-MW01	363831	2485914	25	TT, UCHRBU(?)	7/24/2002	12
[3]TTUST-3524-MW01	362897	2485350	20	TT	7/25/2002	6
[3]TTUST-3546-MW01	362583	2485633	21	TT	7/25/2002	5
[3]TTUST-TTSC-1	361637	2488268	[4]25.7	TT	12/28/1994	10.8
[3]TTUST-TTSC-2	361532	2488246	[4]23.4	TT	12/28/1994	10.1
[3]TTUST-TTSC-3	361589	2488360	[4]23.5	TT	1/9/1994	9.6
					12/28/1994	10.4
[3]TTUST-TTSC-4	361666	2488337	[4]26.5	TT	1/9/1994	10.4
					12/28/1994	11.0
[3]TTUST-TTSC-5	361619	2488355	[4]23.5	TT	12/28/1994	10.6
[3]TTUST-TTSC-6	361552	2488374	[4]23.8	TT	12/28/1994	10.3
[3]TTUST-TTSC-7	361470	2488474	[4]23.8	TT	12/28/1994	9.9
[3]TTUST-TTSC-8	361653	2488577	[4]23.6	TT	12/28/1994	11.1
[3]TTUST-TTSC-9	361328	2488369	[4]23.5	TT	12/28/1994	8.8
[3]TTUST-TTSC-10	361671	2488387	[4]23.7	TT	12/28/1994	11.0
[3]TTUST-TTSC-13	361614	2488404	[4]23.9	UCHRBU	12/28/1994	10.6
[3]TTUST-TTSC-14	361526	2488244	[4]23.5	UCHRBU	12/28/1994	10.0
[3]TTUST-TTSC-15	361657	2488579	[4]23.8	UCHRBU	12/28/1994	11.2
[3]TTUST-TTSC-16	361619	2488397	[4]24.0	TT, UCHRBU	12/28/1994	10.5

[1]See Plate 1 for location

[2]Location coordinates are North Carolina State Plane coordinates, North American Datum of 1983

[3]Because of scale, not shown on Plate 1

[4]Measuring point altitude, in feet NGVD 29

Appendix C2. Construction Data for Selected Wells, Tarawa Terrace and Vicinity, U.S. Marine Corps Base Camp Lejuene, North Carolina

Tables

Sources:

Catlin Engineers and Scientists, 2002a,b

DiGiano et al. 1988

Haliburton NUS Environmental Corporation 1992

Law Engineering and Environmental Services, Inc. 1996, 1998

Law Engineering, Inc. 1994a,b, 1995a,b

Mid-Atlantic Associates, Inc. 2003a,b

Mid-Atlantic Associates, P.A. 2002a,b,c,d,e,f,g

O'Brien & Gere Engineers, Inc. 1992, 1993

OHM Remediation Services Corp 2001

Richard Catlin & Associates, Inc. 1994a,b, 1995a,b, 1996, 1998

U.S. Geological Survey well inventory, written communication, October 21, 1986

Table C2.1. Construction data for Tarawa Terrace water-supply wells, test well T-9, and Civilian Conservation Corps well CCC-1, Tarawa Terrace and vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina.

[NGVD 29, National Geodetic Vertical Datum of 1929; N/A, data not available; AKA, also known as; >, greater than]

Site name[1]	Land-surface altitude, in feet above NGVD 29	Completion date	Borehole depth, in feet	Well depth, in feet	Screen diameter, in inches	Open interval, in feet below land surface
2A	26	5/24/1951	130	130	8	93–130
[2]#6	22	1951(?)	N/A	150–200(?)	N/A	N/A
[2]#7	24	1951(?)	N/A	150–200(?)	N/A	N/A
CCC-1	24.3	9/17/1941	105	75	10	52–75
T-9	28.7	3/1959	202	88	8	37–42
						50–60
						68–72
						83–88
TT-23	23.9	3/14/1983	263	147	10	70–95
						132–42
TT-25	32.0	7/9/1981	200	180	8	70–75
						85–95
						150–75
TT-26, AKA #1	34.0	5/18/1951	180	108	8	91–108
TT-27, AKA #2B	26.4	5/31/1951	90	90	10	77–90
TT-28, AKA #3	26	1951	N/A	50–100(?)	N/A	N/A
TT-29, AKA #4	25	1951	N/A	50–100(?)	N/A	N/A
TT-30, AKA #13	26	1971	N/A	128	N/A	50–70
						98–113
TT-31, AKA #14	25.8	1973	N/A	94	N/A	N/A
TT-45, AKA #5	26	1951	N/A	50–100(?)	N/A	N/A
TT-52, AKA #9	24.9	6/27/1961	102	98	N/A	N/A[3]
TT-53, AKA #10	25	7/22/1961	N/A	90	10	42–62
						68–83
TT-54, AKA #11	22.1	6/30/1961	N/A	104	N/A	N/A[3]
TT-55, AKA #8	26.4	11/1/1961	N/A	>50	N/A	N/A[3]
TT-67, AKA #12	27.5	11/15/1971	200	104	8	70–94

[1]See Plate 1 for location

[2]Out of map area, location not shown. North Carolina State Plane coordinates: #6 (highly approximate) North 369730, East 2481720; #7 (highly approximate) North 370500, East 2481530; and TT-45 North 365688, East 2483352

[3]Construction is probably similar to TT-53

Table C2.2. Construction data for monitor wells installed during ABC One-Hour Cleaners Operable Units 1 and 2 and by the North Carolina Department of Natural Resources and Community Development, Tarawa Terrace and vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina.

[NGVD 29, National Geodetic Vertical Datum of 1929]

Site name[1]	Land-surface altitude, in feet above NGVD 29	Completion date	Borehole depth, in feet	Well depth, in feet	Screen diameter, in inches	Open interval, in feet below land surface
C1	30.6	4/4/1992	104.0	100.6	4	90–100
C2	32.0	4/8/1992	87.0	85	4	74.5–84.5
C3	33.4	4/9/1992	90.5	90.5	4	79.1–89.1
C4	32.2	4/2/1992	200.0	130.4	4	120–130
C5	32.0	4/7/1992	92.5	91	4	80.5–90.5
C9	32.1	9/1993	76	76	4	66–76
C10	32.5	10/1993	175	175	4	165–175
C11	31.0	9/1993	108	108	4	98–108
PZ-01	31.9	9/1993	80	80	2	74.5–79.5
PZ-02	31.9	9/1993	35	35	2	29.5–34.5
PZ-03	32.5	9/1993	80	80	2	74.5–79.5
PZ-04	32.5	9/1993	35	35	2	29.5–34.5
PZ-05	32.0	9/1993	80	80	2	74.5–79.5
PZ-06	32.0	9/1993	35	35	2	29.5–34.5
S1	30.6	3/22/1992	28.0	25.5	4	5.5–25.5
S2	32.5	3/26/1992	39.7	39.7	4	19.7–39.7
S3	33.4	4/2/1992	39.5	39.5	4	19.5–39.5
S4	32.2	4/3/1992	34.0	34	4	14–34
S5	31.9	4/1/1992	30.0	28	4	8–28
S6	31.1	3/26/1992	40.5	40.5	4	20.5–40.5
S7	31.3	4/5/1992	30.3	30.3	4	10–30
S8	30.8	4/4/1992	28.0	28	4	8–28
S9	32.7	3/21/1992	40.0	28.3	4	8–28
S10	31.6	3/19/1992	40.0	35	4	15–35
S11	30.8	9//1993	35	35	4	15–35
[2]X24B4	33.3	9/25/1985	59	59	2	42–52
[2]X24B5	31.4	9/25/1985	59	59	2	42–52
[2]X24B6	33.4	9/25/1985	59	59	2	42–52

[1]See Plate 1 for location

[2]On Plate 1 shown as B4, B5, and B6, respectively

Table C2.3. Construction data for monitor wells installed during investigations of releases of refined-petroleum products to groundwater, Tarawa Terrace and vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina.

[NGVD 29, National Geodetic Vertical Datum of 1929; N/A, data not available]

Site name[1]	Measuring point altitude, in feet above NGVD 29	Completion date	Borehole depth, in feet	Well depth, in feet	Screen diameter, in inches	Open interval, in feet below land surface
STT61to66-MW01	26.9	12/12/1991	15	15	2	5–15
STT61to66-MW02	26.8	12/13/1991	30	30	2	20–30
STT61to66-MW03	27.1	12/12/1991	15	15	2	5–15
STT61to66-MW04	27.0	12/13/1991	30	30	2	20–30
STT61to66-MW05	27.5	12/12/1991	15	15	2	5–15
STT61to66-MW06	27.6	12/13/1991	30	30	2	19–29
STT61to66-MW07	27.7	1/7/1992	15	15	2	5–15
STT61to66-MW08	27.7	1/8/1992	30	30	2	20–30
STT61to66-MW09	27.1	1/8/1992	14	14	2	4–14
STT61to66-MW10	27.0	1/8/1992	30	30	2	20–30
STT61to66-MW11	27.6	1/8/1992	15	15	2	5–15
STT61to66-MW12	27.5	1/9/1992	30	30	2	20–30
STT61to66-MW13	26.2	1/9/1992	12	12	2	2–12
STT61to66-MW14	26.2	1/9/1992	27	27	2	17–27
STT61to66-MW15	26.3	12/9/1992	14	14	2	4–14
STT61to66-MW16	25.6	12/9/1992	30	30	2	20–30
STT61to66-MW17	24.7	12/11/1992	14	14	2	4–14
STT61to66-MW18	25.7	12/9/1992	30	30	2	20–30
STT61to66-MW19	26.4	12/15/1992	14	14	2	4–14
STT61to66-MW20	26.5	12/9/1992	30	30	2	20–30
TTDump-MW01	2.6	6/25/1991	13.0	13.0	2	3.0–13.0
TTDump-MW02	6.4	6/18/1991	15.0	14.0	2	4.0–14.0
TTDump-MW03	2.9	6/24/1991	14.0	5.5	2	2.5–5.5
[2]TTUST-44-MW01	24.4	8/3/1994	N/A	25.8	N/A	15–25
[2]TTUST-44-MW02	24.4	8/3/1994	N/A	25.8	N/A	15–25
[2]TTUST-44-MW03	23.8	8/3/1994	N/A	25.8	N/A	15–25
[2]TTUST-48-MW01	25	8//1997	12	12	N/A	2–12
[2]TTUST-779-MW01	25	7/22/2002	19.5	19.5	2	4.5–19.5
[2]TTUST-2254-MW01	24	7/22/2002	14.5	14.5	2	4.5–14.5
[2]TTUST-2258-MW01	24	7/22/2002	16.5	16.5	2	6.5–16.5
[2]TTUST-2302-MW01	24	7/24/2002	19.5	19.5	2	4.5–19.5
[2]TTUST-2453-A1	26.9	1987	N/A	39.7	2	23.6–39.7
[2]TTUST-2453-A2	25.7	1987	N/A	37.9	2	24.1–37.9
[2]TTUST-2453-A3	26.5	1987	N/A	39.3	2	23.4–39.3
[2]TTUST-2453-A4	26.8	1987	N/A	40.2	2	25.0–40.2
[2]TTUST-2453-A5	25.2	1987	N/A	39.5	2	24.3–39.5
[2]TTUST-2453-A6	26.8	1987	N/A	41.2	2	28.9–41.2
[2]TTUST-2453-A7	26.7	1987	N/A	41.0	2	26.1–41.0
[2]TTUST-2453-A8	26.2	1987	N/A	42.2	2	25.1–26.2
[2]TTUST-2453-A9	26.4	1987	N/A	40.5	2	25.4–40.5
[2]TTUST-2453-OB1	25.2	1989	N/A	N/A	N/A	N/A
[2]TTUST-2453-OB2	27.1	1989	N/A	N/A	N/A	N/A

Table C2.3. Construction data for monitor wells installed during investigations of releases of refined-petroleum products to groundwater, Tarawa Terrace and vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina.—Continued

[NGVD 29, National Geodetic Vertical Datum of 1929; N/A, data not available]

Site name[1]	Measuring point altitude, in feet above NGVD 29	Completion date	Borehole depth, in feet	Well depth, in feet	Screen diameter, in inches	Open interval, in feet below land surface
[2]TTUST-2453-OB3	24.8	1989	N/A	N/A	N/A	N/A
[2]TTUST-2453-OB4	26.6	1989	N/A	N/A	N/A	N/A
[2]TTUST-2453-OB7	[3]26.7	1989	N/A	N/A	N/A	N/A
[2]TTUST-2453-OB8	23.8	1989	N/A	N/A	N/A	N/A
[2]TTUST-2453-OB9	24.4	1989	N/A	N/A	N/A	N/A
[2]TTUST-2453-OB10	24.8	1989	N/A	N/A	N/A	N/A
[2]TTUST-2453-OB11	27.3	1989	N/A	N/A	N/A	N/A
[2]TTUST-2453-RW	26.8	1989	N/A	N/A	N/A	N/A
[2]TTUST-2455-4	22.1	10/14/1993	25	25	2	10–25
[2]TTUST-2455-5	22.9	10/4/1993	25	25	2	10–25
[2]TTUST-2455-6	22.7	10/13/1993	25	25	2	10–25
[2]TTUST-2455-7	24.2	10/4/1993	25	25	2	10–25
[2]TTUST-2455-8	21.5	10/5/1993	25	25	2	10–25
[2]TTUST-2455-9	21.9	10/14/1993	25	25	2	10–25
[2]TTUST-2455-10	22.6	10/5/1993	25	25	2	10–25
[2]TTUST-2455-11	22.8	10/5/1993	25	25	2	10–25
[2]TTUST-2455-12	21.2	10/5/1993	25	25	2	10–25
[2]TTUST-2455-13	23.1	10/14/1993	25	25	2	10–25
[2]TTUST-2455-14	25.5	10/14/1993	25	25	2	10–25
[2]TTUST-2455-15	17.2	11/18/1993	20	20	2	4–20
[2]TTUST-2455-16	25.5	10/8/1993	47	47	2	42–47
[2]TTUST-2455-18	22.0	10/6/1993	47	47	2	42–47
[2]TTUST-2477-MW01	24.0	10/26/1993	N/A	19.5	4	N/A
[2]TTUST-2477-MW06	24.5	10/28/1994	32	32	6	12–32
[2]TTUST-2477-MW07	24.8	11/1/1994	50	50	2	45–50
[2]TTUST-2477-MW08	24.6	11/3/1994	22	22	2	12–22
[2]TTUST-2477-MW09	25.4	11/3/1994	22	22	2	12–22
[2]TTUST-2477-MW10	26.3	11/3/1994	22	22	2	12–22
[2]TTUST-2477-MW11	26.3	11/4/1994	50	50	2	45–50
[2]TTUST-2477-MW12	26.2	11/8/1994	50	50	2	43–50
[2]TTUST-2477-MW13	26.2	11/9/1994	22	22	2	12–22
[2]TTUST-2477-MW14	22.9	11/9/1994	21	21	2	11–21
[2]TTUST-2478-MW08	24.4	11/22/1993	19	19	2	8.5–18.5
[2]TTUST-2478-MW09	22.0	11/23/1993	18	18	2	7.5–17.5
[2]TTUST-2478-MW10	21.8	11/23/1993	18	18	2	7.5–17.5
[2]TTUST-2478-MW11	21.9	11/29/1993	18	18	2	7.5–17.5
[2]TTUST-2478-MW11D	22.0	12/15/1993	50	50	2	45–50
[2]TTUST-2478-MW12	22.6	12/2/1993	18	18	2	8–18
[2]TTUST-2478-MW13	24.9	11/30/1993	18	18	2	7.5–17.5
[2]TTUST-2478-MW14	24.2	11/30/1993	18	18	2	7.5–17.5
[2]TTUST-2478-MW14D	24.3	12/16/1993	50	50	2	45–50
[2]TTUST-2478-MW15	24.6	11/30/1993	18	18	2	7.5–17.5

Table C2.3. Construction data for monitor wells installed during investigations of releases of refined-petroleum products to groundwater, Tarawa Terrace and vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina.—Continued

[NGVD 29, National Geodetic Vertical Datum of 1929; N/A, data not available]

Site name[1]	Measuring point altitude, in feet above NGVD 29	Completion date	Borehole depth, in fee	Well depth, in feet	Screen diameter, in inches	Open interval, in feet below land surface
[2]TTUST-2478-MW16	23.2	12/6/1993	18.5	18.5	2	8.5–18.5
[2]TTUST-2478-MW17	25.6	12/7/1993	22	22	2	11.5–21.5
[2]TTUST-2478-MW17D	25.7	12/14/1993	50	50	2	43–48
[2]TTUST-2478-MW18	26.1	12/7/1993	22.5	22.5	2	12–22
[2]TTUST-2478-MW19	25.4	12/7/1993	20.5	20.5	2	10–20
[2]TTUST-2478-PW01	24.7	N/A	N/A	20.5	N/A	N/A
[2]TTUST-2478-MW20	26.5	9/14/2000	24	24	2	14–24
[2]TTUST-2478-MW21D	27.2	9/12/2000	50	50	2	45–50
[2]TTUST-2478-MW22	20.5	9/13/2000	21	20	2	10–21
[2]TTUST-2478-MW23	19.3	9/13/2000	19	19	2	9–19
[2]TTUST-2478-MW24	23.6	9/13/2000	23.5	23.5	2	13.5–23.5
[2]TTUST-2478-MW25	25.8	9/13/2000	23	23	2	13–23
[2]TTUST-2634-MW01	22	11/1/2001	16	16	2	6–16
[2]TTUST-3140-MW01	26	7/23/2002	19	19	2	4–19
[2]TTUST-3165-MW01	26	7/23/2002	19	19	2	4–19
[2]TTUST-3233-MW01	25	7/23/2002	18	18	2	3–18
[2]TTUST-3524-MW01	20	7/23/2002	17.8	17.8	2	7.8–17.8
[2]TTUST-3546-MW01	21	7/23/2002	18.5	18.5	2	8.5–18.5
[2]TTUST-TTSC-1	25.7	11/21/1994	20	20	2	10–20
[2]TTUST-TTSC-2	23.4	11/21/1994	20	20	2	9–19
[2]TTUST-TTSC-3	23.5	11/21/1994	20	20	2	9.5–19.5
[2]TTUST-TTSC-4	26.5	11/22/1994	20	20	2	10–20
[2]TTUST-TTSC-5	23.5	11/22/1994	20	20	2	10–20
[2]TTUST-TTSC-6	23.8	11/22/1994	20	20	2	5–20
[2]TTUST-TTSC-7	23.8	11/22/1994	20	20	2	10–20
[2]TTUST-TTSC-8	23.6	12/6/1994	20	20	2	10–20
[2]TTUST-TTSC-9	23.5	12/6/1994	20	20	2	10–20
[2]TTUST-TTSC-10	23.7	12/6/1994	20	20	2	10–20
[2]TTUST-TTSC-13	23.9	12/1/1994	50.5	50.5	2	43.5–50.5
[2]TTUST-TTSC-14	23.5	11/28/1994	50	50	2	43–50
[2]TTUST-TTSC-15	23.8	11/29/1994	50	50	2	43–50
[2]TTUST-TTSC-16	24.0	12/1/1994	38	38	2	6.5–38

[1]See Plate 1 for location

[2]Because of scale, not shown on Plate 1

[3]Estimated altitude

Appendix C3. Capacity and Operational History for Selected Wells, Tarawa Terrace, U.S. Marine Corps Base Camp Lejuene, North Carolina

Tables

Table C3.1. Capacity and operational history of water-supply well TT-26[1] (AKA #1), Tarawa Terrace, U.S. Marine Corps Base Camp Lejeune, North Carolina.

[gpm, gallons per minute; do., ditto]

Date	Capacity, in gpm	Operational status	Data source
5/19/1951	215		Well capacity test[2]
1/1952		In service	Estimated date
1/1952	200	do.	Henry Von Oesen & Associates[3]
6/24/1958	182	do.	Well capacity summary
2/7/1966	130	do.	Raw water-supply list
1973 (?)	104	do.	Well capacity summary
3/31977	110	do.	Well survey sheet
1978	175	do.	Henry Von Oesen & Associates[3]
7/1980		Out of service	Operation records
9/1980		In service	do.
5/1982		"Ran all month"	do.
12/28/1982		Out of service	do.
3/1983		In service	do.
3/1/1983	133	do.	Well capacity test
6/20/1984	150	do.	Well survey sheet
2/1985		Out of service	Operation records
2/1985		Service terminated	do.
6/1993		Abandonment	AH Environmental Consultants[4]

[1]See Figure C1 for location

[2]R.E. Peterson, Public Works, written communication, May 31, 1951

[3]Henry Von Oesen and Associates, Inc. 1979

[4]AH Environmental Consultants, Inc., written communication, September 3, 2004

Table C3.2. Capacity and operational history of water-supply wells TT-27, TT-28, TT-29, TT-45, #6, #7, and TT-55, Tarawa Terrace, U.S. Marine Corps Base Camp Lejeune, North Carolina.

[gpm, gallons per minute; —, operational status unknown; USGS, U.S. Geological Survey; do., ditto]

Well name[1]	Date	Capacity, in gpm	Operational status	Data source
TT-27 (AKA #2b)	5/31/1951	100	—	Well capacity test[3]
	1/1952		In service	Estimated date
	1/1952	100	—	Estimated rate[3]
	6/24/1958	75	In service	Well capacity summary
	12/1961		Service terminated	Estimated date
	1/10/1963		Out of service	USGS well schedule
	2/27/1967		Abandonment	List for Mr. Tew[5]
TT-28 (AKA #3)	1/1952		In service	Estimated date
	1/1952	100	—	Estimated rate[6]
	6/24/1958	20	In service	Well capacity summary
	2/7/1966	110	do.	Raw water-supply list
	8/3/1971		do.	Building dimensions list
	12/1971		Service terminated	Estimated date
	3/1973		Abandonment	AH Environmental Consultants[7]
TT-29 (AKA#4)	1/1952		In service	Estimated date
	1/1952	100	—	Estimated rate[6]
	6/24/1958		Out of service	Well capacity summary
	6/1958		Service terminated	Estimated date
	10/1958		"Abandoned"	LeGrand[4]
	2/27/1967		Abandonment	List for Mr. Tew[5]
TT-45 (AKA #5)	1/1952		In service	Estimated date
	1/1952	100	do.	Estimated rate[6]
	6/24/1958	70	do.	Well capacity summary
	2/7/1966	50	do.	Raw water-supply list
	8/3/1971		"Abandoned"	Building dimensions list
	12/1971		Service terminated	Estimated date
	3/1973		Abandonment	AH Environmental Consultants[7]
[2]#6	1/1952		In service	Estimated date
	1/1952	100	—	Estimated rate[6]
	6/24/1958	80	In service	Well capacity summary
	12/1961		Service terminated	Estimated date
[2]#7	1/1952		In service	Estimated date
	1/1952	120	—	Estimated rate[6]
	6/24/1958	100	In service	Well capacity summary
	12/1961		Service terminated	Estimated date
TT-55 (AKA #8)	11/1/1961	100	—	Driller[8]
	1/1962		In service	Estimated date
	1/1962	100	—	Estimated rate[7]
	3/28/1962	100	In service	Well capacity summary
	2/7/1966	95	do.	Raw water-supply list
	8/3/1971		do.	Building dimensions list
	12/1971		Service terminated	Estimated date

[1]See Plate 1 for location

[2]Out of map area, location not shown. North Carolina State Plane coordinates: #6 (highly approximate) North 369730, East 2481720; #7 (highly approximate) North 370500, East 2481530; and TT-45 North 365688, East 2483352

[3]R.E. Peterson, Public Works, written communication, May 31, 1951

[4]H.E. LeGrand, written communication, October 25, 1958

[5]List furnished to Mr. Tew for abandonment, written communication, February 27, 1967

[6]LeGrand (1959)

[7]AH Environmental Consultants, Inc., written communication, September 3, 2004

[8]Hartsfield Water Company, Inc., written communication, November 1, 1961

Table C3.3. Capacity and operational history of water-supply well TT-52[1] (AKA #9A), Tarawa Terrace, U.S. Marine Corps Base Camp Lejeune, North Carolina.

[gpm, gallons per minute; —, operational status unknown; do., ditto]

Date	Capacity, in gpm	Operational status	Data source
10/17/1961	348	—	Driller[2]
1/1962		In service	Estimated date
1/1962	300	—	Henry Von Oesen & Associates[3]
3/28/1962	300	In service	Well capacity summary
2/7/1966	300	—	Raw water-supply list
1973(?)	174	In service	Well capacity summary
3/3/1977		do.	Well survey sheet
1978	200	do.	Henry Von Oesen & Associates[3]
5/1982		"Ran all month"	Operation records
9/14/1982	128	In service	Well capacity test
6/20/1984	200	do.	Well survey sheet
12/27/1984	170	do.	Well capacity test
2/1985		"Running 24 hours"	Operation records
3/1985		do.	do.
9/11/1985	201	In service	Well capacity test
3/1986		Out of service	Operation records
4/1986		In service	do.
4/1987		Service terminated	Water flow records
4/1987		do.	Estimated date
6/1993		Abandonment	AH Environmental Consultants[4]

[1]See Figure C1 for location

[2]Hartsfield Water Company, Inc., written communication, October 17, 1961

[3]Henry Von Oesen and Associates, Inc. 1979

[4]AH Environmental Consultants, Inc., written communication, September 3, 2004

Table C3.4. Capacity and operational history of water-supply well TT-53[1] (AKA #10), Tarawa Terrace, U.S. Marine Corps Base Camp Lejeune, North Carolina.

[gpm, gallons per minute; —, operational status unknown; do., ditto]

Date	Capacity, in gpm	Operational status	Data source
7/22/1961	350	—	Driller[2]
1/1962		In service	Estimated date
1/1962	350	do.	Henry Von Oesen & Associates[3]
3/28/1962	350	do.	Well capacity summary
2/7/1966	320	do.	Raw water-supply list
1973(?)	174	do.	Well capacity summary
1978	75	do.	Henry Von Oesen & Associates[3]
8/3/1971		do.	Building dimensions list
3/3/1977		do.	Well survey sheet
7/1981		Out of service	Operation records
9/1981		In service	do.
5/1982		"Ran all month"	do.
2/1984		Out of service	do.
2/1984		Service terminated	do.
6/1993		Abandonment	AH Environmental Consultants[4]

[1]See Figure C1 for location

[2]Hartsfield Water Company, Inc., written communication, July 22, 1961

[3]Henry Von Oesen and Associates, Inc. 1979

[4]AH Environmental Consultants, Inc., written communication, September 3, 2004

Table C3.5. Capacity and operational history of water-supply well TT-54[1] (AKA #11), Tarawa Terrace, U.S. Marine Corps Base Camp Lejeune, North Carolina.

[gpm, gallons per minute; —, operational status unknown; do., ditto]

Date	Capacity, in gpm	Operational status	Data source
6/30/1961	250	—	Driller[2]
1/1962		In service	Estimated date
1/1962	200	do.	Henry Von Oesen & Associates[3]
3/28/1962	200	do.	Well capacity summary
2/7/1966	200	do.	Raw water-supply list
8/3/1971		do.	Building dimensions list
1973(?)	139	do.	Well capacity summary
3/3/1977		do.	Well survey sheet
1978	170	do.	Henry Von Oesen & Associates[3]
9/14/1982	140	do.	Well capacity test
2/1984		Out of service	Operation records
4/1984		In service	do.
6/20/1984	150	do.	Well survey sheet
3/1985		"Running 24 hours"	Operation records
4/1987		Out of service	Water flow records
4/1987		Service terminated	do.
6/1994		Abandonment	AH Environmental Consultants[4]

[1]See Figure C1 for location

[2]Hartsfield Water Company, Inc., written communication, June 30, 1961

[3]Henry Von Oesen and Associates, Inc. 1979

[4]AH Environmental Consultants, Inc., written communication, September 3, 2004

Table C3.6. Capacity and operational history of water-supply well TT-67[1] (AKA #12) Tarawa Terrace, U.S. Marine Corps Base Camp Lejeune, North Carolina.

[gpm, gallons per minute; —, operational status unknown; do., ditto]

Date	Capacity, in gpm	Operational status	Data source
11/15/1971	140	—	Driller[2]
1/1972		In service	Estimated date
1/1972	168	do.	Henry Von Oesen & Associates[3]
1973(?)	83	do.	Well capacity summary
3/3/1977		do.	Well survey sheet
1978	140	do.	Henry Von Oesen & Associates[3]
9/14/1982	90	do.	Well capacity test
5/18/1983	108	do.	do.
6/20/1984	100	do.	Well survey sheet
8/21/1984	125	do.	Well capacity test
12/23/1984	119	do.	do.
9/13/1985	119	do.	do.
4/1987		Out of service	Water flow records
4/1987		Service terminated	do.
6/1993		Abandonment	AH Environmental Consultants[4]

[1]See Figure C1 for location

[2]Sydnor Hydrodynamics, Inc., written communication, November 15, 1971

[3]Henry Von Oesen and Associates, Inc, 1979

[4]AH Environmental Consultants, Inc., written communication, September 3, 2004

Table C3.7. Capacity and operational history of water-supply well TT-30[1] (AKA #13), Tarawa Terrace, U.S. Marine Corps Base Camp Lejeune, North Carolina.

[gpm, gallons per minute; do., ditto]

Date	Capacity, in gpm	Operational status	Data source
1/1972		In service	Estimated date
1/1972	100	do.	Henry Von Oesen & Associates[2]
1973(?)	76	do.	Well capacity summary
3/3/1977		do.	Well survey sheet
1978	70	do.	Henry Von Oesen & Associates[2]
5/1982		"Ran all month"	Operation records
12/27/1982		"New pump"	do.
6/20/1984	50	In service	Well survey sheet
9/1984		"Well won't pump"	Operation records
2/1985		Out of service	do.
2/1985		Service terminated	do.

[1]See Figure C1 for location

[2]Henry Von Oesen and Associates, Inc. 1979

Table C3.8. Capacity and operational history of water-supply well TT-31[1] (AKA #14), Tarawa Terrace, U.S. Marine Corps Base Camp Lejeune, North Carolina.

[gpm, gallons per minute; do., ditto]

Date	Capacity, in gpm	Operational status	Data source
1/1973		In service	Estimated date
1/1973	145	do.	Henry Von Oesen & Associates[2]
1973(?)	83	do.	Well capacity summary
3/3/1977		do.	Well survey sheet
1978	125	do.	Henry Von Oesen & Associates[2]
5/1982		"Ran all month"	Operation records
9/14/1982	104	In service	Well capacity test
6/1983		"Low on water"	Operation records
6/1984		Out of service	Operation records
6/20/1984	150	do.	Well survey sheet
7/6/1984	119	In service	Well capacity test
2/1985		"Running 24 hours"	Operation records
9/13/1985	111	In service	Well capacity test
3/1986		"Ran all month"	Operation records
4/1987		Out of service	Operation records
4/1987		Service terminated	Water flow records
6/1993		Abandonment	AH Environmental Consultants[3]

[1]See Figure C1 for location

[2]Henry Von Oesen and Associates, Inc. 1979

[3]AH Environmental Consultants, Inc., written communication, September 3, 2004

Table C3.9. Capacity and operational history of water-supply well TT-25,[1] Tarawa Terrace, U.S. Marine Corps Base Camp Lejeune, North Carolina.

[gpm, gallons per minute; —, operational status unknown; do., ditto]

Date	Capacity, in gpm	Operational status	Data source
7/1981	150	—	Driller[2]
12/27/1981	150	—	Well capacity test
1/1982		In service	Operation Records
1/1982	150	do.	Well capacity test[2]
6/1983		"Ran all month"	Operation records
6/20/1984		In service	Well survey sheet
2/1985		"Running 24 hours"	Operation records
3/1985		"Running 24 hours"	do.
9/11/1985	130	In service	Well capacity test
4/1987		Out of service	Operation records
4/1987		Service terminated	Water flow records
6/1993		Abandonment	AH Environmental Consultants[3]

[1]See Figure C1 for location

[2]Carolina Well and Pump Company, written communication, July 9, 1981

[3]AH Environmental Consultants, Inc., written communication, September 3, 2004

Table C3.10. Capacity and operational history of water-supply well TT-23,[1] Tarawa Terrace, U.S. Marine Corps Base Camp Lejeune, North Carolina.

[gpm, gallons per minute; —, operational status unknown; do., ditto; hrs, hours]

Date	Capacity, in gpm	Operational status	Data source
3/15/1983	162	—	Driller[2]
8/1984		In service	Estimated date
9/4/1984	254	do.	Well capacity test
10/4/1984	252	do.	do.
2/1985		Out of service	Operation records
3/11/1985		In service, 24 hrs	CLW documents[3]
3/12/1985		Out of service	do.
4/22/1985		In service, 7 hrs	do.
4/23/1985		do.	do.
4/29/1985		do.	do.
4/30/1985		Out of service	Estimated date
4/1985		Service terminated	do.
6/1993		Abandonment	AH Environmental Consultants[4]

[1]See Figure C1 for location

[2]C.W. Brinkley & Son, Inc., written communication, March 14, 1983

[3]Camp Lejeune water document 1194, written communication, May 1985

[4]AH Environmental Consultants, Inc., written communication, September 3, 2004

Appendix C4. Simulation Stress Periods and Corresponding Month and Year

[Jan, January; Feb, February; Mar, March; Apr, April; Aug, August; Sept, September; Oct, October; Nov, November; Dec, December]

Stress period	Month and year	Stress period	Month and year	Stress period	Month and year	Stress period	Month and year	Stress period	Month and year	Stress period	Month and year
1	Jan 1951	49	Jan 1955	97	Jan 1959	145	Jan 1963	193	Jan 1967	241	Jan 1971
2	Feb 1951	50	Feb 1955	98	Feb 1959	146	Feb 1963	194	Feb 1967	242	Feb 1971
3	Mar 1951	51	Mar 1955	99	Mar 1959	147	Mar 1963	195	Mar 1967	243	Mar 1971
4	Apr 1951	52	Apr 1955	100	Apr 1959	148	Apr 1963	196	Apr 1967	244	Apr 1971
5	May 1951	53	May 1955	101	May 1959	149	May 1963	197	May 1967	245	May 1971
6	June 1951	54	June 1955	102	June 1959	150	June 1963	198	June 1967	246	June 1971
7	July 1951	55	July 1955	103	July 1959	151	July 1963	199	July 1967	247	July 1971
8	Aug 1951	56	Aug 1955	104	Aug 1959	152	Aug 1963	200	Aug 1967	248	Aug 1971
9	Sept 1951	57	Sept 1955	105	Sept 1959	153	Sept 1963	201	Sept 1967	249	Sept 1971
10	Oct 1951	58	Oct 1955	106	Oct 1959	154	Oct 1963	202	Oct 1967	250	Oct 1971
11	Nov 1951	59	Nov 1955	107	Nov 1959	155	Nov 1963	203	Nov 1967	251	Nov 1971
12	Dec 1951	60	Dec 1955	108	Dec 1959	156	Dec 1963	204	Dec 1967	252	Dec 1971
13	Jan 1952	61	Jan 1956	109	Jan 1960	157	Jan 1964	205	Jan 1968	253	Jan 1972
14	Feb 1952	62	Feb 1956	110	Feb 1960	158	Feb 1964	206	Feb 1968	254	Feb 1972
15	Mar 1952	63	Mar 1956	111	Mar 1960	159	Mar 1964	207	Mar 1968	255	Mar 1972
16	Apr 1952	64	Apr 1956	112	Apr 1960	160	Apr 1964	208	Apr 1968	256	Apr 1972
17	May 1952	65	May 1956	113	May 1960	161	May 1964	209	May 1968	257	May 1972
18	June 1952	66	June 1956	114	June 1960	162	June 1964	210	June 1968	258	June 1972
19	July 1952	67	July 1956	115	July 1960	163	July 1964	211	July 1968	259	July 1972
20	Aug 1952	68	Aug 1956	116	Aug 1960	164	Aug 1964	212	Aug 1968	260	Aug 1972
21	Sept 1952	69	Sept 1956	117	Sept 1960	165	Sept 1964	213	Sept 1968	261	Sept 1972
22	Oct 1952	70	Oct 1956	118	Oct 1960	166	Oct 1964	214	Oct 1968	262	Oct 1972
23	Nov 1952	71	Nov 1956	119	Nov 1960	167	Nov 1964	215	Nov 1968	263	Nov 1972
24	Dec 1952	72	Dec 1956	120	Dec 1960	168	Dec 1964	216	Dec 1968	264	Dec 1972
25	Jan 1953	73	Jan 1957	121	Jan 1961	169	Jan 1965	217	Jan 1969	265	Jan 1973
26	Feb 1953	74	Feb 1957	122	Feb 1961	170	Feb 1965	218	Feb 1969	266	Feb 1973
27	Mar 1953	75	Mar 1957	123	Mar 1961	171	Mar 1965	219	Mar 1969	267	Mar 1973
28	Apr 1953	76	Apr 1957	124	Apr 1961	172	Apr 1965	220	Apr 1969	268	Apr 1973
29	May 1953	77	May 1957	125	May 1961	173	May 1965	221	May 1969	269	May 1973
30	June 1953	78	June 1957	126	June 1961	174	June 1965	222	June 1969	270	June 1973
31	July 1953	79	July 1957	127	July 1961	175	July 1965	223	July 1969	271	July 1973
32	Aug 1953	80	Aug 1957	128	Aug 1961	176	Aug 1965	224	Aug 1969	272	Aug 1973
33	Sept 1953	81	Sept 1957	129	Sept 1961	177	Sept 1965	225	Sept 1969	273	Sept 1973
34	Oct 1953	82	Oct 1957	130	Oct 1961	178	Oct 1965	226	Oct 1969	274	Oct 1973
35	Nov 1953	83	Nov 1957	131	Nov 1961	179	Nov 1965	227	Nov 1969	275	Nov 1973
36	Dec 1953	84	Dec 1957	132	Dec 1961	180	Dec 1965	228	Dec 1969	276	Dec 1973
37	Jan 1954	85	Jan 1958	133	Jan 1962	181	Jan 1966	229	Jan 1970	277	Jan 1974
38	Feb 1954	86	Feb 1958	134	Feb 1962	182	Feb 1966	230	Feb 1970	278	Feb 1974
39	Mar 1954	87	Mar 1958	135	Mar 1962	183	Mar 1966	231	Mar 1970	279	Mar 1974
40	Apr 1954	88	Apr 1958	136	Apr 1962	184	Apr 1966	232	Apr 1970	280	Apr 1974
41	May 1954	89	May 1958	137	May 1962	185	May 1966	233	May 1970	281	May 1974
42	June 1954	90	June 1958	138	June 1962	186	June 1966	234	June 1970	282	June 1974
43	July 1954	91	July 1958	139	July 1962	187	July 1966	235	July 1970	283	July 1974
44	Aug 1954	92	Aug 1958	140	Aug 1962	188	Aug 1966	236	Aug 1970	284	Aug 1974
45	Sept 1954	93	Sept 1958	141	Sept 1962	189	Sept 1966	237	Sept 1970	285	Sept 1974
46	Oct 1954	94	Oct 1958	142	Oct 1962	190	Oct 1966	238	Oct 1970	286	Oct 1974
47	Nov 1954	95	Nov 1958	143	Nov 1962	191	Nov 1966	239	Nov 1970	287	Nov 1974
48	Dec 1954	96	Dec 1958	144	Dec 1962	192	Dec 1966	240	Dec 1970	288	Dec 1974

Appendix C4.1. Simulation stress periods and corresponding month and year.—Continued

[Jan, January; Feb, February; Mar, March; Apr, April; Aug, August; Sept, September; Oct, October; Nov, November; Dec, December]

Stress period	Month and year	Stress period	Month and year	Stress period	Month and year	Stress period	Month and year	Stress period	Month and year
289	Jan 1975	337	Jan 1979	385	Jan 1983	433	Jan 1987	481	Jan 1991
290	Feb 1975	338	Feb 1979	386	Feb 1983	434	Feb 1987	482	Feb 1991
291	Mar 1975	339	Mar 1979	387	Mar 1983	435	Mar 1987	483	Mar 1991
292	Apr 1975	340	Apr 1979	388	Apr 1983	436	Apr 1987	484	Apr 1991
293	May 1975	341	May 1979	389	May 1983	437	May 1987	485	May 1991
294	June 1975	342	June 1979	390	June 1983	438	June 1987	486	June 1991
295	July 1975	343	July 1979	391	July 1983	439	July 1987	487	July 1991
296	Aug 1975	344	Aug 1979	392	Aug 1983	440	Aug 1987	488	Aug 1991
297	Sept 1975	345	Sept 1979	393	Sept 1983	441	Sept 1987	489	Sept 1991
298	Oct 1975	346	Oct 1979	394	Oct 1983	442	Oct 1987	490	Oct 1991
299	Nov 1975	347	Nov 1979	395	Nov 1983	443	Nov 1987	491	Nov 1991
300	Dec 1975	348	Dec 1979	396	Dec 1983	444	Dec 1987	492	Dec 1991
301	Jan 1976	349	Jan 1980	397	Jan 1984	445	Jan 1988	493	Jan 1992
302	Feb 1976	350	Feb 1980	398	Feb 1984	446	Feb 1988	494	Feb 1992
303	Mar 1976	351	Mar 1980	399	Mar 1984	447	Mar 1988	495	Mar 1992
304	Apr 1976	352	Apr 1980	400	Apr 1984	448	Apr 1988	496	Apr 1992
305	May 1976	353	May 1980	401	May 1984	449	May 1988	497	May 1992
306	June 1976	354	June 1980	402	June 1984	450	June 1988	498	June 1992
307	July 1976	355	July 1980	403	July 1984	451	July 1988	499	July 1992
308	Aug 1976	356	Aug 1980	404	Aug 1984	452	Aug 1988	500	Aug 1992
309	Sept 1976	357	Sept 1980	405	Sept 1984	453	Sept 1988	501	Sept 1992
310	Oct 1976	358	Oct 1980	406	Oct 1984	454	Oct 1988	502	Oct 1992
311	Nov 1976	359	Nov 1980	407	Nov 1984	455	Nov 1988	503	Nov 1992
312	Dec 1976	360	Dec 1980	408	Dec 1984	456	Dec 1988	504	Dec 1992
313	Jan 1977	361	Jan 1981	409	Jan 1985	457	Jan 1989	505	Jan 1993
314	Feb 1977	362	Feb 1981	410	Feb 1985	458	Feb 1989	506	Feb 1993
315	Mar 1977	363	Mar 1981	411	Mar 1985	459	Mar 1989	507	Mar 1993
316	Apr 1977	364	Apr 1981	412	Apr 1985	460	Apr 1989	508	Apr 1993
317	May 1977	365	May 1981	413	May 1985	461	May 1989	509	May 1993
318	June 1977	366	June 1981	414	June 1985	462	June 1989	510	June 1993
319	July 1977	367	July 1981	415	July 1985	463	July 1989	511	July 1993
320	Aug 1977	368	Aug 1981	416	Aug 1985	464	Aug 1989	512	Aug 1993
321	Sept 1977	369	Sept 1981	417	Sept 1985	465	Sept 1989	513	Sept 1993
322	Oct 1977	370	Oct 1981	418	Oct 1985	466	Oct 1989	514	Oct 1993
323	Nov 1977	371	Nov 1981	419	Nov 1985	467	Nov 1989	515	Nov 1993
324	Dec 1977	372	Dec 1981	420	Dec 1985	468	Dec 1989	516	Dec 1993
325	Jan 1978	373	Jan 1982	421	Jan 1986	469	Jan 1990	517	Jan 1994
326	Feb 1978	374	Feb 1982	422	Feb 1986	470	Feb 1990	518	Feb 1994
327	Mar 1978	375	Mar 1982	423	Mar 1986	471	Mar 1990	519	Mar 1994
328	Apr 1978	376	Apr 1982	424	Apr 1986	472	Apr 1990	520	Apr 1994
329	May 1978	377	May 1982	425	May 1986	473	May 1990	521	May 1994
330	June 1978	378	June 1982	426	June 1986	474	June 1990	522	June 1994
331	July 1978	379	July 1982	427	July 1986	475	July 1990	523	July 1994
332	Aug 1978	380	Aug 1982	428	Aug 1986	476	Aug 1990	524	Aug 1994
333	Sept 1978	381	Sept 1982	429	Sept 1986	477	Sept 1990	525	Sept 1994
334	Oct 1978	382	Oct 1982	430	Oct 1986	478	Oct 1990	526	Oct 1994
335	Nov 1978	383	Nov 1982	431	Nov 1986	479	Nov 1990	527	Nov 1994
336	Dec 1978	384	Dec 1982	432	Dec 1986	480	Dec 1990	528	Dec 1994

Appendix C5. Simulated and Observed Transient Water Levels in Selected Wells and Related Statistics, Tarawa Terrace and Vicinity, U.S. Marine Corps Base Camp Lejuene, North Carolina

Tables

Appendix C5. Simulated and Observed Transient Water Levels in Selected Wells and Related Statistics, Tarawa Terrace

Table C5.1. Simulated and observed transient water levels in supply well TT-25[1] and related statistics, Tarawa Terrace, U.S. Marine Corps Base Camp Lejeune, North Carolina.

[NGVD 29, National Geodetic Vertical Datum of 1929; –, below NGVD 29]

Date	Simulated water level, in feet above or below NGVD 29	Observed water level, in feet above or below NGVD 29	Absolute water-level difference, in feet
10/31/1980	7.5	6.0	1.5
6/30/1981	7.4	0.0	7.4
10/31/1982	–5.0	–13	8.0
12/31/1982	–2.8	–13	10.2
1/31/1983	–3.0	–14	11.0
2/28/1983	–2.6	–13	10.4
3/31/1983	–2.4	–10	7.6
4/30/1983	–2.9	–9	6.1
5/31/1983	–3.7	–9	5.3
7/31/1983	–5.3	–10	4.7
8/31/1983	–5.9	–12	6.1
9/30/1983	–4.4	–12	7.6
10/31/1983	–3.2	–15	11.8
11/30/1983	–3.1	–11	7.9
12/31/1983	–6.0	–9	3.0
1/31/1984	–0.9	–11	10.1
5/31/1984	–2.7	–10	7.3
6/30/1984	–4.1	–11	6.9
7/31/1984	–2.0	–10	8.0
8/31/1984	–1.1	–9	7.9
9/30/1984	–0.9	–5	4.1
10/31/1984	–0.7	–5	4.3
11/30/1984	–0.6	–11	10.4
12/31/1984	–0.2	–10	9.8
1/31/1985	–0.6	–10	9.4
6/30/1985	–3.4	–2	1.4
7/31/1985	–2.7	–3	0.3
8/31/1985	–3.4	–3	0.4
9/30/1985	–3.4	–4	0.6
10/31/1985	–3.4	–6	2.6
11/30/1985	–3.5	3	6.5
12/31/1985	–3.5	–4	0.5
1/31/1986	–2.0	–3	1.0
2/28/1986	–1.9	–3	1.1
3/31/1986	–2.7	–5	2.3
4/30/1986	–1.9	3	4.9
10/31/1986	–1.8	3.0	4.8
3/31/1987	8.5	10.9	2.4

[1]See Figure C1 for location

Statistics:

Average of water-level difference = 5.7 feet
Standard deviation of water-level difference = 3.5 feet
Root-mean-square error of water-level difference = 6.6 feet

Table C5.2. Simulated and observed transient water levels in supply well TT-26[1] and related statistics, Tarawa Terrace, U.S. Marine Corps Base Camp Lejeune, North Carolina.

[NGVD 29, National Geodetic Vertical Datum of 1929; –, below NGVD 29]

Date	Simulated water level, in feet above or below NGVD 29	Observed water level, in feet above or below NGVD 29	Absolute water-level difference, in feet
5/31/1951	14.4	14.0	0.4
1/31/1978	–4.0	7	11.0
2/28/1978	–6.2	7	13.2
3/31/1978	–2.9	6	8.9
4/30/1978	–4.2	7	11.2
5/31/1978	–3.4	7	10.4
6/30/1978	–5.7	6	11.7
7/31/1978	–5.5	6	11.5
8/31/1978	–4.5	7	11.5
9/30/1978	–4.5	6	10.5
10/31/1978	–6.4	6	12.4
11/30/1978	–2.5	6	8.5
12/31/1978	–2.3	6	8.3
1/31/1979	–3.1	5	8.1
2/28/1979	–3.1	6	9.1
3/31/1979	–3.1	8	11.1
4/30/1979	–3.1	6	9.1
6/30/1979	–3.2	6	9.2
7/31/1979	–3.2	5	8.2
9/30/1979	–3.2	5	8.2
2/29/1980	–1.8	6	7.8
3/31/1980	–3.3	2	5.3
4/30/1980	–0.7	–8	7.3
5/31/1980	–1.0	6	7.0
10/31/1980	–1.3	–7	5.7
12/31/1980	–1.1	–8	6.9
1/31/1981	–0.9	0	0.9
2/28/1981	0.5	–2	2.5
3/31/1981	–1.0	0	1.0
4/30/1981	–1.6	2	3.6
6/30/1981	–4.0	0	4.0
7/31/1981	–5.3	2	7.3
8/31/1981	–4.7	–1	3.7
10/31/1981	–2.7	–2	0.7
11/30/1981	–2.7	2	4.7
4/30/1982	–5.4	–10	4.6
6/30/1982	–5.4	–14	8.6
8/31/1982	–5.7	–5	0.7
10/31/1982	–4.8	–15	10.2
12/31/1982	–2.3	2	4.3
1/31/1983	8.1	2	6.1
2/28/1983	8.6	4	4.6
3/31/1983	–1.6	4	5.6
4/30/1983	–2.3	4	6.3
5/31/1983	–3.3	–13	9.7
6/30/1983	–4.4	4	8.4
9/30/1983	–4.1	–22	17.9
10/31/1983	–2.7	3	5.7
11/30/1983	–2.6	–2	0.6
12/31/1983	–5.9	4	9.9
3/31/1984	–6.6	–6	0.6
5/31/1984	–5.0	4	9.0
6/30/1984	–6.9	–2	4.9
9/30/1984	–2.0	8	10.0
10/31/1984	–1.8	8	9.8
11/30/1984	–1.6	3	4.6
12/31/1984	–1.0	3	4.0
1/31/1985	–1.6	1	2.6
6/30/1985	9.0	6	3.0
7/31/1985	9.1	2	7.1
9/30/1985	9.0	2	7.0
10/31/1985	9.0	2	7.0
11/18/1985	8.9	11.1	2.2
11/30/1985	8.9	4	4.9
10/31/1986	9.3	7.4	1.9
3/31/1987	10.6	14.0	3.4

[1]See Figure C2 for location

Statistics:

Average of water-level difference = 6.8 feet
Standard deviation of water-level difference = 3.7 feet
Root-mean-square error of water-level difference = 7.7 feet

Table C5.3. Simulated and observed transient water levels in supply well TT-30[1] and related statistics, Tarawa Terrace, U.S. Marine Corps Base Camp Lejeune, North Carolina.

[NGVD 29, National Geodetic Vertical Datum of 1929; –, below NGVD 29]

Date	Simulated water level, in feet above or below NGVD 29	Observed water level, in feet above or below NGVD 29	Absolute water-level difference, in feet
1/31/1978	8.6	4	4.6
2/28/1978	7.3	4	3.3
3/31/1978	9.2	6	3.2
4/30/1978	8.4	5	3.4
5/31/1978	8.9	4	4.9
6/30/1978	7.5	5	2.5
7/31/1978	7.7	4	3.7
8/31/1978	8.2	–2	10.2
9/30/1978	8.3	0	8.3
10/31/1978	7.1	–2	9.1
11/30/1978	9.5	–1	10.5
12/31/1978	9.5	–3	12.5
1/31/1979	9.0	–2	11.0
2/28/1979	8.9	–2	10.9
3/31/1979	8.9	2	6.9
4/30/1979	8.9	–2	10.9
6/30/1979	8.9	–1	9.9
7/31/1979	8.9	–2	10.9
8/31/1979	8.9	–2	10.9
9/30/1979	8.9	–4	12.9
1/31/1980	7.8	–4	11.8
2/29/1980	9.7	–4	13.7
3/31/1980	8.8	–6	14.8
4/30/1980	10.3	3	7.3
5/31/1980	10.1	–6	16.1
7/31/1980	5.9	–4	9.9
8/31/1980	7.0	–2	9.0
9/30/1980	9.2	–4	13.2
10/31/1980	9.7	–6	15.7
12/31/1980	10.0	–6	16.0
1/31/1981	10.7	–8	18.7
2/28/1981	11.6	–7	18.6
3/31/1981	10.8	–6	16.8
4/30/1981	10.6	–4	14.6
5/31/1981	10.4	–5	15.4
6/30/1981	9.3	–6	15.3
7/31/1981	8.6	–7	15.6
8/31/1981	8.9	–5	13.9
9/30/1981	9.9	–6	15.9
10/31/1981	10.1	–10	20.1
3/31/1982	9.7	16	6.3
4/30/1982	9.6	11	1.4
6/30/1982	9.3	7	2.3
7/31/1982	9.3	9	0.3
8/31/1982	9.3	13	3.7
9/30/1982	9.3	11	1.7
10/31/1982	9.7	10	0.3
12/31/1982	10.8	9	1.8
1/31/1983	10.0	9	1.0
2/28/1983	10.1	9	1.1
3/31/1983	10.9	9	1.9
4/30/1983	10.8	9	1.8
5/31/1983	10.4	13	2.6
6/30/1983	10.2	10	0.2
7/31/1983	9.7	10	0.3
8/31/1983	9.4	10	0.6
9/30/1983	10.2	10	0.2
10/31/1983	10.8	10	0.8
11/30/1983	10.9	-7	17.9
12/31/1983	9.2	11	1.8
1/31/1984	11.6	10	1.6
2/29/1984	9.2	10	0.8
3/31/1984	9.5	15	5.5
4/30/1984	10.7	12	1.3
5/31/1984	10.3	11	0.7
6/30/1984	9.4	11	1.6
7/31/1984	10.8	11	0.2
9/30/1984	17.3	11	6.3
10/31/1984	12.5	11	1.5
11/30/1984	12.5	11	1.5
12/31/1984	12.7	11	1.7
1/31/1985	12.5	11	1.5
3/31/1985	17.8	11	6.8

[1]See Figure C1 for location

Statistics:

Average of water-level difference = 7.3 feet
Standard deviation of water-level difference = 6.1 feet
Root-mean-square error of water-level difference = 9.5 feet

Table C5.4. Simulated and observed transient water levels in supply well TT-31[1] and related statistics, Tarawa Terrace, U.S. Marine Corps Base Camp Lejeune, North Carolina.

[NGVD 29, National Geodetic Vertical Datum of 1929; –, below NGVD 29]

Date	Simulated water level, in feet above or below NGVD 29	Observed water level, in feet above or below NGVD 29	Absolute water-level difference, in feet
10/31/1978	–14.2	–2	12.2
11/30/1978	–10.1	–1	9.1
7/31/1979	–10.4	–3	7.4
8/31/1979	–10.4	–2	8.4
9/30/1979	–10.4	2	12.4
1/31/1980	–12.4	–3	9.4
2/29/1980	–9.1	–2	7.1
3/31/1980	–10.4	–2	8.4
4/30/1980	–7.8	12	19.8
5/31/1980	–7.8	0	7.8
7/31/1980	–15.3	0	15.3
8/31/1980	–14.3	–2	12.3
12/31/1980	–7.9	–4	3.9
1/31/1981	–8.7	–8	0.7
2/28/1981	–7.2	–6	1.2
3/31/1981	–8.8	–8	0.8
5/31/1981	–10.2	–4	6.2
6/30/1981	–12.6	–5	7.6
7/31/1981	–14.3	–3	11.3
10/31/1981	–11.6	–6	5.6
11/30/1981	–11.5	–8	3.5
6/30/1982	–12.1	–6	6.1
7/31/1982	–12.3	–3	9.3
9/30/1982	–12.5	–8	4.5
10/31/1982	–11.6	–4	7.6
12/31/1982	–8.5	3	11.5
1/31/1983	–10.3	4	14.3
2/28/1983	–10.3	2	12.3
3/31/1983	–8.7	4	12.7
4/30/1983	–8.8	8	16.8
5/31/1983	–9.7	8	17.7
10/31/1983	–9.3	3	12.3
11/30/1983	–9.0	6	15.0
12/31/1983	–12.4	–8	4.4
3/31/1984	–11.3	–6	5.3
5/31/1984	–10.9	8	18.9
7/31/1984	–9.2	–4	5.2
9/30/1984	–7.6	–4	3.6
10/31/1984	–7.2	–4	3.2
11/30/1984	–7.0	–6	1.0
12/31/1984	–6.4	–4	2.4
1/31/1985	–6.8	–5	1.8
3/31/1985	–7.2	–5	2.2
6/30/1985	–15.9	–3	12.9
7/31/1985	–14.9	–11	3.9
8/31/1985	–16.0	–3	13.0
9/13/1985	–16.0	–5	11.0
9/30/1985	–16.2	–4	12.2
10/31/1985	–16.3	–3	13.3
11/30/1985	–16.4	–8	8.4
12/31/1985	–16.4	–6	10.4
1/31/1986	–13.7	–5	8.7
2/28/1986	–13.3	–6	7.3
4/30/1986	–12.8	–2	10.8
10/31/1986	–12.9	–0.1	12.8
3/31/1987	3.1	5.2	2.1

[1]See Figure C1 for location

Statistics:

Average of water-level difference = 8.7 feet
Standard deviation of water-level difference = 4.9 feet
Root-mean-square error of water-level difference = 9.9 feet

Table C5.5. Simulated and observed transient water levels in supply well TT-52[1] and related statistics, Tarawa Terrace, U.S. Marine Corps Base Camp Lejeune, North Carolina.

[NGVD 29, National Geodetic Vertical Datum of 1929; –, below NGVD 29]

Date	Simulated water level, in feet above or below NGVD 29	Observed water level, in feet above or below NGVD 29	Absolute water-level difference, in feet
10/31/1961	9.8	12.9	3.1
3/31/1962	–7.4	9	16.4
1/31/1978	–10.1	–5	5.1
2/28/1978	–12.7	–4	8.7
3/31/1978	–9.2	–5	4.2
4/30/1978	–10.5	–5	5.5
5/31/1978	–9.6	–1	8.6
6/30/1978	–12.3	–3	9.3
7/31/1978	–12.2	–1	11.2
8/31/1978	–11.1	–3	8.1
9/30/1978	–11.0	–3	8.0
10/31/1978	–13.2	–3	10.2
11/30/1978	–8.8	–4	4.8
12/31/1978	–8.3	–7	1.3
1/31/1979	–9.2	–7	2.2
2/28/1979	–9.2	–4	5.2
3/31/1979	–9.3	–5	4.3
6/30/1979	–9.3	–4	5.3
7/31/1979	–9.3	–4	5.3
8/31/1979	–9.3	–3	6.3
9/30/1979	–9.3	–4	5.3
1/31/1980	–11.4	–4	7.4
2/29/1980	–7.9	–3	4.9
3/31/1980	–9.4	–4	5.4
4/30/1980	–6.6	–4	2.6
5/31/1980	–6.8	–4	2.8
7/31/1980	–14.7	–5	9.7
8/31/1980	–13.3	–5	8.3
12/31/1980	–6.9	–6	0.9
1/31/1981	–10.2	–7	3.2
2/28/1981	–8.4	–6	2.4
3/31/1981	–10.5	–9	1.5
4/30/1981	–11.4	–9	2.4
5/31/1981	–12.0	–5	7.0
6/30/1981	–15.1	–5	10.1
7/31/1981	–17.2	–7	10.2
10/31/1981	–13.4	–9	4.4
11/30/1981	–13.4	–7	6.4
4/30/1982	–13.7	–5	8.7
6/30/1982	–14.0	–5	9.0
7/31/1982	–14.0	–6	8.0
9/30/1982	–14.2	–9	5.2
12/31/1982	–9.6	–6	3.6
1/31/1983	–11.8	–6	5.8
2/28/1983	–11.7	–9	2.7
3/31/1983	–9.7	–2	7.7
4/30/1983	–9.9	–2	7.9
5/31/1983	–11.0	–1	10.0
10/31/1983	–10.2	–4	6.2
11/30/1983	–10.0	–2	8.0
12/31/1983	–14.3	–2	12.3
3/31/1984	–13.1	–4	9.1
4/30/1984	–10.1	–2	8.1
5/31/1984	–11.3	–2	9.3
6/30/1984	–12.6	–3	9.6
7/31/1984	–9.7	–3	6.7
9/30/1984	–6.8	–2	4.8
10/31/1984	–6.4	3	9.4
11/30/1984	–6.2	3	9.2
12/31/1984	–5.5	–2	3.5
1/31/1985	–4.4	–2	2.4
5/31/1985	–12.9	–5	7.9
6/30/1985	–13.3	2	15.3
7/31/1985	–12.3	0	12.3
8/31/1985	–13.3	–1	12.3
9/30/1985	–13.5	4	17.5
10/31/1985	–13.6	3	16.6
11/30/1985	–13.6	5	18.6
12/31/1985	–13.6	4	17.6
1/31/1986	–11.1	–2	9.1
2/28/1986	–10.9	5	15.9
3/31/1986	3.4	–7	10.4
4/30/1986	–9.8	5	14.8
10/31/1986	–10.6	1.8	12.4
3/31/1987	4.9	5.0	0.1

[1]See Figure C1 for location

Statistics:

Average of water-level difference = 7.7 feet
Standard deviation of water-level difference = 4.3 feet
Root-mean-square error of water-level difference = 8.8 feet

Table C5.6. Simulated and observed transient water levels in supply well TT-53[1] and related statistics, Tarawa Terrace, U.S. Marine Corps Base Camp Lejeune, North Carolina.

[NGVD 29, National Geodetic Vertical Datum of 1929; –, below NGVD 29]

Date	Simulated water level, in feet above or below NGVD 29	Observed water level, in feet above or below NGVD 29	Absolute water-level difference, in feet
7/31/1961	11.9	16	4.1
3/31/1962	–1.3	11	12.3
1/31/1978	1.5	–4	5.5
2/28/1978	0.3	–5	5.3
3/31/1978	1.6	–3	4.6
4/30/1978	1.2	–5	6.2
5/31/1978	1.5	–5	6.5
6/30/1978	0.4	–4	4.4
7/31/1978	0.2	–4	4.2
8/31/1978	0.6	0	0.6
9/30/1978	0.7	–3	3.7
12/31/1978	2.0	–2	4.0
1/31/1979	1.8	–2	3.8
2/28/1979	1.7	–4	5.7
3/31/1979	1.7	–2	3.7
4/30/1979	1.7	–8	9.7
6/30/1979	1.7	–6	7.7
7/31/1979	1.6	–4	5.6
1/31/1980	0.7	–4	4.7
2/29/1980	2.1	–3	5.1
3/31/1980	1.6	–1	2.6
4/30/1980	2.8	–2	4.8
5/31/1980	3.0	–5	8.0
7/31/1980	–0.2	–7	6.8
8/31/1980	0.2	–3	3.2
9/30/1980	1.7	–7	8.7
12/31/1980	3.0	–3	6.0
1/31/1981	2.2	–9	11.2
2/28/1981	3.0	–7	10.0
3/31/1981	2.3	–9	11.3
4/30/1981	1.9	–9	10.9
6/30/1981	0.2	–9	9.2
10/31/1981	0.7	–9	9.7
11/30/1981	0.7	–8	8.7
1/31/1982	0.4	–9	9.4
3/31/1982	–0.4	–13	12.6
4/30/1982	–0.6	–8	7.4
6/30/1982	–0.9	–22	21.1
7/31/1982	–1.0	–15	14.0
8/31/1982	–1.1	–15	13.9
12/31/1982	1.3	–19	20.3
1/31/1983	0.6	–19	19.6
2/28/1983	0.7	–19	19.7
3/31/1983	1.4	–11	12.4
4/30/1983	1.4	–11	12.4
5/31/1983	0.9	–10	10.9
10/31/1983	0.7	–9	9.7
11/30/1983	1.0	–13	14.0
12/31/1983	–0.8	–13	12.2
1/31/1984	1.5	–11	12.5
7/31/1986	6.5	1	5.5
3/31/1987	8.2	10	1.8

[1]See Figure C1 for location

Statistics:

Average of water-level difference = 8.6 feet
Standard deviation of water-level difference = 4.8 feet
Root-mean-square error of water-level difference = 9.9 feet

Table C5.7. Simulated and observed transient water levels in supply well TT-54[1] and related statistics, Tarawa Terrace, U.S. Marine Corps Base Camp Lejeune, North Carolina.

[NGVD 29, National Geodetic Vertical Datum of 1929; –, below NGVD 29]

Date	Simulated water level, in feet above or below NGVD 29	Observed water level, in feet above or below NGVD 29	Absolute water-level difference, in feet
6/30/1961	7.6	12.1	4.5
3/31/1962	–12.3	6	18.3
1/31/1978	–15.8	–7	8.8
2/28/1978	–18.9	–6	12.9
3/31/1978	–14.6	–6	8.6
4/30/1978	–16.1	–5	11.1
5/31/1978	–15.0	–7	8.0
6/30/1978	–18.3	–6	12.3
7/31/1978	–18.2	–7	11.2
8/31/1978	–16.8	–6	10.8
9/30/1978	–16.6	–6	10.6
10/31/1978	–19.4	–6	13.4
11/30/1978	–14.0	–7	7.0
12/31/1978	–13.5	–7	6.5
1/31/1979	–14.5	–7	7.5
2/28/1979	–14.5	–8	6.5
3/31/1979	–14.6	–6	8.6
4/30/1979	–14.6	–7	7.6
6/30/1979	–14.6	–8	6.6
8/31/1979	–14.6	–6	8.6
1/31/1980	–17.1	–7	10.1
2/29/1980	–12.9	–6	6.9
3/31/1980	–14.7	–8	6.7
4/30/1980	–11.3	–10	1.3
5/31/1980	–11.6	–8	3.6
7/31/1980	–21.2	–6	15.2
8/31/1980	–19.2	–8	11.2
12/31/1980	–11.7	–8	3.7
1/31/1981	–13.7	–11	2.7
2/28/1981	–11.7	–11	0.7
3/31/1981	–14.0	–12	2.0
4/30/1981	–15.0	–10	5.0
5/31/1981	–15.6	–8	7.6
7/31/1981	–21.3	–10	11.3
8/31/1981	–20.5	–8	12.5
10/31/1981	–17.2	–12	5.2
11/30/1981	–17.1	–10	7.1
1/31/1982	–16.6	–11	5.6
3/31/1982	–17.3	–10	7.3
4/30/1982	–17.6	–9	8.6
5/31/1982	–7.5	–10	2.5
6/30/1982	–17.1	–10	7.1
7/31/1982	–17.7	–10	7.7
8/31/1982	–17.9	–12	5.9
9/30/1982	–18.0	–10	8.0
10/31/1982	–16.7	–10	6.7
11/30/1982	–11.9	–10	1.9
12/31/1982	–13.1	–9	4.1
1/31/1983	–15.4	–9	6.4
2/28/1983	–15.3	–8	7.3
3/31/1983	–13.2	–8	5.2
4/30/1983	–13.4	–8	5.4
5/31/1983	–14.6	–8	6.6
6/30/1983	–15.7	–8	7.7
10/31/1983	–13.9	–9	4.9
11/30/1983	–13.6	–7	6.6
12/31/1983	–18.3	0	18.3
1/31/1984	–12.0	–9	3.0
2/29/1984	0.3	–8	8.3
5/31/1984	–14.6	–8	6.6
6/30/1984	–16.2	–10	6.2
7/31/1984	–13.3	–8	5.3
9/30/1984	–11.2	–8	3.2
10/31/1984	–10.9	–8	2.9
11/30/1984	–10.7	–9	1.7
12/31/1984	–9.9	–8	1.9
1/31/1985	–10.6	–12	1.4
2/28/1985	–16.9	–14	2.9
4/30/1985	–17.9	–12	5.9
6/30/1985	–21.0	–2	19.0
7/31/1985	–19.7	–13	6.7
8/31/1985	–21.1	–12	9.1
9/13/1985	–21.1	–8	13.1
9/30/1985	–21.2	–8	13.2
10/31/1985	–21.3	–10	11.3
11/30/1985	–21.4	–1	20.4
12/31/1985	–21.4	–8	13.4
1/31/1986	–18.0	–6	12.0
2/28/1986	–17.7	–9	8.7
3/31/1986	–19.2	–10	9.2
4/30/1986	–17.4	–8	9.4
10/31/1986	–17.3	0.4	17.7
3/31/1987	2.3	6.7	4.4

[1]See Figure C1 for location

Statistics:

Average of water-level difference = 7.9 feet
Standard deviation of water-level difference = 4.3 feet
Root-mean-square error of water-level difference = 9.0 feet

Table C5.8. Simulated and observed transient water levels in supply well TT-67[1] and related statistics, Tarawa Terrace, U.S. Marine Corps Base Camp Lejeune, North Carolina.

[NGVD 29, National Geodetic Vertical Datum of 1929; –, below NGVD 29]

Date	Simulated water level, in feet above or below NGVD 29	Observed water level, in feet above or below NGVD 29	Absolute water-level difference, in feet
3/31/1979	–10.5	–14	3.5
4/30/1979	–10.6	–12	1.4
6/30/1979	–10.6	–12	1.4
7/31/1979	–10.6	–10	0.6
8/31/1979	–10.6	–10	0.6
9/30/1979	–10.6	–8	2.6
1/31/1980	–12.7	–8	4.7
2/29/1980	–9.2	–10	0.8
3/31/1980	–10.7	–4	6.7
4/30/1980	–7.8	–12	4.2
5/31/1980	–7.9	–10	2.1
7/31/1980	–15.6	–8	7.6
8/31/1980	–14.2	–10	4.2
10/31/1980	–8.9	–6	2.9
12/31/1980	–8.0	–8	0.0
1/31/1981	–6.5	–10	3.5
2/28/1981	–5.1	–10	4.9
3/31/1981	–6.5	–8	1.5
4/30/1981	–7.2	–6	1.2
6/30/1981	–9.9	–4	5.9
7/31/1981	–10.7	–8	2.7
10/31/1981	–8.9	–6	2.9
11/30/1981	–8.8	–8	0.8
1/31/1982	–8.8	–11	2.2
3/31/1982	–9.5	–7	2.5
4/30/1982	–9.7	–9	0.7
6/30/1982	–9.7	–11	1.3
7/31/1982	–9.9	–12	2.1
8/31/1982	–10.1	–8	2.1
9/30/1982	–10.2	–8	2.2
10/31/1982	–9.4	–6	3.4
12/31/1982	–6.6	–6	0.6
1/31/1983	–9.0	–7	2.0
2/28/1983	–8.9	–6	2.9
3/31/1983	–7.5	–4	3.5
4/30/1983	–7.6	–4	3.6
5/18/1983	–8.5	–5	3.5
5/31/1983	–8.5	–3	5.5
6/30/1983	–9.5	–4	5.5
10/31/1983	–8.2	–3	5.2
11/30/1983	–7.9	–6	1.9
12/31/1983	–11.1	–6	5.1
3/31/1984	–8.2	10	18.2
5/31/1984	–7.9	–4	3.9
6/30/1984	–8.4	–1	7.4
8/21/1984	–6.1	–3	3.1
8/31/1984	–6.1	–3	3.1
9/30/1984	–6.0	–5	1.0
10/31/1984	–5.8	–5	0.8
11/30/1984	–5.6	0	5.6
12/31/1984	–5.0	–1	4.0
1/31/1985	–5.4	–4	1.4
3/31/1985	–5.4	–4	1.4
7/31/1985	–10.8	–2	8.8
8/31/1985	–11.7	–4	7.7
9/13/1985	–11.7	–2	9.7
9/30/1985	–11.8	–4	7.8
10/31/1985	–11.9	–3	8.9
11/30/1985	–11.9	–2	9.9
12/31/1985	–11.9	–4	7.9
1/31/1986	–9.9	–2	7.9
2/28/1986	–9.6	–4	5.6
3/31/1986	–10.3	–5	5.3
4/30/1986	–9.2	–10	0.8
10/31/1986	–9.2	–4	5.2
3/31/1987	4.8	8.4	3.6

[1]See Figure C1 for location

Statistics:

Average of water-level difference = 4.0 feet
Standard deviation of water-level difference = 3.1 feet
Root-mean-square error of water-level difference = 5.0 feet

Table C5.9. Simulated and observed transient water levels in test well T-9 and supply wells TT-23, TT-27, and TT-55 and related statistics, Tarawa Terrace, U.S. Marine Corps Base Camp Lejeune, North Carolina.

[NGVD 29, National Geodetic Vertical Datum of 1929; –, below NGVD 29]

Site name[1]	Measurement date	Simulated water level, in feet above NGVD 29	Observed water level, in feet above or below NGVD 29	Absolute water-level difference, in feet
T-9	9/24/1986	13.1	17.5	4.4
	10/19/1986	13.1	20.3	7.2
	10/21/1986	13.1	19.1	6.0
	4/7/1987	13.4	24.5	11.1
	4/10/1987	13.4	23.4	10.0
TT-23	3/14/1983	3.8	–1.8	5.6
	9/25/1985	4.0	1.1	2.9
	10/21/1986	4.5	2.2	2.3
	4/7/1987	6.4	9.3	2.9
TT-27	1/10/1963	12.1	16.6	4.5
	4/17/1963	11.6	18.4	6.8
	1/16/1964	11.4	19.4	8.0
	7/14/1964	11.3	19.0	7.7
	9/17/1964	11.3	20.6	9.3
	10/14/1964	11.3	21.9	10.6
TT-55	11/1/1961	3.7	18.9	15.2
	3/28/1962	12.3	14.4	2.1

[1]See Plate 1 for location

Statistics:

Average of water-level difference = 6.9 feet
Standard deviation of water-level difference = 3.6 feet
Root-mean-square error of water-level difference = 7.7 feet

Table C5.10. Simulated and observed transient water levels and related statistics in monitor wells installed during ABC One-Hour Cleaners Operable Units 1 and 2 and during similar investigations by the North Carolina Department of Natural Resources and Community Development, Tarawa Terrace and vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina.

[NGVD 29, National Geodetic Vertical Datum of 1929]

Site name[1]	Measurement date	Simulated water level, in feet above NGVD 29	Observed water level, in feet above NGVD 29	Absolute water-level difference, in feet
C1	4/22/1992	18.3	21.5	3.2
	6/2/1992	18.3	20.8	2.5
	6/25/1992	18.3	21.2	2.9
C2	4/22/1992	17.1	19.6	2.5
	6/2/1992	17.1	19.0	1.9
	6/25/1992	17.1	19.6	2.5
C3	4/22/1992	14.6	15.8	1.2
	6/2/1992	14.6	14.7	0.1
	6/25/1992	14.6	15.6	1.0
C4	4/22/1992	11.6	11.9	0.3
	6/2/1992	11.6	11.3	0.3
	6/25/1992	11.6	10.2	1.4
C5	4/22/1992	14.2	15.7	1.5
	6/2/1992	14.2	15.0	0.8
	6/25/1992	14.2	15.9	1.7
C9	10/1/1993	14.8	12.4	2.4
	11/18/1993	14.8	13.0	1.8
C10	11/18/1993	14.4	12.6	1.8
C11	10/1/1993	6.8	6.3	0.5
PZ-01	10/1/1993	17.5	15.9	1.6
	11/18/1993	17.5	16.7	0.8
PZ-02	10/1/1993	17.6	16.0	1.6
	11/18/1993	17.6	16.7	0.9
PZ-03	10/1/1993	17.2	15.6	1.6
	11/18/1993	17.2	16.6	0.6
PZ-04	10/1/1993	17.4	15.8	1.6
	11/18/1993	17.4	16.4	1.0
PZ-05	10/1/1993	17.5	15.7	1.8
PZ-06	10/1/1993	17.7	16.1	1.6
S1	4/22/1992	18.6	23.7	5.1
	6/2/1992	18.6	23.3	4.7
	6/25/1992	18.6	22.6	4.0
	10/1/1993	18.8	17.4	1.4
	11/18/1993	18.8	18.3	0.5
S2	4/22/1992	17.3	19.9	2.6
	6/2/1992	17.3	19.2	1.9
	6/25/1992	17.3	19.8	2.5
	10/1/1993	17.5	16.4	1.1
	11/18/1993	17.5	16.6	0.9
S3	4/22/1992	14.5	16.0	1.5
	6/2/1992	14.5	14.8	0.3
	6/25/1992	14.5	15.8	1.3
	10/1/1993	14.8	13.1	1.7
	11/18/1993	14.8	13.6	1.2

Table C5.10. Simulated and observed transient water levels and related statistics in monitor wells installed during ABC One-Hour Cleaners Operable Units 1 and 2 and during similar investigations by the North Carolina Department of Natural Resources and Community Development, Tarawa Terrace and vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina.—Continued

[NGVD 29, National Geodetic Vertical Datum of 1929]

Site name[1]	Measurement date	Simulated water level, in feet above NGVD 29	Observed water level, in feet above NGVD 29	Absolute water-level difference, in feet
S4	4/22/1992	12.2	13.6	1.4
	6/2/1992	12.2	12.4	0.2
	6/25/1992	12.2	11.9	0.3
	10/1/1993	12.4	11.2	1.2
	11/18/1993	12.4	13.5	1.1
S5	4/22/1992	14.3	16.4	2.1
	6/2/1992	14.3	15.2	0.9
	6/25/1992	14.3	16.2	1.9
	10/1/1993	14.5	13.5	1.0
	11/18/1993	14.5	13.7	0.8
S6	4/22/1992	17.7	20.6	2.9
	6/2/1992	17.7	20.0	2.3
	6/25/1992	17.7	20.5	2.8
	10/1/1993	17.9	16.3	1.6
	11/18/1993	17.9	17.1	0.8
S7	4/22/1992	17.1	19.8	2.7
	6/2/1992	17.1	19.0	1.9
	6/25/1992	17.1	19.4	2.3
	10/1/1993	17.3	15.8	1.5
	11/18/1993	17.3	16.6	0.7
S8	4/22/1992	16.3	20.9	4.6
	6/2/1992	16.3	19.8	3.5
	6/25/1991	16.3	21.1	4.8
	10/1/1993	16.5	18.8	2.3
	11/18/1993	16.5	19.0	2.5
S9	4/22/1992	14.5	15.4	0.9
	6/2/1992	14.5	14.2	0.3
	6/25/1992	14.5	13.3	1.2
	10/1/1993	14.7	12.5	2.2
	11/18/1993	14.7	13.0	1.7
S10	4/22/1992	11.9	12.2	0.3
	6/2/1992	11.9	12.8	0.9
	6/25/1992	11.9	13.3	1.4
	10/1/1993	12.2	12.4	0.2
	11/18/1993	12.2	12.7	0.5
S11	10/1/1993	20.3	17.9	2.4
	11/18/1993	20.3	19.0	1.3
[2]X24B4	9/25/1985	9.8	5.0	4.8
[2]X24B5	9/25/1985	12.2	7.7	4.5
[2]X24B6	9/25/1985	13.7	10.4	3.3

[1]See Plate 1 for location

[2]Shown on Plate 1 as B4, B5, and B6, respectively

Statistics:

Average of water-level difference = 1.8 feet
Standard deviation of water-level difference = 1.2 feet
Root-mean-square error of water-level difference = 2.1 feet

Table C5.11. Simulated and observed transient water levels in monitor wells installed during investigations of releases of refined-petroleum products to groundwater and related statistics, Tarawa Terrace and vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina.

[NGVD 29, National Geodetic Vertical Datum of 1929]

Site name[1]	Measurement date	Simulated water level, in feet above NGVD 29	Observed water level, in feet above NGVD 29	Absolute water-level difference, in feet
STT61to66-MW01	1/8/1992	19.3	20.6	1.3
	1/11/1992	19.3	20.7	1.4
	1/29/1992	19.3	21.6	2.3
	12/17/1992	19.3	21.1	1.8
STT61to66-MW02	1/8/1992	19.3	20.2	0.9
	1/11/1992	19.3	20.1	0.8
	1/29/1992	19.3	21.6	2.3
	12/17/1992	19.3	20.4	1.1
STT61to66-MW03	1/9/1992	19.0	20.4	1.4
	1/11/1992	19.0	20.3	1.3
	1/29/1992	19.0	21.3	2.3
	12/17/1992	18.9	21.0	2.1
STT61to66-MW04	1/9/1992	19.0	20.1	1.1
	1/11/1992	19.0	20.9	1.9
	1/29/1992	19.0	20.7	1.7
	12/17/1992	18.9	20.4	1.5
STT61to66-MW05	1/9/1992	19.1	20.9	1.8
	1/11/1992	19.1	18.9	0.2
	1/29/1992	19.1	19.6	0.5
	12/17/1992	19.1	21.3	2.2
STT61to66-MW06	1/9/1992	19.1	20.4	1.3
	1/11/1992	19.1	20.1	1.0
	1/29/1992	19.1	20.8	1.7
	12/17/1992	19.1	20.5	1.4
STT61to66-MW07	1/9/1992	19.3	20.9	1.6
	1/11/1992	19.3	20.9	1.6
	1/29/1992	19.3	21.5	2.2
	12/17/1992	19.3	21.1	1.8
STT61to66-MW08	1/9/1992	19.3	19.8	0.5
	1/11/1992	19.3	19.9	0.6
	1/29/1992	19.3	20.8	1.5
	12/17/1992	19.3	20.5	1.2
STT61to66-MW09	1/9/1992	19.0	20.9	1.9
	1/11/1992	19.0	20.8	1.8
	1/29/1992	19.0	21.6	2.6
	12/17/1992	19.0	21.4	2.4
STT61to66-MW10	1/9/1992	19.0	20.7	1.7
	1/11/1992	19.0	20.0	1.0
	1/29/1992	19.0	20.7	1.7
	12/17/1992	19.0	20.4	1.4
STT61to66-MW11	1/10/1992	18.8	20.1	1.3
	1/11/1992	18.8	20.9	2.1
	1/29/1992	18.8	21.9	3.1
	12/17/1992	18.8	21.5	2.7
STT61to66-MW12	1/10/1992	18.8	19.7	0.9
	1/11/1992	18.8	19.8	1.0
	1/29/1992	18.8	20.6	1.8
	12/17/1992	18.8	20.3	1.5

Table C5.11. Simulated and observed transient water levels in monitor wells installed during investigations of releases of refined-petroleum products to groundwater and related statistics, Tarawa Terrace and vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina.—Continued

[NGVD 29, National Geodetic Vertical Datum of 1929]

Site name[1]	Measurement date	Simulated water level, in feet above NGVD 29	Observed water level, in feet above NGVD 29	Absolute water-level difference, in feet
STT61to66-MW13	1/10/1992	18.7	20.4	1.7
	1/11/1992	18.7	20.2	1.5
	1/29/1992	18.7	21.8	3.1
	12/17/1992	18.7	21.2	2.5
STT61to66-MW14	1/10/1992	18.7	19.8	1.1
	1/11/1992	18.7	19.7	1.0
	1/29/1992	18.7	20.5	1.8
	12/17/1992	18.7	20.3	1.6
STT61to66-MW15	12/17/1992	18.9	21.0	2.1
STT61to66-MW16	12/17/1992	18.6	20.2	1.6
STT61to66-MW17	12/17/1992	18.9	21.3	2.4
STT61to66-MW18	12/17/1992	18.7	20.2	1.5
STT61to66-MW19	12/17/1992	18.5	20.5	2.0
STT61to66-MW20	12/17/1992	18.5	20.1	1.6
TTDump MW01	6/26/1991	1.8	2.4	0.6
TTDump MW02	6/26/1991	4.3	6.2	1.9
TTDump MW03	6/26/1991	3.0	2.2	0.8
[2]TTUST-2453-A-1	6/7/1989	6.7	8.4	1.7
[2]TTUST-2453-A-2	6/7/1989	5.7	6.6	0.9
[2]TTUST-2453-A-3	6/7/1989	5.7	6.6	0.9
[2]TTUST-2453-A-4	6/7/1989	6.2	7.6	1.4
[2]TTUST-2453-A-5	6/7/1989	6.0	7.4	1.4
[2]TTUST-2453-A-6	6/7/1989	5.7	6.4	0.7
[2]TTUST-2453-A-7	6/7/1989	5.7	6.7	1.0
[2]TTUST-2453-A-8	6/7/1989	5.6	6.5	0.9
[2]TTUST-2453-A-9	6/7/1989	5.7	6.7	1.0
[2]TTUST-2453-OB-1	6/7/1989	5.7	6.8	1.1
[2]TTUST-2453-OB-2	6/7/1989	5.7	6.6	0.9
[2]TTUST-2453-OB-3	6/7/1989	5.5	6.4	0.9
[2]TTUST-2453-OB-4	6/7/1989	6.0	7.3	1.3
[2]TTUST-2453-OB-8	6/7/1989	5.2	6.5	1.3
[2]TTUST-2453-OB-9	6/7/1989	5.7	6.6	0.9
[2]TTUST-2453-OB-1	6/7/1989	5.5	6.3	0.8
[2]TTUST-2453-OB-1	6/7/1989	6.1	7.4	1.3
[2]TTUST-2453-RW	6/7/1989	5.8	6.8	1.0
[2]TTUST-2455-1	10/7/1993	7.8	9.0	1.2
[2]TTUST-2455-2	10/7/1993	7.7	8.5	0.8
[2]TTUST-2455-3	10/7/1993	7.8	8.2	0.4
[2]TTUST-2455-4	10/28/1993	7.9	8.6	0.7
[2]TTUST-2455-5	10/28/1993	8.2	9.0	0.8
[2]TTUST-2455-6	10/28/1993	7.5	8.0	0.5
[2]TTUST-2455-7	10/28/1993	6.8	6.8	0.0
[2]TTUST-2455-8	10/28/1993	7.2	7.6	0.4
[2]TTUST-2455-9	10/28/1993	7.5	7.9	0.4
[2]TTUST-2455-10	10/28/1993	7.1	7.4	0.3
[2]TTUST-2455-11	10/28/1993	7.0	7.3	0.3

Table C5.11. Simulated and observed transient water levels in monitor wells installed during investigations of releases of refined-petroleum products to groundwater and related statistics, Tarawa Terrace and vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina.—Continued

[NGVD 29, National Geodetic Vertical Datum of 1929]

Site name[1]	Measurement date	Simulated water level, in feet above NGVD 29	Observed water level, in feet above NGVD 29	Absolute water-level difference, in feet
[2]TTUST-2455-12	10/28/1993	7.6	8.2	0.6
[2]TTUST-2455-13	10/28/1993	8.4	9.2	0.8
	12/14/1993	8.4	9.2	0.8
[2]TTUST-2455-14	10/28/1993	6.9	7.0	0.1
[2]TTUST-2455-15	10/28/1993	6.1	5.6	0.5
[2]TTUST-2455-16	10/28/1993	7.7	8.3	0.6
[2]TTUST-2455-18	10/28/1993	7.1	7.6	0.5
[2]TTUST-2477-MW01	12/6/1994	9.1	10.0	0.9
[2]TTUST-2477-MW02	12/6/1994	9.1	10.1	1.0
[2]TTUST-2477-MW06	10/26/1994	8.9	10.0	1.1
	12/6/1994	8.9	9.8	0.9
[2]TTUST-2477-MW07	12/6/1994	8.9	9.8	0.9
[2]TTUST-2477-MW08	11/3/1994	8.7	9.8	1.1
	12/6/1994	8.7	9.5	0.8
[2]TTUST-2477-MW09	11/3/1994	8.5	9.5	1.0
	12/6/1994	8.5	9.3	0.8
[2]TTUST-2477-MW10	11/3/1994	7.9	8.8	0.9
	12/6/1994	7.9	8.6	0.7
[2]TTUST-2477-MW11	11/4/1994	8.0	11.6	3.6
	12/6/1994	8.0	8.6	0.6
[2]TTUST-2477-MW12	11/8/1994	7.5	10.0	2.5
	12/6/1994	7.5	8.1	0.6
[2]TTUST-2477-MW13	11/9/1994	7.4	8.1	0.7
	12/6/1994	7.4	8.1	0.7
[2]TTUST-2477-MW14	11/9/1994	7.1	7.9	0.8
	12/6/1994	7.1	7.8	0.7
[2]TTUST-2478-MW08	11/22/1993	10.9	12.6	1.7
	1/9/1994	10.9	12.3	1.4
[2]TTUST-2478-MW09	11/23/1993	9.9	11.8	1.9
	1/9/1994	9.9	11.4	1.5
[2]TTUST-2478-MW10	11/23/1993	9.4	11.4	2.0
	1/9/1994	9.4	11.0	1.6
	12/6/1994	10.0	11.2	1.2
[2]TTUST-2478-MW11	11/29/1993	9.1	9.9	0.8
	1/9/1994	9.1	10.6	1.5
	12/6/1994	9.7	10.9	1.2
[2]TTUST-2478-MW11D	12/15/1993	9.1	11.0	1.9
	1/9/1994	9.1	10.6	1.5
	12/6/1994	9.6	10.8	1.2
[2]TTUST-2478-MW12	12/2/1993	8.3	10.2	1.9
	1/9/1994	8.3	9.7	1.4
	12/6/1994	8.9	9.9	1.0
[2]TTUST-2478-MW13	11/30/1993	9.2	11.1	1.9
	1/9/1994	9.2	10.7	1.5
	12/6/1994	9.8	11.0	1.2

Table C5.11. Simulated and observed transient water levels in monitor wells installed during investigations of releases of refined-petroleum products to groundwater and related statistics, Tarawa Terrace and vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina.—Continued

[NGVD 29, National Geodetic Vertical Datum of 1929]

Site name[1]	Measurement date	Simulated water level, in feet above NGVD 29	Observed water level, in feet above NGVD 29	Absolute water-level difference, in feet
[2]TTUST-2478-MW14	11/30/1993	9.4	11.3	1.9
	1/9/1994	9.4	10.9	1.5
	12/6/1994	10.0	11.2	1.2
[2]TTUST-2478-MW14D	12/16/1993	9.4	11.4	2.0
	1/9/1994	9.4	10.9	1.5
	12/6/1994	10.0	11.2	1.2
[2]TTUST-2478-MW15	11/30/1993	10.0	11.9	1.9
	1/9/1994	10.0	11.6	1.6
[2]TTUST-2478-MW16	12/6/1993	7.9	9.5	1.6
	1/9/1994	8.0	9.1	1.1
	12/6/1994	8.5	9.3	0.8
[2]TTUST-2478-MW17	12/7/1993	7.6	9.1	1.5
	1/9/1994	7.6	8.6	1.0
	12/6/1994	8.1	8.8	0.7
[2]TTUST-2478-MW17D	12/14/1993	7.6	9.1	1.5
	1/9/1994	7.6	8.7	1.1
	12/6/1994	8.1	8.9	0.8
[2]TTUST-2478-MW18	12/7/1993	7.9	9.4	1.5
	1/9/1994	7.9	8.9	1.0
	12/6/1994	8.4	9.2	0.8
[2]TTUST-2478-MW19	12/7/1993	8.4	10.0	1.6
	1/9/1994	8.4	9.6	1.2
	12/6/1994	8.9	9.9	1.0
[2]TTUST-2478-PW01	1/9/1994	10.0	11.6	1.6
[2]TTUST-TTSC-1	12/28/1994	9.5	10.8	1.3
[2]TTUST-TTSC-2	12/28/1994	9.1	10.1	1.0
[2]TTUST-TTSC-3	1/9/1994	8.8	9.6	0.8
	12/28/1994	9.3	10.4	1.1
[2]TTUST-TTSC-4	1/9/1994	9.0	10.4	1.4
	12/28/1994	9.6	11.0	1.4
[2]TTUST-TTSC-5	12/28/1994	9.4	10.6	1.2
[2]TTUST-TTSC-6	12/28/1994	9.2	10.3	1.1
[2]TTUST-TTSC-7	12/28/1994	8.9	9.9	1.0
[2]TTUST-TTSC-8	12/28/1994	9.6	11.1	1.5
[2]TTUST-TTSC-9	12/28/1994	8.3	8.8	0.5
[2]TTUST-TTSC-10	12/28/1994	9.6	11.0	1.4
[2]TTUST-TTSC-13	12/28/1994	9.4	10.6	1.2
[2]TTUST-TTSC-14	12/28/1994	9.0	10.0	1.0
[2]TTUST-TTSC-15	12/28/1994	9.5	11.2	1.7
[2]TTUST-TTSC-16	12/28/1994	9.4	10.5	1.1

[1]See Plate 1 for location

[2]Because of scale, not shown on Plate 1

Statistics:

Average of water-level difference = 1.3 feet
Standard deviation of water-level difference = 0.6 feet
Root-mean-square error of water-level difference = 1.4 feet

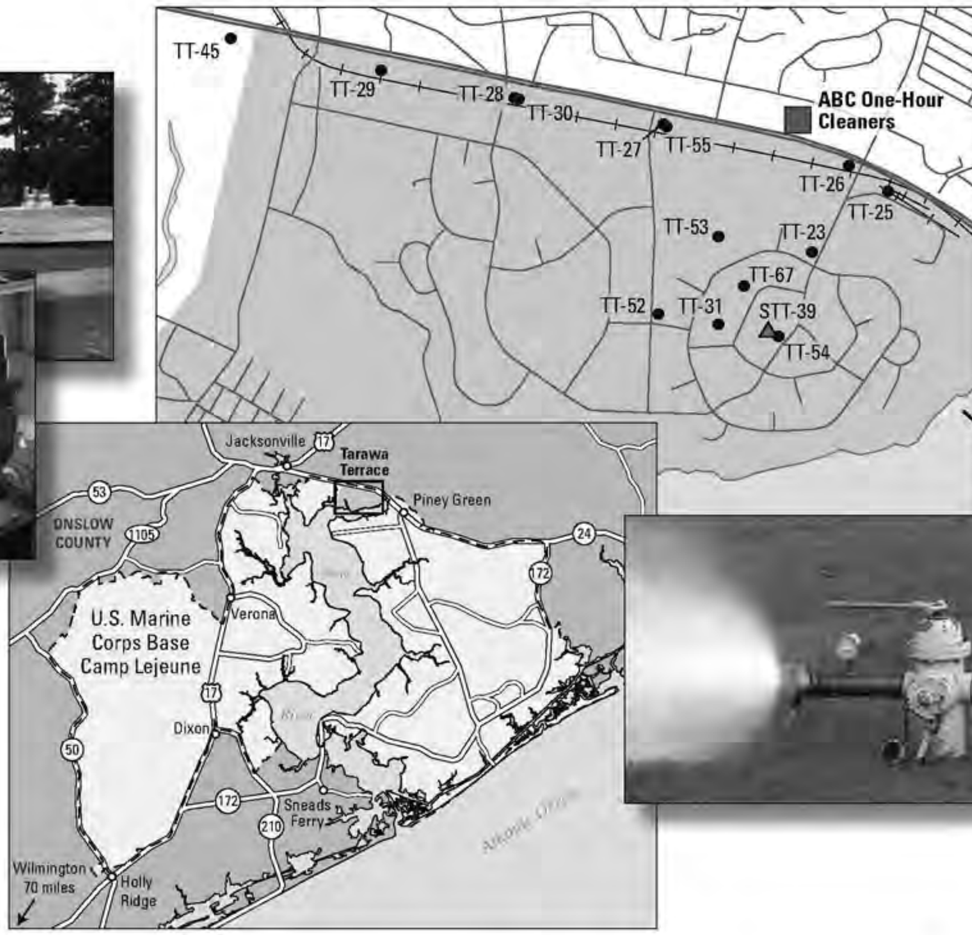
Analyses of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water at Tarawa Terrace and Vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina: Historical Reconstruction and Present-Day Conditions—Chapter C: Simulation of Groundwater Flow

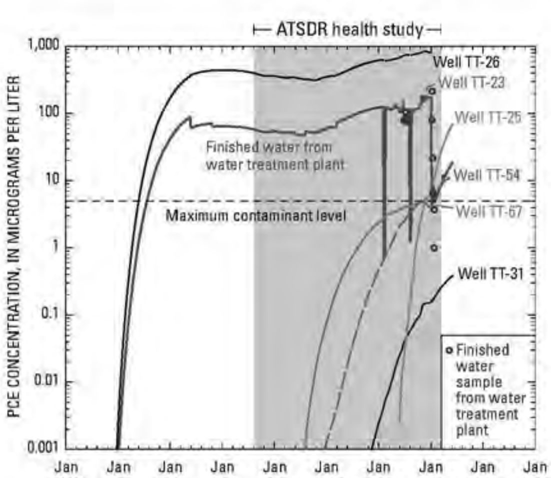
Printed on recycled paper

EXHIBIT 12

Analyses of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water at Tarawa Terrace and Vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina: Historical Reconstruction and Present-Day Conditions

Chapter F: Simulation of the Fate and Transport of Tetrachloroethylene (PCE)





ATSDR
AGENCY FOR TOXIC SUBSTANCES AND DISEASE REGISTRY

Atlanta, Georgia–February 2008

Front cover: Historical reconstruction process using data, information sources, and water-modeling techniques to estimate historical exposures

Maps: U.S. Marine Corps Base Camp Lejeune, North Carolina; Tarawa Terrace area showing historical water-supply wells and site of ABC One-Hour Cleaners

Photographs on left: Ground storage tank STT-39 and four high-lift pumps used to deliver finished water from tank STT-39 to Tarawa Terrace water-distribution system

Photograph on right: Equipment used to measure flow and pressure at a hydrant during field test of the present-day (2004) water-distribution system

Graph: Reconstructed historical concentrations of tetrachloroethylene (PCE) at selected water-supply wells and in finished water at Tarawa Terrace water treatment plant

Analyses of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water at Tarawa Terrace and Vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina: Historical Reconstruction and Present-Day Conditions

Chapter F: Simulation of the Fate and Transport of Tetrachloroethylene (PCE)

By Robert E. Faye

Agency for Toxic Substances and Disease Registry
U.S. Department of Health and Human Services
Atlanta, Georgia

February 2008

Author

Robert E. Faye, MSCE, PE
Civil Engineer/Hydrologist
Robert E. Faye and Associates, Inc.
Consultant to Eastern Research Group, Inc.
Lexington, Massachusetts

For additional information write to:

Project Officer
Exposure-Dose Reconstruction Project
Division of Health Assessment and Consultation
Agency for Toxic Substances and Disease Registry
4770 Buford Highway NE
Mail Stop F59, Room 02-004
Atlanta, Georgia 30341-3717

Suggested citation: Faye RE. Analyses of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water at Tarawa Terrace and Vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina: Historical Reconstruction and Present-Day Conditions—Chapter F: Simulation of the Fate and Transport of Tetrachloroethylene (PCE). Atlanta, GA: Agency for Toxic Substances and Disease Registry; 2008.

Foreword

The Agency for Toxic Substances and Disease Registry (ATSDR), an agency of the U.S. Department of Health and Human Services, is conducting an epidemiological study to evaluate whether in utero and infant (up to 1 year of age) exposures to volatile organic compounds in contaminated drinking water at U.S. Marine Corps Base Camp Lejeune, North Carolina, were associated with specific birth defects and childhood cancers. The study includes births occurring during the period 1968–1985 to women who were pregnant while they resided in family housing at the base. During 2004, the study protocol received approval from the Centers for Disease Control and Prevention Institutional Review Board and the U.S. Office of Management and Budget.

Historical exposure data needed for the epidemiological case-control study are limited. To obtain estimates of historical exposure, ATSDR is using water-modeling techniques and the process of historical reconstruction. These methods are used to quantify concentrations of particular contaminants in finished water and to compute the level and duration of human exposure to contaminated drinking water.

Final interpretive results for Tarawa Terrace and vicinity—based on information gathering, data interpretations, and water-modeling analyses—are presented as a series of ATSDR reports. These reports provide comprehensive descriptions of information, data analyses and interpretations, and modeling results used to reconstruct historical contaminant levels in drinking water at Tarawa Terrace and vicinity. Each topical subject within the water-modeling analysis and historical reconstruction process is assigned a chapter letter. Specific topics for each chapter report are listed below:

- **Chapter A:** Summary of Findings
- **Chapter B:** Geohydrologic Framework of the Castle Hayne Aquifer System
- **Chapter C:** Simulation of Groundwater Flow
- **Chapter D:** Properties and Degradation Pathways of Common Organic Compounds in Groundwater
- **Chapter E:** Occurrence of Contaminants in Groundwater
- **Chapter F:** Simulation of the Fate and Transport of Tetrachloroethylene (PCE) in Groundwater
- **Chapter G:** Simulation of Three-Dimensional Multispecies, Multiphase Mass Transport of Tetrachloroethylene (PCE) and Associated Degradation By-Products
- **Chapter H:** Effect of Groundwater Pumping Schedule Variation on Arrival of Tetrachloroethylene (PCE) at Water-Supply Wells and the Water Treatment Plant
- **Chapter I:** Parameter Sensitivity, Uncertainty, and Variability Associated with Model Simulations of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water
- **Chapter J:** Field Tests, Data Analyses, and Simulation of the Distribution of Drinking Water
- **Chapter K:** Supplemental Information

An electronic version of this report, *Chapter F: Simulation of the Fate and Transport of Tetrachloroethylene (PCE)*, will be made available on the ATSDR Camp Lejeune Web site at *http://www.atsdr.cdc.gov/sites/lejeune/index.html*. Readers interested solely in a summary of this report or any of the other reports should refer to *Chapter A: Summary of Findings* that also is available at the ATSDR Web site.

Contents

Figures

Tables

Conversion Factors

Multiply	By	To obtain
	Length	
inch	2.54	centimeter (cm)
foot (ft)	0.3048	meter (m)
mile (mi)	1.609	kilometer (km)
	Area	
square foot (ft^2)	0.09290	square meter (m^2)
square mile (mi^2)	259.0	hectare (ha)
square mile (mi^2)	2.590	square kilometer (km^2)
acre	0.004047	square kilometer (km^2)
acre	0.4047	hectare (ha)
	Volume	
gallon (gal)	3.785	liter (L)
gallon (gal)	0.003785	cubic meter (m^3)
million gallons (MG)	3,785	cubic meter (m^3)
	Flow rate	
foot per day (ft/d)	0.3048	meter per day (m/d)
foot per year (ft/yr)	0.3048	meter per year (m/yr)
cubic foot per second (ft^3/s)	0.02832	cubic meter per second (m^3/s)
cubic foot per day (ft^3/d)	0.02832	cubic meter per day (m^3/d)
million gallons per day (MGD)	0.04381	cubic meter per second (m^3/s)
inch per year (in/yr)	25.4	millimeter per year (mm/yr)
	Mass	
pound, avoirdupois (lb)	4.535×10^{-4}	gram (g)
pound, avoirdupois (lb)	0.4536	kilogram (kg)
	Hydraulic conductivity	
foot per day (ft/d)	0.3048	meter per day (m/d)
	Transmissivity	
foot squared per day (ft^2/d)	0.09290	meter squared per day (m^2/d)

Concentration Conversion Factors

Unit	To convert to	Multiply by
microgram per liter (µg/L)	milligram per liter (mg/L)	0.001
microgram per liter (µg/L)	milligram per cubic meter (mg/m^3)	1
microgram per liter (µg/L)	microgram per cubic meter ($µg/m^3$)	1,000
parts per billion by volume (ppbv)	parts per million by volume (ppmv)	1,000

Vertical coordinate information is referenced to the National Geodetic Vertical Datum of 1929 (NGVD 29).

Horizontal coordinate information is referenced to the North American Datum of 1983 (NAD 83).

Altitude, as used in this report, refers to distance above the vertical datum.

Glossary and Abbreviations

1,1,1-TCA	1,1,1-trichloroethane
1,1- and 1,2-DCA	1,1- and 1,2-dichloroethane
AKA	also known as
ATSDR	Agency for Toxic Substances and Disease Registry
BTEX	benzene, toluene, ethylbenzene, and xylene
CLP	Clinical Laboratory Program
DCA	dichloroethane
DCE	1,1-DCE 1,1-dichloroethylene or 1,1-dichloroethene 1,2-DCE 1,2-dichloroethylene or 1,2-dichloroethene 1,2-cDCE *cis*-1,2-dichloroethylene or *cis*-1,2-dichloroethene 1,2-tDCE *trans*-1,2-dichloroethylene or *trans*-1,2-dichloroethene
GC/MS	gas chromatograph/mass spectrometer
MCL	maximum contaminant level
MODFLOW	original version of the numerical code for a three-dimensional groundwater-flow model, developed by the U.S. Geological Survey
MODFLOW-96	a three-dimensional groundwater-flow model, 1996 version, developed by the U.S. Geological Survey
MT3DMS	a three-dimensional mass transport, multispecies model developed by C. Zheng and P. Wang on behalf of the U.S. Army Engineer Research and Development Center in Vicksburg, Mississippi
NCDNRCD	North Carolina Department of Natural Resources and Community Development
ND	not detected
PCE	tetrachloroethene, tetrachloroethylene, 1,1,2,2-tetrachloroethylene, or perchloroethylene; also known as PERC® or PERK®
PMWINPro™	Processing MODFLOW Pro, version 7.017
RMS	root mean square
TCE	1,1,2-trichloroethene, 1,1,2-trichloroethylene, or trichloroethylene
USEPA	U.S. Environmental Protection Agency
USGS	U.S. Geological Survey
VOC	volatile organic compound
WTP	water treatment plant

Note: The maximum contaminant level (MCL) is a legal threshold limit set by the USEPA on the amount of a hazardous substance that is allowed in drinking water under the Safe Drinking Water Act; usually expressed as a concentration in milligrams or micrograms per liter. Effective dates for MCLs are as follows: trichloroethylene (TCE) and vinyl chloride (VC), January 9, 1989; tetrachloroethylene (PCE) and *trans*-1,2-dichloroethylene (1,2-tDCE), July 6, 1992 (40 CFR, Section 141.60, Effective Dates, July 1, 2002, ed.)

Analyses of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water at Tarawa Terrace and Vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina: Historical Reconstruction and Present-Day Conditions

Chapter F: Simulation of the Fate and Transport of Tetrachloroethylene (PCE)

By Robert E. Faye[1]

Abstract

Two of three water-distribution systems that have historically supplied drinking water to family housing at U.S. Marine Corps Base Camp Lejeune, North Carolina, were contaminated with volatile organic compounds (VOCs). Tarawa Terrace was contaminated mostly with tetrachloroethylene (PCE), and Hadnot Point was contaminated mostly with trichloroethylene (TCE). Because scientific data relating to the harmful effects of VOCs on a child or fetus are limited, the Agency for Toxic Substances and Disease Registry (ATSDR), an agency of the U.S. Department of Health and Human Services, is conducting an epidemiological study to evaluate potential associations between in utero and infant (up to 1 year of age) exposures to VOCs in contaminated drinking water at Camp Lejeune and specific birth defects and childhood cancers. The study includes births occurring during the period 1968–1985 to women who were pregnant while they resided in family housing at Camp Lejeune. Because limited measurements of contaminant and exposure data are available to support the epidemiological study, ATSDR is using modeling techniques to reconstruct historical conditions of groundwater flow, contaminant fate and transport, and the distribution of drinking water contaminated with VOCs delivered to family housing areas. This report, Chapter F, describes the development and calibration of a digital model applied to the simulation of the fate and transport of tetrachloroethylene (PCE) within the Tarawa Terrace aquifer and Castle Hayne aquifer system at and in the vicinity of the Tarawa Terrace housing area, U.S. Marine Corps Base Camp Lejeune, North Carolina. The analyses and results presented in this chapter refer solely to Tarawa Terrace and vicinity. Future analyses and reports will present information and data about contamination of the Hadnot Point water-distribution system.

[1]Consultant to Eastern Research Group, Inc., Lexington, Massachusetts.

Background

U.S. Marine Corps Base Camp Lejeune is located in the Coastal Plain of North Carolina, in Onslow County, south of the City of Jacksonville and about 70 miles northeast of the City of Wilmington, North Carolina. The major cultural and geographic features of Camp Lejeune are shown in Figure F1 and on [2]Plate 1 (Maslia et al. 2007). A major focus of this investigation is the water-supply and distribution network at Tarawa Terrace, a noncommissioned officers' housing area located near the northwest corner of the base. Tarawa Terrace was constructed during 1951 and was subdivided into housing areas I and II. Areas I and II originally contained a total of 1,846 housing units described as single, duplex, and multiplex, and accommodated a resident population of about 6,000 persons (Sheet 3 of 18, U.S. Marine Corps Base Camp Lejeune, Map of Tarawa Terrace II Quarters, June 30, 1961; Sheet 7 of 34, U.S. Marine Corps Base Camp Lejeune, Tarawa Terrace I Quarters, July 31, 1984). The general area of Tarawa Terrace is bordered on the east by Northeast Creek, to the south by New River and Northeast Creek, and generally to the west and north by drainage boundaries of these streams.

Groundwater is the source of contaminants that occurred in water-distribution networks at Tarawa Terrace and was supplied to the networks via water-supply wells open to one or several water-bearing zones of the Tarawa Terrace aquifer and Castle Hayne aquifer system. Faye (2007) provides a complete description of the geohydrologic framework at and in the vicinity of Tarawa Terrace (Table F1), including data and maps that summarize the geometry of individual aquifers and confining units.

[2] In this report, for any reference to "Plate 1," see the Chapter A report (Maslia et al. 2007). Plate 1 also is available on the ATSDR Camp Lejeune Web site at *http://www.atsdr.cdc.gov/sites/lejeune/docs/Camp_Lejuene_master_plate.pdf*

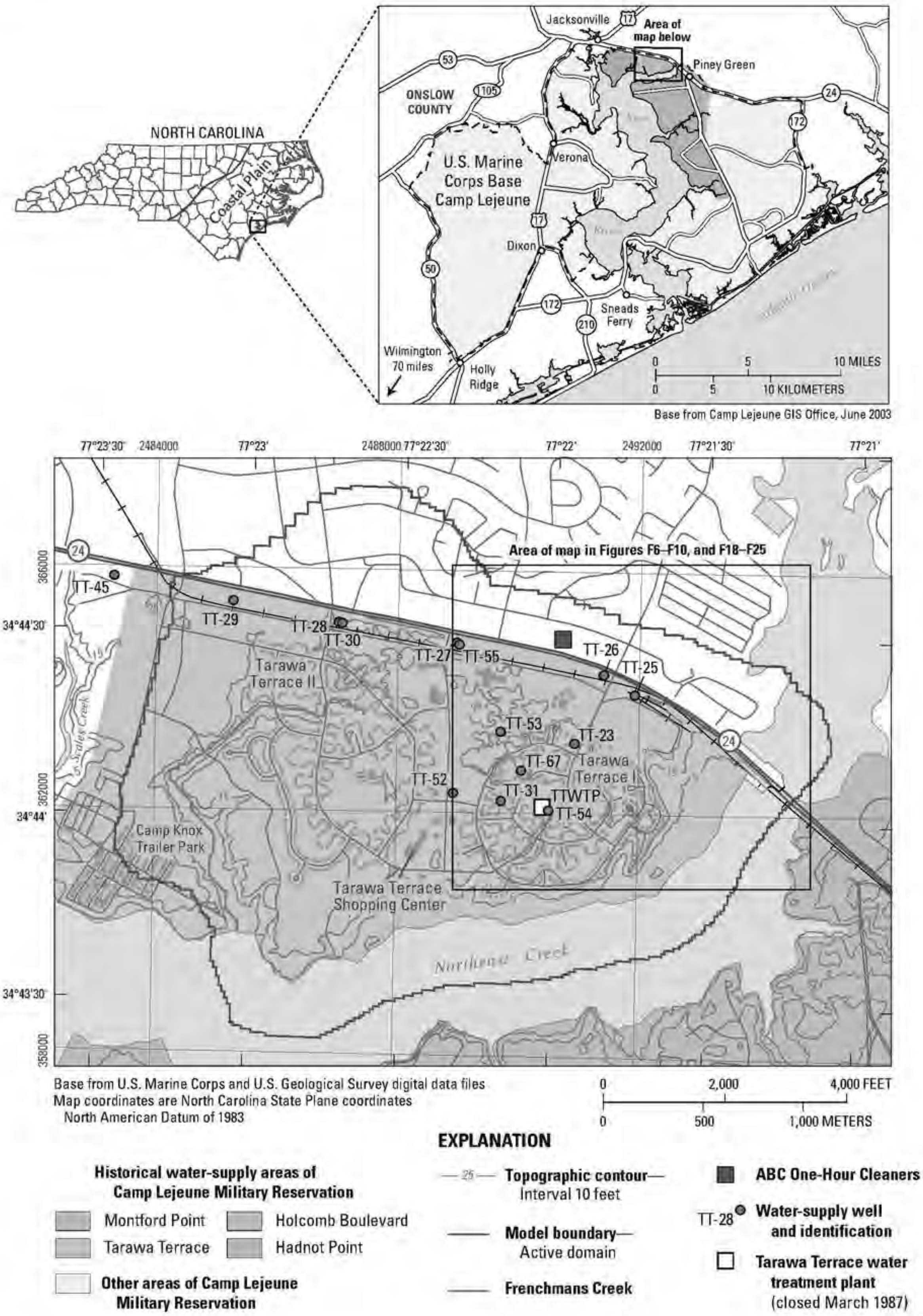


Figure F1. U.S. Marine Corps Base Camp Lejeune, Tarawa Terrace water-supply wells, Tarawa Terrace Shopping Center, and ABC One-Hour Cleaners, Onslow County, North Carolina.

Table F1. Geohydrologic units, unit thickness, and corresponding model layer, Tarawa Terrace and vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina.

[Units are listed shallowest to deepest and youngest to oldest; N/A, not applicable]

Geohydrologic unit	Thickness range, in feet	Model layer
Tarawa Terrace aquifer	8 to 30	1
Tarawa Terrace confining unit	8 to 20	1
Castle Hayne aquifer system		
Upper Castle Hayne aquifer–River Bend unit	16 to 56	1
Local confining unit	7 to 17	2
Upper Castle Hayne aquifer–Lower unit	8 to 30	3
Middle Castle Hayne confining unit	12 to 28	4
Middle Castle Hayne aquifer	32 to 90	5
Lower Castle Hayne confining unit	18 to 30	6
Lower Castle Hayne aquifer	41 to 64	7
Beaufort confining unit	N/A	

Contamination of groundwater by a halogenated hydrocarbon—tetrachloroethylene (PCE)—was first detected in water supplies at Tarawa Terrace during 1982 (Grainger Laboratories, Camp Lejeune water document CLW 0592, written communication, August 10, 1982). The source of contamination was later determined to be ABC One-Hour Cleaners (Figure F1), located on North Carolina Highway 24 (SR 24) and less than a half-mile west and slightly north of several Tarawa Terrace water-supply wells (Shiver 1985, Figure 4). Production at water-supply wells TT-26 and TT-23 (Figure F1) was terminated during February 1985 because of contamination by PCE and related degradation products—trichloroethylene (TCE), and dichloroethylene (DCE) (Table F2). Trichloroethylene degrades to 1,1-dichloroethylene and 1,2-dichloroethylene and its related isomers *trans*-1,2-dichloroethylene (1,2-tDCE), and *cis*-1,2-dichloroethylene, all of which ultimately degrade to vinyl chloride.

Historical reconstruction characteristically includes the application of simulation tools, such as models, to re-create or represent past conditions. At Camp Lejeune, historical reconstruction methods included linking materials mass balance (mixing) and water-distribution system models to groundwater fate and transport models. Groundwater fate and transport models are based to a large degree on groundwater-flow velocities or specific discharges simulated by a groundwater-flow model. The groundwater-flow model is characterized by the vertical and spatial distribution of aquifers and confining units and their respective hydraulic characteristics, such as hydraulic conductivity and specific storage. Calibration of fate and transport models also requires knowledge of temporal, spatial, and vertical occurrences of specific contaminant constituents within the water-bearing units open to water-supply and other observation wells. This report describes the simulation of these contaminant occurrences—to the extent possible—given available data and, based on simulated concentrations, summarizes the occurrence of PCE concentrations within the Tarawa Terrace water-distribution system caused by the migration of PCE in groundwater to Tarawa Terrace water-supply wells.

Purpose and Scope of Study

This study seeks to reasonably simulate the migration of PCE in groundwater from the vicinity of ABC One-Hour Cleaners (Figure F1) to the intrusion of PCE into individual Tarawa Terrace water-supply wells. Concentrations of PCE at Tarawa Terrace water-supply wells are simulated at monthly intervals for their entire period of operation, January 1952 through March 1987.[3] Simulation of PCE migration in groundwater was accomplished by calibrating integrated groundwater-flow and advection-dispersion models. The computation of PCE concentrations in groundwater delivered to the Tarawa Terrace water treatment plant (WTP), and subsequently distributed through a network of pipelines to base housing, also is summarized herein and was accomplished using a flow-weighted mixing model (Masters 1998).

Geologic Framework

Geologic units of interest to this study are those that occur at or near land surface and extend to a depth generally recognized as the base of the Castle Hayne Formation. The lithostratigraphic top of the Castle Hayne Formation has not been definitively identified. In the northern part of Tarawa Terrace, borehole logs collected in conjunction with the drilling of monitor wells by Roy F. Weston, Inc. (1992, 1994) variously identify the top of the Castle Hayne Formation, "Castle Hayne Limestone," or the "Castle Hayne aquifer" at or near the top of the first occurrence of limestone or shell limestone, at depths ranging from about 60 to 70 feet (ft) at most sites but ranging in depth to about 90 ft at one location. Borehole and other drillers' and geophysical logs in the remainder of the study area do not indicate the top of the Castle Hayne Formation. Overlying the limestone or fossiliferous rock in the Roy F. Weston logs is a dark gray silty clay, silt, or sandy silt that ranges in thickness from about 5 to 15 ft. This clay also is identified as a "lean" and sandy clay. For this study, the top of this clay or sandy silt is assigned as the top of the Castle Hayne Formation and is part of a well-recognized, somewhat to highly persistent geohydrologic unit that occurs throughout most of Camp Lejeune east of Northeast Creek (Harned et al. 1989, Sections A–A', B–B', and C–C';

[3]Simulation stress periods and corresponding month and year are listed in Appendix F1

Table F2. Summary of selected analyses for tetrachloroethylene (PCE), trichloroethylene (TCE), and *trans*-1,2-dichloroethylene (1,2-tDCE) in water samples collected at water-supply wells during ABC One-Hour Cleaners Operable Units 1 and 2, by the North Carolina Department of Natural Resources and Community Development, and by the U.S. Navy, Tarawa Terrace and vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina.

[µg/L, microgram per liter; ND, not detected; #, *cis*-1,2-dichloroethylene; —, constituent not determined; J, estimated value]

Site name	Date	PCE concentration, in µg/L	TCE concentration, in µg/L	1,2-tDCE concentration, in µg/L
[1]RW1	7/12/1991	[2]ND	[2]ND	[2]ND#
[1]RW2	7/12/1991	[2]760	[2]ND	[2]ND#
[1]RW3	7/12/1991	[2]ND	[2]ND	[2]ND#
[3,4]TT-23	7/1984	—	[5]37.0	—
	1/16/1985	[6]132	[6]5.8	[6]11.0
	2/12/1985	[6]37.0	[6]1.8	[6]1.9
	2/19/1985	[2]26.2	[2]53.5	[2]Trace
	2/19/1985	[6]ND	[6]ND	[6]13.0
	3/11/1985	**[2]14.9**	**[2]ND**	**[2]ND**
	3/11/1985	**[6]16.0**	**[6]1.3**	**[6]1.2**
	3/12/1985	**[2]40.6**	**[2]ND**	**[2]ND**
	3/12/1985	**[6]48.0**	**[6]2.4**	**[6]2.8**
	4/9/1985	[2]ND	[2]ND	[2]ND
	9/25/1985	[2]4.0	[2]0.2	—
	7/11/1991	[7]ND	[7]ND	[7]ND#
[3]TT-25	7/1984	—	[5]Trace	—
	2/5/1985	[6]ND	[6]ND	[6]ND
	4/9/1985	[2]ND	[2]ND	[2]ND
	9/25/1985	[2]0.43	—	—
	10/29/1985	[6]ND	[6]ND	[6]ND
	11/4/1985	[6]ND	[6]ND	[6]ND
	11/12/1985	[6]ND	[6]ND	[6]ND
	12/3/1985	[6]ND	[6]ND	[6]ND
	7/11/1991	[7]23.0	[7]5.8	[7]1.4J#
[3]TT-26	7/1984	—	[5]3.9	—
	1/16/1985	[6]1,580	[6]57	[6]92.0
	2/12/1985	[6]3.8	[6]ND	[6]ND
	2/19/1985	[2]55.2	[2]3.9	[2]Trace
	2/19/1985	[6]64.0	[6]4.1	[6]9.5
	4/9/1985	[2]630	[2]18.0	[2]1.4
	6/24/1985	[2]1,160	[2]24.0	[2]5
	9/25/1985	[2]1,100	[2]27.0	[2]1.6
	7/11/1991	[7]340	[7]56J	[7]ND#
	7/11/1991	[7]360	[7]62J	[7]15J#
[3]TT-30	2/6/1985	[6]ND	[6]ND	[6]ND
[3]TT-31	2/6/1985	[6]ND	[6]ND	[6]ND
[3]TT-52	2/6/1985	[6]ND	[6]ND	[6]ND
[3]TT-54	2/6/1985	[6]ND	[6]ND	[6]ND
	7/11/1991	[7]ND	[7]ND	[7]ND
[3]TT-67	2/6/1985	[6]ND	[6]ND	[6]ND

[1]See Figure F6 for location
[2]Detection limit = 2 µg/L
[3]See Figure F1 for location
[4]Well TT-23 was operated for 2 hours prior to sampling on 3/11/1985 and 22 hours prior to sampling on 3/12/1985 (**bold**)
[5]Detection limit unknown
[6]Detection limit = 10 µg/L
[7]Detection limit = 5 µg/L

Cardinell et al. 1993, Sections A–A' and B–B'). This unit is designated herein as the Local confining unit. Consequently, contours of equal altitude at the top of the Local confining unit are considered to also approximate the top of the Castle Hayne Formation (Figure F2). As shown, the top of the Castle Hayne Formation occurs near land surface in the northern part of and west of Tarawa Terrace, at altitudes ranging from about –20 to –30 ft, and dips to the east-southeast at a generally uniform rate to the vicinity of Northeast Creek, where the altitude at the top of the formation is less than –50 ft. Harned et al. (1989) and Cardinell et al. (1993) report that the base of the Castle Hayne Formation occurs at the top of the Beaufort Formation, which is capped by a relatively thick unit of clay, silt, and sandy clay. This clay is named in this report the Beaufort confining unit, following similar usage by Harned et al. (1989) and Cardinell et al. (1993), and is a recognizable unit in logs of deep wells at Camp Lejeune.

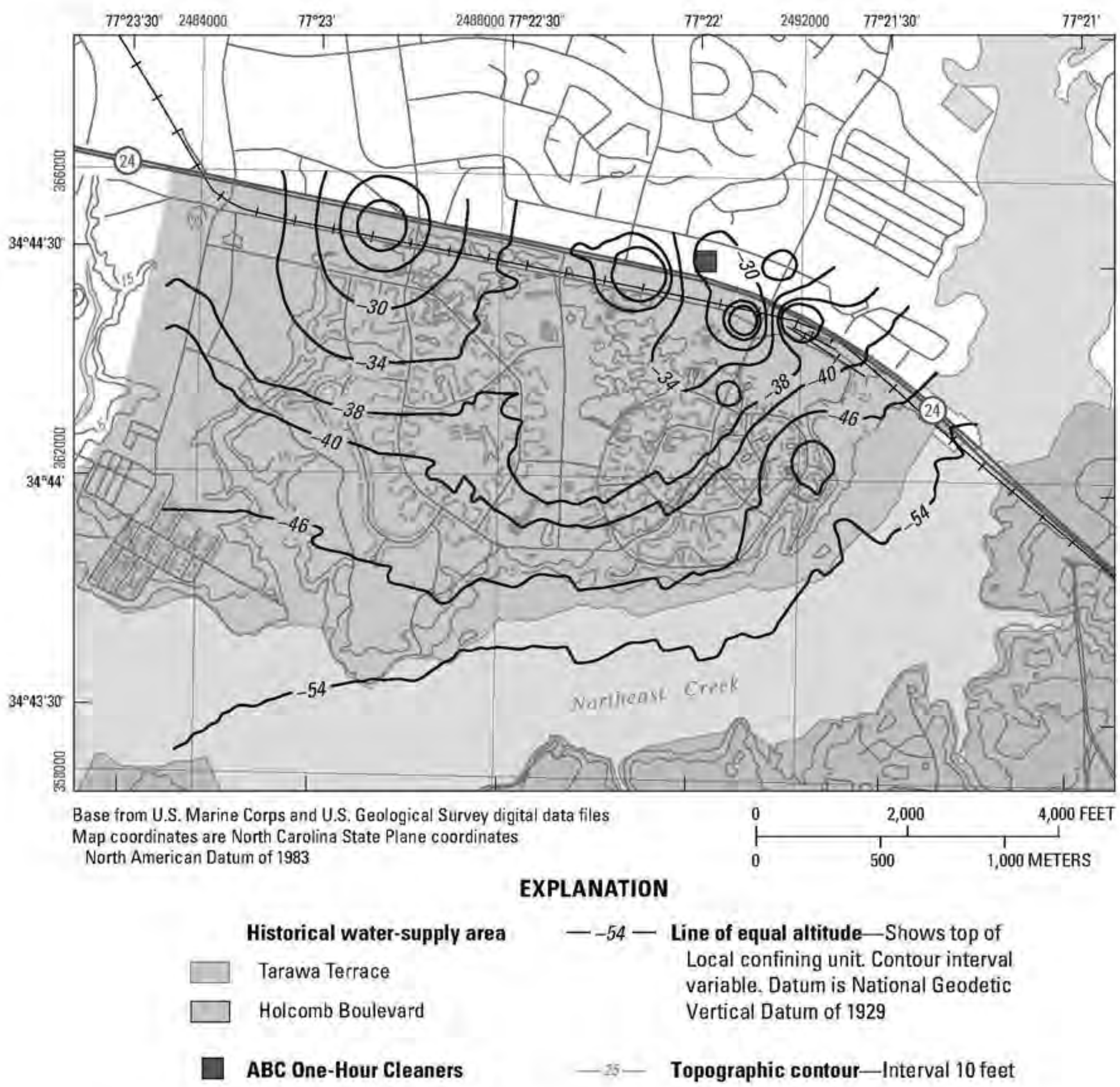


Figure F2. Altitude at the top of the Local confining unit, approximates the lithostratigraphic top of the Castle Hayne Formation, Tarawa Terrace and vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina.

The top of the Beaufort confining unit occurs at about altitude –215 ft in the northern and western parts of the study area and dips gradually to the south and southeast to a minimum altitude of about –250 ft in the vicinity of Northeast Creek (Figure F3). Comparing the maps that show the approximate top and base of the Castle Hayne Formation (Figures F2 and F3), the thickness of the Castle Hayne Formation is shown to range from about 180 ft west of Tarawa Terrace to a maximum thickness of about 200 ft near Northeast Creek (Figure F4). Irregularities of contours shown in Figures F2–F4 are caused by interpolation of the small set of point data used to define the unit altitude or thickness in the study area. The base of the Castle Hayne Formation or the top of the Beaufort confining unit is considered the base of groundwater flow of interest to this study.

In general, the Castle Hayne Formation at Camp Lejeune consists primarily of silty and clayey sand and sandy limestone with interbedded deposits of clay and sandy clay. LeGrand (1959) indicates a "tendency toward layering" with respect to the alternating (with depth) beds of predominantly sandy or clayey sediments. LeGrand (1959) also pointed out that at Tarawa Terrace, Montford Point, and Hadnot Point, the "shellrock is subordinate in quantity to sand" within the Castle Hayne Formation. The sand is fine, often gray in color, and frequently fossiliferous. Much of the limestone is shell limestone, also called "shell hash," "shellrock," or coquina in drillers' logs. Several of the clay deposits, such as the Local confining unit, appear to be continuous and areally extensive (Harned et al. 1989, Sections A–A', B–B'; Cardinell et al. 1993,

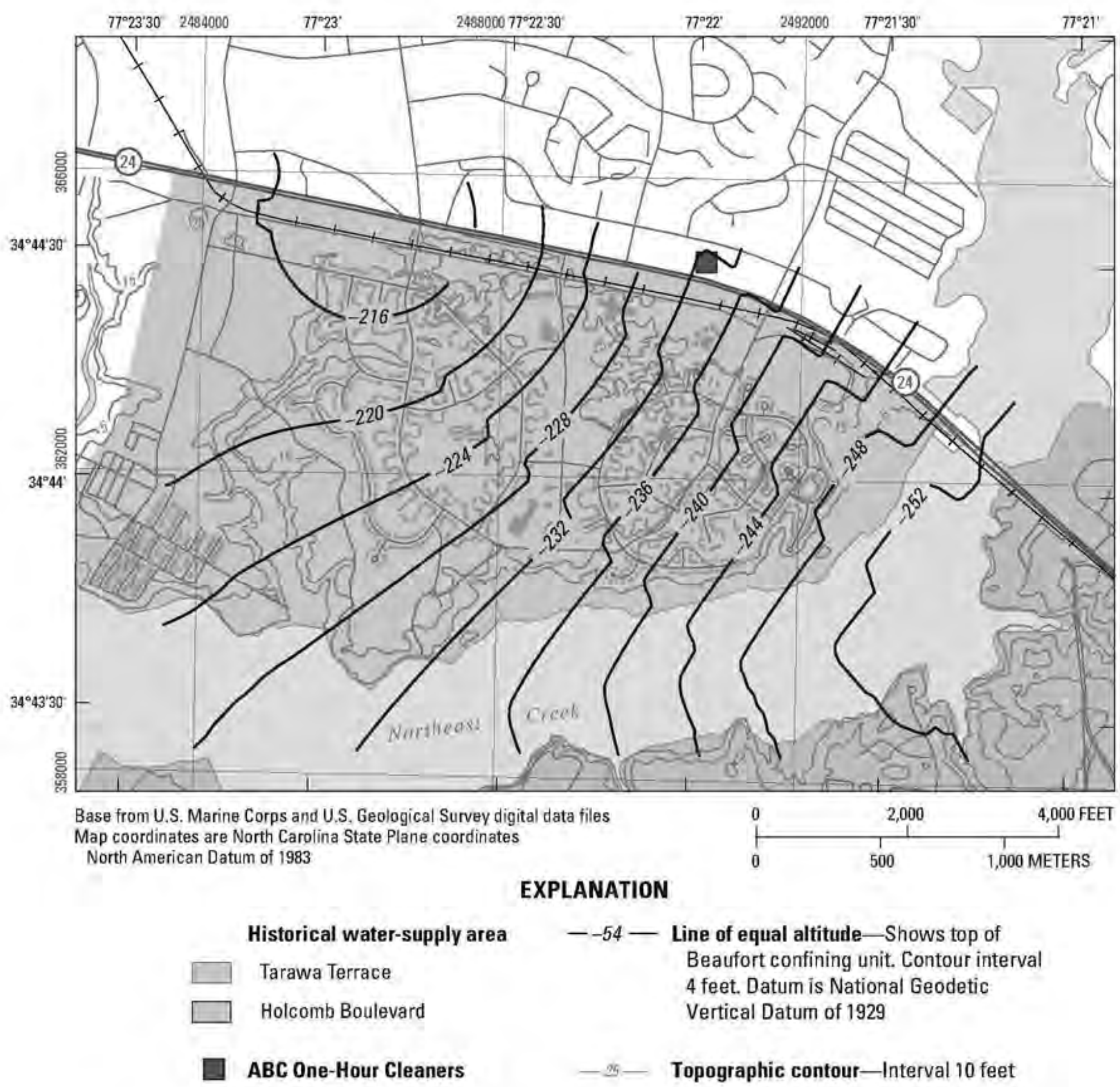


Figure F3. Altitude at the top of the Beaufort confining unit, Tarawa Terrace and vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina.

Sections A–A', B–B') and range in thickness from about 10 ft to more than 30 ft. Lensoidal and discontinuous clay units probably occur frequently. The occurrence of limestone also probably is discontinuous, particularly in the vicinity of Tarawa Terrace. Limestone units of the Castle Hayne Formation at Camp Lejeune are marine and likely were deposited in near-shore environments. Clastic units probably are beach deposits or were formed in deltaic or other near shore transitional environments.

Harned et al. (1989) and Cardinell et al. (1993) assigned an Eocene undifferentiated age to the Castle Hayne Formation, and this age is assigned as well in this report. Similarly, they assigned a Paleocene age to the Beaufort Formation at Camp Lejeune, and this age is adopted as well for this study.

Sediments that occur between land surface and the top of the Castle Hayne Formation are variously referred to as the River Bend Formation of Oligocene age and Belgrade Formation of early Miocene age (Harned et al. 1989; Cardinell et al. 1993). These sediments consist mainly of fine to medium, silty, gray and white sand interbedded with clay and sandy clay. Clays and sands are generally unfossiliferous at Tarawa Terrace but are frequently fossiliferous southeast of Tarawa Terrace in the vicinities of Holcomb Boulevard and Hadnot Point (Plate 1), particularly at depths greater than 30 ft. The base of these units conforms to the top of the Castle Hayne Formation (Figure F2) and dips uniformly to the south and southeast. Unit thickness is zero at land surface and ranges from about 50 to 75 ft within the study area.

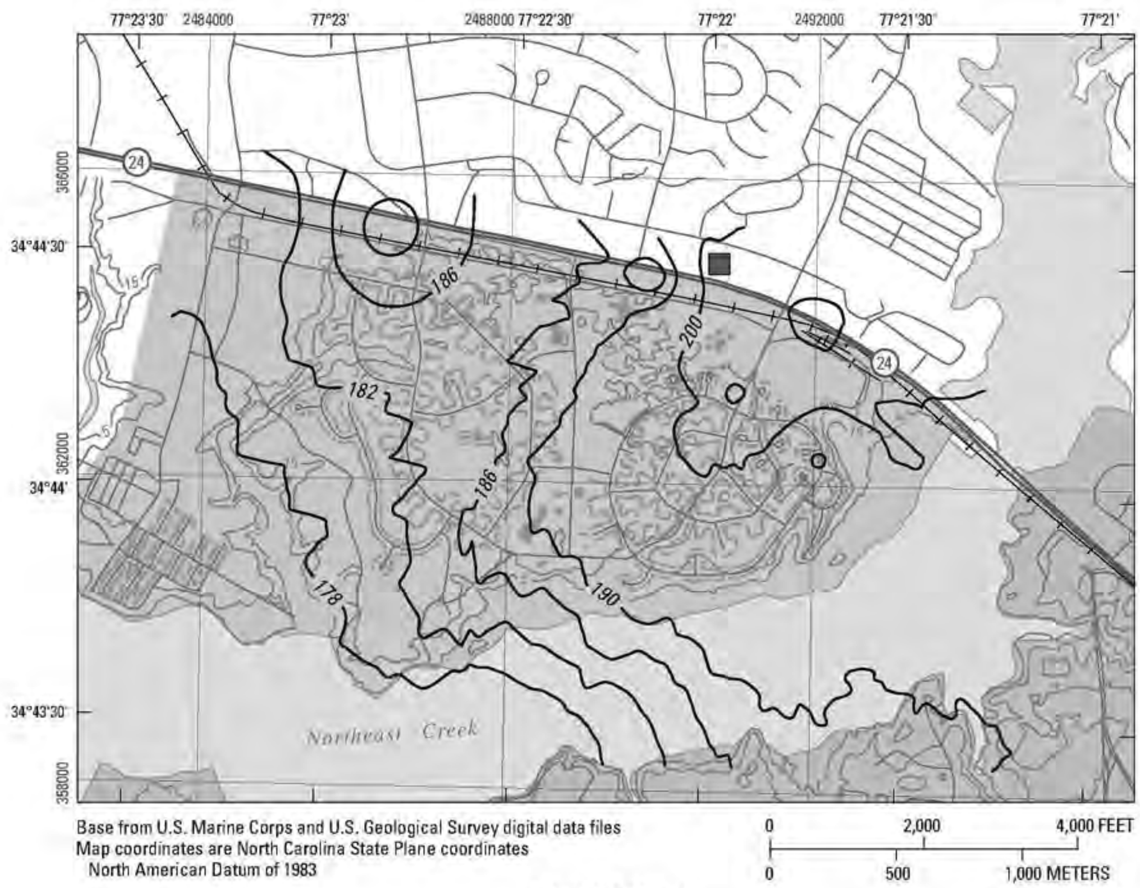


Figure F4. Thickness of the Castle Hayne Formation, Tarawa Terrace and vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina.

Geohydrologic Framework

A total of nine aquifers and confining units that occur between land surface and the top of the Beaufort Formation in the vicinity of Tarawa Terrace were identified and named after local cultural features where the units were first identified or as subdivisions of the Castle Hayne Formation. From shallowest to deepest these units are the Tarawa Terrace aquifer, Tarawa Terrace confining unit, Upper Castle Hayne aquifer–River Bend unit, Local confining unit, Upper Castle Hayne aquifer–Lower unit, Middle Castle Hayne confining unit, Middle Castle Hayne aquifer, Lower Castle Hayne confining unit, and Lower Castle Hayne aquifer (Table F1). The River Bend unit of the Upper Castle Hayne aquifer is so named to conform to the upper part of the "Castle Hayne aquifer" as described by Cardinell et al. (1993). As defined in this study, the River Bend unit probably includes sediments of the Castle Hayne Formation only at the base, if at all. The Local confining unit separates the River Bend and Lower units of the Upper Castle Hayne aquifer and conforms in areal extent and thickness to the silty or sandy clay described previously at the top of the Castle Hayne Formation (Figure F2). The aquifers and confining units ranging from the top of the Upper Castle Hayne aquifer–River Bend unit to the top of the Beaufort confining unit are inclusive of the Castle Hayne aquifer system, as defined for this study. The water table in the northern part of the study area generally occurs near the base of the Tarawa Terrace confining unit or near the top of the Upper Castle Hayne aquifer–River Bend unit. During periods of significant and prolonged rainfall, the water table possibly resides temporarily near the base of the Tarawa Terrace aquifer; however, sediments equivalent to the Tarawa Terrace aquifer are generally unsaturated. Available water-level data from paired wells individually open to the Upper Castle Hayne aquifer–River Bend and Lower units indicate little or no head difference between the aquifers or a slightly downward gradient from the River Bend unit to the Lower unit (Roy F. Weston, Inc. 1992, 1994). In the southern part of the study area, in the vicinity of the Tarawa Terrace Shopping Center, the Tarawa Terrace confining unit is mainly absent and the Tarawa Terrace aquifer and the Upper Castle Hayne aquifer–River Bend unit are undifferentiated. The water table in this area probably occurs consistently within the middle or base of sediments equivalent to the Tarawa Terrace aquifer.

Altitudes at the top of the Local confining unit and the Beaufort confining unit were shown previously in Figures F2 and F3. Point data used for interpolation control when plotting unit top and thickness generally decrease in number and density with unit depth, increasing the subjectivity of interpolated results. Nevertheless, such maps are considered integral elements of the groundwater-flow model necessary for fate and transport simulation and were used to assign layers and layer geometry during flow-model construction. Contour maps showing altitude at the unit top and unit thickness for all flow-model layers and lists of related point data are included in Faye (2007). Most unit surfaces trend to the south and southeast and increase in thickness in the same directions, similar to the contours shown in Figures F2 and F3. The tops of most units exhibit a moderate to high degree of irregularity at one or several locations and probably at one or several times following their deposition were erosional surfaces, exposed to the effects of rain, ice, runoff, weathering, dissolution, and similar agents. Accordingly, surface irregularities may represent relict stream channels or hilltops. Where a unit is mainly limestone in composition, surface irregularities possibly represent the remnants of a karst terrain such as sinkholes or related solution or fracture features.

Previous Investigations

Discussions of previous investigations in this report are limited mainly to summaries of remedial investigations of PCE-contaminated groundwater at and in the immediate vicinity of ABC One-Hour Cleaners and within the northern part of the Tarawa Terrace housing area. Summaries of similar investigations for benzene and toluene in the vicinity of the Tarawa Terrace Shopping Center (Figure F1) and elsewhere within the Tarawa Terrace housing areas can be found in Faye (2007), Faye and Green (2007), and Faye and Valenzuela (2007). These reports summarize, as well, the results of investigations of the geohydrologic framework, groundwater contamination, and simulations of groundwater flow within the study area (Figure F1).

During August 1982, routine gas chromatograph/mass-spectrometer (GC/MS) analyses for trihalomethane in water samples collected from the Tarawa Terrace and Hadnot Point WTPs (Plate 1) at U.S. Marine Corps Base Camp Lejeune were interrupted by interference from constituents in the water samples thought to be halogenated hydrocarbons (Grainger Laboratories, Camp Lejeune water document CLW 0592, written communication, August 10, 1982; Elizabeth A. Betz, written communication, August 19, 1982; AH Environmental Consultants, Inc., written communication, June 18, 2004; Camp Lejeune water documents CLW 0592–0595 and 0606–0607). Subsequent analyses confirmed the presence of PCE in samples of finished water supplies from both locations ranging in concentration from 76 to 104 micrograms per liter (μg/L) at Tarawa Terrace and from 15 μg/L to not detected (ND) at Hadnot Point. Concentrations of TCE determined in samples from the Hadnot Point WTP ranged from 19 to 1,400 μg/L. Samples analyzed were collected during May and July 1982 (Faye and Green 2007, Table E12).

During July 1984, routine sampling and analyses of community water-supply wells at Camp Lejeune, as a part of the Base Naval Assessment and Control of Installation Pollutants Program, indicated the occurrence of TCE in samples obtained from water-supply wells TT-23 (37 μg/L), TT-25 (trace), and TT-26 (3.9 μg/L) (Maslia et al. 2007). Well TT-26 was open only to the Upper Castle Hayne aquifer, whereas wells TT-23 and TT-25 were open to both the Upper and Middle Castle Hayne aquifers (Faye and Green 2007, Table E2).

Beginning during January and continuing into September 1985, the North Carolina Department of Natural Resources and Community Development (NCDNRCD) periodically sampled water-supply wells TT-23, TT-25, and TT-26 and water treated at the Tarawa Terrace WTP for PCE and its degradation products, TCE, DCE, and vinyl chloride (McMorris 1987). On occasion, duplicate samples were analyzed by NCDNRCD and JTC Environmental Consultants, Inc. (Shiver 1985; R.A. Tiebout, Memorandum for the Commanding General, Chief of Staff, written communication, November 6, 1985; J.R. Bailey to U.S. Environmental Protection Agency, written communication, April 25, 1986; Camp Lejeune water documents CLW 1338–1339 and 1475–1483). Concentrations of PCE in samples from well TT-26 ranged from an estimated 3.8 to 1,580 μg/L in seven samples collected during this period (Table F2). Concentrations of PCE in 10 samples from well TT-23 ranged from "not detected" to 132 μg/L. Concentrations also were detected of TCE, 1,2-tDCE, and vinyl chloride. Tarawa Terrace water-supply wells TT-30, TT-31, TT-52, TT-54, and TT-67 (Figure F1) also were sampled once during this period, and subsequent analyses detected no concentrations of PCE or related degradation products above detection limits at these wells (JTC Environmental Consultants Report 85-047, Report 19, written communication, February 5–6, 1985). However, JTC Environmental Consultants detected benzene at a concentration of 6.3 μg/L in a sample collected at well TT-23 on February 19, 1985 (JTC Environmental Consultants Report 85-072, Report 37, written communication, March 1, 1985). An estimated concentration of PCE of 0.43 μg/L was determined in a sample from well TT-25 during September 1985 (Table F2). Results of sampling and analyses for volatile organic compounds (VOCs) during January and February 1985 caused wells TT-23 and TT-26 to be removed from service during February 1985. Well TT-26 was permanently closed at that time; however, well TT-23 was used to deliver water to the Tarawa Terrace WTP for several days during March and April 1985 (Camp Lejeune water document CLW 1182; Camp Lejeune water document CLW 1193, "Direction to Operators at Tarawa Terrace," April 30, 1985; Camp Lejeune water document CLW 1194, "Procedures for operating the 'New Well' at Tarawa Terrace," date unknown). At the time of discovery of PCE and related contaminants at Tarawa Terrace water-supply wells, the Tarawa Terrace WTP provided drinking water to about 6,200 people in the service area (McMorris 1987). A summary of analyses of water samples collected at Tarawa Terrace and nearby water-supply wells is listed in Table F2. Location coordinates of Tarawa Terrace and nearby water-supply wells are listed in Table F3.

During April 1985, the NCDNRCD began a field investigation to determine the source or sources of PCE and related constituents occurring in water-supply wells TT-23 and TT-26. Samples were collected at these wells and at well TT-25 for analyses of VOCs. Three monitor wells were installed in the "Water Table aquifer" northwest of well TT-26 and parallel to SR 24 to collect additional samples and water-level data (Shiver 1985; wells X24B4, X24B5, and X24B6 [shown in Figure F6 and on Plate 1 as B4, B5, and B6, respectively]) (Table F5). Results of analyses of samples collected at supply and monitor wells were sufficient to delineate a highly generalized plume of PCE in groundwater of the aquifer. The northwest apex of the plume was located at monitor well X24B6, immediately opposite the entrance of ABC One-Hour Cleaners at 2127 Lejeune Boulevard (SR 24). The PCE concentration determined in the sample from this well was 12,000 μg/L. These and ancillary water-level data indicating the direction of groundwater flow to the southeast toward well TT-26 pinpointed ABC One-Hour Cleaners as the source of PCE in Tarawa Terrace water-supply wells (Shiver 1985, Figure 4).

Table F3. Location coordinates of water-supply wells, Tarawa Terrace and vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina.

[AKA, also known as]

Site name	Location coordinates[1]	
	North	East
[2]2A	364625	2489025
[3]RW1	365150	2489880
[3]RW2	364930	2490770
[3]RW3	364170	2493350
[4]#6	369730	2481720
[4]#7	370500	2481530
[5]TT-23	363208	2491024
[5]TT-25	364042	2491984
[5]TT-26, AKA #1	364356	2491461
[5]TT-27, AKA #2B	364794	2489026
[5]TT-28, AKA #3	365058	2487071
[5]TT-29, AKA #4	365352	2485328
[5]TT-30, AKA #13	365044	2487130
[5]TT-31, AKA #14	362224	2489843
[5]TT-45, AKA #5	365688	2483352
[5]TT-52, AKA #9	362321	2489060
[5]TT-53, AKA #10	363360	2489800
[5]TT-54, AKA #11	362090	2490630
[5]TT-55, AKA #8	364767	2489070
[5]TT-67, AKA #12	362730	2490160

[1]Location coordinates are North Carolina State Plane coordinates, North American Datum of 1983

[2]See Plate 1 in the Chapter A report (Maslia et al. 2007) for location. Plate 1 also is available on the ATSDR Camp Lejeune Web site at *http://www.atsdr.cdc.gov/sites/lejeune/docs/Camp_Lejeune_master_plate.pdf*

[3]See Figure F6 for location

[4]Out of map area, location not shown. North Carolina State Plane coordinates: #6 (highly approximate) North 369730, East 2481720; #7 (highly approximate) North 370500, East 2481530; and TT-45 North 365688, East 2483352

[5]See Figure F1 for location

Table F4. Summary of selected analyses for tetrachloroethylene (PCE) in soil samples collected at ABC One-Hour Cleaners by Law Engineering and Testing Company, Inc., and during ABC One-Hour Cleaners Operable Units 1 and 2.

[µg/kg, microgram per kilogram; ND, not detected; detection limits are unknown; data source: Roy F. Weston 1994, Table 2-4, Figures 2-4, 3-1, and 5-2]

Site name	Location coordinates[1]		Date	Sample depth, in feet	PCE concentration, in µg/kg
	North	East			
[2]Law #3	364918	2490707	9/10/1986	8.00	5,900
[2]Law #9	364932	2490717	9/10/1986	4.00	106,000
				8.00	450,000
				12.00	22,000
				16.00	12,000
[2]Law #10	364927	2490703	9/10/1986	4.00	1,300
				8.00	110
[2]Law #11	364927	2490731	9/10/1986	4.00	450,000
				8.00	170,000
[2]Law #12	364918	2490717	9/10/1986	4.00	720,000
				8.00	860,000
				10.00	820,000
[2]Law #13	364914	2490731	9/10/1986	4.00	630,000
				8.00	260,000
[2]Law #14	364906	2490731	9/10/1986	4.00	24,000
				8.00	280,000
[2]Law #15	364901	2490724	9/10/1986	4.00	12,000
				8.00	18,000
[2]Law #17	364893	2490719	9/10/1986	4.00	5,600
				8.00	5,800
[2]Law #18	364901	2490707	9/10/1986	4.00	17,000
				8.00	6,000
[3]SB-1	364874	2490691	6/26/1991	6.00	640
				10.00	37
				14.00	440
[3]SB-2	364930	2490697	6/26/1991	2.00	10
				6.00	19
				10.00	27
				14.00	ND
[3]SB-3	364981	2490754	6/27/1991	6.00	ND
				10.00	ND
				14.00	ND
[3]SB-4	364985	2490736	6/27/1991	12.00	ND
				16.00	ND
[3]SB-5	364795	2490714	6/27/1991	6.00	3
				12.00	ND
[3]SB-6	364798	2490696	6/27/1991	12.00	ND
				14.00	ND
[3]SB-10	364857	2490750	6/30/1991	6.00	2,100
				10.00	210
				14.00	90
[3]SB-12	364922	2490767	6/30/1991	4.00	ND
				6.00	ND
				12.00	ND
[2]SB-13	364841	2490658	9/9/1993	1.00	ND
				4.00	ND
				9.00	ND
				14.00	ND
[2]SB-14	364930	2490664	9/9/1993	1.00	90
				4.00	570
				9.00	210
				14.00	ND
[3]SB-15	364938	2490675	9/9/1993	1.00	20
				4.00	ND
				9.00	ND
				14.00	ND
[2]SB-16	364855	2490726	9/10/1993	1.00	49,000
				4.00	27,000
				9.00	200
				14.00	390

Table F4. Summary of selected analyses for tetrachloroethylene (PCE) in soil samples collected at ABC One-Hour Cleaners by Law Engineering and Testing Company, Inc., and during ABC One-Hour Cleaners Operable Units 1 and 2.—Continued

[µg/kg, microgram per kilogram; ND, not detected; detection limits are unknown; data source: Roy F. Weston 1994, Table 2-4, Figures 2-4, 3-1, and 5-2]

Site name	Location coordinates[1]		Date	Sample depth, in feet	PCE concentration, in µg/kg
	North	East			
[2]SB-17	364834	2490744	9/12/1993	1.00	14
				4.00	1,400
				9.00	650
				14.00	1,400
[2]SB-18	364859	2490753	9/12/1993	1.00	2,100,000
				4.00	110,000
				9.00	Not sampled
				14.00	Not sampled
[2]SB-19	364886	2490731	9/15/1993	1.00	300,000
				4.00	4,900
				9.00	16
				14.00	5,100
[2]SB-20	364918	2490695	9/16/1993	1.00	56
				4.00	Not sampled
				9.00	Not sampled
				14.00	Not sampled
[2]SB-21	364859	2490703	9/16/1993	1.00	170
				4.00	Not sampled
				9.00	Not sampled
				14.00	Not sampled
[2]SB-22	364909	2490705	9/17/1993	1.00	580,000
				4.00	210,000
				9.00	26,000
				14.00	2,900
[2]SB-23	364933	2490738	9/18/1993	1.00	41,600
				4.00	120
				9.00	20
				14.00	44
[3]SB-24	364889	2490752	9/21/1993	1.00	ND
				4.00	ND
				9.00	ND
				14.00	ND
[3]SPM1	364906	2490730	9/17/1993	1.00	49,000
				4.00	7,500
				9.00	7,100
				14.00	8,900
[3]SPM2	364910	2490730	9/15/1993	1.00	4,400
				4.00	14,000
				9.00	15,000
				14.00	6,000
[3]SPM5	364902	2490716	9/14/1993	1.00	43,000
				4.00	11,000
				9.00	3,000
				14.00	13,000
[3]V1	364899	2490730	9/17/1993	1.00	Not sampled
				4.00	Not sampled
				9.00	33,000
				14.00	180,000
[3]V2	364929	2490730	9/17/1993	1.00	180,000
				4.00	5,400
				9.00	2,300
				14.00	800

[1]Location coordinates are North Carolina State Plane coordinates, North American Datum of 1983

[2]Roy F. Weston, Inc. 1994, Table 2-4, Figure 2-4

[3]See Figure F5 for location

Table F5. Summary of selected analyses for tetrachloroethylene (PCE), trichloroethylene (TCE), and total dichloroethylene (DCE) in water samples collected at monitor wells during ABC One-Hour Cleaners Operable Units 1 and 2 and by the North Carolina Department of Natural Resources and Community Development, Tarawa Terrace and vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina.

[µg/L, microgram per liter; ND, not detected; J, estimated value; #, *cis*-1,2-dichloroethylene; —, constituent not determined]

Site name[1]	Date	Concentration, in µg/L		
		PCE	TCE	Total DCE
C1	4/24/1992	ND	ND	ND
	9/21/1993	ND	ND	ND
C2	4/23/1992	1J	3J	9J
	10/21/1993	ND	ND	ND
C3	4/29/1992	7J	28	14
	9/23/1993	120	43	21
C4	4/22/1992	ND	ND	ND
	9/22/1993	ND	ND	ND
C5	4/23/1992	ND	17J	ND
	9/22/1993	ND	ND	ND
C9	9/1/1993	0.2J	0.1J	NA
C10	9/1/1993	4.8J	ND	ND
C11	9/1/1993	0.64J	ND	ND
S1	4/24/1992	10	ND	ND
	9/20/1993	27	0.6J	0.2J#
S2	4/23/1992	880	690	1,200
	10/21/1993	490	280	467
S3	4/29/1992	5,400	640	1,200
	9/23/1993	380	24	46J
S4	4/22/1992	ND	ND	ND
	9/20/1993	ND	ND	—
S5	4/23/1992	3	3	ND
	9/22/1993	0.8J	ND	—
S6	4/29/1992	4J	ND	ND
	9/29/1993	0.5J	0.1J	—
S7	4/28/1992	ND	ND	ND
	9/28/1993	0.2J	ND	ND
S8	4/24/1992	ND	ND	ND
	9/28/1993	ND	ND	ND
S9	4/22/1992	ND	ND	ND
	9/23/1993	ND	ND	ND
S10	4/28/1992	ND	ND	ND
	9/22/1993	ND	ND	—
S11	9/29/1993	0.3J	46	ND
[2]X24B4	9/25/1985	2.2	—	—
[2]X24B5	9/25/1985	4.9	0.98	—
[2]X24B6	9/25/1985	12,000	2.7	—

[1]See Figure F6 for location

[2]See Plate 1, Chapter A report, for location (Maslia et al. 2007). X24B4, X24B5, and X24B6 are shown as B4, B5, and B6, respectively

Detection limit at "C" and "S" sites = 10 µg/L, 5 µg/L, or 1 µg/L

Detection limit at "X24" sites = 2 µg/L

ABC One-Hour Cleaners always used PCE in its dry-cleaning operations, beginning during 1953 when the business opened (Hopf & Higley, P.A., Deposition of Victor John Melts, written communication, April 12, 2001). A primary pathway of contaminants from the dry-cleaning operations at ABC One-Hour Cleaners to the soil and subsequently to groundwater was apparently through a septic tank–soil absorption system to which ABC One-Hour Cleaners discharged waste and wastewater. Shiver (1985) reported that an inspection of the PCE storage area at ABC One-Hour Cleaners indicated that PCE releases could and did enter the septic system through a floor drain, probably as a result of spillage in the storage area (Roy F. Weston, Inc. 1994). In addition, spent PCE was routinely reclaimed using a filtration-distillation process that produced dry "still bottoms" which, until about 1982 (Hopf & Higley, P.A., Deposition of Victor John Melts, written communication, April 12, 2001) or 1984/1985 (McMorris 1987), were disposed of onsite, generally by filling potholes in a nearby alleyway. When ABC One-Hour Cleaners totally discontinued the use of the floor drain and the onsite disposal of still bottoms is not known exactly, but such practices probably terminated completely during 1985.

The disposal of dry-cleaning solvents to the septic system and subsequently to groundwater placed ABC One-Hour Cleaners in violation of various State laws and statutes. During January 1986, the owners were ordered by the State of North Carolina to cease such disposal and propose a plan to restore the quality of affected groundwater to an acceptable level as determined by the State (Roy F. Weston, Inc. 1994). Pursuant to this plan, ABC One-Hour Cleaners hired Law Engineering and Testing Company, Inc., to investigate the septic tank and the surrounding soil for contaminant content. Samples collected and analyzed by Law Engineering and Testing Company, Inc., indicated PCE concentrations of the septic tank sludge were as high as 1,400 milligrams per liter (mg/L) and that soil 4 ft below the tank contained PCE concentrations as high as 400 milligrams per kilogram (mg/kg) (Law Engineering and Testing Company, Inc. 1986a; Roy F. Weston, Inc. 1992). Subsequently, Law Engineering and Testing Company, Inc., conducted additional investigations to determine the vertical and horizontal extent of contamination within the soil profile. These investigations were completed by December 1986 and indicated the depth of PCE contamination in the vicinity of the septic tank to be in excess of 16 ft. PCE concentration at a depth of 8 ft was 860 mg/kg (Law Engineering and Testing Company, Inc. 1986b; Roy F. Weston, Inc. 1992). A summary of PCE concentrations in soil in the vicinity of ABC One-Hour Cleaners is listed in Table F4.

By March or April 1987, all water-supply wells at Tarawa Terrace were removed from service. During March 1989, the ABC One-Hour Cleaners site was placed on the U.S. Environmental Protection Agency's (USEPA) National Priority List (Final List). During June 1990, USEPA hired Roy F. Weston, Inc., to conduct a remedial investigation at the site aimed at determining the areal and vertical extent of contaminant plumes (Operable Unit 1) and characterizing the source of contaminants in the unsaturated soils beneath and in the vicinity of the septic disposal system at ABC One-Hour Cleaners (Operable Unit 2) (Roy F. Weston, Inc. 1992, 1994).

Operable Unit 1 of the remedial investigation included the installation of eight soil borings to depths ranging from 16 to 20 ft surrounding and in the immediate vicinity of ABC One-Hour Cleaners (SB-1–SB-6, SB-10, and SB-12; Figure F5, Table F4). These borings occurred entirely within the unsaturated zone. Ten shallow and five deep monitor wells also were installed during Operable Unit 1, not only in the immediate vicinity of ABC One-Hour Cleaners but northwest of the site as well as proximate to water-supply wells TT-25 and TT-26. Several monitor wells also were located between SR 24 (Lejeune Boulevard) and the Tarawa Terrace housing area (Figure F6). The shallow wells, S1–S10, were constructed to depths ranging from 28 to 40 ft and were open at the base of the well to the Upper Castle Hayne aquifer–River Bend unit (Faye 2007). Four of the deep wells—C1, C2, C3, and C5—ranged in depth from about 90 to 100 ft and were open at the base to the Upper Castle Hayne aquifer–Lower unit. Well C4 was constructed to a depth of about 200 ft and was open to the Middle Castle Hayne aquifer.

Operable Unit 2 included the construction of an additional shallow well (S11) about 1,000 ft northwest of ABC One-Hour Cleaners. Two additional deep wells, C9 and C10, were constructed east and south of the cleaners. An additional well, C11, was located in the northeast part of the Tarawa Terrace housing area (Figure F6). Depths of the additional deep wells ranged from about 75 to 175 ft. Wells C9 and C11 were open to the Upper Castle Hayne aquifer–Lower unit. Well C10 was open to the Middle Castle Hayne aquifer. Also installed as part of Operable Unit 2 were six piezometers, three shallow (PZ-02, -04, -06) and three deep (PZ-01, -03, -05), in the immediate vicinity of ABC One-Hour

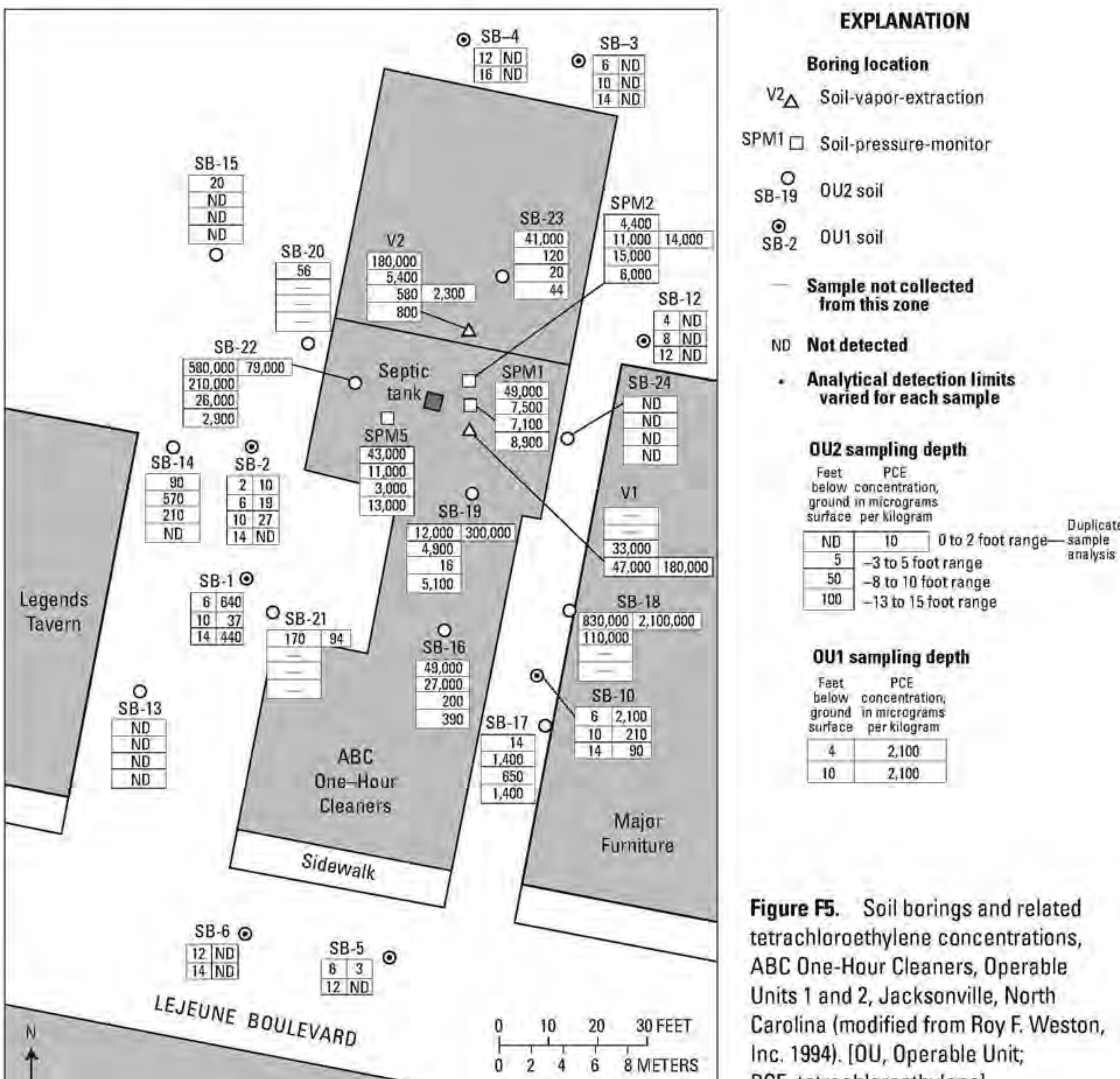
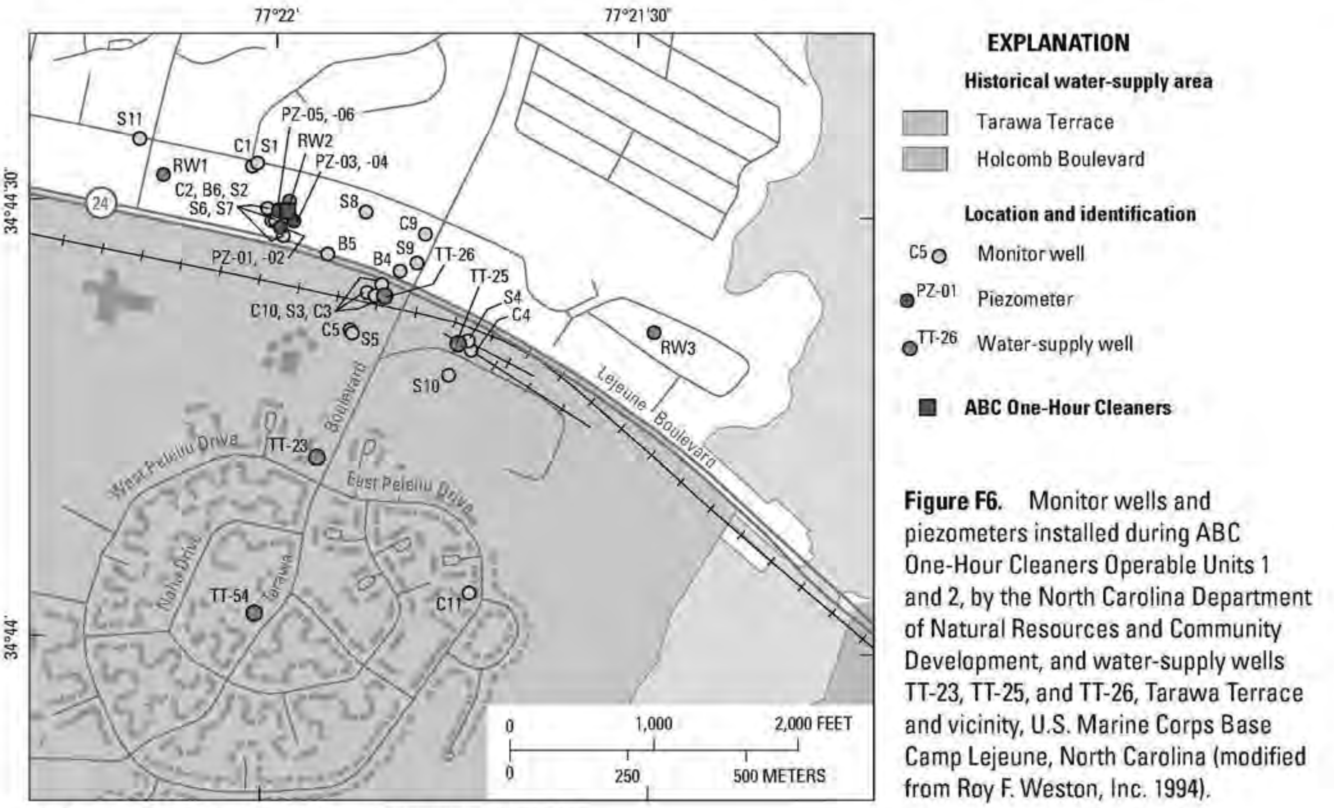


Figure F5. Soil borings and related tetrachloroethylene concentrations, ABC One-Hour Cleaners, Operable Units 1 and 2, Jacksonville, North Carolina (modified from Roy F. Weston, Inc. 1994). [OU, Operable Unit; PCE, tetrachloroethylene]



Base from U.S. Marine Corps and U.S. Geological Survey digital data files

Figure F6. Monitor wells and piezometers installed during ABC One-Hour Cleaners Operable Units 1 and 2, by the North Carolina Department of Natural Resources and Community Development, and water-supply wells TT-23, TT-25, and TT-26, Tarawa Terrace and vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina (modified from Roy F. Weston, Inc. 1994).

Cleaners and open to the Upper Castle Hayne aquifer–River Bend and Lower units, respectively. The depths of PZ-02, -04, and -06 ranged from 29.5 to 34.5 ft. Depths of PZ-01, -03, and -05 ranged from 74.5 to 79.5 ft.

Results of analyses of periodic water samples obtained from monitor wells during Operable Units 1 and 2 are summarized in Table F5. Concentrations of PCE ranged from not detected at several wells to 5,400 µg/L at well S3. Samples from monitor wells also were analyzed for various metals and semivolatile compounds. Location coordinates of monitor wells and piezometers constructed during Operable Units 1 and 2 are listed in Table F6.

During Operable Unit 2, similar constituent analysis schedules were used during analyses of effluent from the septic tank at ABC One-Hour Cleaners and of soil samples obtained from the unsaturated zone in the vicinity of the tank. The PCE concentration in the tank effluent was 6,800 µg/L during June 1991. Concentrations of PCE in soil borings at various depths in the immediate vicinity of ABC One-Hour Cleaners ranged from not detected to more than 2,000,000 micrograms per kilogram (µg/kg) (Figure F5, Table F4).

Deep monitor wells C1–C5 were paired with their respective shallow well counterparts S1–S5. Piezometers with odd and even numbers were likewise paired, in an effort to determine vertical hydraulic gradients. Water levels at paired wells and piezometers were measured to hundredths of a foot periodically during 1992 and 1993. Vertical head gradients were downward at all paired wells at all times with the exception of slightly upward gradients at piezometer sites PZ-01/-02 and PZ-03/-04 during November 1993. A maximum head difference of 2.23 ft occurred at paired wells S1/C1 during April 1992. Head differences between the Upper Castle Hayne aquifer–River Bend unit and the Middle Castle Hayne aquifer were always less than 2 ft. These and similar water-level measurements at all monitor wells were used to map local potentiometric surfaces in the vicinity and downgradient of ABC One-Hour Cleaners. Potentiometric surface maps of the Upper Castle Hayne aquifer–River Bend and Lower units based on these data are shown in Figures F7 and F8. Potentiometric levels in the Tarawa Terrace and Upper Castle Hayne aquifers are similar and range from about 23 to 10 ft, National Geodetic Vertical Datum 1929 (NGVD 29). Potentiometric levels trend from northwest to southeast, from greater to lesser, and generally correspond to groundwater-flow directions. The potentiometric gradient of the Upper Castle Hayne aquifer–River Bend unit ranged from about 0.006 to 0.007 foot per foot (ft/ft) (Roy F. Weston, Inc. 1992). Corresponding gradients for the Upper Castle Hayne aquifer–Lower unit were from 0.005 to 0.006 ft/ft. Aquifer tests were conducted in conjunction with several monitoring wells. Test results indicated that values of horizontal hydraulic conductivity ranged from about 10 to 30 feet per day (ft/d) for the "surficial aquifer" (Upper Castle Hayne aquifer–River Bend unit). Corresponding storativity ranged from magnitude 10^{-4} to 10^{-3}.

Table F6. Location coordinates of monitor wells installed during ABC One-Hour Cleaners Operable Units 1 and 2 and by the North Carolina Department of Natural Resources and Community Development, Tarawa Terrace and vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina.

Site name[1]	Location coordinates[2]	
	North	East
C1	365232	2490503
C2	364902	2490793
C3	364437	2491433
C4	364045	2492080
C5	364107	2491233
C9	364800	2491730
C10	364360	2491380
C11	362300	2492130
S1	365251	2490534
S2	364883	2490787
S3	364357	2491413
S4	364065	2492060
S5	364081	2491244
S6	364938	2490617
S7	364753	2490732
S8	364938	2491312
S9	364593	2491682
S10	363818	2491922
S11	365390	2489710
[3]X24B4	364530	2491570
[3]X24B5	364640	2491050
[3]X24B6	364810	2490710

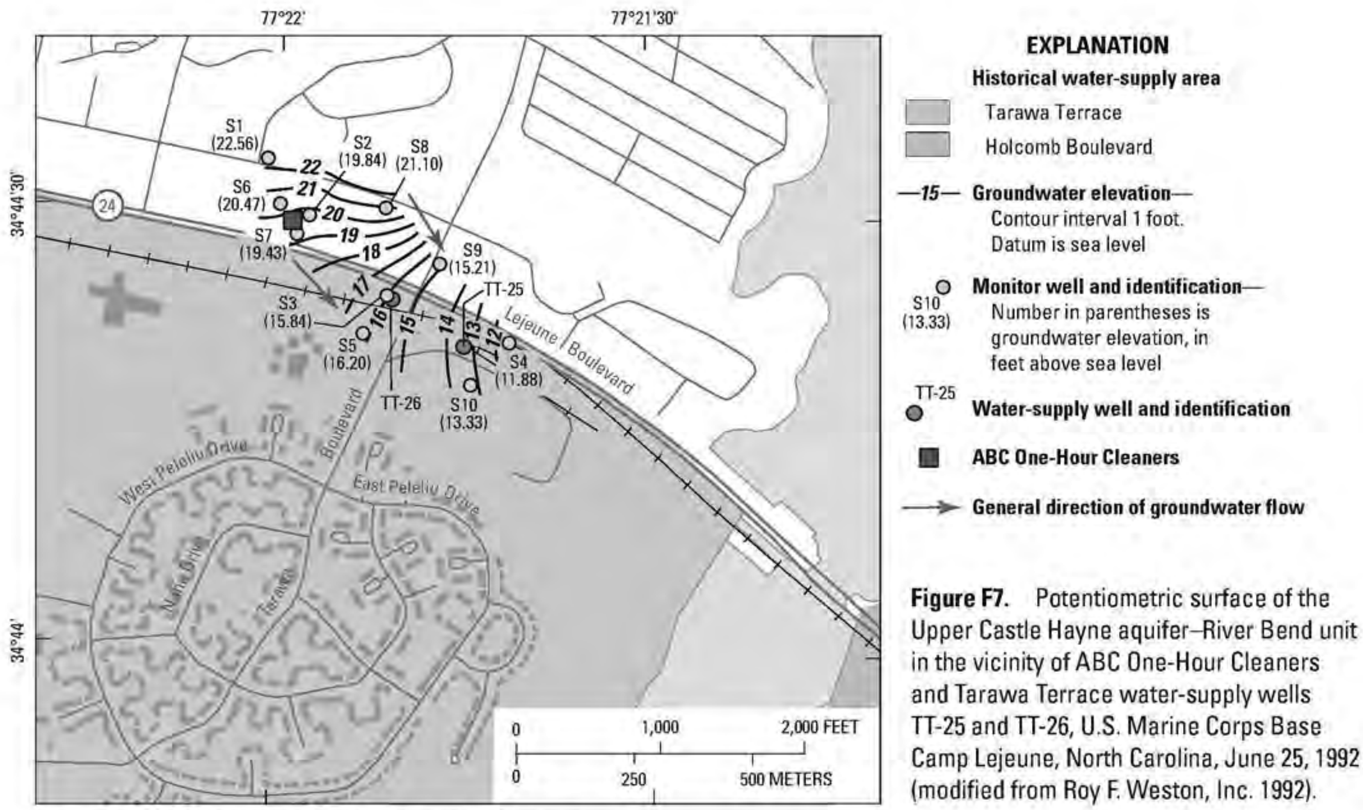
[1]See Figure F6 for location

[2]Location coordinates are North Carolina State Plane coordinates, North American Datum of 1983

[3]See Plate 1, Chapter A report, for location (Maslia et al. 2007). X24B4, X24B5, and X24B6 are shown as B4, B5, and B6, respectively

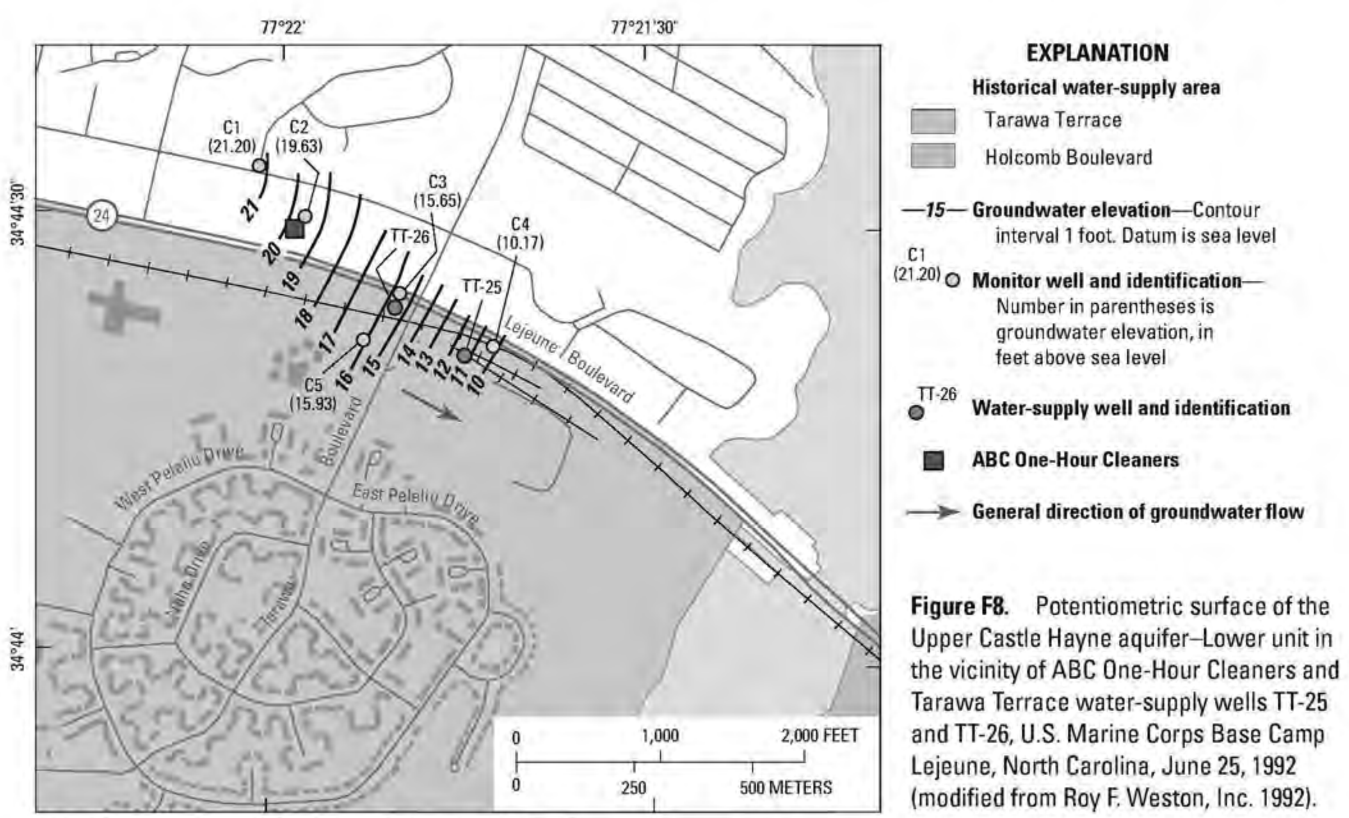
In order to characterize the depth, areal extent, and water quality of the contaminant plumes emanating from the vicinity of ABC One-Hour Cleaners, hydrocone penetrations using direct-push technology were accomplished at 47 sites near, east, and south of the cleaners (Figure F9). Two levels of samples were collected at each site, generally at about 20 and 40 ft. The constituent analysis schedule used for hydrocone sample analyses included PCE, TCE, 1,2-tDCE, and vinyl chloride, as well as 1,1,1-trichloroethane (1,1,1-TCA), 1,1- and 1,2-dichloroethane (1,1-DCA, 1,2-DCA), and carbon tetrachloride. Samples were analyzed in the field using a mobile laboratory. Several duplicate samples were submitted to "CLP" laboratories for quality assurance of results. Although not defined in the respective Operable Unit reports, CLP probably refers to "Clinical Laboratory Program," a process of inspection of State and Federal public health laboratories for purposes of certification. The CLP laboratories also determined concentrations of benzene, toluene, ethylbenzene, and total xylenes (BTEX compounds), in addition to the constituents discussed previously. Benzene and related toluene, ethylbenzene, and total xylenes were detected infrequently in the hydrocone samples. Benzene concentrations ranged from not detected to 12 μg/L. Results of mobile and CLP laboratory analyses were not highly consistent (Roy F. Weston, Inc 1992, Table 5-12); however, most constituents were noted in one or more samples. PCE was detected most frequently and was found in 75 samples at concentrations ranging from 1 to nearly 30,000 μg/L. The maximum depth of PCE occurrence determined by hydrocone penetration was 64 ft (sample HC-6-64), which is near the base of or slightly below the Upper Castle Hayne aquifer—River Bend unit at the sample location. Results of analyses of water samples collected during hydrocone penetration investigations are summarized in Table F7. Location coordinates of hydrocone penetration sites are listed in Table F8. Construction data for Tarawa Terrace water-supply wells are listed in Table F9. Similar data for monitor wells and piezometers constructed during ABC One-Hour Cleaners Operable Units 1 and 2 are listed in Table F10. A contour map based on PCE concentrations observed at Tarawa Terrace water-supply wells, monitor wells, and hydrocone penetration sites during 1991 and 1993 is shown in Figure F10. Concentrations represent data from the Upper Castle Hayne aquifer–River Bend and Lower units. The center of PCE mass at the time occurred southeast of ABC One-Hour Cleaners near the intersection of SR 24 and Tarawa Boulevard. This center of mass originally occurred in the immediate vicinity of ABC One-Hour Cleaners, and its location during 1991 and 1993 indicates that migration of the PCE mass apparently occurred advectively, mainly along potentiometric gradients (Figures F7 and F8).

During 1990, ATSDR completed an assessment of public health effects related to groundwater contamination at ABC One-Hour Cleaners and expressed a public health concern that off-site (namely Tarawa Terrace) exposure of contaminants to humans had occurred through the groundwater pathway. During 1997, ATSDR conducted a comprehensive Public Health Assessment of U.S. Marine Corps Base Camp Lejeune, which included an assessment of human exposure to contaminated groundwater at Tarawa Terrace. Maximum contaminant concentrations for PCE (215 μg/L), TCE (8 μg/L), and DCE (12 μg/L) determined from samples obtained within the Tarawa Terrace water-distribution system were listed, and a definitive exposure timeframe was identified for the period 1982–1985. The period 1954–1982 was identified as an unknown exposure time frame (ATSDR 1997).



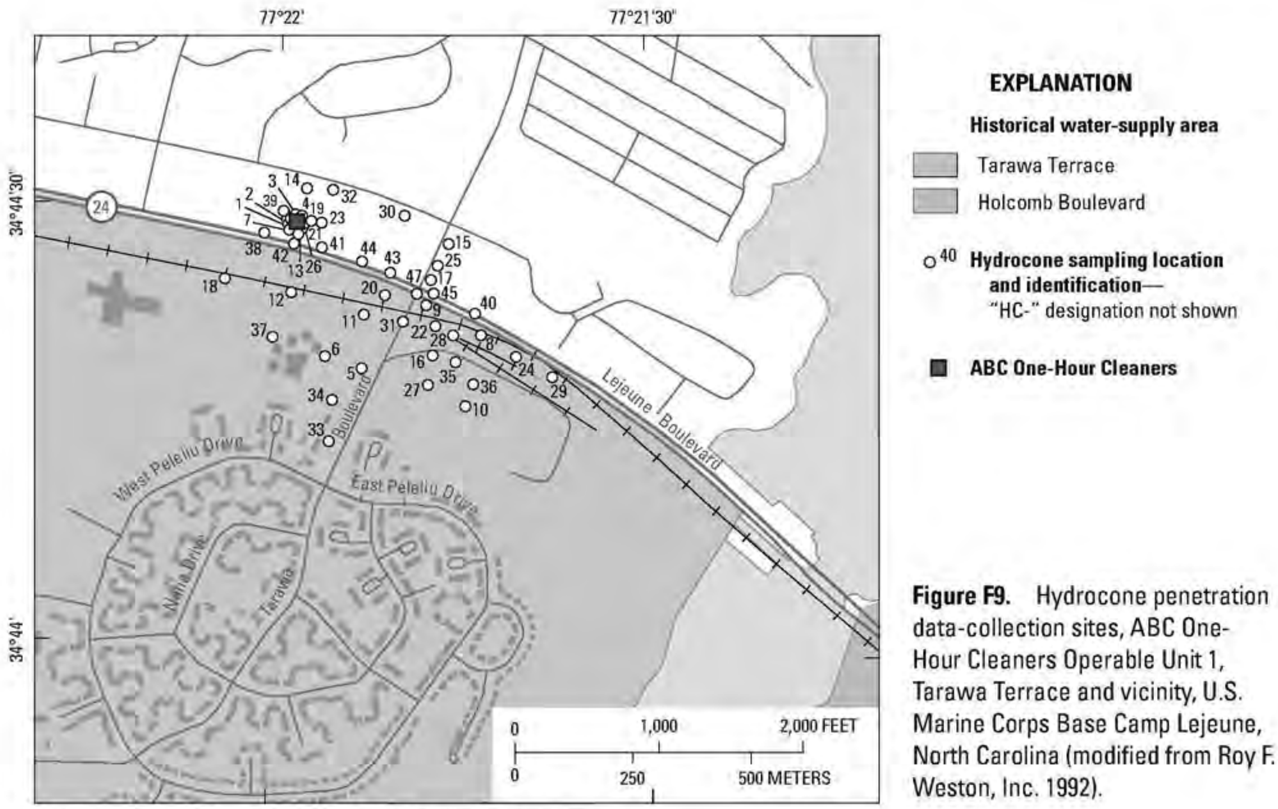
Base from U.S. Marine Corps and U.S. Geological Survey digital data files

Figure F7. Potentiometric surface of the Upper Castle Hayne aquifer–River Bend unit in the vicinity of ABC One-Hour Cleaners and Tarawa Terrace water-supply wells TT-25 and TT-26, U.S. Marine Corps Base Camp Lejeune, North Carolina, June 25, 1992 (modified from Roy F. Weston, Inc. 1992).



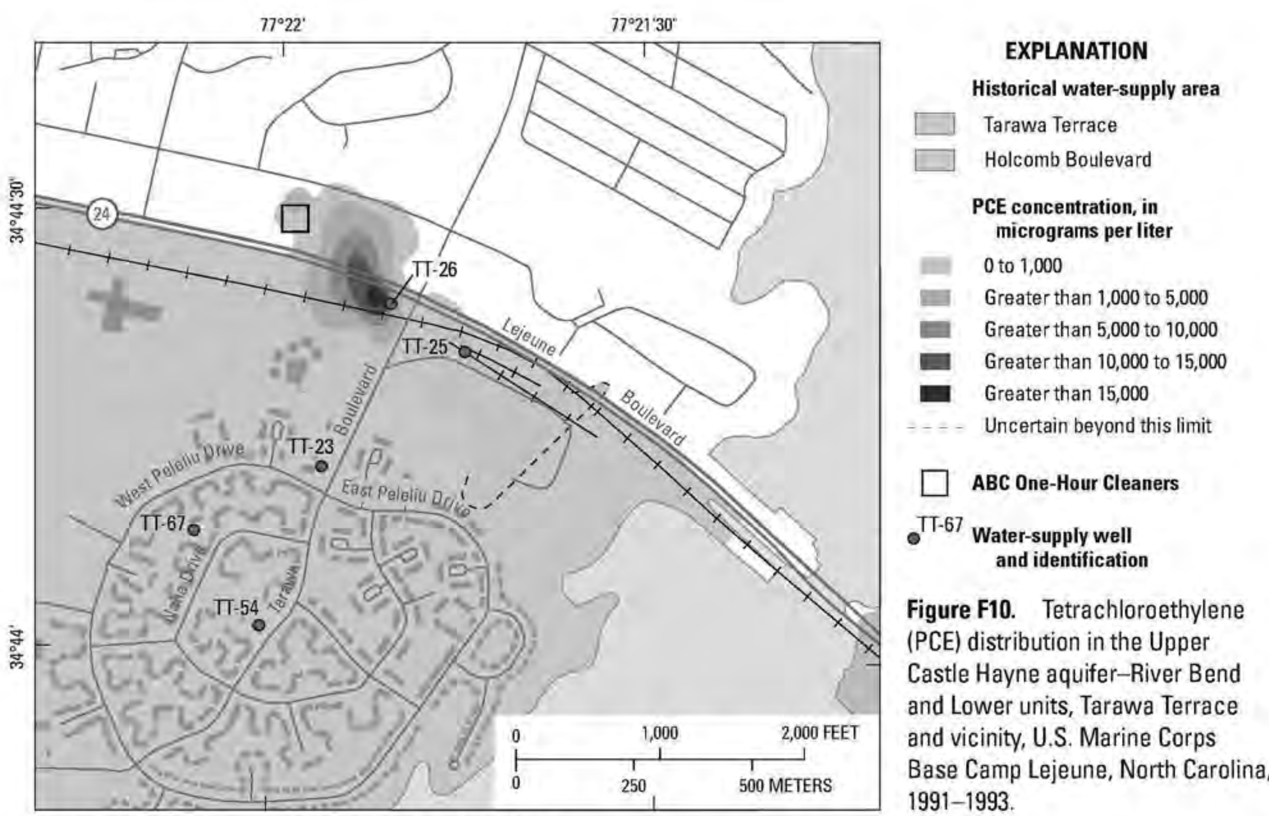
Base from U.S. Marine Corps and U.S. Geological Survey digital data files

Figure F8. Potentiometric surface of the Upper Castle Hayne aquifer–Lower unit in the vicinity of ABC One-Hour Cleaners and Tarawa Terrace water-supply wells TT-25 and TT-26, U.S. Marine Corps Base Camp Lejeune, North Carolina, June 25, 1992 (modified from Roy F. Weston, Inc. 1992).



Base from U.S. Marine Corps and U.S. Geological Survey digital data files

Figure F9. Hydrocone penetration data-collection sites, ABC One-Hour Cleaners Operable Unit 1, Tarawa Terrace and vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina (modified from Roy F. Weston, Inc. 1992).



Base from U.S. Marine Corps and U.S. Geological Survey digital data files

Figure F10. Tetrachloroethylene (PCE) distribution in the Upper Castle Hayne aquifer–River Bend and Lower units, Tarawa Terrace and vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina, 1991–1993.

Table F7. Summary of selected analyses for tetrachloroethylene (PCE), trichloroethylene (TCE), and *trans*-1,2-dichloroethylene (1,2-tDCE) in water samples collected at hydrocone penetration sites during ABC One-Hour Cleaners Operable Unit 1, Tarawa Terrace and vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina, December 15, 1991.

[µg/L, microgram per liter; ND, not detected; —, constituent not determined; J, estimated value; unless noted by superscript "2," detection limit is unknown]

Site name[1]	PCE concentration, in µg/L	TCE concentration, in µg/L	1,2-tDCE concentration, in µg/L
HC-1-17.5	4	ND	—
HC-1-39	1.7	ND	—
HC-2-21.5	1.5J	0.13J	—
HC-2-44.5	5	ND	—
HC-3-21	2.5J	ND	—
HC-3-40.5	ND	ND	—
HC-4-19	ND	ND	—
HC-4-40	0.16J	ND	—
HC-5-25	0.38J	ND	—
HC-5-25	2J	ND	ND
HC-5-42.5	ND	ND	—
HC-6-30	5	ND	—
HC-6-41	9.4	ND	—
HC-6-64	0.6J	ND	—
HC-7-26.5	0.93J	ND	—
HC-7-26.5A	[2]4	[2]ND	[2]ND
HC-7-39	8.1	ND	—
HC-7-39	[2]2J	[2]ND	—
HC-8-28	5	ND	—
HC-8-35	6.8	ND	—
HC-8-35	[2]27	[2]3J	[2]ND
HC-9-31	175.7	ND	—
HC-9-36.5	6.3	ND	—
HC-10-24	2.5J	ND	—
HC-10-40	0.8J	ND	—
HC-10-40	[2]ND	[2]ND	[2]ND
HC-11-24	12.2	ND	—
HC-11-34	2.8J	ND	—
HC-11-34	[2]8J	[2]ND	[2]ND
HC-12-24	ND	ND	—
HC-12-24	[2]ND	[2]ND	[2]ND
HC-12-40	3.4J	ND	—
HC-13-19.5	0.76J	0.19J	—
HC-13-19.5	[2]2J	[2]ND	[2]ND
HC-13-32	0.4J	ND	—
HC-14-20	0.22J	ND	—
HC-14-20	[2]ND	[2]ND	[2]ND
HC-14-40	ND	ND	—
HC-14-40	[2]ND	[2]ND	[2]ND
HC-15-24	ND	ND	—
HC-15-24	[2]ND	[2]ND	[2]ND
HC-15-36.5	ND	2.8J	—
HC-15-36.5	[2]ND	[2]ND	[2]ND
HC-16-30	0.23J	ND	—
HC-17-24	ND	ND	—
HC-17-24	[2]ND	[2]ND	[2]ND
HC-17-44	ND	ND	—
HC-17-44	[2]ND	[2]ND	[2]ND
HC-18-24	1J	ND	—
HC-18-36	ND	ND	—
HC-18-36	[2]ND	[2]ND	[2]ND
HC-19-25	53.3	ND	—
HC-19-35.5	157	ND	—
HC-19-35.5	[2]200	[2]100	[2]170
HC-20-34	500	ND	—
HC-20-34	[2]30,000	[2]2,900	[2]5,700
HC-20-41	196	ND	—
HC-20-41	[2]43	[2]29	[2]89
HC-21-22	96	ND	—
HC-21-22	[2]6,900	[2]1,100	[2]2,300
HC-21-31.5	13.5	ND	—
HC-22A-30	740	ND	—
HC-22-41	5.2	ND	—
HC-23-19	2.2J	ND	—
HC-23-45	11	ND	—
HC-24-28	14	ND	—
HC-24-38	13	ND	—
HC-25-18	8.2	ND	—
HC-25-27	6	ND	—
HC-26-42	5	ND	—
HC-27-27	4	ND	—
HC-27-37.5	3.2	0.34J	—
HC-28-28	2.7J	ND	—
HC-28-41	2.2J	ND	—
HC-29-23	1.4J	ND	—
HC-29-26.5	5	ND	—
HC-30-24	2	0.2	—
HC-30-40	2J	ND	—
HC-31-29	1.2J	ND	—
HC-31-39	1.4J	ND	—
HC-32-26	1.3J	ND	—
HC-32-38	1.1J	ND	—
HC-33-28	2J	ND	—
HC-33-36	1.5J	ND	—
HC-34-21.5	2J	0.3J	—
HC-34-34	2J	ND	—
HC-35-30	133	ND	—
HC-35-42	7.5	ND	—

Table F7. Summary of selected analyses for tetrachloroethylene (PCE), trichloroethylene (TCE), and *trans*-1,2-dichloroethylene (1,2-tDCE) in water samples collected at hydrocone penetration sites during ABC One-Hour Cleaners Operable Unit 1, Tarawa Terrace and vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina, December 15, 1991.—Continued

[μg/L, microgram per liter; —, constituent not determined; J, estimated value; ND, not detected; unless noted by superscript "2," detection limit is unknown]

Site name[1]	PCE concentration, in μg/L	TCE concentration, in μg/L	1,2-tDCE concentration, in μg/L
HC-36-30	ND	ND	—
HC-36-30	[2]ND	[2]ND	[2]ND
HC-36-41	1J	ND	—
HC-37-27	0.3J	ND	—
HC-37-48	1.4J	ND	—
HC-38-24	0.5J	ND	—
HC-38-40	1.2J	ND	—
HC-39-23	0.9J	ND	—
HC-39-23	[2]ND	[2]ND	[2]ND
HC-39-35	2.4J	ND	—
HC-40-26	ND	ND	—
HC-40-40	ND	ND	—
HC-41-27	82	ND	—
HC-41-27	[2]120	[2]4J	[2]4J
HC-41-45	2J	ND	—
HC-42-24	ND	ND	—
HC-42-40	ND	ND	—
HC-43-24	33	ND	—
HC-43-34	1,060	ND	—
HC-44-28	6	ND	—
HC-44-28	[2]13	[2]5J	[2]17
HC-44-39	12,860	ND	—
HC-45-28	ND	ND	—
HC-45-38	2J	ND	—
HC-47-26	18	ND	—
HC-47-38	30	ND	—

[1]See Figure F9 for location

[2]Detection limit = 10 μg/L

Site name key: Example HC-20-34
HC Hydrocone site
20 Site location number
34 Sample depth

Table F8. Location coordinates of hydrocone penetration sites, ABC One-Hour Cleaners Operable Unit 1, Tarawa Terrace and vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina.

Site name[1]	Location coordinates[2] North	Location coordinates[2] East
HC-1	364830	2490670
HC-2	364980	2490675
HC-3	365020	2490700
HC-4	365010	2490750
HC-5	363870	2491230
HC-6	363850	2490960
HC-7	364800	2490680
HC-8	364080	2492020
HC-9	364310	2491690
HC-10	363604	2491940
HC-11	364250	2491230
HC-12	364350	2490730
HC-13	364790	2490730
HC-14	365050	2490810
HC-15	364740	2491810
HC-16	363946	2491690
HC-17	364470	2491670
HC-18	364410	2490280
HC-19	364975	2490850
HC-20	364370	2491372
HC-21	364970	2490770
HC-22	364130	2491710
HC-23	364960	2490910
HC-24	363960	2492270
HC-25	364590	2491750
HC-26	364820	2490750
HC-27	363738	2491680
HC-28	363080	2491836
HC-29	363810	2492550
HC-30	364950	2491520
HC-31	364170	2491510
HC-32	365060	2490980
HC-33	363365	2491045
HC-34	363640	2491090
HC-35	363884	2491860
HC-36	363756	2491996
HC-37	364050	2490590
HC-38	364770	2490550
HC-39	365040	2490650
HC-40	364250	2492010
HC-41	364700	2490920
HC-42	364720	2490730
HC-43	364500	2491410
HC-44	364610	2491200
HC-45	364390	2491730
HC-47	364400	2491600

[1]See Figure F9 for location

[2]Location coordinates are North Carolina State Plane coordinates, North American Datum of 1983

Table F9. Construction data for Tarawa Terrace water-supply wells, test well T-9, and Civilian Conservation Corps well CCC-1, Tarawa Terrace and vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina.

[NGVD 29, National Geodetic Vertical Datum of 1929; N/A, data not available; AKA, also known as; >, greater than]

Site name	Land-surface altitude, in feet above NGVD 29	Completion date	Borehole depth, in feet	Well depth, in feet	Screen diameter, in inches	Open interval, in feet below land surface
[1]2A	26	5/24/1951	130	130	8	93–130
[2]#6	22	1951(?)	N/A	150–200(?)	N/A	N/A
[2]#7	24	1951(?)	N/A	150–200(?)	N/A	N/A
[1]CCC-1	24.3	9/17/1941	105	75	10	52–75
[1]T-9	28.7	3/1959	202	88	8	37–42
						50–60
						68–72
						83–88
[3]TT-23	23.9	3/14/1983	263	147	10	70–95
						132–42
[3]TT-25	32.0	7/9/1981	200	180	8	70–75
						85–95
						150–75
[3]TT-26, AKA #1	34.0	5/18/1951	180	108	8	91–108
[3]TT-27, AKA #2B	26.4	5/31/1951	90	90	10	77–90
[3]TT-28, AKA #3	26	1951	N/A	50–100(?)	N/A	N/A
[3]TT-29, AKA #4	25	1951	N/A	50–100(?)	N/A	N/A
[3]TT-30, AKA #13	26	1971	N/A	128	N/A	50–70
						98–113
[3]TT-31, AKA #14	25.8	1973	N/A	94	N/A	N/A
[3]TT-45, AKA #5	26	1951	N/A	50–100(?)	N/A	N/A
[3]TT-52, AKA #9	24.9	6/27/1961	102	98	N/A	N/A[4]
[3]TT-53, AKA #10	25	7/22/1961	N/A	90	10	42–62
						68–83
[3]TT-54, AKA #11	22.1	6/30/1961	N/A	104	N/A	N/A[4]
[3]TT-55, AKA #8	26.4	11/1/1961	N/A	>50	N/A	N/A[4]
[3]TT-67, AKA #12	27.5	11/15/1971	200	104	8	70–94

[1]See Plate 1, Chapter A report, for location (Maslia et al. 2007)

[2]Out of map area, location not shown. North Carolina State Plane coordinates: #6 (highly approximate) North 369730, East 2481720; #7 (highly approximate) North 370500, East 2481530; and TT-45 North 365688, East 2483352

[3]See Figure 1 for location

[4]Construction is probably similar to TT-53

Table F10. Construction data for monitor wells installed during ABC One-Hour Cleaners Operable Units 1 and 2 and by the North Carolina Department of Natural Resources and Community Development, Tarawa Terrace and vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina.

[NGVD 29, National Geodetic Vertical Datum of 1929]

Site name[1]	Land-surface altitude, in feet above NGVD 29	Completion date	Borehole depth, in feet	Well depth, in feet	Screen diameter, in inches	Open interval, in feet below land surface
C1	30.6	4/4/1992	104.0	100.6	4	90–100
C2	32.0	4/8/1992	87.0	85	4	74.5–84.5
C3	33.4	4/9/1992	90.5	90.5	4	79.1–89.1
C4	32.2	4/2/1992	200.0	130.4	4	120–130
C5	32.0	4/7/1992	92.5	91	4	80.5–90.5
C9	32.1	9/1993	76	76	4	66–76
C10	32.5	10/1993	175	175	4	165–175
C11	31.0	9/1993	108	108	4	98–108
PZ-01	31.9	9/1993	80	80	2	74.5–79.5
PZ-02	31.9	9/1993	35	35	2	29.5–34.5
PZ-03	32.5	9/1993	80	80	2	74.5–79.5
PZ-04	32.5	9/1993	35	35	2	29.5–34.5
PZ-05	32.0	9/1993	80	80	2	74.5–79.5
PZ-06	32.0	9/1993	35	35	2	29.5–34.5
S1	30.6	3/22/1992	28.0	25.5	4	5.5–25.5
S2	32.5	3/26/1992	39.7	39.7	4	19.7–39.7
S3	33.4	4/2/1992	39.5	39.5	4	19.5–39.5
S4	32.2	4/3/1992	34.0	34	4	14–34
S5	31.9	4/1/1992	30.0	28	4	8–28
S6	31.1	3/26/1992	40.5	40.5	4	20.5–40.5
S7	31.3	4/5/1992	30.3	30.3	4	10–30
S8	30.8	4/4/1992	28.0	28	4	8–28
S9	32.7	3/21/1992	40.0	28.3	4	8–28
S10	31.6	3/19/1992	40.0	35	4	15–35
S11	30.8	9/1993	35	35	4	15–35
[2]X24B4	33.3	9/25/1985	59	59	2	42–52
[2]X24B5	31.4	9/25/1985	59	59	2	42–52
[2]X24B6	33.4	9/25/1985	59	59	2	42–52

[1]See Figure F6 for location

[2]See Plate 1, Chapter A report, for location (Maslia et al. 2007). X24B4, X24B5, and X24B6 are shown as B4, B5, and B6, respectively

Conceptual Model of Groundwater Flow

A conceptual model of groundwater-flow directions and budget quantities is a necessary element of flow-model development and calibration. The source of water to the Tarawa Terrace and underlying aquifers in the study area is recharge from precipitation. Recharge to the Castle Hayne aquifer system occurs originally as infiltration of precipitation to the water table. Average annual effective recharge, defined herein as recharge to the water table remaining after discharge to evapotranspiration, is described in previous investigations as ranging from about 11 to about 19 inches per year (in/yr) in the study area (LeGrand 1959; Heath 1994; Giese and others 1997; Baker Environmental, Inc. 1998). These rates conform well to maps of average annual rainfall and annual potential evaporation by Heath (1994, Figures 9 and 12), which indicate rates from about 56 to 60 in/yr and 42 in/yr, respectively, for Onslow County. Within the study area (Figure F1), surface soils generally are sands or silty sands, and the land surface largely is undissected by streams, indicating little or minimal runoff. Thus, long-term, average annual effective recharge rates in the study area could be as much as 18 in/yr, the maximum difference between rates of average annual rainfall and annual potential evaporation (Heath 1994, Figures 9 and 12).

The spatial configuration of the water table prior to development of local aquifers by wells probably resembled, to a large degree, a subdued replica of surface topography (Figure F1). Consequently, precipitation recharged to the water table flowed laterally from highland to lowland areas and eventually discharged to surface-water bodies. Northeast Creek and New River are partially or completely incised within the Tarawa Terrace aquifer and Upper Castle Hayne aquifer–River Bend unit and receive water directly from these aquifers. Frenchmans Creek, near the western limit of the study area, is apparently a perennial stream through most of its reach and probably also derives baseflow directly from the Tarawa Terrace aquifer and the Upper Castle Hayne aquifer–River Bend unit.

Lateral flow directions within the Upper, Middle, and Lower Castle Hayne aquifers probably mimic, to a large degree, corresponding directions within the Upper Castle Hayne aquifer–River Bend unit, except in the immediate vicinity of discharge areas such as Northeast Creek and New River, where flow directions within the deeper confined aquifers are vertically upward. Diffuse vertical leakage across confining units and between aquifers probably is pronounced in the vicinity of pumping wells, where vertical hydraulic gradients are relatively large, but is limited elsewhere by small vertical head gradients and the thickness and vertical hydraulic conductivity of confining units. Groundwater probably flows vertically downward through the Upper and Middle Castle Hayne aquifers in areas of recharge in the northern part of the study area near and somewhat south of Lejeune Boulevard (SR 24) and probably is vertically upward within these same aquifers in the vicinity of New River and Northeast Creek. Paired observations that measure water levels in individual aquifers of the Castle Hayne aquifer system are not available for the study area; however, long-term measurements are available for the Upper and Lower Castle Hayne aquifers at site X24S located just north of Wallace Creek (Plate 1). These data are possibly influenced by local pumping but indicate less than a 3-ft head difference occurred between the Upper and Lower Castle Hayne aquifers during 1987–2004. The head gradient was vertically upward (North Carolina Division of Water Resources, written communication, August 30, 2005). Similar flow conditions probably occurred within the study area during the period of interest to this investigation in the vicinities of Northeast Creek and New River.

Following the onset of pumping at water-supply wells during 1952, groundwater flow that under predevelopment conditions was entirely directed toward Northeast Creek, New River, and Frenchmans Creek was partially diverted to pumping wells. Consequently, (1) predevelopment potentiometric levels near and in the vicinity of pumping wells declined in the aquifers open to the wells, (2) predevelopment flow directions changed preferentially toward wells from natural points of discharge such as Northeast Creek, and (3) potentiometric levels possibly declined near groundwater/topographic divides resulting in the migration of boundaries farther west or north of predevelopment locations. Water-level declines near or in the vicinity of Northeast Creek or New River possibly caused a complete reversal in the direction of groundwater flow such that saltwater or brackish water from these surface-water bodies intruded landward into the Tarawa Terrace or Upper Castle Hayne aquifers.

Conceptual Model of Tetrachloroethylene (PCE) Migration

Migration of PCE to the water table in the immediate vicinity of ABC One-Hour Cleaners and subsequently to Tarawa Terrace water-supply wells probably began with the onset of dry-cleaning operations during 1953. The floor drain used to discharge waste streams and spillage from ABC One-Hour Cleaners was apparently in place at this time as was the septic tank–soil absorption system that received the drain discharge. The septic tank–soil absorption system also was connected to and was used by several other businesses proximate to ABC One-Hour Cleaners (Hopf & Higley, P.A., Deposition of Victor John Melts, written communication, April 12, 2001). The drain laterals and drain field related to the septic tank–soil absorption system were probably located to the rear of ABC One-Hour Cleaners but were never traced during ABC One-Hour Cleaners Operable Unit 2. Neither the depth nor length of drain laterals was determined (Roy F. Weston, Inc. 1994). However, the sandy soils noted in soil boring logs obtained in the immediate vicinity of ABC One-Hour Cleaners (Roy F. Weston, Inc. 1994) probably are characterized by a relatively high infiltration capacity, and drain laterals were probably placed between 5 and 10 ft below ground level. Waste streams discharged to the septic tank–soil absorption system were probably composed mostly of water, by volume, in substantially larger quantities than corresponding discharges of PCE mass. Accordingly, PCE concentrations in the mixed waste streams were probably always below solubility limits (150 mg/L), and PCE occurred in solution in the subsurface, rather than as "pure product."

Once discharged to the drain field, wastewater containing PCE and PCE spillage in solution migrated downward through the unsaturated zone to the water table or was lost to evapotranspiration in the immediate vicinity of the drain field. Thickness of the unsaturated zone in the vicinity of ABC One-Hour Cleaners ranges from about 20 to 25 ft, and the water table probably fluctuates seasonally across a range of 2 or 3 ft (Roy F. Weston, Inc. 1992, 1994; Harned and others 1989). Analyses of core samples collected during ABC One-Hour Cleaners Operable Units 1 and 2 at numerous locations surrounding ABC One-Hour Cleaners (Figure F5) indicated PCE occurrences to a depth of 14 or 15 ft at several sites. Concentrations ranged to 580,000 mg/kg west of and adjacent to the septic tank. The maximum concentration noted in these core samples of 2,100,000 mg/kg occurred at a depth range from 0 to 2 ft in the alley east of the building housing ABC One-Hour Cleaners and may have been the result of "still bottom" disposal practices. Samples were collected during 1992 and 1993 (Roy F. Weston, Inc. 1994, Figure 5-2).

At the water table, the wastewater stream containing the PCE mass mixed with groundwater, and PCE was transported advectively along potentiometric gradients and by diffusion along declining concentration gradients. Transport velocity under each condition was dependent on the magnitude of the respective gradients and, with respect to advection, the lateral and vertical hydraulic conductivities of the Tarawa Terrace aquifer and the Upper Castle Hayne aquifer–River Bend unit. Lateral potentiometric contours within the Upper Castle Hayne aquifer–River Bend unit during June 1992 are shown in Figure F7 and correspond to gradients ranging from about 0.005 to 0.007 ft/ft to the southeast (Roy F. Weston, Inc. 1992, Figure 4-6). Such gradients probably closely resemble predevelopment conditions as groundwater pumping at Tarawa Terrace was terminated during March or April 1987. Note that groundwater-flow directions and, thus, lateral advection is southeast toward Tarawa Terrace water-supply wells TT-25 and TT-26 and Northeast Creek (Figure F1). Vertical head gradients within the Upper Castle Hayne aquifer in the vicinity of ABC One-Hour Cleaners were small but generally downward during 1992 and 1993 (Roy F. Weston, Inc. 1992, 1994), and PCE probably was transported downward along these gradients. However, lateral advection was probably the primary mechanism of PCE transport in groundwater at Tarawa Terrace and vicinity.

The onset of pumping at Tarawa Terrace water-supply wells during 1952 substantially increased lateral and vertical groundwater-flow gradients in the vicinity of ABC One-Hour Cleaners compared to natural gradients (Figures F7 and F8). Such changes increased lateral and downward groundwater-flow velocities and, hence, advective transport velocities, and preferentially altered flow and PCE transport directions toward the pumping wells. Water-supply well TT-26 began operation during 1952 and was located along a direct groundwater flowpath from ABC One-Hour Cleaners. The proximity of this well to the source of PCE (about 900 ft), its relatively shallow construction (Table F9), and its location with respect to preferential groundwater-flow directions indicate that the first occurrence of PCE breakthrough at a Tarawa Terrace water-supply well probably occurred at well TT-26. Nearby water-supply well TT-25 was located about 1,400 ft southeast from ABC One-Hour Cleaners (Figure F1) and began operation during 1981. The location and relatively shallow open intervals of this well indicate possible breakthroughs of PCE and related degradation products also occurred at this site following the onset of pumping. Four water-supply wells were located northwest of ABC One-Hour Cleaners and probably also began operation during 1952 (TT-27, TT-28, TT-29, and TT-45). The discharge of these wells during their period of operation was limited to about 100 gallons per minute (gal/min) or less (LeGrand 1959), and their limited radius of influence combined with their location upstream of the PCE source probably minimized or eliminated the possibility of PCE breakthrough at these sites. Water-supply well TT-55 began operation about 1961 and was located near well TT-27. Construction information regarding this well is not available; however, construction was probably similar to that reported for water-supply well TT-53. Water-supply well TT-30 began operation during 1972 and was located near well TT-28. Considerations of a location upstream of the PCE source and a limited radius of influence described for wells TT-27 and TT-28 probably also applied to wells TT-30 and TT-55, and any breakthrough of PCE or related degradation products was probably minimal or did not occur at all at these sites. Water-supply wells generally south of ABC One-Hour Cleaners and located within the Tarawa Terrace housing areas included, in order of year of beginning operation, TT-52 (1962), TT-53 (1962), TT-54 (1962), TT-67 (1972), TT-31 (1973), and TT-23 (1984). The most proximate of these wells to ABC One-Hour Cleaners was TT-23, at a distance of about 1,700 ft. The farthest of these wells from ABC One-Hour Cleaners was TT-31 at a distance of about 3,000 ft. With the exception of well TT-23, all of these wells were in operation for a minimum of 12 years prior to the termination of operations at wells TT-23 and TT-26. Because of their proximity to one another and similar depth, cones of depression created by pumping at individual wells from the same water-bearing units possibly coalesced and created a large single cone of depression when three or more of these wells were operating at the same time. Drawdown related to this large single cone of depression was probably most extreme in the Upper Castle Hayne aquifer–River Bend and Lower units, the same units open to well TT-26, and possibly caused groundwater to flow generally south from the direction of ABC One-Hour Cleaners toward Tarawa Terrace housing. Accordingly, PCE probably migrated south and was available in sufficient quantities in the vicinity of well TT-23 to contaminate the water supply at the onset of operations at this well during 1984.

In addition to dilution and diffusion, PCE concentrations during migration were altered by (1) adsorption onto soil particles, particularly silts and clays, (2) degradation by biological processes sequentially into TCE, DCE, and finally vinyl chloride, and (3) dispersion. Biodegradation is the only one of these processes actually observed at Tarawa Terrace and vicinity and had occurred completely at water-supply well TT-26 by January 1985, about 1 month prior to the termination of well operations because of contamination. The reported concentrations of PCE, TCE, DCE, and vinyl chloride at TT-26 at this time were, respectively, 1,580, 57, 92, and 27 μg/L (Shiver 1985). The DCE concentration was reported as the isomer 1,2-tDCE. Biodegradation of PCE in the unsaturated zone in the immediate vicinity of ABC One-Hour Cleaners also was noted in soil cores during 1992 (Roy F. Weston, Inc. 1992, Table 2-4). Concentrations of TCE in 22 core samples from 10 individual boreholes ranged from about 0.1 to 860 mg/kg. Concentrations of 1,2-dichloroethylene in every sample were less than 0.1 mg/kg. These data indicate that the vicinity of ABC One-Hour Cleaners probably also was a source of TCE to groundwater.

Simulation of Tetrachloroethylene (PCE) Migration

The original version of the numerical code used in this study to simulate groundwater flow was written by McDonald and Harbaugh (1984) and was designated a modular finite-difference groundwater-flow model (MODFLOW). The code used to simulate contaminant transport is designated MT3DMS, version 4, written by Zheng and Wang (1998).

The MODFLOW code simulates groundwater flow in a three-dimensional heterogeneous and anisotropic porous medium. Updates to the original MODFLOW code were developed periodically along with various modules to expand simulation capability and computational performance. The MT3DMS code is a modular, three-dimensional transport model that simulates advection, dispersion, and chemical reactions of contaminants in groundwater. The MODFLOW version used in this study is known as MODFLOW 96 (Harbaugh and McDonald 1996). The MT3DMS code used is version 4.00. Both codes are part of a highly integrated simulation system called PMWINPro (Processing MODFLOW Pro, version 7.017), which also includes codes that support and augment groundwater-flow and transport simulation using techniques such as particle tracking and inverse modeling (Chiang and Kinzelbach 2001). The capability to simulate advective transport also is integrated within PMWINPro and is based on techniques and codes first published by Pollock (1989, 1994). Two flow models were calibrated: (1) a predevelopment flow model representing long-term average, steady-state groundwater-flow conditions prior to the development of the Castle Hayne aquifer system and (2) a transient flow model representing pumping of the Castle Hayne aquifer system as a water supply for Tarawa Terrace. The transient flow model was subdivided into 528 stress periods, representing monthly conditions beginning during January 1951 and ending during December 1994 (Appendix F1). A single month corresponded to a single stress period, and each stress period represented a single time step. The unit of time was days. Thus, the appropriate number of days representing a particular month was assigned as the time interval of the stress period. The fate and transport model, the subject of this report, was linked directly to the transient flow model with an equivalent time unit (days), equal stress periods (months), and equal time discretization within stress periods. The active model domain, model grid, model boundary conditions, model geometry, hydraulic characteristic arrays, pumpage arrays, recharge arrays, and all other model elements common to the calibrated predevelopment flow model, transient flow model, and fate and transport model were identical. The model domain and geometry are briefly described in the following section. All flow model arrays and flow model calibrations are described in detail in Faye and Valenzuela (2007).

Model Domain and Boundary Conditions

The total domain of the Tarawa Terrace groundwater-flow and fate and transport models comprises most of the area north and west of the mid-channel line of Northeast Creek. The total area represented by the model domain is shown in Figure F11. For modeling purposes, the total domain was subdivided into active and inactive domains. The active domain, which corresponds to the area pertinent to the simulation of groundwater flow and PCE fate and transport, is the blue gridded area shown in Figure F11, and also includes the adjacent dark blue area that extends to the mid-channel of Northeast Creek. The remaining area within the total model domain but outside the gridded area is the inactive domain. The total model domain was subdivided into 270 columns and 200 rows of square cells representing a length of 50 ft per side ($\Delta x = \Delta y = 50$ ft). The model was subdivided vertically into seven layers. Model layer 1 corresponds to the combined Tarawa Terrace aquifer, the Tarawa Terrace confining unit, and the Upper Castle Hayne aquifer–River Bend unit (Table F1). The remaining six layers correspond, respectively, to the Local confining unit, the Upper Castle Hayne aquifer–Lower unit, the Middle Castle Hayne confining unit, the Middle Castle Hayne aquifer, the Lower Castle Hayne confining unit, and the Lower Castle Hayne aquifer. The area represented by the total model domain is about 135,000,000 square feet (ft^2) or about 4.8 square miles (mi^2). The active model domain corresponds to an area of about 59,400,000 ft^2, about 2.1 mi^2 or about 1,360 acres. Model layer 1 was specified as an unconfined aquifer and contains the water table. All other model layers were specified as confined.

The base of simulated groundwater flow and PCE mass transport corresponds to the top of the Beaufort confining unit and is implicitly a no-flow boundary. Boundaries assigned to the eastern, western, southwestern, and southern perimeters of the active model domain were all no-flow and are equal in location and condition for each layer. The southern boundary and most of the eastern boundary conform to the mid-channel line of Northeast Creek. The western boundary conforms to

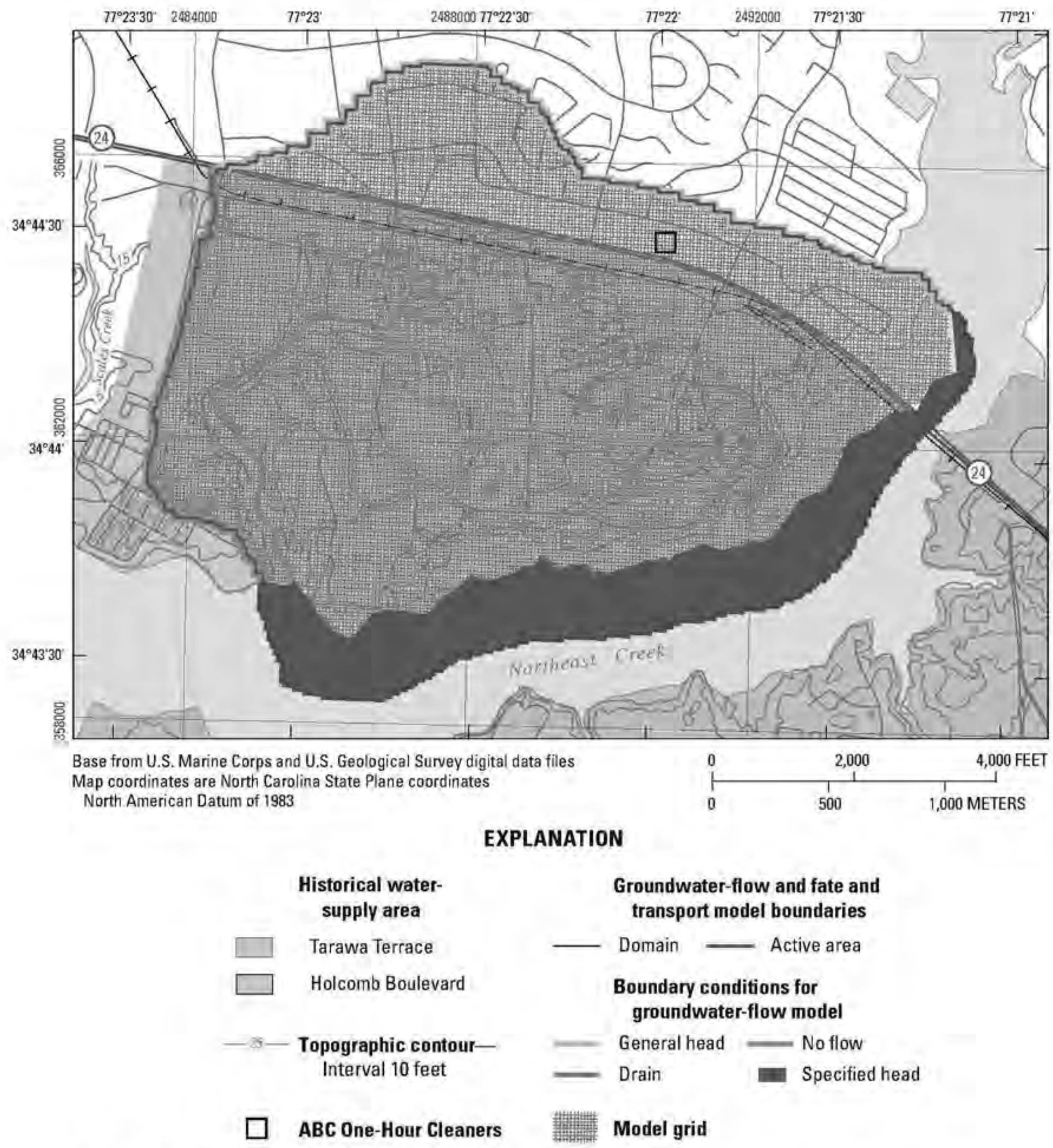


Figure F11. Groundwater-flow model grid and model boundaries, Tarawa Terrace and vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina.

the topographic divide that separates the drainage areas of Scales and Frenchmans Creeks (Figure F1). The northern boundary also generally conforms to a topographic divide but was assigned as a general-head (head-dependent) boundary in all model layers because of the proximity of water-supply wells to the boundary in the northeastern and north-central parts of the active model domain (Figures F1 and F11). The surface of Northeast Creek within the active domain was assigned a specified head of zero in model layer 1, corresponding to sea level. A drain also was assigned to model layer 1 along the channel of Frenchmans Creek in the western part of the model area. Drain altitudes were interpolated to the center of drain cells using detailed topographic maps and ranged from zero to about 16 ft.

Boundaries assigned exclusively to the fate and transport model were (1) a mass loading rate for PCE of 1,200 grams per day (g/d) applied to the model cell that corresponds to layer 1, row 47, column 170; and (2) a no-contaminant flux boundary along the eastern, western, southern, and northern perimeters of the active model domain. Mass loading occurred continuously from stress period 26 (January 1953) to stress period 408 (December 1984). Prior to stress period 25 and after stress period 408, the assigned mass loading rate was 0.0 g/d.

Model Input Data and Initial Conditions

Other than advection, the subsurface fate and transport of PCE at Tarawa Terrace and vicinity probably was most affected by the various hydrodynamic, geochemical, and biological processes that relate, respectively, to dispersion, sorption, and biodegradation. Accordingly, simulation of PCE migration using MT3DMS required a variety of input data descriptive of these processes. Dispersion was accounted for using assigned dispersivities parallel to the longitudinal, transverse, and vertical-flow directions. Longitudinal dispersivity is in the principal direction of flow. Transverse dispersivity is orthogonal to and generally smaller than longitudinal dispersivity. Longitudinal dispersivity was assigned to MT3DMS as an array. Transverse and vertical dispersivities were computed as ratios or percentages of longitudinal dispersivity. Sorption was probably the primary geochemical process affecting PCE migration. Sorption processes are commonly determined using results of sorption equilibrium experiments conducted in laboratory columns using soil samples obtained from the area or areas of interest and solutes representative of actual or presumed subsurface contaminants. The net effect of all sorption processes is the removal of solute, in this case PCE, from solution to the porous media. Neither laboratory nor field-scale estimates of PCE dispersivity or sorption unique to the Tarawa Terrace area were available for this study, and initial estimates of these parameters were obtained from literature sources. A first-order rate of biodegradation of PCE was computed using concentration data listed in Table F2 and was applied as an initial condition to the MT3DMS model. Detailed discussions of these and related model input parameters are provided in the following sections.

Hydrodynamic Dispersion

To compute directional values of the hydrodynamic dispersion coefficients, MT3DMS requires the cell-by-cell assignment of the effective molecular diffusion coefficient for PCE in water, longitudinal dispersivity, and the ratios of transverse and vertical dispersivity to longitudinal dispersivity. Coefficients of molecular diffusion of PCE as a solute in water examined for this study ranged from 7.0×10^{-4} square feet per day (ft^2/d) (Lucius and others 1990) to 9.5×10^{-4} ft^2/d (California Environmental Protection Agency 1994). A mid-range value of 8.5×10^{-4} ft^2/d was assigned to all model layers for all stress periods for this study and was not varied during model calibration.

Estimates of longitudinal dispersivity were obtained from a variety of sources. Anderson (1984, Figure 2.4) and Fetter (1999, Figure 2.17) show a graph originally published by Lallemand-Barrès and Peaudecerf (1978) indicating that field-scale or longitudinal dispersivity is about one-tenth of a characteristic length or apparent length scale. Neuman (1990) extended the work of Lallemand-Barrès and Peaudecerf and others to derive a universal scaling rule. Neuman related longitudinal dispersivity to scales of investigation within a variety of porous media under diverse conditions of groundwater flow and solute transport. Data were derived from laboratory and field-scale investigations. The most general equation derived by Neuman (1990) using 131 of 134 possible data pairs and representing a large range of scales of investigation is

$$\alpha_L = 0.0175 L_s^{1.46} \qquad (1)$$

where,

α_L = longitudinal macrodispersivity, and
L_s = a characteristic or apparent scale length.

The characteristic length or scale length is unique to the distribution of hydraulic conductivity within a particular aquifer or groundwater-flow regime and is commonly defined as the minimum length of groundwater flowpaths at which all possible variations in hydraulic conductivity are encountered by migrating solutes (paraphrased from Fetter 1999, p. 84). The characteristic length is apparently also proportional to aquifer heterogeneity and anisotropy.

The characteristic length of aquifers at Tarawa Terrace and vicinity is unknown. However, boring logs of the Tarawa Terrace and Upper Castle Hayne aquifers collected at Tarawa Terrace (Roy F. Weston, Inc. 1992, 1994) indicate that fine sands, which compose the vast majority of aquifer sediments, are uniform to highly uniform. A particle-size distribution of a single composite sample of sand collected from the Tarawa Terrace aquifer at Tarawa Terrace indicated a uniformity coefficient of about 1.6 (Miller et al. 1989). Uniformity also is indicated by the results of aquifer tests reported in Faye and Valenzuela (2007, Tables C2–C4), wherein horizontal hydraulic conductivity determined from 13 tests conducted at wells completed generally in the Upper Castle Hayne aquifer–River Bend unit ranged from 10 to 50 ft/d and averaged 22 ft/d. Standard deviation of these test results was 11 ft/d. The horizontal hydraulic conductivity determined from 14 tests conducted at wells largely open to the Upper Castle Hayne aquifer–River Bend and Lower units ranged from 8 to 40 ft/d and averaged 18 ft/d. Standard deviation of these test results was 10 ft/d. Such results indicate that substantial macro- or field-scale hydraulic heterogeneities probably do not occur within the Tarawa Terrace and Upper Castle Hayne aquifers within the study area and the heterogeneities that are present are probably statistically homogeneous on a scale equal to or smaller than the scale of investigation (Neuman 1990). With respect to aquifer tests, the scale of investigation corresponds to distances equal to or less than the radius of influence of the pumped well, which at Tarawa Terrace water-supply wells probably equals several hundred feet.

Longitudinal dispersivity applied to numerical model codes based on finite-difference methods, such as MODFLOW and MT3DMS, also is dependent on the scale of the model. Model scale is commonly represented by cell size and grid discretization. Discretization of the Tarawa Terrace MODFLOW and MT3DMS models is uniform. Thus, cell dimensions (50 ft by 50 ft) determine the scale of investigation and the approximate order of magnitude of longitudinal dispersivity. Assigning a hypothetical longitudinal dispersivity of 50 ft to Equation 1 yields a characteristic length of about 230 ft, which approximates the combined length of 5 model cells (250 ft). Gelhar et al. (1992) published several scatter diagrams, similar to those of Neuman (1990), comparing longitudinal dispersivity to observation scale. At a given scale, the longitudinal dispersivity values ranged across 2 to 3 orders of magnitude. Data within the lower part of a range were described as probably the most reliable (Gelhar et al. 1992, Figure 2). Projecting a measurement scale of 250 ft to the approximate center of the scatter data of Gelhar et al. (1992) corresponds to a longitudinal dispersivity of about 10 meters (about 30 ft). Gelhar et al (1992) also point out that vertical dispersivities are typically an order of magnitude or more smaller than transverse dispersivities and that transverse dispersivities are typically an order of magnitude less than longitudinal dispersivities.

The uniformity of sand particle-size distributions and aquifer-test results indicate that substantial macro-scale hydraulic heterogeneities probably do not occur within the Tarawa Terrace and Upper Castle Hayne aquifers of the study area. Accordingly, a characteristic length for groundwater flowpaths of 250 ft and equal to 5 model cell lengths was initially assigned and used to estimate field-scale longitudinal dispersivity. This characteristic length when combined with the results of Lallemand-Barrès and Peaudecerf (1978) cited previously indicates that a longitudinal dispersivity of about 25 ft is appropriate (0.10×250 ft). The relations between scale length and longitudinal dispersivity described by Neuman (1990) and Gelhar et al. (1992) indicate longitudinal dispersivity values of about 55 and 30 ft, respectively, using a characteristic length of 250 ft. These data provided a magnitude and range of longitudinal dispersivity considered appropriate for calibration of the Tarawa Terrace fate and transport model (25–55 ft). Accordingly, a longitudinal dispersivity of 50 ft was initially assigned uniformly to all layers of the MT3DMS model for all stress periods. The final calibrated longitudinal dispersivity was 25 ft, similarly assigned. Ratios of transverse and vertical dispersivities to longitudinal dispersivity were assigned as 0.1 and 0.01, respectively, to all model layers uniformly for all stress periods and were not varied during calibration.

Sorption

Sorption in MT3DMS is assumed to be an equilibrium-partitioning process between the PCE in solution within the groundwater-flow regime and the sands, clays, and silts that compose the porous media of the aquifers and confining units. Sorption within aquifers and confining units at Tarawa Terrace and vicinity is probably greatly influenced by the fraction of organic matter within the porous media. Boring logs at monitor wells installed during ABC One-Hour Cleaners Operable Units 1 and 2 (Roy F. Weston, Inc. 1992, 1994) qualitatively indicate the occurrence of silt and clay fractions in sediments that compose the Tarawa Terrace and Upper Castle Hayne aquifers. Many of the silts and fine sands are described as gray or black, indicating a relatively high organic composition. Charcoal was noted infrequently at depth. On the other hand, the sand sample collected at Tarawa Terrace from the Tarawa Terrace aquifer and described previously in the context of a particle-size distribution was analyzed for the fraction of organic carbon and cation exchange capacity (Miller et al. 1989). The organic carbon fraction of the sand was small, only 0.024 percent, and the cation exchange capacity was about 5.5 milliequivalents per 100 grams. The intent of the project described by Miller et al. (1989) required the deliberate selection of a sand low in organic material, and the selected sample was probably only partly representative of the Tarawa Terrace aquifer or the Upper Castle Hayne aquifer–River Bend unit.

The MT3DMS code accounts for the sorption process by computing a retardation factor, which is determined by selecting a sorption type: either (1) a linear equilibrium isotherm, (2) a Freundlich nonlinear equilibrium isotherm, or (3) a Langmuir nonlinear equilibrium isotherm. The application of equilibrium isotherms assumes that sorption occurs relatively rapidly in relation to groundwater-flow velocity. Sorption as defined by the linear equilibrium isotherm is possibly the dominant sorption process within the aquifers and confining units of interest to this study. The linear equilibrium isotherm assumes that the sorbed concentration is directly proportional to the dissolved concentration at the model cell and, for modeling purposes, is computationally the most straightforward and efficient of the three isotherm-retardation factor relations accommodated by MT3DMS. The linear equilibrium isotherm also is the least data intensive of the three available sorption types and, accordingly, was the sorption type selected for this study.

The retardation factor is related to the linear equilibrium isotherm by the following formula:

$$R = V_w / V_c = 1 + K_d \rho_b / \theta, \tag{2}$$

where

R = the retardation factor, dimensionless,
K_d = the distribution coefficient, in L^3/M,
ρ_b = the bulk density of the porous media, in M/L^3,
θ = the effective porosity of the porous media, dimensionless,
V_w = linear groundwater velocity, in L/T, and
V_c = solute velocity, in L/T.
(M, L, T = mass, length, time)

The distribution coefficient is the slope of the linear approximation of the equilibrium adsorption isotherm and is unique to a solute and the porous media through which a solute is migrating.

Estimates of retardation factors and distribution coefficients for PCE migration within the Tarawa Terrace aquifer or Castle Hayne aquifer are unknown, and initial estimates applied to the MT3DMS model were based on literature sources. Roberts et al. (1986) reported retardation factors determined from a field-scale investigation of PCE migration through a sand aquifer that ranged from 2.7 to 5.9, based on the collection of high-resolution synoptic data during a period of about 2 years. Retardation factors increased directly with increasing time but at a decreasing rate. Hoffman (1995) reported highly controlled laboratory column determinations of distribution coefficients for PCE migration through gravels, sands, and silt. Of the approximately 150 samples analyzed, the distribution coefficient for sand ranged from 0.25 to 0.76 milliliter per gram (mL/g) and averaged 0.39 mL/g.

Corresponding values for silts ranged from 0.21 to 0.71 mL/g and averaged 0.40 mL/g. Although neither the field-scale experiments reported by Roberts et al. (1986) nor the laboratory results of Hoffman (1995) related to Camp Lejeune or even to North Carolina, the solute investigated in both studies was PCE, and PCE migration was observed through porous media of sand and sands and silts, similar to Camp Lejeune. In addition, the organic carbon content of the porous media selected for the experiments of Hoffman (1995) was less than 0.1 percent, which also is similar to the organic carbon content of sands within part of the Tarawa Terrace aquifer and Upper Castle Hayne aquifer–River Bend unit (Miller et al. 1989). Given these similarities to groundwater conditions at Tarawa Terrace and vicinity, the range of reported retardation factors by Roberts et al. (1986) and distribution coefficients by Hoffman (1995) were considered reasonable initial values for the aquifers and confining units of this study. An initial distribution coefficient of 0.4 mL/g (0.000014 cubic feet per gram [ft^3/g]) was applied uniformly to all layers of the MT3DMS model for all stress periods. The final calibrated value was 0.14 mL/g (0.000005 ft^3/g), similarly applied. The calibrated retardation factor was 2.9.

The lithology of the Castle Hayne aquifer system and the Tarawa Terrace aquifer and confining unit at Tarawa Terrace and vicinity is characterized by fine silty to clayey sand and sandy to silty clay. The specific gravity of 356 samples of fine sand, as reported by Morris and Johnson (1967), ranged from 2.54 to 2.77 and averaged 2.67. The specific gravity of clay (104 samples) and silt (388 samples) ranged from 2.47 to 2.79 and averaged 2.67 and 2.62, respectively (Morris and Johnson 1967). In addition, two 3-inch undisturbed soil samples collected during soil boring investigations in the vicinity of ABC One-Hour Cleaners were used to determine a variety of geotechnical data including specific gravity and total porosity. The samples were classified as a clayey sand and a silty sand. Specific gravity of the clayey sand was 2.69 and of the silty sand was 2.68. Total porosity of the clayey sand was 32.9 percent; of the silty sand, 36.5 percent (Roy F. Weston, Inc. 1994, Appendix B) Based on these data, a specific gravity of 2.7 was assigned to all sediments represented by the seven layers of the MT3DMS model. Model input requires a conversion of specific gravity to a bulk density. Accordingly a bulk density of sediments of 170 pounds per cubic foot (lbs/ft^3) or 77,100 grams per cubic foot (g/ft^3) was assigned uniformly to all layers of the MT3DMS model.

The effective porosity of a porous media is that porosity directly related to the volume of connected interstices. Because porosity of unconsolidated sediments is largely primary, effective porosity is probably somewhat to substantially less than total porosity, particularly where silts and clays compose a significant percentage of the media. Effective porosity is closely related to laboratory determinations of specific yield and also is equated with drainage porosity (Brady and Kunkel no date). Published data, primarily Morris and Johnson (1967), were the primary sources of estimates of effective porosity for this study. With respect to fine sand, Morris and Johnson (1967) reported the specific yield of 287 samples ranged from 1 to about 46 percent and averaged 33 percent. Total porosity of fine sand ranged from 26 to about 53 percent and averaged 43 percent, based on the analyses of 243 samples. With respect to silt, total porosity ranged from about 34 to 61 percent and averaged 46 percent, based on the analyses of 281 samples. The specific yield of 266 silt samples ranged from about 1 to 39 percent and averaged 20 percent. The range and average specific yield of 27 clay samples were substantially smaller than corresponding values for fine sand and silt. The specific yield of clay ranged from about 1 to 18 percent and averaged 6 percent. Total porosity of 74 clay samples ranged from about 34 to 57 percent and averaged 42 percent. Drainage porosity of fine sand, reported by Brady and Kunkel (no date) ranged from about 1 to 40 percent and averaged about 19 percent. The average drainage porosity of silt reported by Brady and Kunkel (no date) was about 14 percent and ranged from about 4 to 29 percent.

The primary lithology of the sediments that compose the Castle Hayne aquifer system and the Tarawa Terrace aquifer is fine silty and clayey sand. The mean of the average specific yield values reported for fine sand, silt, and clay by Morris and Johnson (1967) is about 20 percent. This value also closely corresponds to the average drainage porosity of fine sand (about 19 percent) reported by Brady and Kunkel (no date). Accordingly, an effective porosity of 20 percent was initially assigned uniformly to all model layers for all stress periods. The final calibrated effective porosity also was 20 percent, similarly applied.

Biodegradation

Reductions of PCE concentration reported at water-supply well TT-26 between September 1985 and July 1991 (Table F2) probably occurred largely by microbially mediated degradation such as reductive dechlorination. Knowing the initial and final PCE concentrations at well TT-26 for this period and the number of days between measurements, a first-order degradation rate can be computed using the relation

$$C = C_0 e^{-kt}, \qquad (3)$$

where

- C = the PCE concentration at well TT-26 on July 11, 1991,
- C_0 = the PCE concentration at well TT-26 on September 25, 1985,
- e = the base of Naperian or Natural logarithms,
- k = the degradation rate constant, in $days^{-1}$, and
- t = the elapsed time, in days.

The PCE concentrations at water-supply well TT-26 on September 25, 1985, and July 11, 1991, were 1,100 and 350 μg/L, respectively, and the elapsed time was 2,151 days (Table F2). Applying these data to Equation 3 yields a degradation rate of 0.00053 per day. Potentiometric levels shown in Figures F7 and F8 indicate that well TT-26 is located on a direct advective pathway from ABC One-Hour Cleaners. Thus, PCE mass migrates downgradient toward and away from well TT-26. To the extent that migration of PCE mass toward and away from well TT-26 occurred at about equal rates from 1985 to 1991, the computed degradation rate of 0.00053 per day approximates a long-term average degradation rate. On the other hand, if a significant quantity of the PCE degraded in the vicinity of well TT-26 was replaced by advection, then the degradation rate computed using Equation 3 is probably a minimum rate.

Half-lives of PCE reported in the literature range from about 360 to 720 days (Lucius and others 1990). Applying these half-lives to Equation 3 yields first-order degradation rates ranging between 0.001 and 0.002 per day, about twice to four times the rate computed using concentrations at water-supply well TT-26. An initial first-order degradation rate of 0.00053 per day was applied to the MT3DMS model uniformly to every layer for all stress periods. The final calibrated degradation rate was 0.00050 per day, similarly applied.

Mass-Loading Rate

The concentrations of PCE at monitor wells, at Tarawa Terrace water-supply wells, and at hydrocone locations determined by Roy F. Weston, Inc. (1992, 1994) during Operable Units 1 and 2 (Tables F2–F3, F5–F8) also were used to calculate the mass of PCE still contained in the Tarawa Terrace and Upper Castle Hayne aquifers at the time the Operable Units were in progress (1991–1993). With only three exceptions, the water samples collected by hydrocone were collected at two depths at each location. The collection depth for the majority of the "shallow" samples ranged from about 15 to 25 ft. These data and data from the "S" monitor wells were assigned to an "upper shell." The collection depth for the majority of the "deep" samples ranged from about 35 to 45 ft. These data and data from the "C" monitor wells and Tarawa Terrace water-supply wells were assigned to a "lower shell." An altitude also was assigned to each sampling interval. At monitor wells and Tarawa Terrace water-supply wells, altitude was assigned at the mid-point of the open or screened interval. At hydrocone locations, altitude was assigned at the reported sample depth. Using gridding and interpolation techniques, contour maps of PCE concentration and altitude were constructed for the upper and lower shells. The individual shell maps of PCE concentration closely resembled the map shown in Figure F10. The contour maps of altitude of the upper and lower shells were used to compute the volume of aquifer materials between shells. This volume equaled about 186×10^6 cubic feet (ft^3) or about 5.3×10^9 liters. The total volume of aquifer materials was multiplied by an effective porosity of 20 percent to estimate the volume of connected interstices between shells, which equaled about 1.1×10^9 liters (Table F11). The shell contour maps of PCE concentration were first used to determine contours of PCE concentration representing an average condition between the upper and lower shells, termed herein the *average PCE shell*. Contours representing the average PCE shell were constructed at concentration intervals of 2,000 μg/L of PCE. The area between each concentration contour was determined using Geographic Information System (GIS) techniques and is termed herein a *subarea*. A total of nine subareas were identified and a representative PCE concentration was assigned to each subarea, representing the average concentration of the two contours that bounded the subarea. The product of each subarea and its representative concentration was then determined. These products were summed, and the total divided by the total area of PCE contamination represented by the average PCE shell, or about 42 acres. The result of this computation is an area-weighted average PCE concentration for the entire volume of aquifer material between the upper and lower shells, which equaled about 1.4×10^{-3} grams per liter (g/L). The product of this weighted average concentration and the estimated volume of connected interstices between the shells (1.1×10^9 liters) equals the mass of PCE within the volume of aquifer materials between the upper and lower shells, or about 1.5×10^6 grams. This mass in grams was converted to a weight of 3.2×10^3 pounds, or 1.6 tons. The unit weight of PCE is about 1.6 times that of water, or about 101 lbs/ft^3. Accordingly, the estimated volume of PCE within the aquifer materials between the upper and lower shells at Tarawa Terrace and vicinity equals about 32 ft^3, or about 240 gallons (gal).

Shell computations similar to those previously described were applied in conjunction with PCE concentration-depth data listed in Table F4 to estimate the PCE mass occurring within the unsaturated zone at and in the vicinity of ABC One-Hour Cleaners from 1987 to 1993. Three data "shells" were created representing PCE concentrations at depths ranging from 1 to 4 ft, from 4 to 9 ft, and from 9 to 14 ft. The soil mass contained within each shell was computed as the product of the estimated volume of each shell and the unit weight of silty sand, estimated to be 170 lbs/ft^3. Subareas for the uppermost shell were computed based on PCE concentration contours plotted at intervals of 50,000 μg/kg. Subareas for the middle and bottom shells were computed using concentration contours plotted at intervals of 20,000 μg/kg. The computed area-weighted PCE concentration within each shell was 156,900 μg/kg, 88,400 μg/kg, and 78,100 μg/kg, respectively. Total computed sediment volume of each shell was 29,640 ft^3, 52,860 ft^3, and 70,560 ft^3, respectively. Total PCE mass occurring within the unsaturated zone in the vicinity of ABC One-Hour Cleaners was thus estimated to be about 2,500 lbs, or about 190 gal. This mass and the PCE mass computed previously in solution in groundwater represent a minimum loss of PCE to the subsurface of about 430 gal at ABC One-Hour Cleaners during the period 1953–1985, or an average loss of about 13 gal per year or 230 g/d. This contribution rate must necessarily be considered a minimum because (1) the quantity of PCE removed from the aquifers at Tarawa Terrace water-supply wells from 1953 to 1985 is unknown; (2) the mass of PCE degraded to TCE from 1953 to 1993 was probably large and was not accounted for by the computation of PCE mass; and (3) similarly, the mass of PCE sorbed onto the porous media from 1953 to 1993 also was probably substantial and was not accounted for by the computation of PCE mass. Water-quality data applied to the computation of PCE mass refer only to PCE mass in solution in groundwater. Pankow and Cherry (1996) indicated that computations of contaminant mass similar to those described in the preceding sections possibly represent only a small part

Table F11. Computation of tetrachloroethylene (PCE) mass in the Upper Castle Hayne aquifer, Tarawa Terrace and vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina, 1991–1993.

[μg/L, microgram per liter; ft², square foot]

PCE contour range, in μg/L	Cumulative area, in ft²	Subarea, in ft²	Subarea PCE concentration, in μg/L	Subarea-weighted PCE concentration, in μg/L × ft²
12,000+	2,536.4	2,536.4	12,000	30,436,342
10,000 to 12,000	8,327.7	5,791.3	11,000	63,704,515.1
8,000 to 10,000	19,214.3	10,886.6	9,000	97,979,539.6
6,000 to 8,000	46,394.4	27,180.1	7,000	190,260,492.8
4,000 to 6,000	103,822.4	57,428	5,000	287,139,951.1
2,000 to 4,000	238,065.4	134,243	3,000	402,730,048.4
0 to 2,000	1,793,827.4	1,555,762.1	1,000	1,555,762,094
2.2	1,812,259.5	18,432	2.2	40,660.3
3.4	1,834,571.1	22,311.6	3.4	75,859.4
Total area	**1,834,571.0**			
Total subarea		**1,834,571.0**		
Total area-weighted PCE concentration				**2,628,129,503**

Area-weighted PCE concentration = 1.433 μg/L = 0.0014 gram per liter (sum of PCE subarea-weighted concentrations/total area)

Aquifer volume between shells = 186,072,994 cubic feet

Aquifer volume between shells × effective porosity (20 percent) = 37,214,599 cubic feet

Volume of connected interstices, in liters = 1,053,173,152 (1 cubic foot = 28.3 liters)

PCE mass, in grams = 1,474,442 (product of area-weighted PCE concentration and volume of connected interstices)

PCE weight, in pounds = 3,244 (1 gram = 0.0022 pound)

PCE volume, in cubic feet = 32 (unit weight of PCE = 101 pounds/cubic foot)

PCE volume, in gallons = 240 (1 cubic foot = 7.5 gallons)

of the total contaminant mass in the subsurface. Note that the computations of PCE mass within the Upper Castle Hayne aquifer and the unsaturated zone in the immediate vicinity of ABC One-Hour Cleaners are necessarily highly interpretive and somewhat subjective because of poor data density and some uncertainty regarding water-quality analytical methods and results. Nevertheless, the computed loading rate of about 230 g/d was used as a minimum mass-loading rate and assigned as an initial condition to begin model calibration.

The MT3DMS code requires that a contaminant mass be loaded directly to the water table. Mass loading was assigned to the MT3DMS model in layer 1 at cell 47, 170 and was applied continuously during stress periods 25–408. The location of the septic tank–soil absorption system and related drain field was not specifically determined during ABC One-Hour Cleaners (Roy F. Weston, Inc. 1994); however, legal depositions indicate the drain field probably was located to the rear and slightly northeast of the ABC One-Hour Cleaners building (Hopf & Higley, P.A., Deposition of Victor John Melts, written communication, April 12, 2001, p. 62–63). Accordingly, cell 47, 170 was located within the active model domain slightly east and behind the building that houses ABC One-Hour Cleaners in order to approximate the probable location of the septic system drain field used by the cleaners. The initial mass loading rate applied to the model was 230 g/d and was adjusted upward during model calibration. The final calibrated mass-loading rate was 1,200 g/d. Distributed arrays of initial PCE concentrations were populated with zero values at all cells for all layers. Thus, the PCE concentration at cell 47, 170 in layer 1 immediately prior to the beginning of mass loading was 0.0 g/ft³.

The primary loss of PCE from operations at ABC One-Hour Cleaners probably was through volatilization. Loss of PCE to the subsurface during operations was probably substantially less than losses to volatilization. Legal depositions (Hopf & Higley, P.A., Deposition of Victor John Melts, written communication, April 12, 2001) indicate that ABC One-Hour Cleaners replenished its PCE supply at a rate of two or three 55-gal drums per month. The unit weight of PCE is about 100 lbs/ft^3. Using two drums per month, or 110 gal of PCE, ABC One-Hour Cleaners replaced about 1,470 pounds or about 670,000 grams of PCE monthly. The calibrated mass-loading rate (1,200 g/d) applied to the model represents about 36,000 grams of PCE per month, or about 5 percent of total usage. Using three drums per month, this percentage drops to 3.6 percent. These percentages represent loss not only to wastewater but to filter and still residues that were disposed to the land surface in the immediate vicinity of the cleaners as well as spills from a 250-gal PCE storage tank external and adjacent to the cleaners' building. Because PCE is a high-expense item, efficient use of PCE is critical to a profitable dry-cleaning operation. Thus, the calibrated mass-loading rate indirectly reflects a reasonable operational efficiency and PCE loss rate at ABC One-Hour Cleaners.

PCE lost to the subsurface through operations migrated vertically through the unsaturated zone to the water table. Soil-boring data in the vicinity of ABC One-Hour Cleaners (Figure F5) indicate that PCE occurred vertically through much or all of the unsaturated zone. Aerobic biodegradation of PCE to TCE also occurred within the unsaturated zone at these boring sites (Roy F. Weston, Inc. 1994, Table 5-2). Thus, the actual PCE loss rate to the subsurface from operations at ABC One-Hour Cleaners was possibly somewhat greater than indicated by the calibrated mass-loading rate of 1,200 g/d to the water table.

Model Calibration

Calibration of the Tarawa Terrace fate and transport model was accomplished in a hierarchical process consisting of four successive stages or levels. Simulation results achieved for each calibration level were compared to simulation results of previous levels until results at all levels satisfactorily conformed to appropriate conceptual models and calibration standards. Hydraulic characteristic arrays and model boundary conditions were equivalent at all calibration levels following the final calibration at level 4. In hierarchical order, calibration levels consisted of (1) simulation of predevelopment (steady-state) groundwater-flow conditions, (2) simulation of transient or pumping groundwater-flow conditions, (3) simulation of the fate and transport of a PCE source at ABC One-Hour Cleaners, and (4) computation of concentrations of PCE at the Tarawa Terrace WTP and within the Tarawa Terrace water-distribution network. Calibration levels 1 and 2 are described in detail in Faye and Valenzuela (2007). Calibration levels 3 and 4 are described in this report. Numerical computations performed by MT3DMS for this study used the upstream finite-difference method.

Level 3 Calibration

Hydraulic characteristic and recharge arrays of the MODFLOW flow model assigned following the level 2 calibration were not adjusted during level 3 calibration. Initial values of several transport parameters were modified during trial-and-error calibration and were previously described herein. Final calibrated parameter values are listed in Table F12. Level 3 model calibration was achieved by comparing simulated PCE concentrations at Tarawa Terrace water-supply wells to corresponding observed concentrations. Simulated PCE concentrations were computed at the end of each stress period and were considered representative of an average concentration for the respective month. Field data (observed PCE concentrations) were compared to the simulated concentration closest in time (days) to the simulated day.

Observed PCE concentrations at monitor wells and hydrocone locations were not used for model calibration because of substantial scale differences between the volume of aquifer sampled at monitor wells and the corresponding volume represented by a single cell of the fate and transport model. The volume of sediments represented by a typical model cell located in layer 1 is about 100,000 ft^3 and corresponds to a volume of connected interstices of about 20,000 ft^3. In contrast, the volume of aquifer sediments sampled by hydrocone was little more than several cubic inches. The volume sampled at a typical monitor well was probably several dozen or perhaps several hundred cubic feet, at most. In addition, PCE mass simulated at a model cell is distributed uniformly and instantaneously throughout the available interstitial volume of the cell at the end of every stress period. Thus, the simulated PCE concentration at the end of every stress period is equal throughout the volume of sediments represented by the model cell. Compare this condition to the highly variable distribution of PCE with depth at hydrocone penetration sites listed in Table F7. Similar or comparable variations in PCE concentration likely occurred across the screened interval of the "S" monitor wells (Table F6). Although mixing occurred during the sampling process, highly variable PCE concentrations determined in monitor wells at various times possibly reflect similar but unobserved variability with depth caused by local heterogeneity and relate to only a tiny percentage of the volume of a model cell. Only by the most unique and rarest of coincidences could one expect highly variable PCE concentrations within an aquifer volume of several dozen or several hundred cubic feet to equal or be comparable to a corresponding simulated concentration uniformly distributed throughout an aquifer volume of 20,000 ft^3 in the same area. On the other hand, samples obtained from operating supply wells are composite samples obtained from a large volume of the contributing aquifer or aquifers and reflect well-mixed or average conditions within the water-bearing units. Thus, samples collected at supply wells conform to a considerable degree to the assumptions and limitations that apply to simulated results from the Tarawa Terrace fate and transport model.

Table F12. Calibrated model parameter values used for simulating groundwater flow and contaminant fate and transport, Tarawa Terrace and vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina.

[ft/d, foot per day; ft³/d, cubic foot per day; ft³/g, cubic foot per gram; g/ft³, gram per cubic foot; d⁻¹, 1/day; g/d, gram per day; ft, foot; ft²/d, square foot per day; —, not applicable]

Model parameter[1]	Model layer number[2]						
	1	2	3	4	5	6	7
Predevelopment groundwater-flow model (conditions prior to 1951)							
Horizontal hydraulic conductivity, K_H (ft/d)	12.2–53.4	1.0	4.3–20.0	1.0	6.4–9.0	1.0	5.0
Ratio of vertical to horizontal hydraulic conductivity, K_V/K_H[3]	1:7.3	1:10	1:8.3	1:10	1:10	1:10	1:10
Infiltration (recharge), I_R (inches per year)	13.2	—	—	—	—	—	—
Transient groundwater-flow model, January 1951–December 1994							
Specific yield, S_y	0.05	—	—	—	—	—	—
Storage coefficient, S	—	4.0×10^{-4}	4.0×10^{-4}	4.0×10^{-4}	4.0×10^{-4}	4.0×10^{-4}	4.0×10^{-4}
Infiltration (recharge), I_R (inches per year)	6.6–19.3	—	—	—	—	—	—
Pumpage, Q_k (ft³/d)	See footnote[4]	—	See footnote[4]	—	0	—	0
Fate and transport of tetrachloroethylene (PCE) model, January 1951–December 1994							
Distribution coefficient, K_d (ft³/g)	5.0×10^{-6}	5.0×10^{-6}	5.0×10^{-6}	5.0×10^{-6}	5.0×10^{-6}	5.0×10^{-6}	5.0×10^{-6}
Bulk density, ρ_b (g/ft³)	77,112	77,112	77,112	77,112	77,112	77,112	77,112
Effective porosity, n_E	0.2	0.2	0.2	0.2	0.2	0.2	0.2
Reaction rate, r (d⁻¹)	5.0×10^{-4}	5.0×10^{-4}	5.0×10^{-4}	5.0×10^{-4}	5.0×10^{-4}	5.0×10^{-4}	5.0×10^{-4}
Mass-loading rate[5], $q_S C_S$ (g/d)	1,200	—	—	—	—	—	—
Longitudinal dispersivity, α_L (ft)	25	25	25	25	25	25	25
Transverse dispersivity, α_T (ft)	2.5	2.5	2.5	2.5	2.5	2.5	2.5
Vertical dispersivity, α_V (ft)	0.25	0.25	0.25	0.25	0.25	0.25	0.25
Molecular diffusion coefficient, D^* (ft²/d)	8.5×10^{-4}	8.5×10^{-4}	8.5×10^{-4}	8.5×10^{-4}	8.5×10^{-4}	8.5×10^{-4}	8.5×10^{-4}

[1] Symbolic notation used to describe model parameters obtained from Chiang and Kinzelbach (2001)

[2] Refer to Chapter B (Faye 2007) and Chapter C (Faye and Valenzuela 2007) reports for geohydrologic framework corresponding to appropriate model layers; aquifers are model layers 1, 3, 5, and 7; confining units are model layers 2, 4, and 6

[3] For model cells simulating water-supply wells, vertical hydraulic conductivity (K_V) equals 100 feet per day to approximate the gravel pack around the well

[4] Pumpage varies by month, year, and model layer; refer to Chapter K report (Maslia et al. In press 2008) for specific pumpage data

[5] Introduction of contaminant mass began January 1953 and terminated December 1984

Simulated and corresponding observed PCE concentrations at Tarawa Terrace and local water-supply wells are listed in Table F13 and are portrayed in this report as a scatter diagram (Figure F12) and as time-series graphs at individual wells (Figures F13–F17). The calibration target range for observed PCE concentrations was ±½-order of magnitude of the observed concentration. For concentrations that are reported as not detected (ND), the lower calibration target was selected as 1 μg/L; the upper limit selected was the analytical detection limit (Table F2).

Simulated concentrations and observed concentrations reported as not detected do not compare favorably at water-supply well TT-23. Faye and Green (2007) described an enhanced rate of biodegradation of PCE at well TT-23 possibly caused by the occurrence of BTEX compounds in conjunction with PCE in the groundwater. This local enhancement in the rate of biodegradation at well TT-23, and, possibly at other wells, was not accounted for in MT3DMS simulations and possibly explains at least part of the disparity between observed and simulated PCE concentrations.

All simulated PCE concentrations in local water-supply wells labeled as "RW" compared favorably to calibration target limits. Of the 18 paired data that corresponded to Tarawa Terrace water-supply wells and included an observed value for PCE concentration, 11 comparisons of simulated to observed concentrations failed the ½-order of magnitude calibration

Table F13. Simulated and observed tetrachloroethylene (PCE) concentrations at water-supply wells and calibration target range, Tarawa Terrace and vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina.

[µg/L, microgram per liter; ND, not detected; J, estimated]

Site name	Date	PCE concentration, in µg/L		Calibrated target range, in µg/L
		Observed	Simulated	
[1]RW1	7/12/1991	ND	0.0	0.0–2.0
[1]RW2	7/12/1991	760	1,804	240–2,403
[1]RW3	7/12/1991	ND	0.0	0.0–2.0
[2]TT-23	1/16/1985	132	254	41.7–417
	2/12/1985	37.0	254	11.7–117
	2/19/1985	26.2	253	8.3–82.8
	2/19/1985	ND	253	0.0–10.0
	3/11/1985	14.9	253	4.7–47.1
	3/11/1985	16.0	253	5.2–52.5
	3/12/1985	40.6	253	12.8–128
	3/12/1985	48.0	253	15.4–154
	4/9/1985	ND	265	0.0–2.0
	9/25/1985	4.0	279	0.3–12.6
	7/11/1991	ND	193	0.0–5.0
[2]TT-25	2/5/1985	ND	6.2	0.0–10.0
	4/9/1985	ND	8.6	0.0–2.0
	9/25/1985	0.43J	18.1	0.14–1.4
	10/29/1985	ND	20.4	0.0–10.0
	11/4/1985	ND	20.4	0.0–10.0
	11/13/1985	ND	20.4	0.0–10.0
	12/3/1985	ND	22.8	0.0–10.0
	7/11/1991	23.0	72.6	7.3–72.7
[2]TT-26	1/16/1985	1,580	804	500–5,000
	2/12/1985	3.8	804	1.2–12
	2/19/1985	55.2	798	17.5–175
	2/19/1985	64.0	798	20.2–202
	4/9/1985	630	801	199–1,999
	6/24/1985	1,160	732	367–3,668
	9/25/1985	1,100	788	348–3,478
	7/11/1991	340	670	111–1,107
[2]TT-30	2/6/1985	ND	0.0	0.0–10.0
[2]TT-31	2/6/1985	ND	0.15	0.0–10.0
[2]TT-52	2/6/1985	ND	0.0	0.0–10.0
[2]TT-54	2/6/1985	ND	5.8	0.0–10.0
	7/11/1991	ND	30.4	0.0–5.0
[2]TT-67	2/6/1985	ND	3.9	0.0–10.0

[1]See Figure F6 for location

[2]See Figure F1 for location

Note: Calibration target ranges for analyses listed as not detected are detection limits noted in Table F2

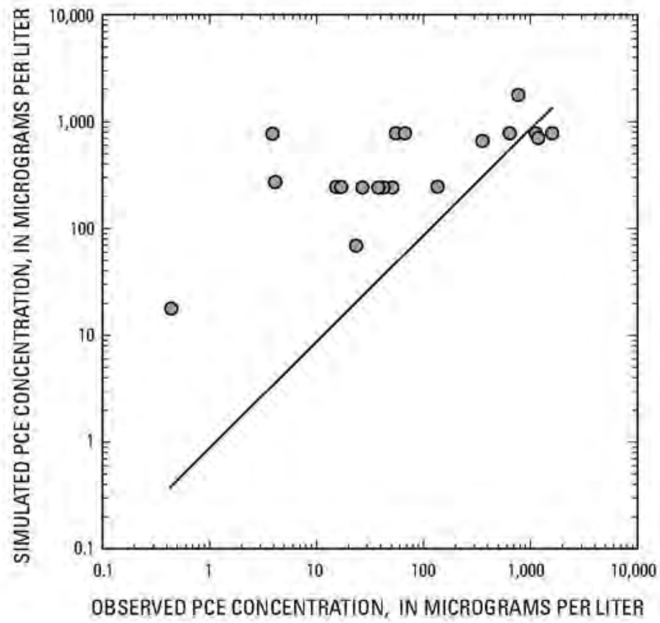


Figure F12. Simulated and observed tetrachloroethylene (PCE) concentrations at selected water-supply wells, Tarawa Terrace, U.S. Marine Corps Base Camp Lejeune, North Carolina, January 1985–July 1991.

standard (Table F13). Of the total of 36 comparisons of simulated to observed PCE concentrations in all water-supply wells used to calibrate the Tarawa Terrace fate and transport model (Table F13), including "not detected" results, 17 comparisons or 47 percent conformed to the calibration standard, and 19 comparisons or 53 percent violated the standard. A scatter diagram of simulated and observed PCE concentrations is shown in Figure F12 and indicates that simulated PCE concentrations mainly exceeded corresponding observed concentrations. A geometric bias that compares simulated and observed concentrations also was computed. An inclusive bias was computed using all 19 paired data at water-supply wells and equaled 5.9. A selected bias also was computed that excluded paired data at water-supply well TT-23 and equaled 3.9 (Maslia et al. 2007). Both results indicate that simulated PCE concentrations moderately to substantially overpredicted observed concentrations at water-supply wells.

Time-series graphs of simulated PCE concentrations in water-supply wells RW2, TT-23, TT-25, TT-26, and TT-54 indicate that PCE concentrations in these wells equaled or exceeded the current maximum contaminant level (MCL) for PCE of 5 µg/L (USEPA 2003) during the service periods of the wells (Faye and Valenzuela 2007) (Figures F13–F17). Well RW2 was located in a commercial building (furniture store) adjacent to ABC One-Hour Cleaners on SR 24. Simulated PCE concentrations at this site probably resemble

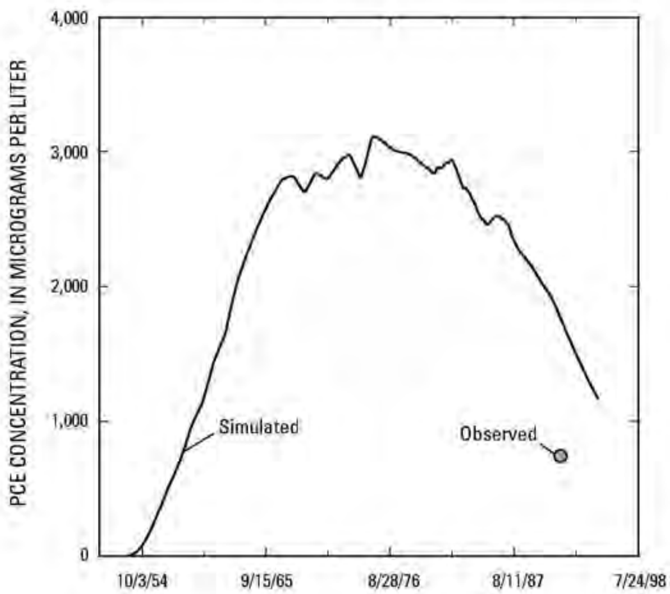


Figure F13. Simulated and observed tetrachloroethylene (PCE) concentrations at local water-supply well RW2, near ABC One-Hour Cleaners, Jacksonville, North Carolina, January 1951–December 1994 (see Figure F6 for location).

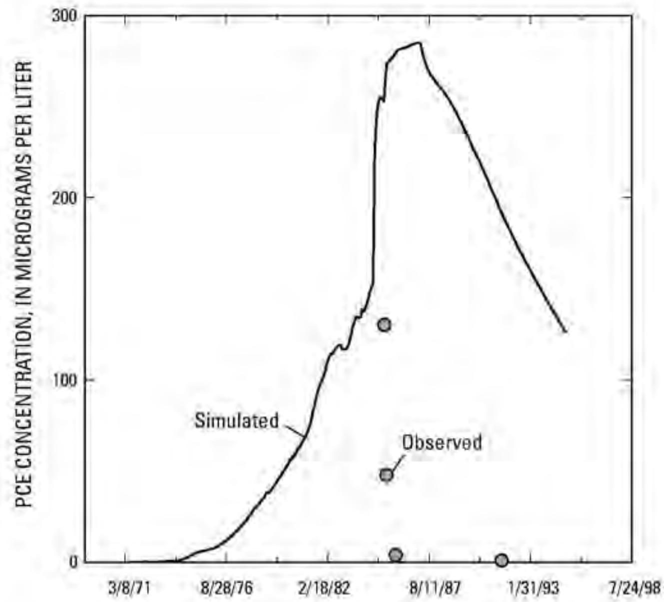


Figure F14. Simulated and observed tetrachloroethylene (PCE) concentrations at water-supply well TT-23, Tarawa Terrace, U.S. Marine Corps Base Camp Lejeune, North Carolina, January 1969–December 1994 (see Figure F6 for location).

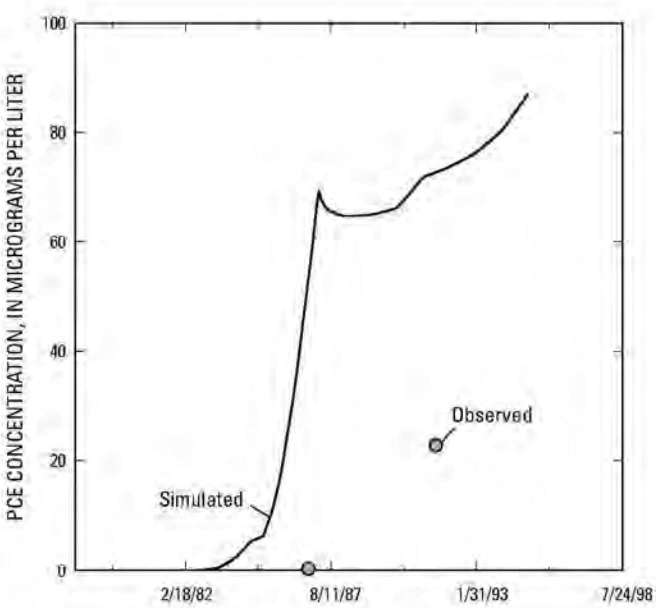


Figure F15. Simulated and observed tetrachloroethylene (PCE) concentrations at water-supply well TT-25, Tarawa Terrace, U.S. Marine Corps Base Camp Lejeune, North Carolina, January 1978–December 1994 (see Figure F6 for location).

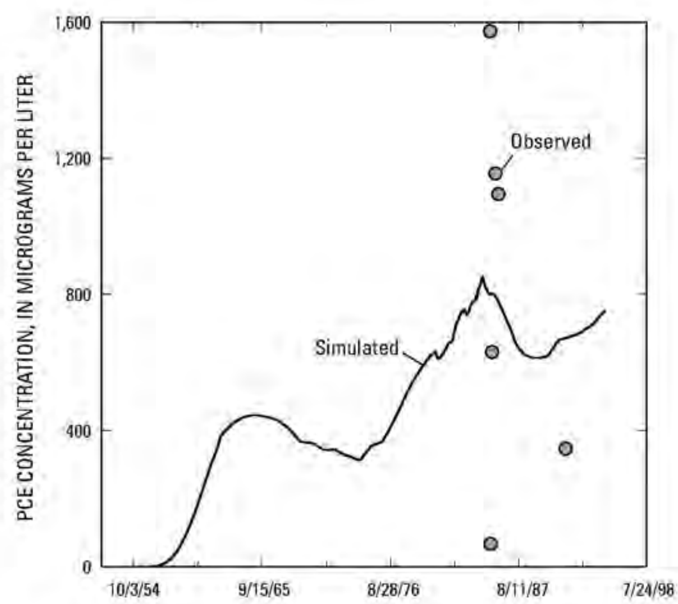


Figure F16. Simulated and observed tetrachloroethylene (PCE) concentrations at water-supply well TT-26, Tarawa Terrace, U.S. Marine Corps Base Camp Lejeune, North Carolina, January 1952–December 1994 (see Figure F6 for location).

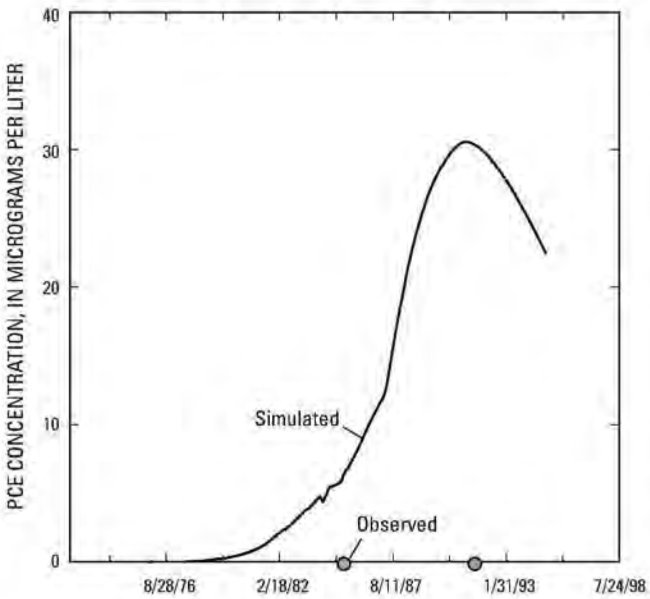


Figure F17. Simulated and observed tetrachloroethylene (PCE) concentrations at water-supply well TT-54, Tarawa Terrace, U.S. Marine Corps Base Camp Lejeune, North Carolina, January 1970–December 1994 (see Figure F6 for location).

groundwater contamination in the immediate vicinity of the cleaners. Pumpage and operation data were not available for well RW2. Regardless, pumpage from well RW2 was considered insignificant for modeling purposes, and simulated pumpage was assigned as 0.0 ft^3/d for the entire period of simulation. Simulated PCE concentrations at Tarawa Terrace water-supply wells approximate an historical record of contaminated groundwater delivered to the Tarawa Terrace WTP, as well as the attenuation of PCE concentrations subsequent to the termination of pumping at the wells. Of the water-supply wells contributing PCE to the Tarawa Terrace WTP, well TT-26 was the earliest and by far the dominant contributor (Figure F16). Simulated breakthrough of PCE at a concentration above 5 μg/L occurs at about December 1956 or January 1957. The simulated PCE concentration increases rapidly following breakthrough to 100 μg/L at about April 1959. Simulated PCE concentrations remain greater than 100 μg/L during the remainder of the simulation period and peak at about 850 μg/L during July 1984, several months prior to the termination of operations at well TT-26 during February 1985. At the time well TT-23 was placed in service, at or about August 1984, the simulated PCE concentration of the discharge water is about 150 μg/L and increases gradually to this level following a breakthrough of 5 μg/L at about December 1974 at the well site (Figure F14). Following the onset of pumping at well TT-23, the simulated PCE concentration increases rapidly to about 280 μg/L by April 1985, when the well was probably removed from service. The simulated PCE concentration at well TT-25 increases to 5 μg/L about June or July 1984 and gradually increases to a maximum concentration of about 87 μg/L at the end of the simulation period during December 1994 (Figure F15). The simulated MCL occurs at well TT-54 (Figure F17) during June 1984. The maximum simulated PCE concentration of about 31 μg/L at well TT-54 occurs during February 1991; however, this condition is not supported by field data (Tables F2 and F13).

Plan views of PCE concentration plumes simulated within model layer 1 (the combined Tarawa Terrace aquifer and Upper Castle Hayne aquifer–River Bend unit) during December 1960, December 1968, December 1975, December 1984, March 1987, and December 1994 are shown in Figures F18–F23. Simulated potentiometric levels also are shown for the respective months and layer. Simulated pumping at original Tarawa Terrace water-supply wells TT-26, TT-27, TT-28, TT-29, and TT-45 begins during January 1952. Operation of well TT-29 was terminated about 1958 (Faye and Valenzuela 2007). Available construction data for the original Tarawa Terrace wells are incomplete (Table F9) but indicate that each of the wells probably was open to the Upper Castle Hayne aquifer–River Bend unit and the Upper Castle Hayne aquifer–Lower unit, the Lower unit either directly by open interval or indirectly by gravel or sand packing within the annular space of the well bore. Accordingly, simulated pumpage at these wells was assigned entirely to either the Upper Castle Hayne aquifer–River Bend unit or Lower unit. Simulated mass loading of PCE to model layer 1 at cell 47, 170 begins during January 1953. By December 1960, a small continuous PCE plume develops along descending hydraulic gradients between ABC One-Hour Cleaners and well TT-26 (Figure F18). Simulated breakthrough of PCE at well TT-26 at the MCL concentration occurs by January 1957, and the concentration increases to about 265 μg/L by December 1960 (Figure F16). Drawdown caused by pumping at water-supply wells west of ABC One-Hour Cleaners significantly flattened the potentiometric surface and related hydraulic gradients between the cleaners and wells TT-27, TT-28, and TT-29, and no simulated breakthrough of PCE occurs at these wells during their assigned periods of operation (Faye and Valenzuela 2007). The simulated PCE concentration during December 1960 at the mass-loading cell (47, 170) equals about 88,000 μg/L. Simulated PCE concentrations in water delivered to the Tarawa Terrace WTP from well TT-26 during 1960 ranges from about 169 to 265 μg/L. Computed breakthrough of PCE at the Tarawa Terrace WTP at the MCL concentration occurs by November 1957 (Maslia et al. 2007).

The areal extent of the simulated PCE plume within model layer 1 approximately doubles between December 1960 and December 1968 (Figures F18 and F19), and plume migration diverts partially southward toward water-supply wells operating near and within the Tarawa Terrace housing areas (Figure F19). Water-supply wells TT-52, TT-53, and TT-54 began operation during 1962. Pumpage at these wells was assigned either entirely to the Upper Castle Hayne aquifer or was equally divided between the

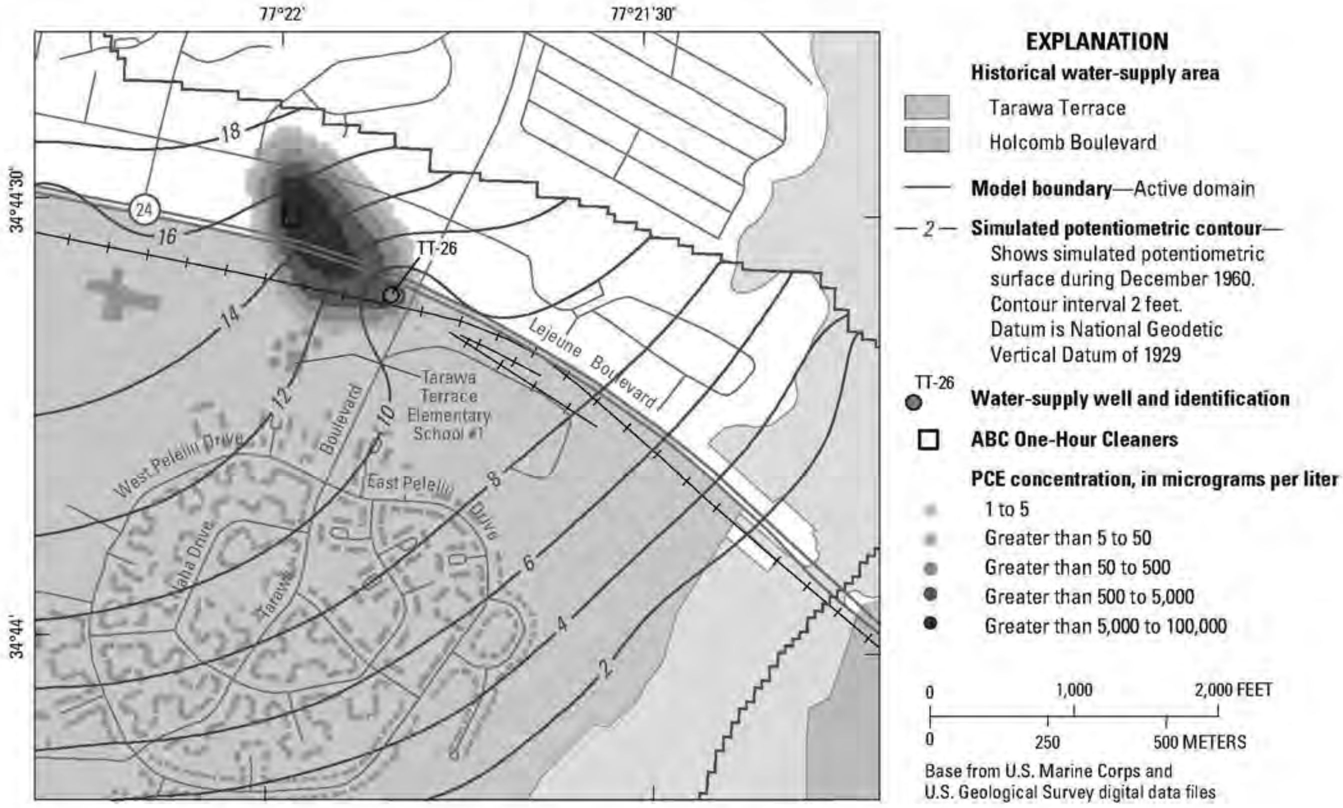


Figure F18. Simulated distribution of tetrachloroethylene (PCE) and potentiometric levels within part of model layer 1, Tarawa Terrace and vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina, December 1960.

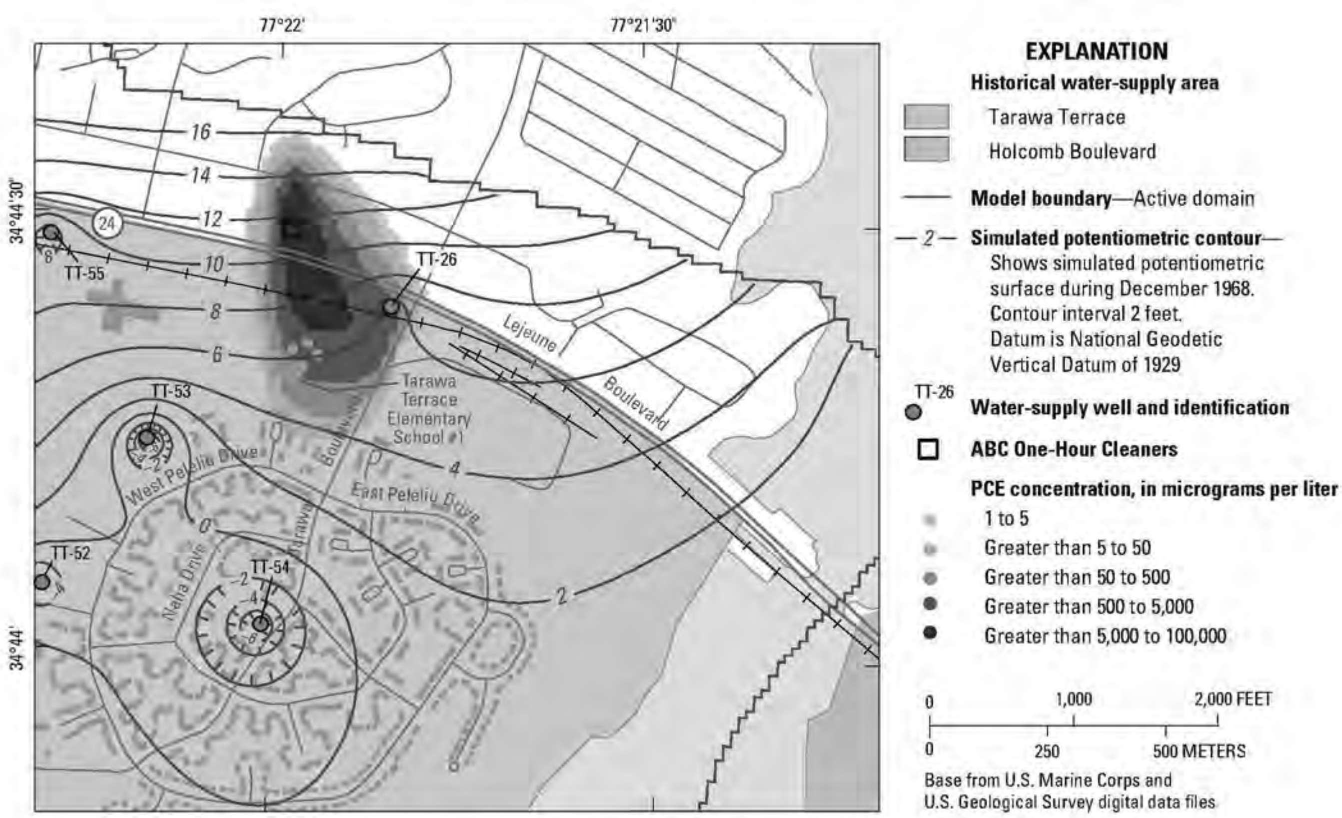


Figure F19. Simulated distribution of tetrachloroethylene (PCE) and potentiometric levels within part of model layer 1, Tarawa Terrace and vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina, December 1968.

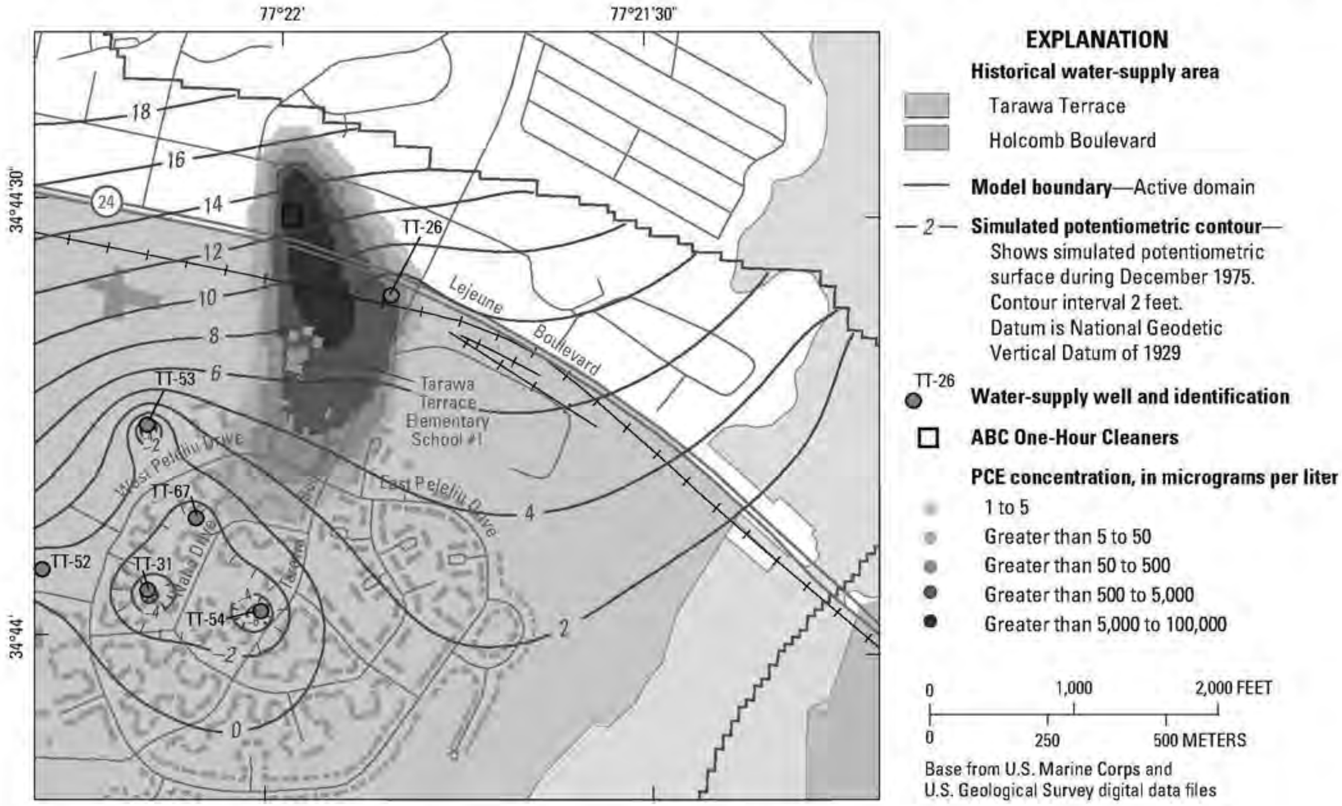


Figure F20. Simulated distribution of tetrachloroethylene (PCE) and potentiometric levels within part of model layer 1, Tarawa Terrace and vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina, December 1975.

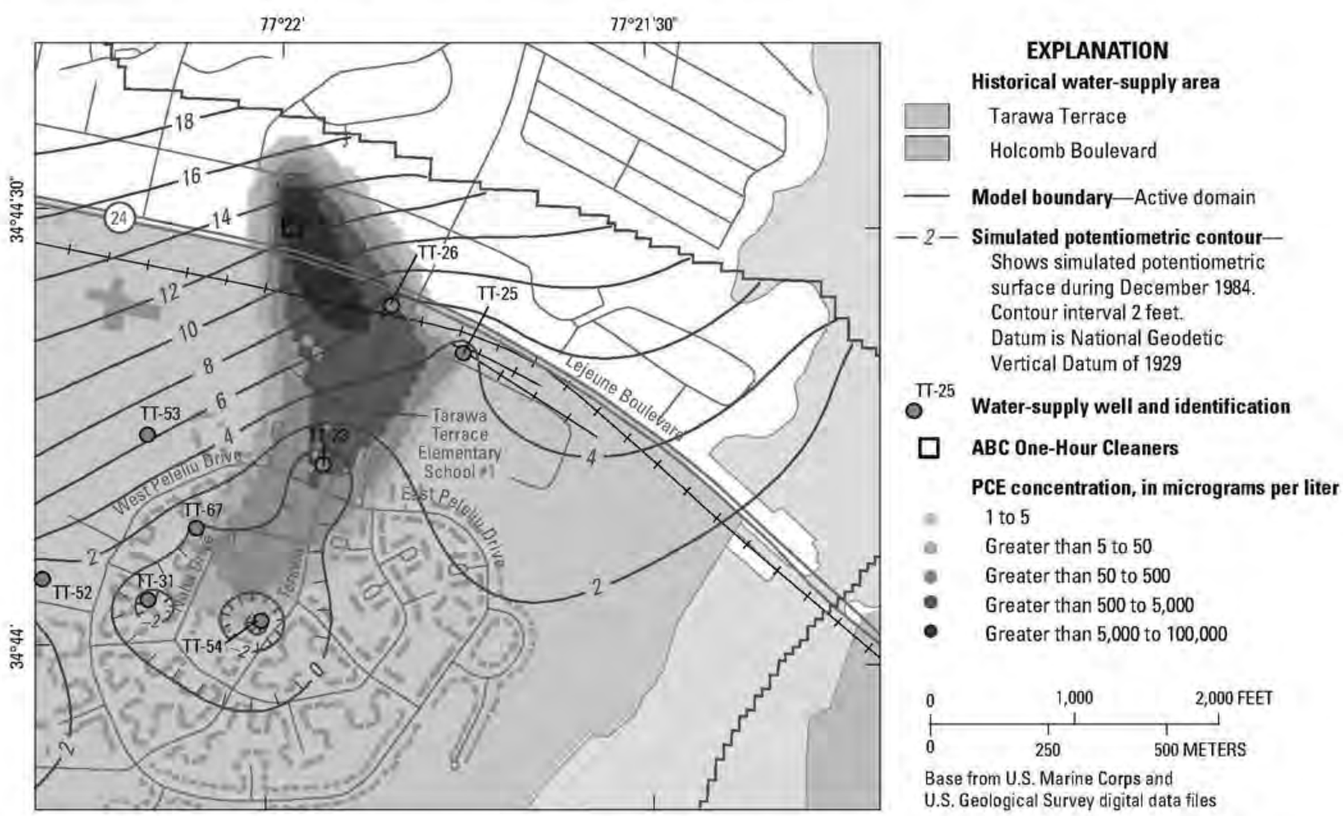


Figure F21. Simulated distribution of tetrachloroethylene (PCE) and potentiometric levels within part of model layer 1, Tarawa Terrace and vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina, December 1984.

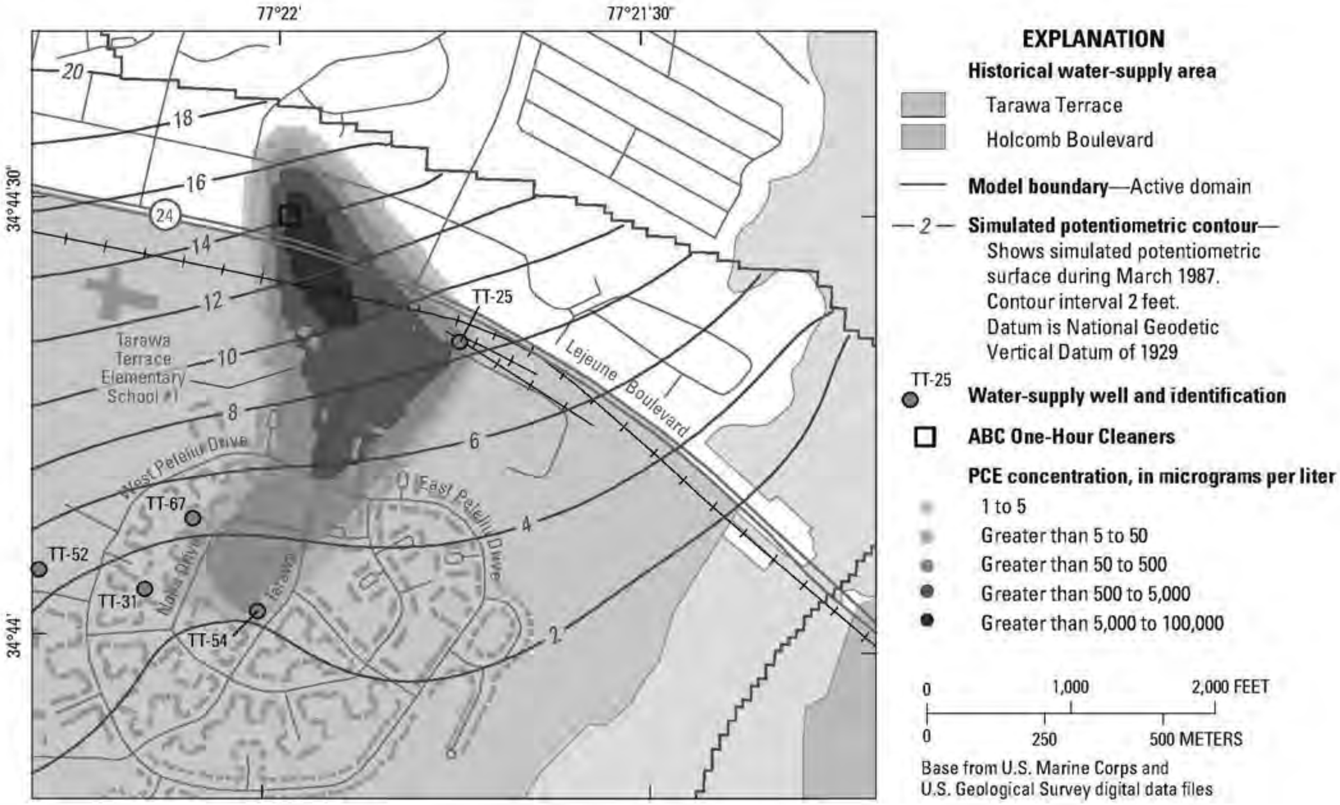


Figure F22. Simulated distribution of tetrachloroethylene (PCE) and potentiometric levels within part of model layer 1, Tarawa Terrace and vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina, March 1987.

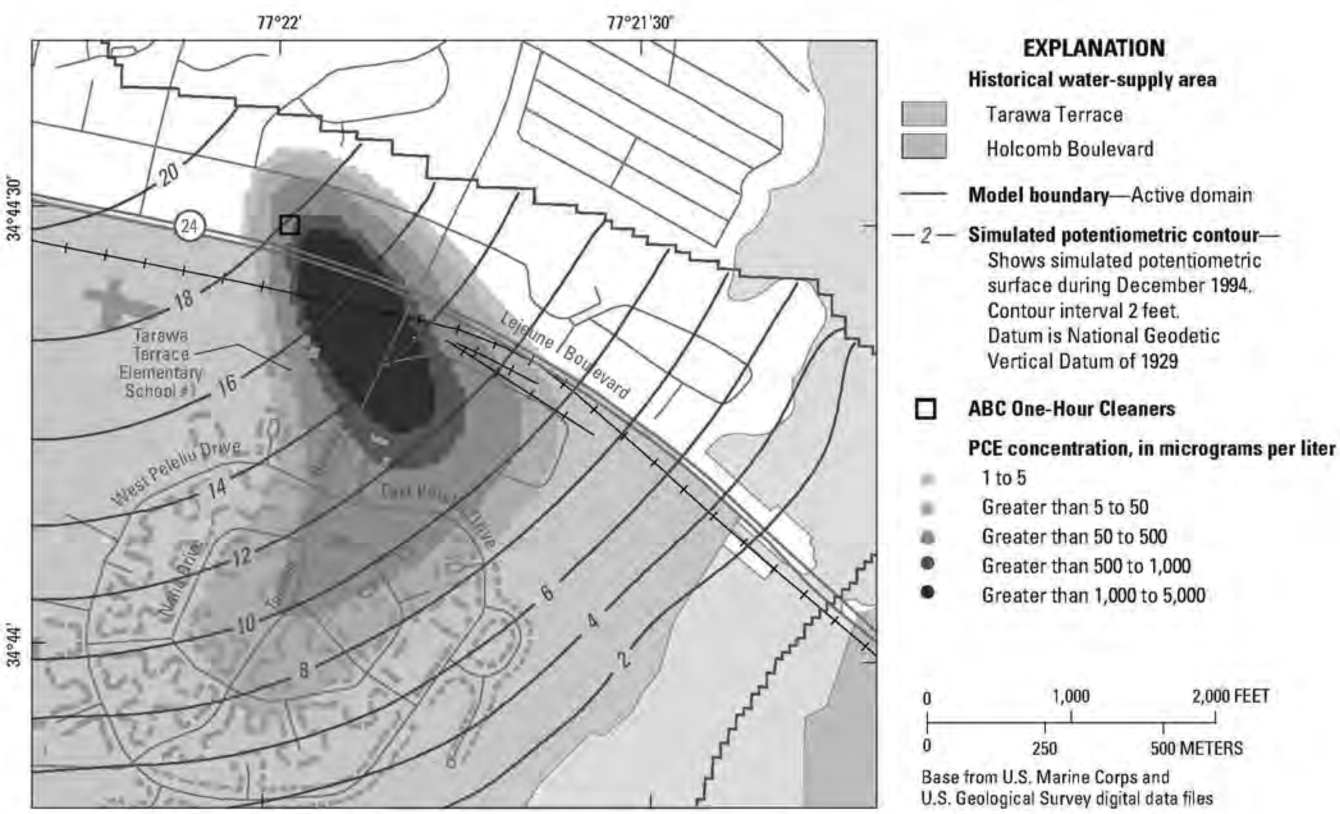


Figure F23. Simulated distribution of tetrachloroethylene (PCE) and potentiometric levels within part of model layer 1, Tarawa Terrace and vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina, December 1994.

River bend and Lower units of the Upper Castle Hayne aquifer (Faye and Valenzuela 2007), and caused hydraulic gradients in the vicinity of ABC One-Hour Cleaners to shift gradually from generally southeast during December 1960 to generally southward by December 1968 (Figures F18 and F19). This shift in hydraulic gradients also caused PCE mass to be diverted southward away from water-supply well TT-26 and probably caused the downward trend in PCE concentration at this well beginning at about January 1965 (Figure F16). During the same period, the simulated concentration of PCE at the mass-loading site in layer 1 (cell 47, 170) decreases from about 88,000 μg/L to about 86,900 μg/L, possibly as a result of dilution from uncontaminated ground-water flowing along hydraulic gradients from the northwestern part of the active model domain (general-head boundary) toward ABC One-Hour Cleaners (Figure F19). Original water-supply wells TT-28 and TT-45 were still in service during December 1968. Original water-supply well TT-27 was removed from service, probably about 1963 and was replaced by water-supply well TT-55 (Faye and Valenzuela 2007). Construction data for well TT-55 are not available, and construction and contributing aquifers were assumed similar to other original Tarawa Terrace water-supply wells. No simulated breakthrough of PCE occurs at wells TT-27 or TT-55 during their assigned periods of operation. Simulated PCE concentrations in water delivered to the Tarawa Terrace WTP from well TT-26 during 1968 ranges from about 367 to 402 μg/L.

By December 1975, southward migration and expansion of the PCE plume within model layer 1 had extended to the northern part of the Tarawa Terrace housing area I (Figure F20). Water-supply wells TT-31 and TT-67 began operation, probably during 1972 and 1973 (Faye and Valenzuela 2007), which further increased the southward-trending hydraulic gradients noted during December 1968 (Figures F19 and F20). Water-supply well TT-30, located near water-supply well TT-28 and substantially west of water-supply well TT-26, probably began operation during 1972 following the termination of service at well TT-28 during 1971. No simulated breakthrough of PCE at well TT-30 occurs during its assigned period of operation. With the exception of well TT-26, service at all of the original Tarawa Terrace water-supply wells, including TT-55, was abandoned by December 1975, and water supplied to the Tarawa Terrace WTP was entirely from wells TT-26, TT-30, TT-31, TT-52, TT-53, TT-54, and TT-67. The simulated PCE concentration at the mass-loading site (cell 47, 170) had decreased to about 80,700 μg/L by December 1975. Simulated PCE concentrations in water delivered to the Tarawa Terrace WTP from well TT-26 during 1975 ranges from about 355 to 367 μg/L.

The southward migration of the PCE plume within model layer 1 continued after December 1975 and, by December 1984, had terminated near the center of Tarawa Terrace housing area I (Figure F21). An additional water-supply well, TT-23, was placed in service during 1984, and service at water-supply well TT-30 was terminated shortly afterward (Faye and Valenzuela 2007). During 1984, wells TT-23 and TT-26 delivered water to the Tarawa Terrace WTP at simulated PCE concentrations ranging from about 224 to 255 μg/L and 791 to 805 μg/L, respectively. Well TT-23 was constructed with screens open to the Upper and Middle Castle Hayne aquifers, and PCE-contaminated water from the Upper Castle Hayne aquifer was diluted with water from the Middle Castle Hayne aquifer that contained little or no PCE. Water-supply well TT-25 was placed in service probably during 1982 and was located about 500 ft southeast of well TT-26. Pumping at this well in conjunction with the operation of well TT-26 further diverted PCE mass toward well TT-26. The simulated PCE concentrations at well TT-26 continue to increase during most of the period December 1975–December 1984 (Figures F16 and F21). The simulated PCE plume migrates to the vicinity of well TT-25 by December 1984 (Figure F21); however, PCE concentrations in the discharge water were below the MCL concentration at this time (Figure F15). In addition, well TT-25 was constructed as a multiaquifer well, similar to well TT-23, causing dilution of PCE-contaminated water obtained from the Upper Castle Hayne aquifer. During 1984, simulated PCE concentrations in discharge water from well TT-25 ranges from about 2.5 to 6.0 μg/L. Simulated breakthrough at the PCE MCL concentration at well TT-25 occurs about June or July 1984. The simulated PCE concentration at the mass-loading cell (47, 170) declines to about 72,200 μg/L by December 1984.

Service at water-supply wells TT-23 and TT-26 was terminated during early 1985 because of PCE contamination. Service at all Tarawa Terrace water-supply wells was terminated by March or April 1987. Concentrations of PCE and potentiometric levels in model layer 1 during March 1987 are shown in Figure F22. The simulated distribution of PCE is similar to that shown for December 1984 (Figure F21), with the exception of additional migration of PCE toward water-supply well TT-31 and a slight shift in migration of the PCE plume center of mass from south to southeast.

Simulated mass loading of PCE to model layer 1 at cell 47, 170 terminates after December 1984. Accordingly, a supply of additional PCE mass to model layer 1 is no longer available beginning January 1985. In addition, (1) substantial quantities of PCE mass are no longer removed from model layers 1 and 3 by wells, following the termination of service at these wells during 1985, and (2) PCE migration is no longer influenced by pumping at wells after March or April 1987. These simulated conditions prevail during most of the period December 1984–December 1994, the end of groundwater-flow and fate and transport simulations (Figure F23). By December 1994, the center of mass of PCE has migrated about 700 ft southeast of ABC One-Hour Cleaners and maximum PCE concentrations at the center of mass have decreased to about 3,300 μg/L. Conversely, simulated PCE concentrations in the vicinity of water-supply wells TT-25 and TT-54 have increased to about 87 μg/L and 22 μg/L, respectively, by December 1994. Increases in simulated PCE concentration at both wells occur mostly as a result of PCE migration along natural groundwater-flow gradients between December 1984 and December 1994.

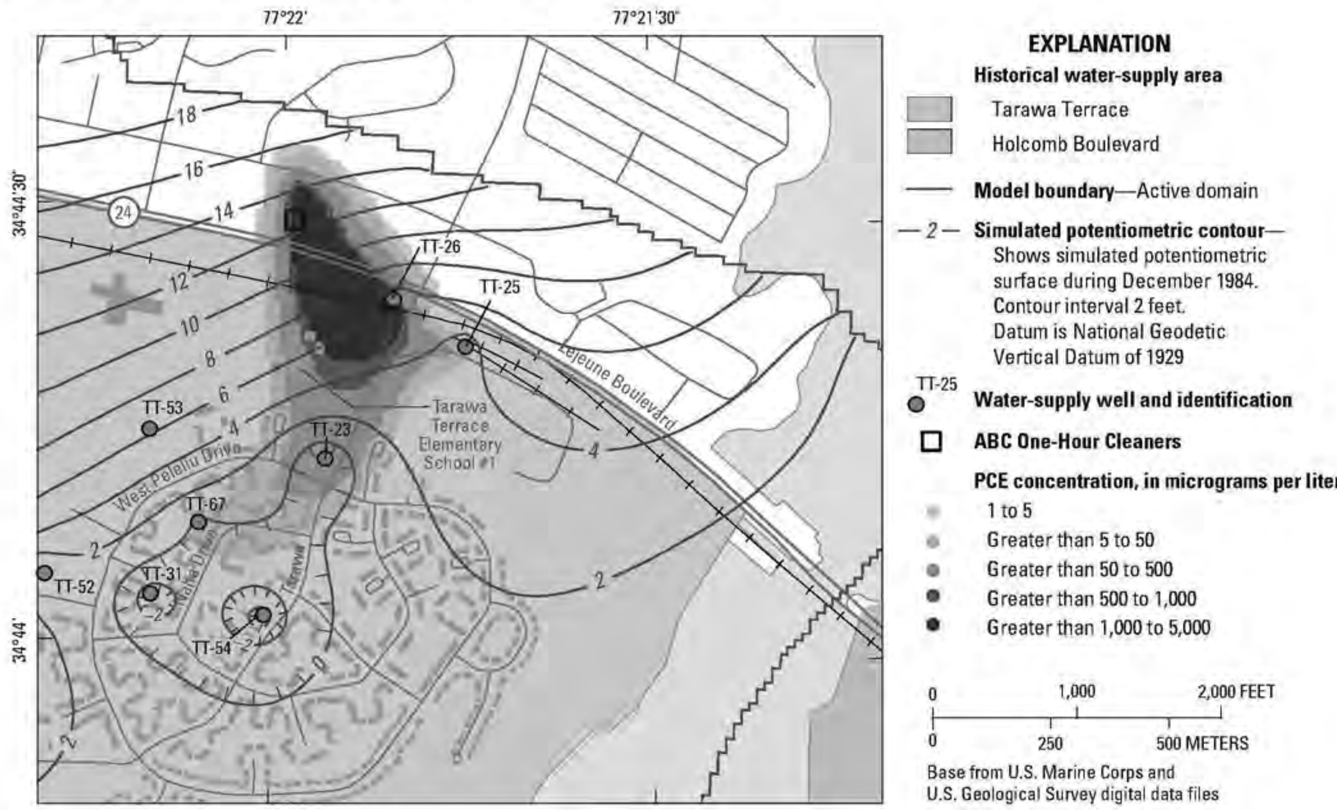


Figure F24. Simulated distribution of tetrachloroethylene (PCE) and potentiometric levels within part of model layer 3, Tarawa Terrace and vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina, December 1984.

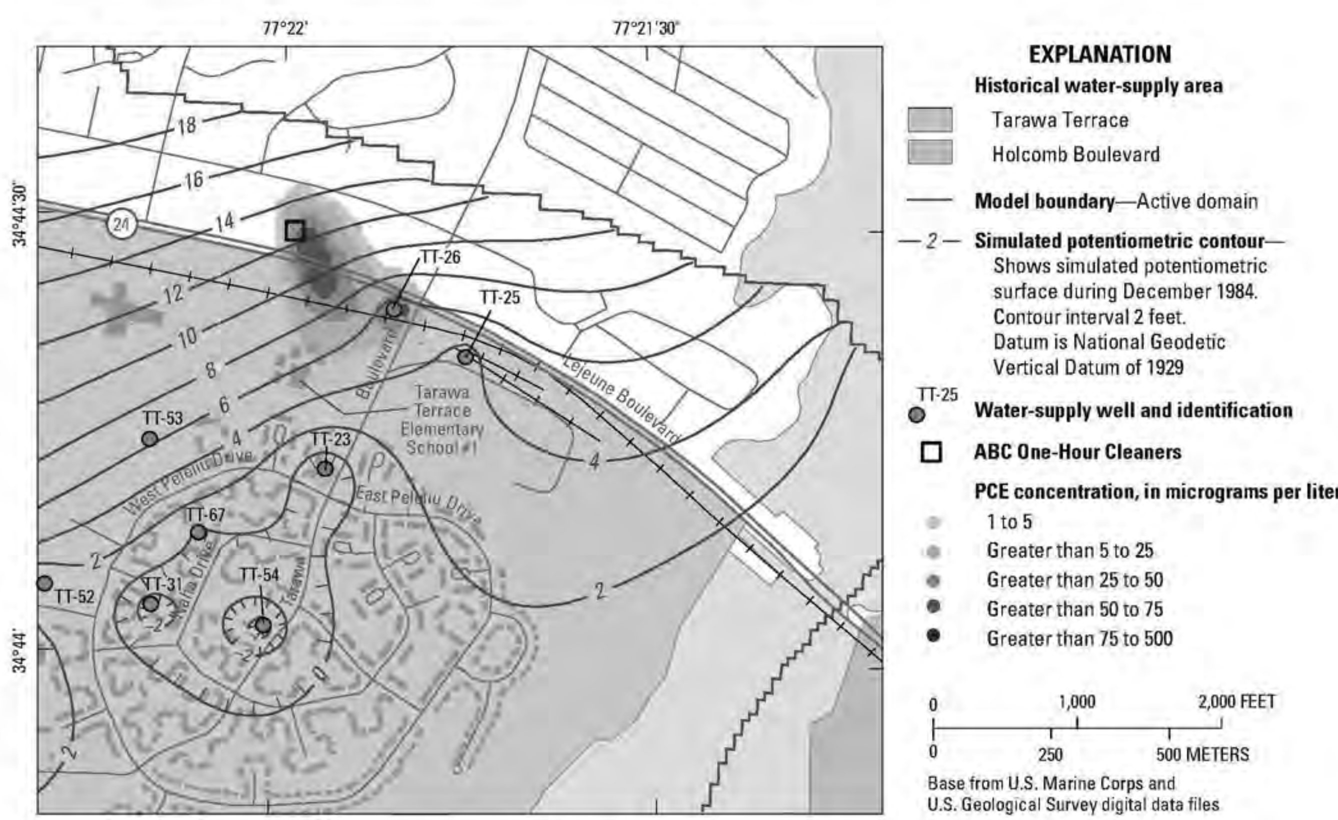


Figure F25. Simulated distribution of tetrachloroethylene (PCE) and potentiometric levels within part of model layer 5, Tarawa Terrace and vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina, December 1984.

Downward vertical migration of PCE to model layers 3 and 5 also was simulated. By December 1984, the distribution of PCE within layer 3 (Figure F24) closely resembles the corresponding distribution within layer 1 (Figure F21), albeit with substantially lower concentrations. The maximum PCE concentration of about 3,600 µg/L occurs slightly east and south of the mass-loading cell. Simulated migration of PCE occurs to the south and southeast largely along hydraulic gradients caused by pumping from model layers 1 and 3 and to the north and northwest along concentration gradients. Potentiometric gradients within model layer 5 are similar to those in layers 3 and 1; however, concentrations of PCE are substantially lower (Figure F25). The occurrence of PCE is limited largely to the area between ABC One-Hour Cleaners and water-supply well TT-26, with minor occurrences southward toward water-supply well TT-23. Simulated contamination within model layer 5 also occurs in the immediate vicinity of water-supply well TT-23, indicating possible "capture" of contaminated water from the well bore caused by pumping at this well and water-supply wells TT-31, TT-54, and TT-67, and the subsequent lowering of heads in model layers 3 and 5. The maximum simulated concentration of PCE in model layer 5 is about 140 µg/L and occurs slightly east of the mass-loading cell—cell 47, 170.

Results of mass balance simulations by the calibrated model are summarized in Figure F26. Of the total PCE mass removed from all model layers during the period of fate and transport simulation (January 1953–December 1994), wells are shown to have removed the least mass (2.4×10^6 grams) and biodegradation the most (9.2×10^6 grams). The simulated sorbtion process removed about 5.8×10^6 grams of PCE. Residual PCE mass still present in the model aquifers and confining units during December 1994 totals about 2.8×10^6 grams. Total PCE mass loaded to the model from January 1953 to December 1984 equals about 14.0×10^6 grams. Mass sorbed also is biodegraded. Thus, total mass removed from the model is the sum of total mass removed by wells and by biodegradation. The algebraic difference between mass loaded to, remaining in, and removed from the model of 4.0×10^5 grams is the result of rounding error and simulation discrepancy.

Mass balance calculations also can be used to determine the quantity of PCE mass in solution in all model layers at the end of any stress period. Most of the data used to compute the quantity of PCE mass in solution (Table F11) were collected during December 1991 and April 1992 (Tables F7 and F5). These months are represented in the model by stress periods 492 and 496, respectively. Algebraic manipulation of mass balance data computed for stress period 494, representing February 1992, indicate the simulated PCE mass in solution at that time equals about 1.0×10^6 grams. The computed PCE mass in solution (Table F11) equals 1.5×10^6 grams and represents, for the most part, PCE quantities in the most contaminated parts of the Upper Castle Hayne aquifer–River Bend and Lower units (model layers 1 and 3). Model simulations indicate that the vast majority of PCE mass occurring in the model during stress period 494 also resided in layers 1 and 3. Although the PCE mass calculation is interpretive and somewhat subjective, the reasonably close agreement between simulated and computed mass in solution within the active model domain at the same time further corroborates the calibration of the fate and transport model.

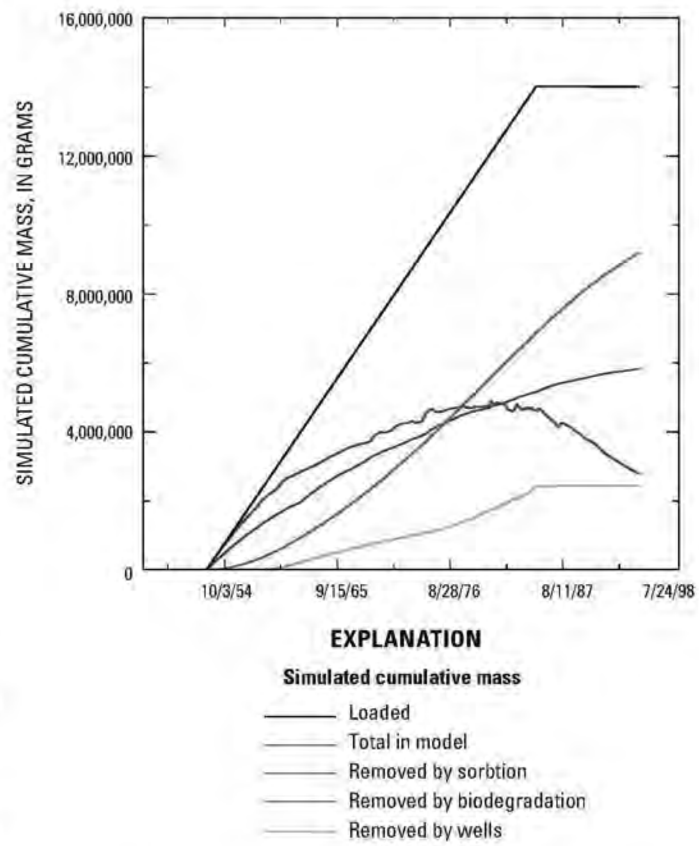


Figure F26. Simulated cumulative mass balance of tetrachloroethylene (PCE), Tarawa Terrace and vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina, January 1953–December 1994.

Level 4 Calibration

The final stage of model calibration employed a simple mixing (flow-weighted average) model to compute PCE concentrations delivered to the Tarawa Terrace WTP from all active water-supply wells and subsequently to the Tarawa Terrace water-supply network. For each stress period (month) of the simulation period (from January 1951 to December 1994), the PCE concentration simulated at each active water-supply well is weighted by the respective well discharge to compute a weighted-average PCE concentration. This weighted-average concentration was considered the monthly average PCE concentration delivered to the Tarawa Terrace WTP. The results of these computations compared to an analysis of a water sample collected at a point in time, either at the Tarawa Terrace WTP or at a location within the Tarawa Terrace water-supply network, such as an outdoor or indoor faucet, are summarized in Table F14. The computed PCE concentration is compared to the observed PCE concentration on a same-month basis; that is, if a sample date was reported as May 1, 1982, then the corresponding computed PCE concentration was the weighted-average concentration for the month of May 1982. The calibration standard applied to the comparisons of computed and observed PCE concentrations was ±½-order of magnitude of the observed value. Many observed analyses were reported as "not detected," and corresponding detection limits were assigned as the calibration standard, similar to the standard applied to water-supply well concentration data. Detection limits pertinent to the 1982 analyses are unknown but probably were not greater than 10 µg/L. Detection limits for the analyses of February 19, 1985, and March 11–12, 1985, were 2 µg/L. Detection limits for all other analyses listed in Table F14 were 10 µg/L. Of the 25 PCE concentrations listed in Table F14 (including the "not detected" analyses), only 3 computed WTP concentrations or about 12 percent failed the calibration standard. The computed PCE concentration used to compare the PCE concentration determined for the tank sample collected on February 11, 1985, was the January 1985 concentration (176 µg/L). The source of the PCE in the tank at a concentration of 215 µg/L could have only been water-supply well TT-23 or TT-26 or both. Service at wells TT-23 and TT-26 was discontinued during February 1985 on an unknown day. Simulated contributions from these wells to the Tarawa Terrace WTP are zero for the entire month of February 1985. Accordingly, the computed WTP PCE concentration for January 1985, prior to removal of wells TT-23 and TT-26 from service, was used as a reasonable surrogate for February 1985. A similar argument is forwarded regarding the analysis of the tap-water sample dated February 2, 1985. The computed WTP PCE concentration for January 1985 is compared to the observed PCE concentration of 80 µg/L.

Table F14. Computed and observed tetrachloroethylene (PCE) concentrations in water samples collected at the Tarawa Terrace water treatment plant and calibration target range, U.S. Marine Corps Base Camp Lejeune, North Carolina.

[µg/L, microgram per liter; TTWTP, Tarawa Terrace water treatment plant; ND, not detected]

Date	PCE concentration, in µg/L		Calibration target range, in µg/L
	Computed[1]	Observed	
[2]TTWTP Building TT-38			
5/27/1982	148	180	25–253
7/28/1982	112	[3]104	33–329
7/28/1982	112	[3]76	24–240
7/28/1982	112	[3]82	26–259
2/5/1985	176	[3,4]80	25–253
2/13/1985	3.6	[5]ND	0–10
2/19/1985	3.6	[6]ND	0–2
2/22/1985	3.6	[5]ND	0–10
3/11/1985	8.7	[6]ND	0–2
3/12/1985	8.7	[6,7]6.6	2.1–21
3/12/1985	8.7	[6,8]21.3	6.7–67
4/22/1985	8.1	[5]1	0.3–3.2
4/23/1985	8.1	[5]ND	0–10
4/29/1985	8.1	[5]3.7	1.2–11.7
5/15/1985	4.8	[5]ND	0–10
7/1/1985	5.5	[5]ND	0–10
7/8/1985	5.5	[5]ND	0–10
7/23/1985	5.5	[5]ND	0–10
7/31/1985	5.5	[5]ND	0–10
8/19/1985	6.0	[5]ND	0–10
9/11/1985	6.0	[5]ND	0–10
9/17/1985	6.0	[5]ND	0–10
9/24/1985	6.0	[5]ND	0–10
10/29/1985	6.0	[5]ND	0–10
[2]TTWTP Tank STT-39			
2/11/1985	176	[5]215	0–10

[1]Weighted-average computation

[2]See Plate 1, Chapter A report, for location (Maslia et al. 2007)

[3]Detection limit is unknown

[4]Analysis of tap water sample for Tarawa Terrace, address unknown

[5]Detection limit = 10 µg/L

[6]Detection limit = 2 µg/L

[7]Sample collected downstream of TTWTP reservoir after operating well TT-23 for 24 hours

[8]Sample collected upstream of TTWTP reservoir after operating well TT-23 for 22 hours

An example of a flow-weighted average computation of PCE concentration is shown in Table F15 for May 1982. Similar computations were accomplished for simulated pumpage and PCE concentrations for all 528 stress periods and are plotted in Figure F27. Computed breakthrough of PCE at the MCL concentration of 5 µg/L occurs at the Tarawa Terrace WTP about October or November 1957 and, except when water-supply well TT-26 was temporarily removed from service, continues above 40 µg/L from about December 1959 until the termination of operations at well TT-26 during February 1985. The precipitous declines in PCE concentration noted in Figure F27 represent periods when well TT-26 was temporarily removed from service during July and August 1980 and January and February 1983. The last decline in PCE concentration corresponds to the final removal of well TT-26 from service. The points indicating "observed" PCE concentrations on Figure F27 correspond to the numerical concentrations listed in Table F14.

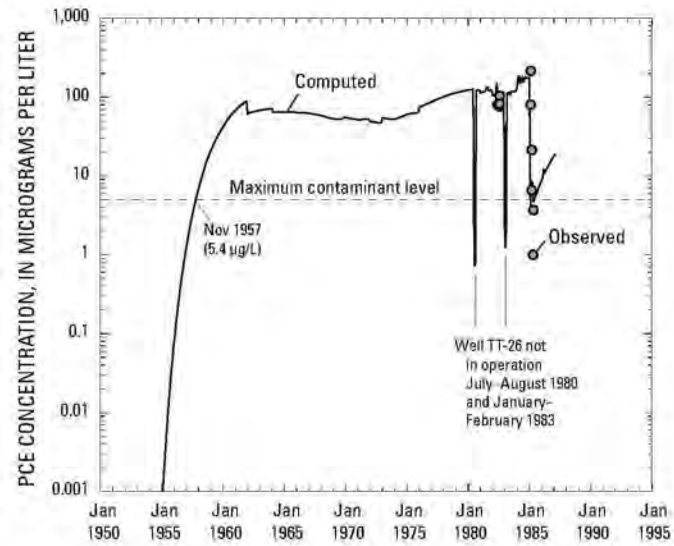


Figure F27. Computed and observed concentrations of tetrachloroethylene (PCE) in finished water at the water treatment plant, Tarawa Terrace, U.S. Marine Corps Base Camp Lejeune, North Carolina, January 1951–December 1984. [µg/L, microgram per liter]

Table F15. Example computation of flow-weighted average tetrachloroethylene (PCE) concentration at the Tarawa Terrace water treatment plant, U.S. Marine Corps Base Camp Lejeune, North Carolina, May 1982.

[ft^3/d, cubic foot per day; g/ft^3, gram per cubic foot; g/d, gram per day; µg/L, microgram per liter]

Site name[1]	Simulated pumping rate, in ft^3/d	Simulated PCE concentration, in g/ft^3	Simulated PCE flow rate, in g/d	Weighted average PCE concentration, in g/ft^3	Weighted-average PCE concentration, in µg/L
TT-26	25,604	0.02046	523.83		
TT-52	21,000	3.82×10^{-16}	8.027×10^{-12}		
TT-53	14,438	1.93×10^{-8}	0.00028		
TT-54	10,223	6.62×10^{-5}	0.68		
TT-67	10,223	0.00011	1.15		
TT-31	20,021	1.035×10^{-6}	0.021		
TT-25	13,865	$4.88 \times ^{-7}$	0.0068		
TT-30	9,626	0.0	0.0		
Total	**125,000**		**525.68**		
				0.00420	**148**

[1]See Figure F1 for location

Sensitivity Analysis

Sensitivity analysis of the fate and transport model compared the root mean square error (RMS) related to specified changes in fate and transport model parameters to the RMS of the calibrated model. Calibrated model parameters were changed by factors ranging from 0.5 to 4.0. The parameter change factor of the calibrated model was 1.0 (Figure F28). A total of 29 PCE concentrations were used to compute the RMS and are the numerical concentrations listed in Tables F13 and F14. Analytical results listed as "not detected" were disregarded. Results of the sensitivity analyses are summarized in Figure F28. The RMS of the calibrated model was 337 µg/L.

Simulation results are shown to be least sensitive to changes to dispersivity and distribution coefficient. The total change in RMS related to changes in dispersivity across the range of change factors applied to the sensitivity analysis equaled about 13 µg/L. Simulation results also are relatively insensitive to changes in distribution coefficient until distribution coefficient values exceed about twice the calibrated value. The maximum change in RMS related to changes in distribution coefficient occurred between parameter change factors 2.0 and 4.0 and equaled about 48 µg/L. Simulation results with respect to changes in the mass-loading rate were highly sensitive when the mass-loading rate exceeded the calibrated rate. A maximum change in RMS of about 156 µg/L occurred when the mass-loading rate changed by factors ranging from 0.9 to 1.5 of the calibrated value. Simulation results also were highly sensitive to changes in effective porosity and biodegradation rate. The RMS related to changes in effective porosity declined rapidly from 533 to 311 µg/L when change factors ranged from 0.5 to 1.5 of the calibrated value. Similarly, the RMS related to changes in biodegradation rate increased from 312 to 429 µg/L when change factors ranged from 1.5 to 4.0 of the calibrated value. With the exception of the mass-loading rate, the maximum change in RMS for all parameters between change factors 0.9 and 1.5 was 47 µg/L and related to effective porosity. The average RMS for all parameters, including mass loading, between change factors 0.9 and 1.5 equals 343 µg/L and compares favorably to the RMS of 337 µg/L related to the calibrated model.

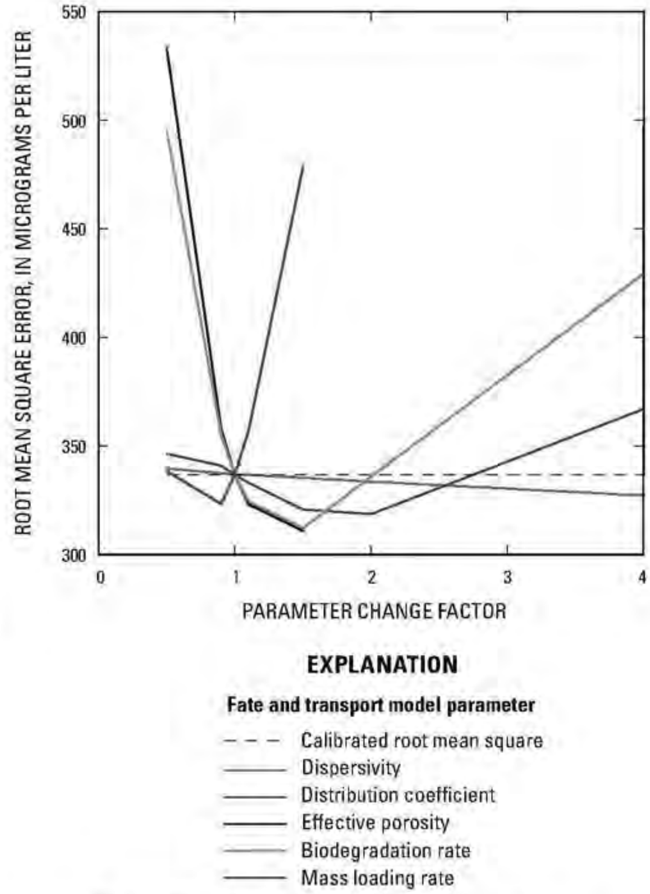


Figure F28. Sensitivity of simulation results to changes in fate and transport model parameters, Tarawa Terrace, U.S. Marine Corps Base Camp Lejeune, North Carolina.

Discussion

Results and interpretations described in this report are substantially dependent on the accuracy of water-quality data. Substantial differences, if not outright contradictions, characterize many analyses of duplicate samples collected during various investigations of groundwater and supply-well water quality. During ABC One-Hour Cleaners Operable Unit 1, duplicate groundwater samples collected at hydrocone penetration sites were analyzed using a field mobile laboratory and by a CLP laboratory (Roy F. Weston, Inc. 1992). Results of these analyses are listed in Table F7. Duplicate samples are indicated by the sequential repetition of site names. The mobile laboratory result is listed first in the sequence followed by the CLP laboratory result. Probably the "best" example of analytical "confusion" occurs at site HC-20-34 where the CLP laboratory reported a PCE concentration of 30,000 µg/L and the corresponding mobile laboratory result was 500 µg/L. Similar differences obtained to corresponding analyses of TCE at this site. Large differences in PCE concentration determined by the mobile and CLP laboratories also occurred at site HC-21-22, and, to a lesser degree, at several other sites sampled. Such differences in analytical results may have been the result of different or poorly applied analytical techniques but also could be caused by extremely large, in-situ concentration gradients in the subsurface, such that sequential samples of even small quantities of water would contain significantly different quantities of constituent. Substantial vertical concentration gradients are indicated at several sites, including site HC-20, cited previously, and sites HC-21 and HC-44. Reported concentrations of PCE at these locations changed by several orders of magnitude over depth intervals ranging from about 7 to 11 ft.

At water-supply well TT-23, duplicate samples collected on February 19, 1985 (Table F2) were analyzed by JTC Environmental Consultants, Inc., for the U.S. Navy and by the NCDNRCD Laboratory (Camp Lejeune water document CLW 1482, written communication, April 25, 1986). The reported concentration of PCE in the sample analyzed by JTC Environmental Consultants, Inc., was 26.17 µg/L. A PCE concentration in the sample analyzed by the North Carolina laboratory was "not detected."

Analyses of water samples collected at water-supply well TT-26 (Table F2, Figure F16) indicate changes in PCE concentration of several orders of magnitude during relatively short intervals of time. The first available analysis of PCE at well TT-26 was obtained from a sample obtained on January 16, 1985. The well was probably operating in a routine manner at this time and was still supplying water to the Tarawa Terrace WTP. The reported PCE concentration was 1,580 µg/L (Shiver 1985). The PCE concentration reported for a sample obtained on February 12, 1985, at well TT-26 had decreased to an estimated 3.8 µg/L, a change of about 2.5 orders of magnitude in only 27 days (Report 29, JTC Environmental Consultants Report 85-052, written communication, February 14, 1985). Seven days later, on February 19, 1985, the reported PCE concentration had increased to about 60 µg/L (Camp Lejeune water document CLW 1482, written communication, April 25, 1986). Although well TT-26 was removed from service some time during February 1985, such radical changes in PCE concentration during this and the previous month are difficult to explain, other than as a result of poor sampling technique or analytical error. The PCE concentrations reported in samples collected at well TT-26 during April, June, and September 1985 ranged from about 600 to 1,200 µg/L and were apparently all determined from analyses at the NCDNRCD Laboratory, as was the sample collected on January 16, 1985. For this study, these analyses are considered the most accurate and representative of PCE concentrations at well TT-26 during 1985.

The accuracy of various analytical methods and technologies used by different laboratories at this time possibly also contributed significantly to conflicting analytical results. Most if not all water-quality analyses cited herein were probably accomplished using GC/MS methodologies. The accuracy of such methods in the 1980s was about ± 20 percent (AH Environmental Consultants, Inc., written communication, June 18, 2004), which possibly explains a number of the conflicting results indicated in Tables F2 and F7.

Sampling methods and techniques probably also affected water-quality results. Little or no information is available regarding sampling methods used at Tarawa Terrace and other Camp Lejeune water-supply wells from 1982 to 1985. In contrast, sampling methods applied at water-supply wells and monitor wells during ABC One-Hour Cleaners Operable Units 1 and 2 are described in detail by Roy F. Weston, Inc. (1992, 1994). These methods included purging water-supply wells from three to five casing volumes before sampling to assure that only aquifer water was sampled. All purge waters were containerized onsite using 500-gal tanks and subjected to regulated disposal. Depending on well construction, 500 gal represented one to about three casing volumes at Tarawa Terrace water-supply wells. Although such methods are generally appropriate, they do not compare to the routine operation of a water-supply well when pumping occurs continuously for several hours or days. Sampling of discharge water from water-supply wells beyond the accepted sampling protocols may have been necessary to obtain a truly representative sample of aquifer water. For example, water-supply well TT-23 was initially pumped for about 2 hours, beginning March 11, 1985 (Table F2). Capacity of the well at the time was about 250 gal/min. Water samples collected after 2 hours of pumping contained PCE concentrations of about 15 µg/L. The well continued pumping for another 22 hours. Water samples collected after this interval contained PCE concentrations of about 41 µg/L (Camp Lejeune water document CLW 1482, written communication, April 25, 1986). Such comparisons indicate that just purging several casing volumes at Tarawa Terrace water-supply wells prior to sampling for PCE and related constituents may not have provided samples representative of the aquifer volume affected during routine operation of the wells and, consequently, possibly contributed to much of the disparity noted between simulated and observed PCE concentrations (Tables F13 and F14).

Comparisons of simulated PCE concentrations at wells to observed concentrations also are not straightforward. Simulated PCE concentrations represent average monthly conditions; whereas, an observed concentration probably represents a condition that occurred during a single day for several minutes or perhaps, at most, an hour. The temporal resolution of flow and MT3DMS simulations was regulated to a substantial degree by project objectives and available data. Monthly resolution was the prescribed protocol for historical reconstruction investigations at U.S. Marine Corps Base Camp Lejeune (ATSDR, Exposure to Volatile Organic Compounds in Drinking Water and Specific Birth Defects and Childhood Cancers, p. 22, written communication, September 2004). Consider, as well, that pumpage quantities used during calibration of the transient flow model (level 2 calibration) were not available for individual water-supply wells at any time and were only available as an annual average of total water supply from 1975 to 1987. Monthly pumpage totals were sporadically available from 1978 to 1987. In addition, monthly water-level data used for transient flow model calibration were generally available at active water-supply wells from 1978 to 1984. Earlier water-level data for water-supply wells were few or none (Faye and Valenzuela 2007). Thus, data limitations and historical reconstruction protocols prescribed a monthly stress period as a rational and appropriate condition for transient flow and MT3DMS model simulations; however, a monthly concentration is not directly comparable to reported PCE concentrations.

The PCE concentrations simulated by the MT3DMS model also were possibly affected by numerical dispersion and the discretization of the time derivative. Substantial numerical dispersion may impart a false accuracy to simulated results. Similarly, an inappropriate discretization of the time derivative frequently causes oscillation of results from time step to time step or from stress period to stress period. Although numerical dispersion cannot be accurately accounted for when using the MT3DMS code, numerical dispersion can be deliberately minimized by accommodating a Peclet number ($\Delta x/\alpha_L$) less than 2.0 during the design and calibration of the flow and fate and transport models. The Peclet number was uniformly 2.0 throughout the Tarawa Terrace fate and transport model. Numerical instabilities related to inappropriate time discretization are minimized when the Courant number ($v\Delta t/\Delta x$) is less than 1.0: where v = simulated groundwater-flow velocity, in feet per day; Δt = stress period length, in days; and Δx is as previously defined. The minimum time discretization was a stress period and equaled the number of days in a single month; that is, 28, 29, 30, or 31 days. Stress periods were not subdivided into time steps. Simulated flow velocities ranged between 0.01 and 1.0 ft/d everywhere within the active model domain, except in the immediate vicinity of wells where flow velocities were as great as 8.0 ft/d. Thus, out of a total of about 28,000 active cells per layer, the Courant number was less than 1.0 at all but a few dozen cells near pumping wells. In addition, the sensitivity of simulated concentrations to time discretization was tested by assigning 1-day stress periods to the calibrated fate and transport model from November 1, 1984, to January 31, 1985, and comparing the concentrations simulated by the modified model to those of the calibrated model. Comparisons were made for the days November 30, 1984, December 31, 1984, and January 31, 1985. Pumpage assigned to the months of interest of the calibrated model was assigned to every day of the respective month of the modified model.

Field data and the calibrated model indicated that water-supply wells TT-23 and TT-26 were substantially contaminated with PCE during the test period. Also, concentration gradients simulated by the calibrated model were large in the vicinity of wells TT-23 and TT-26 at this time. Concentrations simulated by the calibrated and modified models were identical prior to stress period 407 (November 1984). The PCE concentrations simulated by the modified and calibrated models during the test period at wells TT-23 and TT-26 are listed in the following table. Simulated concentrations at these wells were similar to the third or fourth significant figure at the designated times whether or not the stress period length was 1 day or 30 days or 31 days. Thus, PCE concentrations simulated by the Tarawa Terrace fate and transport model were demonstrably unaffected by numerical instabilities caused by inappropriate time discretization.

Site name	Simulated elapsed time, in days	Date	Simulated tetrachloroethylene (PCE) concentration, in gram per cubic foot	
			Δt=1 day	Δt=30 or 31 days
TT-23	12,388	Nov. 30, 1984	0.007183956	0.007182317
	12,419	Dec. 31, 1984	0.007214860	0.007211736
	12,450	Jan. 31, 1985	0.007200035	0.007198663
TT-26	12,388	Nov. 30, 1984	0.02297354	0.02298510
	12,419	Dec. 31, 1984	0.02276520	0.02279888
	12,450	Jan. 31, 1985	0.02275406	0.02276190

Summary

Migration of PCE from the vicinity of ABC One-Hour Cleaners to Tarawa Terrace water-supply wells TT-23 and TT-26 was simulated using the code MT3DMS integrated with a calibrated groundwater-flow model based on the code MODFLOW96. Simulated mass loading occurred at a constant rate of 1,200 grams per day using monthly stress periods representing the period January 1953 to December 1984. Mass loading occurred at a single cell in the uppermost model layer representing the approximate location of ABC One-Hour Cleaners. Total simulation represented the period January 1951 to December 1994. Until 1984, the vast majority of simulated tetrachloroethylene (PCE) supplied to the Tarawa Terrace water treatment plant (WTP) was contributed by well TT-26. During 1984, well TT-23 was placed in service and also contributed significant quantities of PCE to the Tarawa Terrace WTP. Simulated breakthrough of PCE at well TT-26, the nearest water-supply well to ABC One-Hour Cleaners, occurs during January 1957 at the maximum contaminant level (MCL) concentration of 5 micrograms per liter (µg/L). Corresponding breakthrough at well TT-23 occurs during December 1974. Simulated average and maximum PCE concentrations at well TT-26 following breakthrough are 487 µg/L and 851 µg/L, respectively. Corresponding concentrations at well TT-23 subsequent to the onset of operations are 219 µg/L and 285 µg/L. Concentrations of PCE in finished water at the Tarawa Terrace WTP were computed using a simple mixing model. Flow-weighted PCE concentrations were computed using simulated flow and PCE concentrations at active wells and assigned as the average PCE concentration at the WTP for the appropriate month. Simulated breakthrough of PCE at the Tarawa Terrace WTP occurs at the MCL concentration of 5 µg/L during October or November 1957 and remains at 40 µg/L or more from December 1959 until the termination of pumping at well TT-26 during February 1985. From November 1957 to February 1985, computed maximum and average PCE concentrations at the Tarawa Terrace WTP are 183 µg/L and 74 µg/L, respectively.

Acknowledgments

A study of this complexity and magnitude is dependent upon the assistance, input, and suggestions of many colleagues. Thus, the authors of this report and all chapter reports acknowledge the managers and staff of the U.S. Geological Survey Water Science Centers in Raleigh, North Carolina, and Atlanta, Georgia. In particular, the contributions of Melinda J. Chapman, Douglas A. Harned, and Stephen S. Howe are acknowledged for providing the majority of well, water-level, and pumpage data used in this study. Keith W. McFadden and Jonathan W. Musser are acknowledged for assistance with spatial analyses in preparing illustrations and with developing geodatabases, Web-based applications, and the querying system contained on the electronic media accompanying Chapters A and K. Gregory C. Mayer and Edward H. Martin also are acknowledged for their administrative assistance.

The author acknowledges the staff of the Environmental Management Division, U.S. Marine Corps Base Camp Lejeune, North Carolina. In particular, Scott A. Brewer, Brynn Ashton, Scott R. Williams, and Rick Cheng for their assistance and cooperation during the course of this study, especially for providing a large number of technical reports, maps, and historical documents, which summarize the results of groundwater remedial investigations at and in the vicinity of Tarawa Terrace. The author also acknowledges Joel Hartsoe and Danny E. Hill of the Camp Lejeune Public Works Department Utility Section.

The author acknowledges the contributions of the USEPA, Region IV, Atlanta, Georgia, for providing reports and documents summarizing the results of investigations of groundwater contamination in the vicinity of ABC One-Hour Cleaners and in the northern part of Tarawa Terrace.

The author acknowledges colleagues at ATSDR, Eastern Research Group, Inc., the Multimedia Environmental Simulations Laboratory at the Georgia Institute of Technology, and the Oak Ridge Institute for Science and Education for providing assistance and advice with all aspects of this study.

Thomas M. Plummer, Commander, U.S. Public Health Service, Indian Health Service, U.S. Department of Health and Human Services, assisted with planning, field instrumentation, and conducting tests of water-distribution systems serving Camp Lejeune, August 18–28, 2004.

Caryl J. Wipperfurth, Bonnie J. Turcott, Patricia L. Nobles, and Kimberly A. Waltenbaugh, U.S. Geological Survey Enterprise Publishing Network, assisted with the preparation of text, illustrations, and electronic media.

Availability of Input Data Files, Models, and Simulation Results

Calibrated model input data files developed for simulating predevelopment groundwater flow, transient groundwater flow, the fate and transport of PCE as a single specie, and the distribution of water and contaminants in a water-distribution system are provided with Chapter A (Morris et al. 2007) of this report in a digital video disc (DVD) format. Public domain model codes used with these input files are available on the Internet at the following Web sites:

- Predevelopment and transient groundwater flow
  - Model code: MODFLOW-96
  - Web site: *http://water.usgs.gov/nrp/gwsoftware/modflow.html*
- Fate and transport of PCE as a single specie
  - Model code: MT3DMS
  - Web site: *http://hydro.geo.ua.edu/*
- Distribution of water and contaminants in a water-distribution system
  - Model code: EPANET 2
  - Web site: *http://www.epa.gov/nrmrl/wswrd/epanet.html*

Specialized model codes and model input data files were developed specifically for the Tarawa Terrace analyses by the MESL at the School of Civil and Environmental Engineering, Georgia Institute of Technology. These specialized codes and input data files were developed for simulating three-dimensional multispecies, multiphase, mass transport (TechFlowMP) and pumping schedule optimization (PSOpS) and are described in detail in the Chapter G (Jang and Aral In press 2008) and Chapter H (Wang and Aral In press 2008) reports, respectively. Contact information and questions related to these codes are provided on the Internet at the MESL Web site at: *http://mesl.ce.gatech.edu.*

Readers desiring information about the model input data files or the simulation results contained on the DVDs also may contact the Project Officer of ATSDR's Exposure-Dose Reconstruction Project at the following address:

Morris L. Maslia, MSCE, PE, D.WRE, DEE
Exposure-Dose Reconstruction Project
Division of Health Assessment and Consultation
Agency for Toxic Substances and Disease Registry
4770 Buford Highway NE
Mail Stop F59, Room 02-004
Atlanta, Georgia 30341-3717
Tel: (770) 488-3842
Fax: (770) 488-1536
E-mail: mmaslia@cdc.gov

References

Agency for Toxic Substances and Disease Registry. Preliminary Public Health Assessment for ABC One Hour Cleaners, Jacksonville, Onslow County, North Carolina. Atlanta, GA: U.S. Department of Health and Human Services; 1990. Report No.: NCD024644494.

Agency for Toxic Substances and Disease Registry. Public Health Assessment for U.S. Marine Corps Base at Camp Lejeune, Military Reservation, Camp Lejeune, Onslow County, North Carolina. Atlanta, GA: U.S. Department of Health and Human Services; 1997. Report No.: NC6170022580.

Anderson MP. Movement of Contaminants in Groundwater: Groundwater Transport-Advection and Dispersion, *in* Studies in Geophysics, Groundwater Contamination: National Academy Press; 1984.

Baker Environmental, Inc. Basewide Remediation Assessment, Groundwater Study (BRAGS), Marine Corps Base, Camp Lejeune, North Carolina; 1998.

Brady MM, and Kunkel LA. A Practical Technique for Quantifying Drainage Porosity: PTS Laboratories; no date.

California Environmental Protection Agency. Final Draft Report, Intermedia Transfer Factors for Contaminants Found at Hazardous Waste Sites, Tetrachloroethylene (PCE); 1994.

Cardinell AP, Berg SA, and Lloyd OB Jr. Hydrogeologic Framework of U.S. Marine Corps Base at Camp Lejeune, North Carolina. Raleigh, NC: U.S. Geological Survey Water-Resources Investigations Report 93-4049; 1993.

Chiang W-H, and Kinzelbach W. 3D-Groundwater Modeling with PMWIN: Springer-Verlag; 2001.

CLW, Camp Lejeune Water Documents, 0001–8761 (not consecutively available), provided on DVD format, in Maslia ML, Sautner JB, Faye RE, Suárez-Soto RJ, Aral MM, Grayman WM, Jang W, Wang J, Bove FJ, Ruckart PZ, Valenzuela C, Green JW Jr, and Krueger AL. Analyses of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water at Tarawa Terrace and Vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina: Historical Reconstruction and Present-Day Conditions—Chapter A: Summary of Findings. Atlanta, GA: Agency for Toxic Substances and Disease Registry; 2007.

Faye RE. Analyses of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water at Tarawa Terrace and Vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina: Historical Reconstruction and Present-Day Conditions— Chapter B: Geohydrologic Framework of the Castle Hayne Aquifer System. Atlanta, GA: Agency for Toxic Substances and Disease Registry; 2007.

Faye RE, and Green JW Jr. Analyses of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water at Tarawa Terrace and Vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina: Historical Reconstruction and Present-Day Conditions—Chapter E: Occurrence of Contaminants in Groundwater. Atlanta, GA: Agency for Toxic Substances and Disease Registry; 2007.

Faye RE, and Valenzuela C. Analyses of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water at Tarawa Terrace and Vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina: Historical Reconstruction and Present-Day Conditions—Chapter C: Simulation of Groundwater Flow. Atlanta, GA: Agency for Toxic Substances and Disease Registry; 2007.

Fetter CW. Contaminant Hydrogeology: Prentice Hall; 1999.

Gelhar LW, Welty C, and Rehfeldt KR. A Critical Review of Data on Field-Scale Dispersion in Aquifers: Water Resources Research. 1992;28(7).

Giese GL, and Mason RR Jr. Low-Flow Characteristics of Streams in North Carolina: U.S. Geological Survey Open-File Report 90-399; 1991.

Giese GL, Eimers JL, and Coble RW. Simulation of Groundwater Flow in the Coastal Plain Aquifer System of North Carolina: U.S. Geological Survey Professional Paper 1404-M; 1997.

Harbaugh AW, and McDonald MG. User's Documentation for MODFLOW-96, and Update to the U.S. Geological Survey Modular Finite-Difference Groundwater Flow Model: U.S. Geological Survey Open-File Report 96-458; 1996.

Harbaugh AW, Banta ER, Hill MC, and McDonald MG. MODFLOW-2000, The U.S. Geological Survey Modular Groundwater Model—User Guide to Modularization Concepts and the Groundwater Flow Process: U.S. Geological Survey Open-File Report 00-92; 2000.

Harned DA, Lloyd OB Jr. and Treece MW Jr. Assessment of Hydrologic and Hydrogeologic Data at Camp Lejeune Marine Corps Base, North Carolina. Raleigh, NC: U.S. Geological Survey Water-Resources Investigations Report 89-4096; 1989.

Heath RC. Groundwater Recharge in North Carolina: Groundwater Section, Division of Environmental Management, North Carolina Department of Environment, Health, and Natural Resources; 1994.

Hoffman F. Retardation of Volatile Organic Compounds in Ground Water in Low Organic Carbon Sediments: Informal Report—Lawrence Livermore National Laboratory, U.S. Department of Energy; 1995.

Jang W, and Aral MM. Analyses of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water at Tarawa Terrace and Vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina: Historical Reconstruction and Present-Day Conditions—Chapter G: Simulation of Three-Dimensional Multispecies, Multiphase Mass Transport of Tetrachloroethylene (PCE) and Associated Degradation By-Products. Atlanta, GA: Agency for Toxic Substances and Disease Registry; In press 2008.

Lallemand-Barrès A, and Peaudecerf P. Recherche des Relations Entre la Valeur de la Dispersivité Macroscopique d'un Milieu Aquifère, Ses Autres Caractéristiques et les Conditions de Mesure: Bulletin de BRGM. 1978;25:45–61.

Law Engineering and Testing Company, Inc. On-Site Sampling—Septic Tank and Outlying Area, ABC One-Hour Cleaners, Jacksonville, North Carolina, LETCO Job; 1986a. Report No.: J-473-86-1623.

Law Engineering and Testing Company, Inc. On-Site Sampling ABC One-Hour Cleaners, Jacksonville, North Carolina; 1986b.

LeGrand HE. Evaluation of Well-Water Supply, Marine Corps Base, Camp Lejeune, North Carolina: Project Report, Contract NBy-7595; 1959.

Lucius JE, Olhoeft GR, Hill PL, and Duke SK. Properties and Hazards of 108 Selected Substances: U.S. Geological Survey Open-File Report 90-408; 1990.

Maslia ML, Sautner JB, Faye RE, Suárez-Soto RJ, Aral MM, Grayman WM, Jang W, Wang J, Bove FJ, Ruckart PZ, Valenzuela C, Green JW Jr, and Krueger AL. Analyses of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water at Tarawa Terrace and Vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina: Historical Reconstruction and Present-Day Conditions—Chapter A: Summary of Findings. Atlanta, GA: Agency for Toxic Substances and Disease Registry; 2007.

Maslia ML, Sautner JB, Faye RE, Suárez-Soto RJ, Aral MM, Grayman WM, Jang W, Wang J, Bove FJ, Ruckart PZ, Valenzuela C, Green JW Jr, and Krueger AL. Analyses of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water at Tarawa Terrace and Vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina: Historical Reconstruction and Present-Day Conditions—Chapter K: Supplemental Information, Atlanta, GA: Agency for Toxic Substances and Disease Registry; In press 2008.

Masters GM. Introduction to Environmental Engineering and Science. 2nd ed: Prentice Hall; 1998.

McDonald MG, and Harbaugh AW. A Modular Three-Dimensional Finite-Difference Groundwater Flow Model: U.S. Geological Survey Open-File Report 83-875; 1984.

McMorris CA. Site Inspection Report—ABC One Hour Cleaners, NC DO24644494, 2127 Lejeune Boulevard, Jacksonville, NC, 28340: North Carolina Solid and Hazardous Waste Branch, Environmental Health Section; 1987.

Miller CT, Joseph AP, Staes EG, and Gilbertsen RH. Modeling Organic Contaminant Sorption Impacts on Aquifer Restoration: Water Resources Research Institute of the University of North Carolina; 1989.

Morris DA, and Johnson AI. Summary of Hydrologic and Physical Properties of Rock and Soil Materials, as Analyzed by the Hydrologic Laboratory of the U.S. Geological Survey, 1948–60: U.S. Geological Survey Water-Supply Paper 1839-D; 1967.

Neuman SP. Universal Scaling of Hydraulic Conductivities and Dispersivities in Geologic Media: Water Resources Research. 1990;26(8).

References

Pankow JF, and Cherry JA. Dense Chlorinated Solvents and Other DNAPLs in Groundwater: History, Behavior, and Remediation: Waterloo Press; 1996.

Pollock DW. Documentation of Computer Programs to Compute and Display Pathlines Using Results from the U.S. Geological Survey Modular Three-Dimensional Finite-Difference Groundwater Model: U.S. Geological Survey Open-File Report 89-381; 1989.

Pollock DW. User's Guide for MODPATH/MODPATH-PLOT, Version 3: A Particle Tracking Post-Processing Package for MODFLOW, The U.S. Geological Survey Finite-Difference Groundwater Flow Model: U.S. Geological Survey Open-File Report 94-464; 1994.

Roberts PV, Goltz MN, and Mackay DM. A Natural Gradient Experiment on Solute Transport in a Sand Aquifer 3. Retardation Estimates and Mass Balances for Organic Solutes: Water Resources Research. 1986;23(13).

Roy F. Weston, Inc. Remedial Investigation Report, ABC One-Hour Cleaners, Jacksonville, North Carolina: Roy F. Weston, Inc.; 1992.

Roy F. Weston, Inc. Remedial Investigation, ABC One-Hour Cleaners, Operable Unit 2, Jacksonville, North Carolina: Roy F. Weston, Inc.; 1994.

Shiver R. A Groundwater Investigation to Define the Source(s) of Tetrachloroethylene that Have Contaminated Three Community Water Supply Wells at Tarawa Terrace I, Camp Lejeune Marine Corps Base, Onslow County: North Carolina Department of Natural Resources and Community Development; 1985.

U.S. Environmental Protection Agency. National Primary Drinking Water Standards. Report No.: EPA 816-F-03-016. 2003. [cited 2007 January 25]; available from *http://www.epa.gov/water/*

Wang J, and Aral MM. Analyses of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water at Tarawa Terrace and Vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina: Historical Reconstruction and Present-Day Conditions—Chapter H: Effect of Groundwater Pumping Schedule Variation on Arrival of Tetrachloroethylene (PCE) at Water-Supply Wells and the Water Treatment Plant. Atlanta, GA: Agency for Toxic Substances and Disease Registry; In press 2008.

Zheng C, and Wang PP. MT3DMS, A Modular Three-Dimensional Multispecies Transport Model for Simulation of Advection, Dispersion, and Chemical Reactions of Contaminants in Groundwater Systems: Department of Geology and Mathematics University of Alabama; 1998.

Appendix F1. Simulation Stress Periods and Corresponding Month and Year

Appendix F1. Simulation Stress Periods and Corresponding Month and Year

Appendix F1. Simulation stress periods and corresponding month and year.

[Jan, January; Feb, February; Mar, March; Apr, April; Aug, August; Sept, September; Oct, October; Nov, November; Dec, December]

Stress period	Month and year	Stress period	Month and year	Stress period	Month and year	Stress period	Month and year	Stress period	Month and year	Stress period	Month and year
1	Jan 1951	49	Jan 1955	97	Jan 1959	145	Jan 1963	193	Jan 1967	241	Jan 1971
2	Feb 1951	50	Feb 1955	98	Feb 1959	146	Feb 1963	194	Feb 1967	242	Feb 1971
3	Mar 1951	51	Mar 1955	99	Mar 1959	147	Mar 1963	195	Mar 1967	243	Mar 1971
4	Apr 1951	52	Apr 1955	100	Apr 1959	148	Apr 1963	196	Apr 1967	244	Apr 1971
5	May 1951	53	May 1955	101	May 1959	149	May 1963	197	May 1967	245	May 1971
6	June 1951	54	June 1955	102	June 1959	150	June 1963	198	June 1967	246	June 1971
7	July 1951	55	July 1955	103	July 1959	151	July 1963	199	July 1967	247	July 1971
8	Aug 1951	56	Aug 1955	104	Aug 1959	152	Aug 1963	200	Aug 1967	248	Aug 1971
9	Sept 1951	57	Sept 1955	105	Sept 1959	153	Sept 1963	201	Sept 1967	249	Sept 1971
10	Oct 1951	58	Oct 1955	106	Oct 1959	154	Oct 1963	202	Oct 1967	250	Oct 1971
11	Nov 1951	59	Nov 1955	107	Nov 1959	155	Nov 1963	203	Nov 1967	251	Nov 1971
12	Dec 1951	60	Dec 1955	108	Dec 1959	156	Dec 1963	204	Dec 1967	252	Dec 1971
13	Jan 1952	61	Jan 1956	109	Jan 1960	157	Jan 1964	205	Jan 1968	253	Jan 1972
14	Feb 1952	62	Feb 1956	110	Feb 1960	158	Feb 1964	206	Feb 1968	254	Feb 1972
15	Mar 1952	63	Mar 1956	111	Mar 1960	159	Mar 1964	207	Mar 1968	255	Mar 1972
16	Apr 1952	64	Apr 1956	112	Apr 1960	160	Apr 1964	208	Apr 1968	256	Apr 1972
17	May 1952	65	May 1956	113	May 1960	161	May 1964	209	May 1968	257	May 1972
18	June 1952	66	June 1956	114	June 1960	162	June 1964	210	June 1968	258	June 1972
19	July 1952	67	July 1956	115	July 1960	163	July 1964	211	July 1968	259	July 1972
20	Aug 1952	68	Aug 1956	116	Aug 1960	164	Aug 1964	212	Aug 1968	260	Aug 1972
21	Sept 1952	69	Sept 1956	117	Sept 1960	165	Sept 1964	213	Sept 1968	261	Sept 1972
22	Oct 1952	70	Oct 1956	118	Oct 1960	166	Oct 1964	214	Oct 1968	262	Oct 1972
23	Nov 1952	71	Nov 1956	119	Nov 1960	167	Nov 1964	215	Nov 1968	263	Nov 1972
24	Dec 1952	72	Dec 1956	120	Dec 1960	168	Dec 1964	216	Dec 1968	264	Dec 1972
25	Jan 1953	73	Jan 1957	121	Jan 1961	169	Jan 1965	217	Jan 1969	265	Jan 1973
26	Feb 1953	74	Feb 1957	122	Feb 1961	170	Feb 1965	218	Feb 1969	266	Feb 1973
27	Mar 1953	75	Mar 1957	123	Mar 1961	171	Mar 1965	219	Mar 1969	267	Mar 1973
28	Apr 1953	76	Apr 1957	124	Apr 1961	172	Apr 1965	220	Apr 1969	268	Apr 1973
29	May 1953	77	May 1957	125	May 1961	173	May 1965	221	May 1969	269	May 1973
30	June 1953	78	June 1957	126	June 1961	174	June 1965	222	June 1969	270	June 1973
31	July 1953	79	July 1957	127	July 1961	175	July 1965	223	July 1969	271	July 1973
32	Aug 1953	80	Aug 1957	128	Aug 1961	176	Aug 1965	224	Aug 1969	272	Aug 1973
33	Sept 1953	81	Sept 1957	129	Sept 1961	177	Sept 1965	225	Sept 1969	273	Sept 1973
34	Oct 1953	82	Oct 1957	130	Oct 1961	178	Oct 1965	226	Oct 1969	274	Oct 1973
35	Nov 1953	83	Nov 1957	131	Nov 1961	179	Nov 1965	227	Nov 1969	275	Nov 1973
36	Dec 1953	84	Dec 1957	132	Dec 1961	180	Dec 1965	228	Dec 1969	276	Dec 1973
37	Jan 1954	85	Jan 1958	133	Jan 1962	181	Jan 1966	229	Jan 1970	277	Jan 1974
38	Feb 1954	86	Feb 1958	134	Feb 1962	182	Feb 1966	230	Feb 1970	278	Feb 1974
39	Mar 1954	87	Mar 1958	135	Mar 1962	183	Mar 1966	231	Mar 1970	279	Mar 1974
40	Apr 1954	88	Apr 1958	136	Apr 1962	184	Apr 1966	232	Apr 1970	280	Apr 1974
41	May 1954	89	May 1958	137	May 1962	185	May 1966	233	May 1970	281	May 1974
42	June 1954	90	June 1958	138	June 1962	186	June 1966	234	June 1970	282	June 1974
43	July 1954	91	July 1958	139	July 1962	187	July 1966	235	July 1970	283	July 1974
44	Aug 1954	92	Aug 1958	140	Aug 1962	188	Aug 1966	236	Aug 1970	284	Aug 1974
45	Sept 1954	93	Sept 1958	141	Sept 1962	189	Sept 1966	237	Sept 1970	285	Sept 1974
46	Oct 1954	94	Oct 1958	142	Oct 1962	190	Oct 1966	238	Oct 1970	286	Oct 1974
47	Nov 1954	95	Nov 1958	143	Nov 1962	191	Nov 1966	239	Nov 1970	287	Nov 1974
48	Dec 1954	96	Dec 1958	144	Dec 1962	192	Dec 1966	240	Dec 1970	288	Dec 1974

Appendix F1. Simulation stress periods and corresponding month and year.—Continued

[Jan, January; Feb, February; Mar, March; Apr, April; Aug, August; Sept, September; Oct, October; Nov, November; Dec, December]

Stress period	Month and year	Stress period	Month and year	Stress period	Month and year	Stress period	Month and year	Stress period	Month and year
289	Jan 1975	337	Jan 1979	385	Jan 1983	433	Jan 1987	481	Jan 1991
290	Feb 1975	338	Feb 1979	386	Feb 1983	434	Feb 1987	482	Feb 1991
291	Mar 1975	339	Mar 1979	387	Mar 1983	435	Mar 1987	483	Mar 1991
292	Apr 1975	340	Apr 1979	388	Apr 1983	436	Apr 1987	484	Apr 1991
293	May 1975	341	May 1979	389	May 1983	437	May 1987	485	May 1991
294	June 1975	342	June 1979	390	June 1983	438	June 1987	486	June 1991
295	July 1975	343	July 1979	391	July 1983	439	July 1987	487	July 1991
296	Aug 1975	344	Aug 1979	392	Aug 1983	440	Aug 1987	488	Aug 1991
297	Sept 1975	345	Sept 1979	393	Sept 1983	441	Sept 1987	489	Sept 1991
298	Oct 1975	346	Oct 1979	394	Oct 1983	442	Oct 1987	490	Oct 1991
299	Nov 1975	347	Nov 1979	395	Nov 1983	443	Nov 1987	491	Nov 1991
300	Dec 1975	348	Dec 1979	396	Dec 1983	444	Dec 1987	492	Dec 1991
301	Jan 1976	349	Jan 1980	397	Jan 1984	445	Jan 1988	493	Jan 1992
302	Feb 1976	350	Feb 1980	398	Feb 1984	446	Feb 1988	494	Feb 1992
303	Mar 1976	351	Mar 1980	399	Mar 1984	447	Mar 1988	495	Mar 1992
304	Apr 1976	352	Apr 1980	400	Apr 1984	448	Apr 1988	496	Apr 1992
305	May 1976	353	May 1980	401	May 1984	449	May 1988	497	May 1992
306	June 1976	354	June 1980	402	June 1984	450	June 1988	498	June 1992
307	July 1976	355	July 1980	403	July 1984	451	July 1988	499	July 1992
308	Aug 1976	356	Aug 1980	404	Aug 1984	452	Aug 1988	500	Aug 1992
309	Sept 1976	357	Sept 1980	405	Sept 1984	453	Sept 1988	501	Sept 1992
310	Oct 1976	358	Oct 1980	406	Oct 1984	454	Oct 1988	502	Oct 1992
311	Nov 1976	359	Nov 1980	407	Nov 1984	455	Nov 1988	503	Nov 1992
312	Dec 1976	360	Dec 1980	408	Dec 1984	456	Dec 1988	504	Dec 1992
313	Jan 1977	361	Jan 1981	409	Jan 1985	457	Jan 1989	505	Jan 1993
314	Feb 1977	362	Feb 1981	410	Feb 1985	458	Feb 1989	506	Feb 1993
315	Mar 1977	363	Mar 1981	411	Mar 1985	459	Mar 1989	507	Mar 1993
316	Apr 1977	364	Apr 1981	412	Apr 1985	460	Apr 1989	508	Apr 1993
317	May 1977	365	May 1981	413	May 1985	461	May 1989	509	May 1993
318	June 1977	366	June 1981	414	June 1985	462	June 1989	510	June 1993
319	July 1977	367	July 1981	415	July 1985	463	July 1989	511	July 1993
320	Aug 1977	368	Aug 1981	416	Aug 1985	464	Aug 1989	512	Aug 1993
321	Sept 1977	369	Sept 1981	417	Sept 1985	465	Sept 1989	513	Sept 1993
322	Oct 1977	370	Oct 1981	418	Oct 1985	466	Oct 1989	514	Oct 1993
323	Nov 1977	371	Nov 1981	419	Nov 1985	467	Nov 1989	515	Nov 1993
324	Dec 1977	372	Dec 1981	420	Dec 1985	468	Dec 1989	516	Dec 1993
325	Jan 1978	373	Jan 1982	421	Jan 1986	469	Jan 1990	517	Jan 1994
326	Feb 1978	374	Feb 1982	422	Feb 1986	470	Feb 1990	518	Feb 1994
327	Mar 1978	375	Mar 1982	423	Mar 1986	471	Mar 1990	519	Mar 1994
328	Apr 1978	376	Apr 1982	424	Apr 1986	472	Apr 1990	520	Apr 1994
329	May 1978	377	May 1982	425	May 1986	473	May 1990	521	May 1994
330	June 1978	378	June 1982	426	June 1986	474	June 1990	522	June 1994
331	July 1978	379	July 1982	427	July 1986	475	July 1990	523	July 1994
332	Aug 1978	380	Aug 1982	428	Aug 1986	476	Aug 1990	524	Aug 1994
333	Sept 1978	381	Sept 1982	429	Sept 1986	477	Sept 1990	525	Sept 1994
334	Oct 1978	382	Oct 1982	430	Oct 1986	478	Oct 1990	526	Oct 1994
335	Nov 1978	383	Nov 1982	431	Nov 1986	479	Nov 1990	527	Nov 1994
336	Dec 1978	384	Dec 1982	432	Dec 1986	480	Dec 1990	528	Dec 1994

Analyses of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water at Tarawa Terrace and Vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina: Historical Reconstruction and Present-Day Conditions—Chapter F: Simulation of the Fate and Transport of Tetrachloroethylene (PCE)

Printed on recycled paper

EXHIBIT 13

Predictive Accuracy of a Ground-Water Model — Lessons from a Postaudit

by Leonard F. Konikow[a]

ABSTRACT

Hydrogeologic studies commonly include the development, calibration, and application of a deterministic simulation model. To help assess the value of using such models to make predictions, a postaudit was conducted on a previously studied area in the Salt River and lower Santa Cruz River basins in central Arizona. A deterministic, distributed-parameter model of the ground-water system in these alluvial basins was calibrated by Anderson (1968) using about 40 years of data (1923-64). The calibrated model was then used to predict future water-level changes during the next 10 years (1965-74). Examination of actual water-level changes in 77 wells from 1965-74 indicates a poor correlation between observed and predicted water-level changes. The differences have a mean of −73 ft—that is, predicted declines consistently exceeded those observed—and a standard deviation of 47 ft. The bias in the predicted water-level change can be accounted for by the large error in the assumed total pumpage during the prediction period. However, the spatial distribution of errors in predicted water-level change does not correlate with the spatial distribution of errors in pumpage. Consequently, the lack of precision probably is not related only to errors in assumed pumpage, but may indicate the presence of other sources of error in the model, such as the two-dimensional representation of a three-dimensional problem or the lack of consideration of land-subsidence processes. This type of postaudit is a valuable method of verifying a model, and an evaluation of predictive errors can provide an increased understanding of the system and aid in assessing the value of undertaking development of a revised model.

[a]U.S. Geological Survey, Mail Stop 431, National Center, Reston, Virginia 22092.

Received May 1985, revised August 1985, accepted September 1985.

Discussion open until September 1, 1986.

INTRODUCTION

Hydrogeologic studies commonly include the use of deterministic, distributed-parameter, ground-water models to predict responses of an aquifer system to changes in stresses. The extreme example of using such models for predictions may be in the planning of high-level radioactive waste repositories, where regulators desire and require projections of ground-water flow and transport for 1,000 to 10,000 years into the future. Is there any evidence, either on the basis of a postaudit of the outcome of past predictive efforts or otherwise, that deterministic simulation models can indeed accurately predict future responses in ground-water systems? Is forecasting the only or primary motivation for applying a deterministic ground-water model, or does the modeling exercise have some other value?

The underlying philosophy of process-simulating deterministic-modeling approaches is that, given a comprehensive understanding of the processes by which stresses on a system produce subsequent responses in that system, the system's response to any set of stresses can be defined or predetermined through that understanding of the governing (or controlling) processes, even if the magnitude of the new stresses falls outside of the range of historically observed stresses. Predictions made this way assume an understanding of cause-and-effect relations. The accuracy of such deterministic forecasts thus depends, in part, upon how closely our concepts of the governing processes reflect the processes that actually control the system's behavior. But more is involved. Even if we have an accurate conceptual model of the governing processes, and if the processes were represented accurately in a deterministic simulation model, we also need (1) a definition of the properties and boundaries of the domain over which these processes and stresses are acting; (2) the state of the system at some point in time (either past or present); and (3) an estimate (or prediction) of what the future stresses will be, which, though it is an obvious requirement, is not necessarily a trivial matter. Thus, the "model" of an aquifer system incorporates processes, specifications for parameters, and stresses.

Ground-water hydrologists are becoming increasingly aware that inadequate and insufficient data limit the reliability of traditional deterministic ground-water models. The data may be inadequate because aquifer heterogeneities occur on a scale smaller than can be defined on the basis of available data, time-dependent variables are monitored too infrequently, and measurement errors exist.

The purpose of this paper is to review the use and reliability of deterministic models for predicting future changes in ground water by examining the outcome of a past predictive effort. A model study of an area in central Arizona was selected as an example because it represents one of the first well-documented deterministic, distributed-parameter, model analyses of a ground-water system. Consequently, it was also done sufficiently long ago that a long-term (10-year) forecast period has passed. Furthermore, there are now available historical observations of the aquifer for the time for which the forecast was made. The purposes of this example are: (1) to illustrate how accurate (or inaccurate) a prediction made with a supposedly well-calibrated model can be, recognizing that only limited generalizations should be drawn on the basis of a single example; (2) to try to isolate the sources of predictive error; and (3) to evaluate the importance of conducting a postaudit of model predictions.

DESCRIPTION OF STUDY AREA

The Salt River Valley and the lower Santa Cruz River basin are located near Phoenix, Arizona (see Figure 1) and are the two largest agricultural areas in Arizona. According to Anderson (1968), about 1,250 mi^2 (800,000 acres) are under cultivation. Because of the arid climate (rainfall averages about 8 inches per year), the agricultural economy is dependent on a reliable source of irrigation water. Since the early 1900's, the ground-water system has been developed extensively in the area. By the mid-1960's, ground water was providing approximately 80 percent (3.2 million ac-ft) of the total annual water supply. Summarizing the discussion of Anderson (1968), such withdrawals greatly exceed the rate of ground-water recharge and resulted in water-level declines of as much as 20 ft per year in some places. Maximum declines from 1923 to 1964 were about 360 ft. Because of the economic importance of ground water in this area, there was much concern that continued declines would cause significantly increased pumping costs and decreased well yields. As part of an analysis of the ground-water resources of the area, Anderson (1968) constructed and calibrated an electric-analog model of the aquifer system, partly ". . . to determine the probable future effects of continued ground-water withdrawals in central Arizona."

The hydrogeologic setting of this area is described in detail by Anderson (1968) and Davidson (1979). A summary of their descriptions follows. The central Arizona area lies in the Basin and Range lowlands water province (Figure 1). The area is characterized by broad and gently sloping valleys or basins that surround and separate steep and rugged mountains. The mountains are composed mainly of low-permeability crystalline rocks, although some sedimentary rocks are present. The valleys are underlain by thousands of feet of unconsolidated to consolidated alluvial deposits, including thick permeable sand and gravel units. In general, coarser material is found near the mountains, which border the margins of the basins, and fine-grained material is deposited in the central, deeper parts of the basins. Most ground water used in the basin is derived from the uppermost unit of the alluvium, which is a highly permeable sand and gravel as much as 600 ft in thickness. Below this unit is the middle silt and clay unit, which is discontinuous, less permeable, and as much as 2,000 ft in thickness. Below that lies the more consolidated lower sand and gravel unit, which is intermediate in permeability.

The water-table configuration in 1923, prior to extensive development of the ground-water resource, is indicated in Figure 2. At that time, ground-water flow was predominantly to the west and northwest, generally paralleling the flow directions of the Santa Cruz, Gila, and Salt Rivers. Anderson (1968) considered the ground-water system to be in an approximate equilibrium condition prior to 1923. He further states, "Since the early 1920's, pumping has exceeded replenishment in central Arizona. Beginning in the early 1940's,

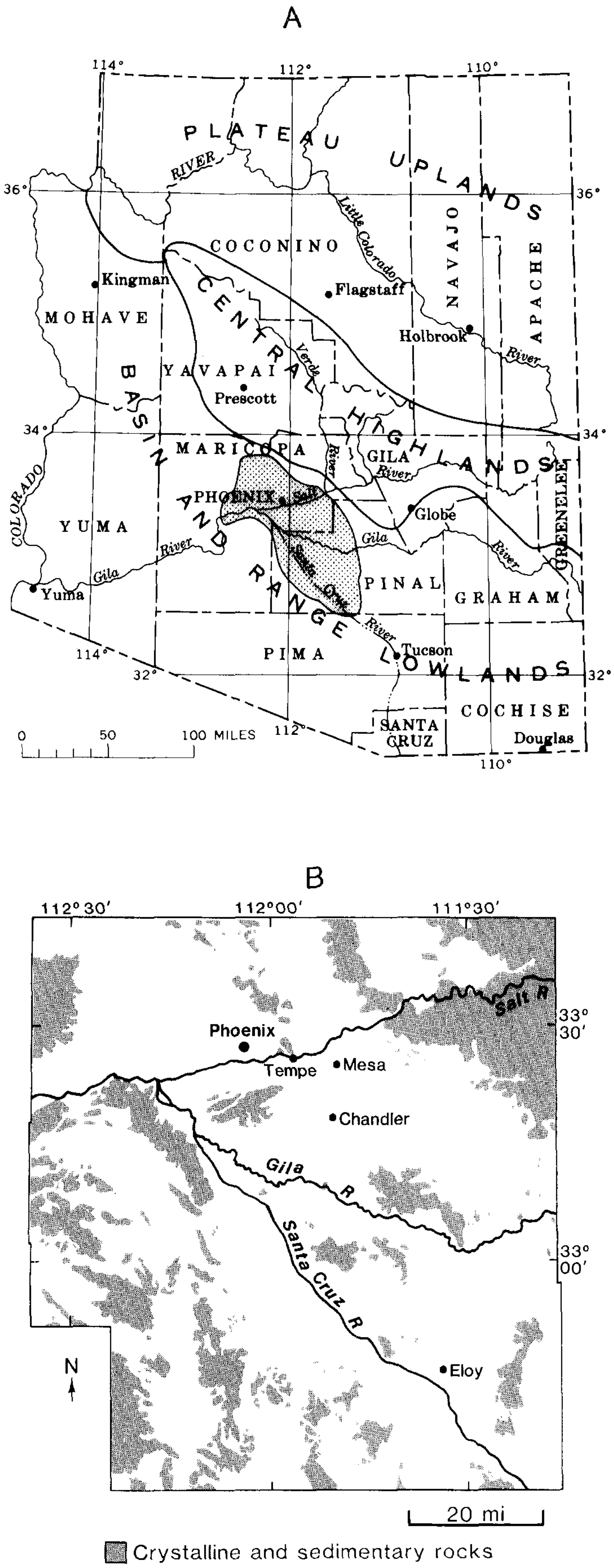
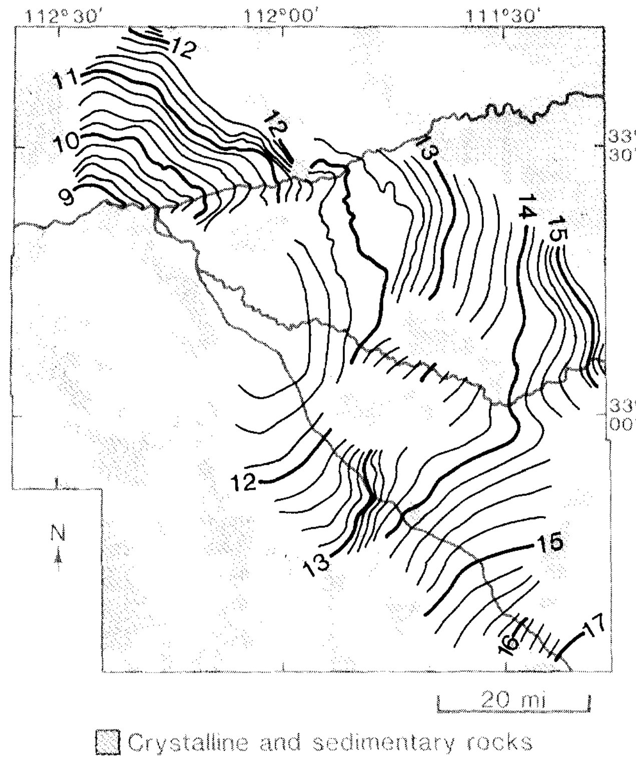


Fig. 1. Location of study area in Arizona (from Anderson, 1968) (A), and main geographic and physiographic features within the study area (B).



1923 water-table altitude, 100s ft

Fig. 2. Altitude of the water table, spring 1923, in central Arizona (from Anderson, 1968).

pumping was greatly accelerated and within a few years reached a rate many times greater than the rate of recharge. Water levels have declined in the entire area, and the rate of decline in some places is as much as 20 feet per year."

The annual water use in the study area during 1923-64 is shown in Figure 3. Because all the flow

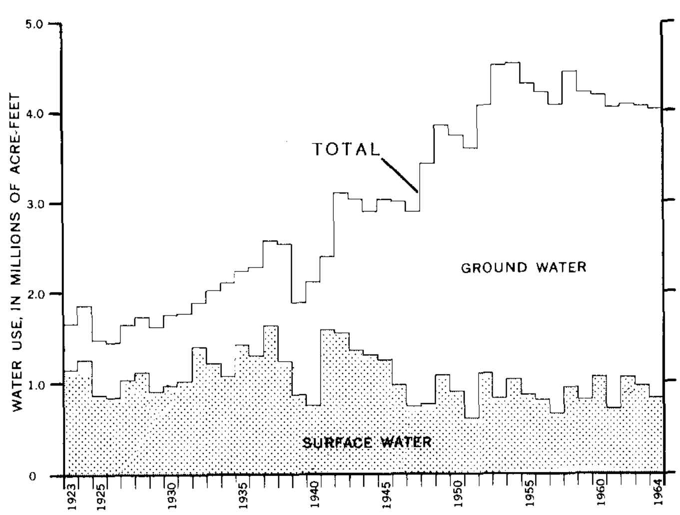


Fig. 3. Annual water use in study area, 1923-64 (from Anderson, 1968). Ground-water use is the difference between total and surface-water use.

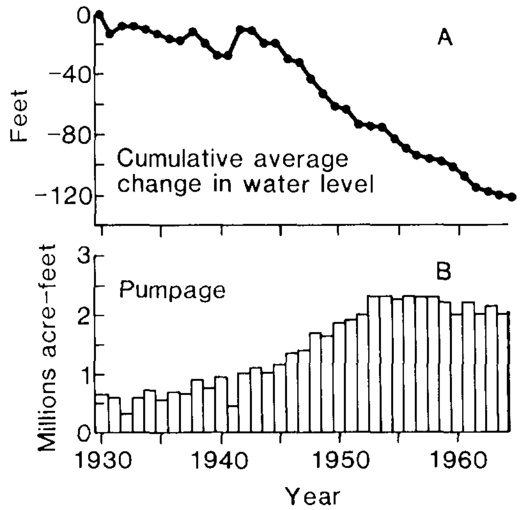
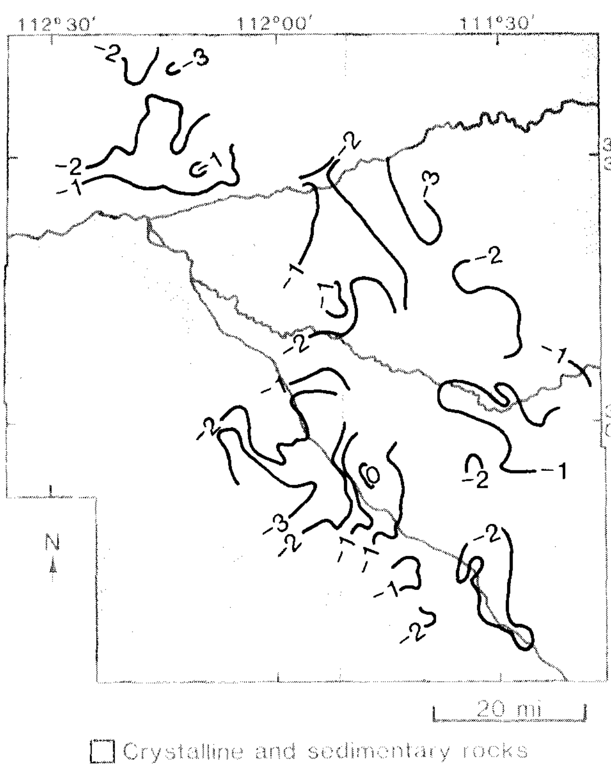


Fig. 4. Average water-level change in the Tempe-Mesa-Chandler area of the Salt River Valley (A), and annual ground-water withdrawals in the Salt River Valley (B), 1930-64 (modified from Babcock, 1970).

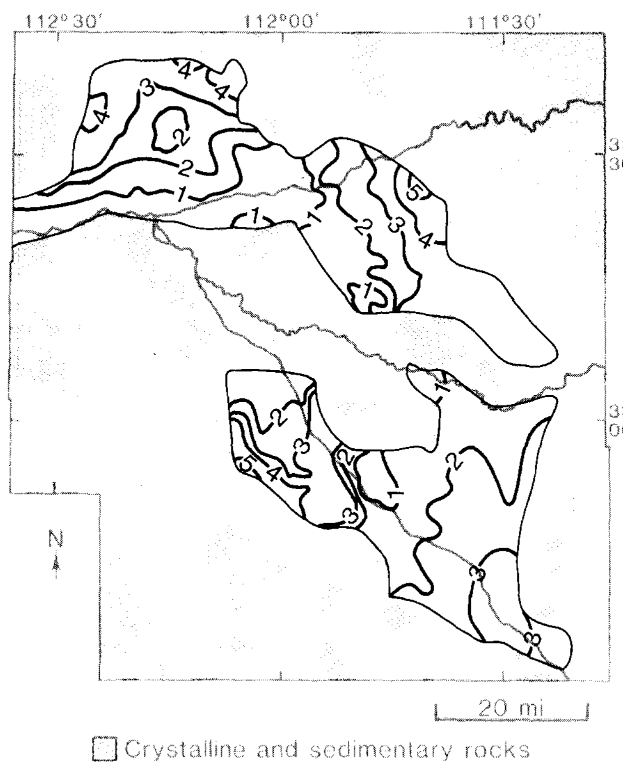
in the Gila and Salt Rivers, except for floodwaters, is diverted for irrigation, increasing demands for water have been met primarily by increases in ground-water withdrawals. The greatest increase in ground-water use occurred during the 1940's and early 1950's. As indicated in Figure 4 by the data for Tempe-Mesa-Chandler area in the Salt River basin, the onset of the major water-level declines generally coincides with the increased ground-water withdrawals, although changes in the rate of decline appear to be lagging behind changes in the pumpage. Anderson (1968) reports that the total volume of ground water withdrawn from this aquifer system during 1923-64 was 80 million ac-ft, and that in 1964 the pumpage was about 3.2 million ac-ft, of which approximately 2.2 million ac-ft were from the Salt River Valley and 1.0 million ac-ft were from the lower Santa Cruz basin.

By the end of 1964 these large ground-water withdrawals, far in excess of recharge, had a major impact on the aquifer system. Anderson (1968) states, "A general regional flow pattern no longer exists, and the flow is directed radially toward the center of the large cones of depression." Figure 5 shows the magnitude of the water-level declines that occurred from 1923 to 1964; the declines exceeded 300 ft in places and exceeded 100 ft in most of the study area. Thus, by 1964 the depth to the water table exceeded 300 ft in parts of the area and exceeded 100 ft in most of the study area (see Figure 6). The increased pumping lifts increased



1923-64 water-level change, 100s ft

Fig. 5. Water-level declines, spring 1923 to spring 1964 (from Anderson, 1968).



1964 depth to water, 100s ft below land surface

Fig. 6. Observed depth to water, spring 1964, in central Arizona (from Anderson, 1968).

the costs of withdrawing ground water, hence was of great concern to the users of ground water (mostly agricultural). Anderson (1968) further notes that another consequence of the increased pumping since 1923 is a reduction in natural discharge, including less evapotranspiration losses and less discharge to rivers, exemplified by the observation that "the Gila River no longer flows as it once did in the reach downstream from its confluence with the Salt."

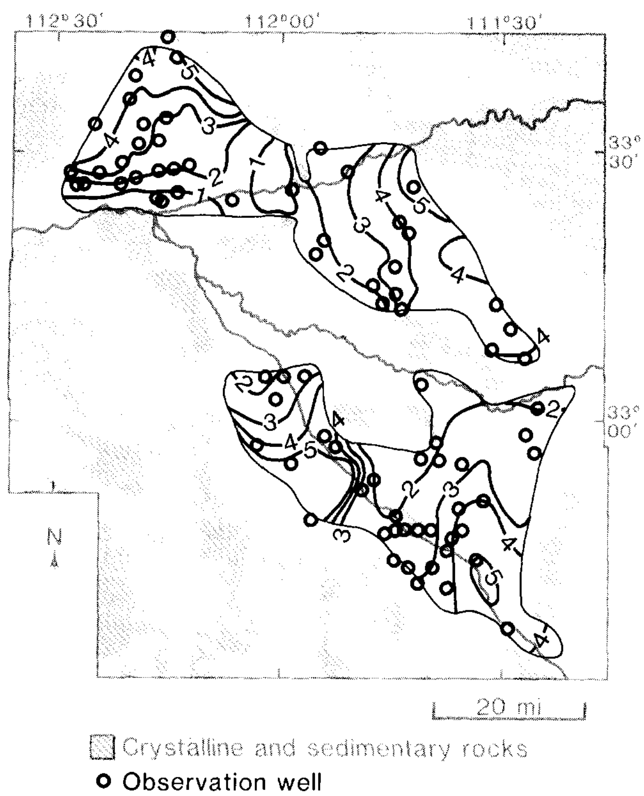
MODEL CALIBRATION AND PREDICTION

Anderson (1968) used a two-dimensional electric-analog model to simulate the uppermost 1200 ft of the aquifer system. Although the technology of electric-analog models of ground-water systems has generally been superseded by numerical (digital computer) models, the principles are the same, and the results of both would be essentially identical. The analog model constitutes a deterministic, distributed-parameter, simulation model and hence provides an appropriate example for analyzing the predictive accuracy of deterministic ground-water models.

The model was based on the assumption that, prior to 1923, an equilibrium existed in the aquifer in which recharge balanced discharge. The analog model then simulates changes in hydraulic head that occur in response to changes in stresses since the assumed steady-state time. The model was calibrated by adjusting aquifer properties, stresses, and boundary conditions to reproduce observed historical changes in ground-water levels during 1923-64 (as shown in Figure 5). The model was constructed at a scale of 1 inch equals 1 mile, with nodes (resistor junctions) placed at 1-inch intervals. Values of the storage coefficient varied spatially in the model from 0.10 to 0.19. One limitation of the model is that it is a two-dimensional approximation of a three-dimensional system. Furthermore, although the transmissivity and storage coefficient are proportional to saturated thickness, a limitation of the model noted by Anderson was that values of these two aquifer properties were not corrected with time to transient changes in water levels. Also, significant land subsidence is known to be occurring within the modeled area, although this process was not explicitly represented in the model. Anderson concluded that the model was a valid representation of the actual hydrologic system for 1923-64, and states, "The close comparison of the field and model data for these periods is the basis for the assumption that the electrical-analog system can be used to predict future ground-water conditions."

Although the model is used to predict future responses, first the future stresses must also be assumed or predicted. In this case, past trends provided the basis for the simplifying assumption that the future amount and areal distribution of pumping would remain about the same as during the most recent six-year period (1958-64). Thus, the future pumpage was assumed to equal 3.2 million ac-ft per year. However, Anderson cautions that, "The amount of water pumped probably will be less because the ever-increasing pumping lifts will make pumping increasingly expensive, and economically marginal lands may be withdrawn from cultivation." He then states that this assumed continuation of the most recent pumpage patterns ". . . will cause the predicted water-level declines to be greater than are actually probable."

The model was thereby used to predict changes in water levels for 10 years into the future. The prediction is illustrated in Figure 7 as the predicted depth to water in 1974. Comparison with Figure 6 shows that the predicted depth to water in 1974 is consistently greater than the depth to water in 1964, in many places by more than 100 ft.



1974 predicted depth to water, 100s ft below land surface

Fig. 7. Predicted depths to water in central Arizona, spring 1974 (modified from Anderson, 1968).

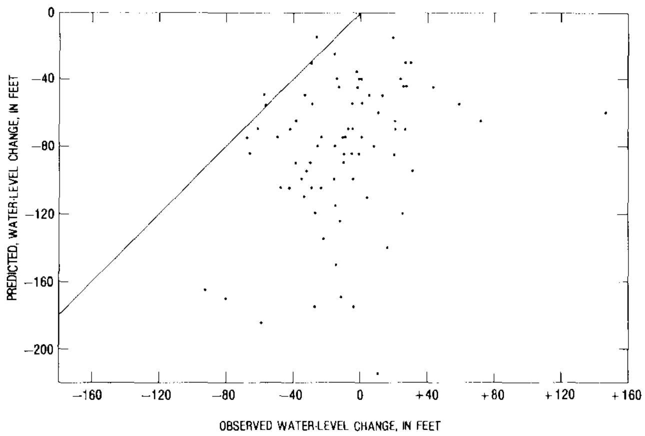


Fig. 8. Relation between predicted and observed changes in water level in the Tempe-Mesa-Chandler area of the Salt River basin, Arizona, 1964-74. Solid line shows where predicted equals observed values.

ASSESSMENT OF PREDICTION

Water-level records are available for 77 wells in the study area for both 1964 and 1974; the locations of these wells are shown in Figure 7. These wells are distributed fairly uniformly throughout the basins; that is, their locations are not clustered in any single subarea or environment. A comparison of the predicted and observed changes in water level at those 77 points provides a basis for evaluating the accuracy of the model prediction. For the entire study area, the predicted water-table decline averages about 50 ft after 10 years. For the 77 available wells, the predicted 10-year decline averages about 82 ft and ranges from 15 ft to 215 ft. However, 10 years after the end of the model-calibration period, measurements of the actual change in water level in the same wells declined an average of only 9 ft, and the observed change ranged from a decline of 92 ft to a rise of 146 ft.

The relationship between the predicted and observed changes in water levels is illustrated in Figure 8. If the predictions were relatively accurate, the data should plot along (or close to) the 45° line connecting equal values of predicted and observed changes. Instead, data from all but three wells fall below that line, indicating poor accuracy and the presence of a bias in the model predictions. Also, the data show a relatively wide scatter, indicating that the model prediction is imprecise. The correlation coefficient is 0.29; although this is statistically significant at the $\alpha = 0.05$ level for a one-sided test, it is low and indicates a poor correlation between the predicted and observed water-level changes. It is further evidence of the relatively poor accuracy of the prediction of the future water levels in this aquifer system.

If there are any lessons to be learned from looking back at this prediction, we must try to ascertain and differentiate among the many possible sources of error. The most obvious question focuses on how much of the error can be attributed simply to errors in the assumed future stresses. In other words, if the future stresses had been estimated accurately and precisely, would the water-level changes have been predicted more closely? This question could best be answered by rerunning the model for the 1965-74 period under an imposition of the stresses that actually occurred. Unfortunately, the original analog model no longer exists and the necessary detailed data on the spatial distribution of pumpage and recharge in the entire study area for 1965-74 are not available. So we are limited to inferring and deducing as much as possible about the sources of error based on the nature and distribution of the errors and our knowledge of the hydrogeologic system.

A frequency distribution of the differences between the observed and predicted changes (that is, the residuals or errors) is presented in Figure 9. The errors are approximately normally distributed [based on the Kolmogorov D statistic (SAS Institute, 1982, p. 580); probability level: $p = 0.043$] and have a mean of −73 ft, a standard deviation of 47 ft, and range from 11 to −226 ft. Ideally, the central tendency of the error distribution should be near zero and the standard deviation should be much smaller than it is.

From Figure 8 it is clear that declines were predicted everywhere, but the changes that occurred turned out to be either much smaller

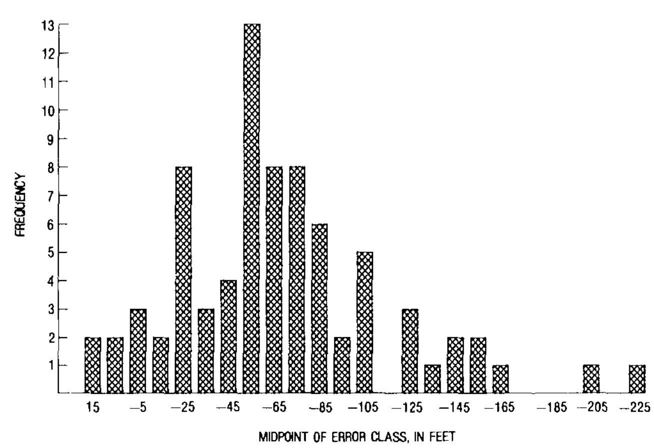


Fig. 9. Histogram showing frequency distribution of errors for the flow model of the Tempe-Mesa-Chandler area of the Salt River basin, Arizona, 1964-74.

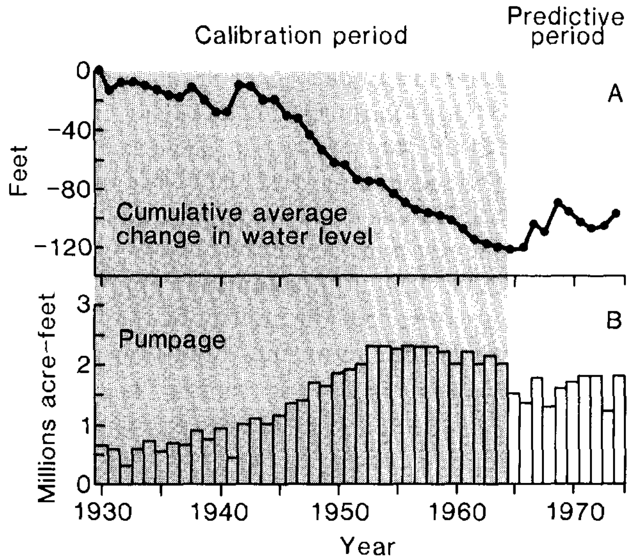


Fig. 10. Average water-level change in the Tempe-Mesa-Chandler area (A) and annual ground-water withdrawals in the Salt River Valley, Arizona (B), 1930-74 (modified from Babcock, 1970).

declines or actual rises, which is a significant deviation from previous long-term trends. This is illustrated in Figure 10, which shows the cumulative average change in water level in wells in the Tempe-Mesa-Chandler area of the Salt River Valley and estimated annual pumpage in the Salt River Valley for 1930-74, which includes most of the calibration period and, in contrast to Figure 4, all of the predictive period. A fairly uniform trend in water-level change prevailed from the early 1940's through the early 1960's, which represented the last 20 years of the model calibration period. But a marked break in this trend occurred very soon after the end of the calibration period. This break corresponds closely with the change to a regime of lesser withdrawal that prevailed since 1964, after a nearly constant and high rate of withdrawal that prevailed from 1953-64. Because the prediction was based on the assumption that stresses observed during the latter few years of the calibration period would continue unchanged, the model basically could do nothing else but extrapolate the water-level trends observed during the latter part of the calibration period.

Estimated actual withdrawals during 1965-74 averaged about 2.5 million ac-ft per year for the entire model area (T. W. Anderson, U.S. Geological Survey, written communication, 1984). The difference between the assumed and actual rates of withdrawal, 0.7 million ac-ft per year, represents an error in the predicted future withdrawals of only about 22 percent of the estimated value. Because the analog model was based on the principle of superposition of solutions and assumed a background withdrawal of 0.5 million ac-ft per year, the difference between the observed and predicted withdrawals actually imposed on the model is about 26 percent of the predicted value (T. W. Anderson, U.S. Geological Survey, written communication, 1985). Regardless, over the 10-year period, the cumulative error then becomes 7.0 million ac-ft. Over the entire modeled area of 1.1 million acres this is equivalent to 6.4 ft of water, and over the cultivated area of 0.8 million acres this is equivalent to 8.8 ft of water. Assuming that the storage coefficient (or specific yield) might be between 0.10 and 0.19, these amounts of water are equivalent to a saturated thickness in the aquifer of between 34 and 64 ft over the entire modeled area and 46 to 88 ft over the cultivated area. In assessing the range of effects of the error in 1965-74 withdrawals, we consider the cultivated area separately because most of the water-level observations, as well as withdrawals, are in these parts of the basins. Therefore, it is possible that the gross error in assumed pumpage can account for a large part of the average bias in the predicted water-level changes.

However, there still remains a relatively large spread in the error distribution shown in Figure 9, which will not be reduced by removing the bias. To help assess whether this lack of precision is also related to errors in the assumed pumpage, we would like to evaluate whether the spatial distribution of errors in assumed pumpage correlates with the spatial distribution of errors in predicted water-level change. Data on actual withdrawals by township (36 mi^2 area) during 1965-74 are available only for the Salt River Valley (T. W. Anderson, U.S. Geological Survey, written communication, 1984, from data prepared by M. R. Long, Arizona Department of Water Resources). Figure 11 shows the relation between the error in pumpage for 1965-74 in each township in both the upper and lower basins (that is, the eastern and western parts, respectively) of the Salt River Valley and the average error in the predicted water-level change (or drawdown) for the same township. The very low correlation between these two factors ($r = -0.086$) indicates that the relatively large spread in errors in predicted water-level change is probably not attributable, either solely or in any large part, to a variance in the accuracy of pumpage estimates. Hence, it appears that there are other sources of error in the model that have not yet been ascertained.

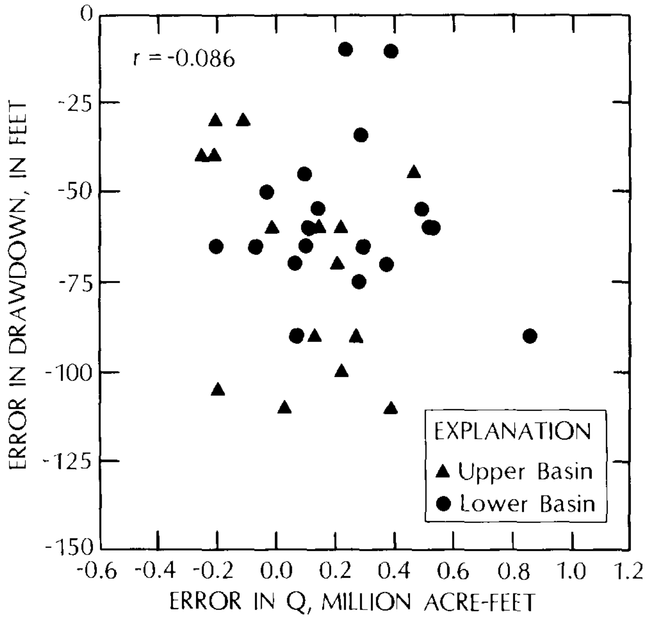


Fig. 11. Relation between the error in the predicted water-level change and the error in the estimated pumpage per township in the upper (eastern) and lower (western) basins of the Salt River Valley, central Arizona, 1965-74.

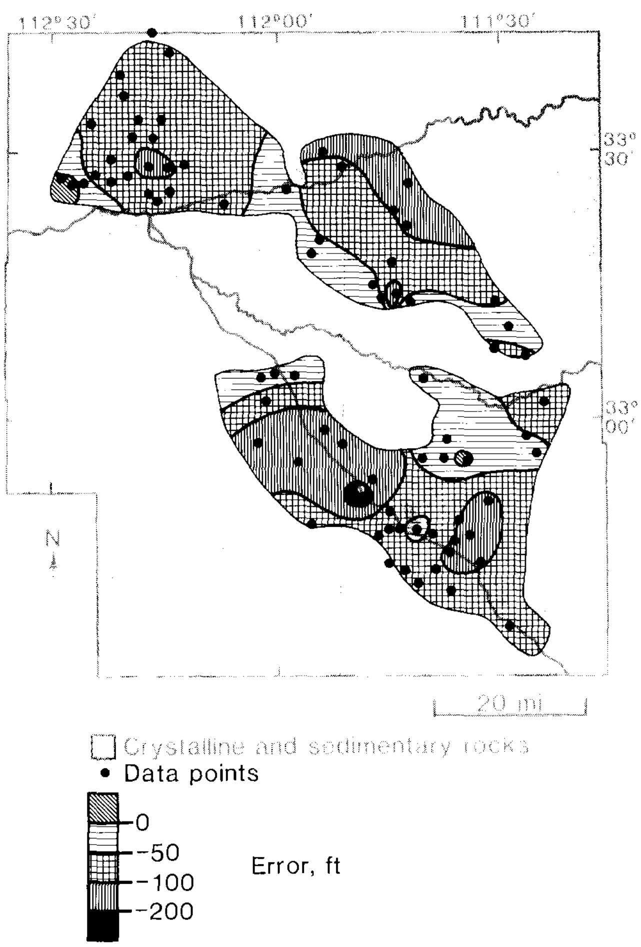


Fig. 12. Map showing the spatial distribution of errors in predicted water-level change, 1965-74, in the Salt River and lower Santa Cruz River basins, Arizona.

The error in the predicted water level for 1974 was plotted on a map of the area and contoured. As shown in Figure 12, it appears that the errors are not just randomly distributed in space, but rather exhibit some persistent patterns in which the errors at nearby data points are usually close in value. However, the error pattern does not correspond closely with the pattern for any single factor for which data are available. In general, the errors seem greatest near the centers of the basins and least near their margins, but exceptions exist. In the southeastern part of the modeled area, the error appears to correlate somewhat closely with depth to water and water-level decline, but elsewhere does not. For the area as a whole, the correlation coefficients for the relationships between the predicted water-level change and the observed water level in 1964 and in 1974 are 0.46 and 0.47, respectively, which are both significant at the 0.05 level for a sample size of 77. However, the correlation coefficients between the errors in predicted water-level change and the two sets (1964 and 1974) of observed water levels are only 0.14 and 0.04, which are not significant at the 0.05 level. Thus, the errors are not strongly associated with water-table elevations. Also, the absence of any important relation between the predictive error and either predicted pumpage or observed pumpage is reflected by the relatively low correlation coefficient of −0.20 for both relationships, and overlaying the transmissivity distribution map on the error map indicates no important association between these two factors.

There are a number of factors that contributed to the reduction in the net withdrawals during 1965-74. Perhaps some of these could have been anticipated and their effects incorporated into the predictive analysis. As noted previously, Anderson did recognize the possibility that net withdrawals would decrease, but he did not account for this in his prediction.

Reexamining the history of the study area for the 1965-74 period, it is believed that the following factors contributed to lower than anticipated net withdrawals: (1) Farmers in certain parts of the area ceased operations because of economic or other reasons, thereby eliminating their withdrawals for irrigation; (2) other farmers took measures, such as leveling their fields, to increase irrigation efficiency, thereby reducing their water requirements; (3) in some areas many wells were deepened to obtain water from deeper permeable zones, thereby reducing the drawdown relative to that resulting from equivalent withdrawals from wells that penetrate less of the aquifer; (4) additional surface water was available for irrigation, reducing the dependence on ground water for supply; (5) in April 1965 an unusual flow event resulted in about 20,000 ac-ft of recharge from infiltration in the channel of the Salt River, which is otherwise normally dry (Briggs and Werho, 1966); and (6) significantly greater than average precipitation occurred in the Salt River watershed in 1972-73, and the subsequent unusually large runoff resulted in the direct recharge of about 0.5 million ac-ft of water along the river channels during 1973-74 (Babcock, 1975). Local variations in these same factors also could have contributed to the variability in the error distribution.

It is also possible that errors in the observed data could be contributing to this variability in the errors. For example, individual water-level measurements may not reflect the local static water level, perhaps due either to recent prior pumping in the observation well or to transient effects from pumps in nearby wells going on or off. These sources of error could not be accurately assessed from existing historical records. Of course, it should not be expected that long-term predictions based on long-term average stresses would predict fluctuations or short-term variations in response to short-cycle stresses (such as local transient well effects) or to unusual hydrologic conditions (such as seasonal recharge from a usually dry river channel).

Because significant land subsidence is known to be occurring in parts of this study area (Schumann, 1974; Laney and others, 1978), the possibility was considered that this process, which was not explicitly represented in the model, could account for some of the error in predicted water-level change. The land subsidence is caused by the compaction of the unconsolidated or partly consolidated sediments in the alluvial-fill basins. The compaction, in turn, is related to the compressibility of the sediments and to the decline in head in the aquifer, the latter of which is obviously induced by the major ground-water withdrawals in the area. Schumann (1974) shows the land subsidence that occurred within the study area from 1948-67; Laney and others (1978) present maps of the study area showing the extent of observed land subsidence in the lower Santa Cruz River basin from 1905 to 1977. Their data indicate that the greatest subsidence within the study area occurred in the lower Santa Cruz basin, where as much as 12.5 ft of subsidence were observed, whereas less than 5 ft of subsidence are reported for the Salt River Valley. Within the lower Santa Cruz basin, Laney and others show that most (more than 90 percent) of the subsidence occurred since 1948; as seen in Figure 10, withdrawals since 1948 were consistently greater than those prior to 1948, except for a few years during the 1965-74 predictive period. Furthermore, they show that the greatest subsidence (between 7.0 and 12.5 ft) occurred in two areas that total about 120 mi^2. The largest of these two areas is about 110 mi^2 and is located in the southwestern part of the basin near Eloy.

Hydrologically, the compaction that causes land subsidence also in effect acts as a source of water to the aquifer system. If this fluid source were not accounted for in the model, then the water produced by compaction might cause the actual drawdowns to be less than would occur otherwise, which is indeed the nature of the predictive error observed here. However, if this hypothesis were correct, we would expect to see some spatial correlation between the amount of subsidence (as shown by Shumann, 1974, and Laney and others, 1978) and the magnitude of the error (as shown in Figure 12). Comparison of these two factors shows that the maximum subsidence zone near Eloy corresponds closely with a high error (> 100 ft) zone in that same area, but that elsewhere there is no obvious association between patterns of errors and subsidence. As much as 4 ft of subsidence were observed in the Eloy area during 1965-74. As a first approximation, if we assume that 4 ft of subsidence generate 4 ft of water and if the specific yield of the aquifer in that area averages 0.15, then the subsidence may cause the water level to be 27 ft higher than it would have been otherwise. In the remainder of the study area the subsidence during 1965-74 averaged about 1 ft, which may similarly be equivalent to about 7 ft of head. These estimates are equivalent to about 20 percent of the error around Eloy and less elsewhere. Furthermore, if the compacting sediments are disseminated and distributed fairly uniformly with depth, then both land subsidence and the storage coefficient are linear functions of aquifer compressibility. Because much of the total subsidence through 1974 occurred during the model calibration period, much of its impact would have been implicitly incorporated into the model parameters during the calibration process, most likely through compensating errors in estimated aquifer properties and stresses. Then if the rate of subsidence (or ratio of rate of subsidence to rate of water-level decline) were essentially the same during the calibration period as during the predictive period, the predictive errors resulting from not explicitly considering the subsidence process in the model would probably be negligible.

Laney and others (1978) present subsidence data at various times from 1905 through 1977 along a northwest-southeast cross section that passes through Eloy. These data indicate that subsidence during the 10-year predictive period on the average represented about 33 percent of the total subsidence that occurred through 1974, although the percentage ranged from 12 to 71 percent. However, although ground-water levels declined fairly steadily during 1948-64, on the average the water level did not decline during 1965-74, yet subsidence continued at a significant or even accelerated rate, at least near Eloy. This could be explained if the compacting low-permeability sediments were restricted to just a few discrete but perhaps relatively thick layers within the total vertical profile of the alluvium. In such a case, the compaction and subsidence would be related to the compressibility of just these low-permeability sediments, rather than to an effective compressibility for the entire aquifer thickness, and the sediments within the low-permeability beds could continue to compact for years after ground-water levels had stabilized. The water produced by the compaction process would act as a delayed-yield or transient-leakage phenomena, which would cause long-term water-level declines to unit stresses to be less than they would otherwise if there were no leakage. It thus appears that, for the Eloy area, the lack of consideration of the land-subsidence process in the model contributed to the error in predicted water-level changes during 1965-74. For the rest of the modeled area, there is no evidence to indicate that this could have been a significant factor.

It also follows that such a significant lack of uniformity with depth in the properties of the sediments would imply the existence of significant variations in hydraulic conductivity and specific storage with depth. This could induce significant vertical components of flow in places, which obviously could not be represented in the two-dimensional model of Anderson, and might thus be a contributor to the predictive error. In fact, Laney (R. L. Laney, U.S. Geological Survey, written communication, 1985) states that in much of this area at least three layers of differing transmissivity would be required to adequately describe the system. For example, the uppermost and highest transmissivity layer has gradually been dewatered since the 1940's and now is saturated only in parts of the basin (R. L. Laney, U.S. Geological Survey, written communication, 1985). This implies that the effective transmissivity may have changed significantly when and where dewatering has occurred. A rigorous test of this hypothesis would require the construction of alternative two- and three-dimensional models, which is beyond the scope of this study.

This example from central Arizona illustrates the weakness of basing a prediction of aquifer responses on a single set of assumed future stresses. Because the uncertainty of the 1965-74 stresses was not assessed, we do not know whether the actual 1965-74 responses fall within some associated confidence interval; hence, we cannot make a judgment based solely on these predictive errors as to whether the model is "good" or "bad." In cases like this, it would be preferable to assess the uncertainty in estimated (or assumed) future stresses and then present the forecasts as a range of responses with associated probabilities of occurrence or confidence intervals. Because Anderson had indicated (correctly) that the assumed stresses were probably greater than would occur, the predictions can be viewed as a "worst-case" estimate. From that perspective, the model predictions are reasonably accurate.

CONCLUSIONS

There is no sure way to reliably predict the future, but, because management decisions must be made, predictions of future conditions are needed and will be made in one manner or another. To make the most reliable prediction for a given ground-water problem, all relevant information should be considered and evaluated in order to arrive at the best estimate of the future behavior of the system. Deterministic simulation models can help accomplish this quantitatively by providing a format to integrate and synthesize all available information in a manner consistent with theories describing the governing processes. Our present understanding of the many processes affecting ground water is sufficiently adequate to allow us, in theory, to forecast the behavior of a ground-water system. In practice, we are severely limited by the inadequacy of available data to describe aquifer properties and historical stresses and responses, and by an inability to predict future stresses.

Overall, extreme caution is required in making, presenting, and accepting predictions of future ground-water behavior. Partly because the confidence in estimates of future stresses decreases with length of predictive time, and partly because historically observed system behavior may not reflect the relative dominance or strengths of different governing processes under a new set of stresses, forecasts will have greater uncertainty with increasing predictive time. The example discussed in this paper showed that calibrating a model with more than 40 years of data, in itself, did not provide a reliable basis for predicting changes in ground-water levels for a 10-year period. This example, although certainly neither exhaustive in scope nor firmly conclusive in implication, at least tends to raise serious questions concerning our ability to forecast the future state of ground-water systems. At a minimum it can be called on to question the credibility and validity of predictions of waste transport in ground water for perhaps thousands of years in areas where there may be no historical observations of flow or transport phenomena. Regardless, all ground-water predictions should be accompanied by some indication of their uncertainty; confidence intervals and explicit statements of probabilities of occurrence should be estimated.

In light of the predictive accuracy demonstrated by the model in the example presented in this paper, one might legitimately question the value of deterministic ground-water models. Although, in general, deterministic ground-water simulation models represent a valuable tool for analyzing aquifer systems and for predicting responses to specific stresses, the predictive accuracy of these models does not necessarily represent their primary value. Rather, they provide a means to quantitatively assess and assure the consistency within and between (1) concepts of the governing processes, and (2) data describing the relevant coefficients. In this manner, a model helps the investigators improve their understanding of the factors controlling ground-water flow.

An aquifer-simulation model is no more than an approximation of a complex field situation. Improvements in the approximation are always possible; thus, models should be considered as dynamic representations of nature, subject to further refinement and improvement. As new information becomes available, previous forecasts could and should be modified. Feedback from preliminary models not only helps an investigator to set improved priorities for the collection of additional data, but also helps test hypotheses concerning governing processes in order to develop an improved conceptual model of the system and problem of concern. In summary, the primary value of deterministic ground-water models in many analyses is in providing a disciplined format to improve one's understanding of the aquifer system. This, in turn, should allow better management of ground-water resources of an area, regardless of the predictive accuracy of the model.

It is fairly common now for comprehensive and intensive hydrogeologic investigations to include the development, application, and calibration of a simulation model, as well as to use that model to make predictions. It is also not unusual for data collection and monitoring efforts in the study area to be curtailed after the project has ended. This will inevitably result in a future deficiency in data on actual stresses and responses during the forecast period. The uncertainty in the natural and man-imposed stresses may be so large (as in this example from Arizona) that it appears impossible to separate out the other sources of error in a postaudit. Although in the Arizona case it is possible that errors in assumed stresses can account for all predictive errors, it is more likely that errors in conceptualization and in estimated values of hydraulic parameters have also contributed. But the significance of these factors remains largely elusive. It seems reasonable to infer that the use of a more finely discretized two-dimensional model would not have improved the predictive capabilities for that aquifer system, but that a three-dimensional model or the inclusion of the land subsidence process might have helped.

It should be recognized that when model parameters have been adjusted during calibration to obtain a "best fit" to historical data, there is a bias towards extrapolating existing trends when predicting future conditions, in part because predictions of future stresses are often based on existing trends. Thus, although one advantage of deterministic models is that they represent processes and thus have cause-and-effect relationships built into them, careful attention must be paid to the accuracy with which future "causes" (stresses) can be predicted (or estimated), because that can be the major source of error in the predictions of future "effects" (system responses). Furthermore, concepts inherent in a given model (for example, two-dimensional flow and vertically-averaged parameter values, or assumed geometry and boundary conditions) may be adequate over the observed range of stresses, but may prove to be oversimplified or invalid approximations under a new and previously inexperienced type or magnitude of stresses.

The example also clearly demonstrates that if a model is to be used for prediction, it should be periodically postaudited, or recalibrated, to incorporate new information, such as changes in imposed stresses or revisions in the assumed conceptual model. In the example, in spite of the inconclusiveness in pinpointing the exact sources of error, the postaudit pointed out the large predictive error and the major change in withdrawal trends that fortuitously occurred immediately after the end of the calibration period. The original forecasts had been extended to 1984, and subsequent to this type of postaudit, the extended prediction could have been revised to more accurately account for the change in pumping patterns and the occurrence of occasional but significant recharge events.

Thus, in general, predictions should not be made and accepted but then forgotten; plans should next focus on conducting a postaudit. Sufficient data should continue to be collected after a prediction is made so that the model can continue to be tested and evaluated as the stress history in the area continues to evolve. A postaudit offers the only true way to "verify" a model, in the sense of demonstrating its predictive accuracy for a particular field application. But more important, the evaluation of the nature and magnitude of predictive errors may itself lead to a large increase in the understanding of the system and in the value of a subsequently revised model. Revised predictions can then be made with greater reliability.

ACKNOWLEDGMENTS

Thomas W. Anderson kindly provided assistance and recent data from Arizona. William M. Alley, Richard L. Cooley, Jurate M. Landwehr, Robert L. Laney, and E. P. Patten, Jr. provided many helpful comments and suggestions during the course of this investigation. Mark A. Person assisted in data analysis.

REFERENCES CITED

Anderson, T. W. 1968. Electric analog analysis of ground-water depletion in central Arizona. U.S. Geological Survey Water-Supply Paper 1860. 21 pp.

Babcock, H. M. 1970. Annual report on ground water in Arizona, spring 1969 to spring 1970. Arizona State Land Department Water-Resources Report 43. 44 pp.

Babcock, H. M. 1975. Annual report on ground water in Arizona with special emphasis on Gila Bend Basin and McMullen Valley and the southeast part of the Harquahala Plains, spring 1973 to spring 1974. Arizona Water Commission Bull. 9. 45 pp.

Briggs, P. C. and L. L. Werho. 1966. Infiltration and recharge from the flow of April 1965 in the Salt River near Phoenix, Arizona. Arizona State Land Dept. Water-Resources Report 29. 12 pp.

Davidson, E. S. 1979. Summary appraisal of the nation's ground-water resources—lower Colorado region. U.S. Geological Survey Professional Paper 813-R. 23 pp.

Laney, R. L., R. H. Raymond, and C. C. Winikka. 1978. Maps showing water-level declines, land subsidence, and earth fissures in south-central Arizona. U.S. Geological Survey Water-Resources Investigations 78-83. 2 sheets.

SAS Institute, Inc. 1982. SAS User's Guide: Basics. Cary, North Carolina. 921 pp.

Schumann, H. H. 1974. Land subsidence and earth fissures in alluvial deposits in the Phoenix area, Arizona. U.S. Geological Survey Misc. Inv. Ser. Map I-845-H. 1 sheet.

* * * * *

Leonard F. Konikow received a B.A. in Geology in 1966 from Hofstra University. His graduate studies were at The Pennsylvania State University, where he received an M.S. and a Ph.D. in Geology in 1969 and 1973, respectively. He has worked for the Water Resources Division of the U.S. Geological Survey since 1972, and presently is a Research Hydrologist in their Reston, Virginia office.

EXHIBIT 14

From:	Prabhakar Clement
To:	Maslia, Morris (ATSDR/DHAC/EISAB)
Cc:	Susan Martel
Subject:	Re: Tarawa Terrace Chapter I Report available on ATSDR web site
Date:	Wednesday, February 18, 2009 12:41:28 PM

Dear Morris,
Nice report, I wish we would had more time to review this work as a panel. May not have the time to digest and incorporate this information at this late stage, however.
I also noticed that you have an interesting meeting coming up:
Camp Lejeune Water-Modeling Expert Panel Meeting - April 29–30, 2009, 8:30 am - 5:00 pm, Atlanta, Georgia.
I hope you and your experts will have a copy of our report before this meeting. I will be very interested in following up how the experts viewed some of our suggestions. Our panel's goal was to help you guys ATSDR/CLJ to make a quick policy decision, hope we contributed to this cause.
I and my exposure group members have thought and debated this problem a lot. It has fundamentally changed my own thinking on modeling and policy making. Let me know if I can be of help to you guys in any way to speed-up the resolution process. I or perhaps even others may be glad to help with your April panel if we can do this without violating any conflict of interest.
Regards,
Prabhakar

PS: I am copying this email to Susan at NAS

--

Prabhakar Clement, Ph.D., P.E.
Professor and Arthur H. Feagin Chair of Civil Engineering
Department of Civil Engineering
212 Harbert Engineering Center
Auburn University, AL 36849-5337
+1 (334) 844-6268 telephone
+1 (334) 844-6290 facsimile
Email: clement@auburn.edu
Home page: http://www.eng.auburn.edu/users/clemept/
Dept page: http://www.eng.auburn.edu/department/ce/
RT3D webpage: http://bioprocess.pnl.gov/rt3d.htm

>>> On 2/18/2009 at 10:39 AM, in message
<2FE93DA9114E7E4A9A2EB70A77C9FFD3057C5383@LTA3VS003.ees.hhs.gov>,
"Maslia,
Morris (ATSDR/DHAC/EISAB)" <mfm4@cdc.gov> wrote:
> ATSDR's Tarawa Terrace Chapter I report,
>
>
>
> "Analyses of Groundwater Flow, Contaminant Fate and Transport, and
> Distribution of Drinking Water at Tarawa Terrace and Vicinity, U.S.
> Marine Corps Base Camp Lejeune, North Carolina: Historical
> Reconstruction and Present-Day Conditions, Chapter I: Parameter
> Sensitivity, Uncertainty, and Variability Associated with Model
> Simulations of Groundwater Flow, Contaminant Fate and Transport, and

> Distribution of Drinking Water" by M.L. Maslia, R.J. Suarez-Soto, J.
> Wang, M.M. Aral, R.E. Faye, J.B. Sautner, C. Valenzuela, and W.M.
> Grayman
>
>
>
> is now available for download on the ATSDR web site:
> http://www.atsdr.cdc.gov/sites/lejeune/index.html
>
>
>
> (look under the heading of "SELECTED RESOURCES")
>
>
>
> There also is an accompanying CD-ROM containing model input files
that
> can be down loaded from the site.
>
>
>
>
>
> Printed copies of the report should be available after March 20,
2009.
>
>
>
>
>
> Best regards
>
>
>
> Morris L. Maslia
>
>
>
> ==================================
> Morris L. Maslia, P.E., D.WRE, DEE
> Research Environmental Engineer
> Agency for Toxic Substances and Disease Registry
> National Center for Environmental Health
>
> TEL: +1 770.488.3842
> FAX: +1 770.488.1536
> Email: mmaslia@cdc.gov
> Web: http://www.atsdr.cdc.gov/edrp/
>
> Mail and Package Address
> 4770 Buford Highway
> Mail Stop F-59, Room 02-004
> Atlanta, Georgia 30341-3717, USA
> ==================================
> P Please only print this e-mail if necessary
>
>

EXHIBIT 15

Expert Report of

Morris L. Maslia, P.E., D.WRE, DEE, Fellow EWRI

Prepared by:

Morris L. Maslia

____

M. L. Maslia Consulting Engineer
Registered Professional Engineer, GA #PE012689

3360 Norfolk Chase Drive, Peachtree Corners, GA 30092
Mobile: +1 (404) 431-0035 — Email: H2OBoy54@gmail.com
https://www.linkedin.com/in/mlmaslia/

Table of Contents

List of Figures[1]

[1] In this Expert Report and in all published ATSDR reports and journal articles on Camp Lejeune, chemical names are referred to by their Common Name (e.g., tetrachloroethylene for PCE). Tables listing complete names for volatile organic compounds in groundwater are provided in Lawrence (2007).

Figure 7.14. Reconstructed (simulated) and observed tetrachloroethylene (PCE) concentrations at water-supply well TT-26, Tarawa Terrace (Faye 2008).

Figure 7.15. Conceptual framework for (a) a deterministic analysis and (b) a probabilistic analysis (Maslia and Aral 2004).

Figure 7.16a. Ratio of pumping rate to pumping capacity ($Q_{TT\text{-}26}$ / $QC_{TT\text{-}26}$) for water-supply well TT-26 for calibrated model and Monte Carlo simulation, Tarawa Terrace (Maslia et al. 2009b).

Figure 7.16b. Concentrations of tetrachloroethylene (PCE) in finished water at the water treatment plant derived from the calibrated MT3DMS model, probabilistic analysis using Monte Carlo simulation for scenario 1 (pumping uncertainty excluded) and scenario 2 (pumping uncertainty included), Tarwa Terrace study area (Maslia et al. 2009b).

Figure 7.17. Locations of historically contaminated water-supply wells, Installation Restoration Program (IRP) sites, and above-ground and underground storage tank (AST/UST) sites, Hadnot Point–Holcomb Boulevard study areas (map area figures refer to the Chapter A report [Maslia et al. 2013]).

Figure 7.18. Steady-state groundwater-flow model results shown as observed and simulated potentiometric levels, and observed potentiometric levels and corresponding residuals, steady-state groundwater-flow model calibration, Hadnot Point–Holcomb Boulevard study area (Suárez-Soto et al. 2013).

Figure 7.19. Comparison of observed water-level altitude and simulated water-level altitude for well X24S6 for two cases of the transient groundwater-flow model: *case a* with temporal variability of recharge, and *case b* without temporal variability of recharge, Hadnot Point–Holcomb Boulevard study area (Suárez-Soto et al. 2013). [Note: Date range for measured and simulated water-level altitude for *cases a* and *b* is March 1988 to June 2008].

Figure 7.20. Reconstructed (simulated) and measured concentrations of trichloroethylene (TCE) at selected water-supply wells within the Hadnot Point Industrial Area, Handot Point-Holcomb Boulevard study area. Groundwater-flow simulation using MODFLOW (Harbaugh 2005) and contaminant fate and transport simulation using MT3DMS (Zheng and Wang 1999), see Figure 7.17 for well location(from Jones et al. 2013).

Figure 7.21. Reconstructed (simulated) and measured observed concentrations of trichloroethylene (TCE) and tetrachloroethylene (PCE) at water supply well HP-651 and extraction wells 82-DRW01, 82-DRW02, 82- DRW03, and 82-DRW04, model layer 5, Hadnot Point landfill area, Hadnot Point–Holcomb Boulevard study area (Jones et al. 2013).

Figure 7.22. *(A)* Line of section *A–A′* and *(B)* simulated water levels within the Hadnot Point landfill area fate and transport model subdomain, model layer 5, Hadnot Point–Holcomb Boulevard study area (Jones et al. 2013).

Figure 7.23. Reconstructed (simulated) and measured concentrations of benzene at selected water-supply wells within the Hadnot Point Industrial Area, Hadnot Point study area, U.S. Marine Corps Base Camp Lejeune, North Carolina (Maslia et al. 2013).

Figure 7.24. Reconstructed (simulated) and measured concentrations of tetrachloroethylene (PCE) and trichloroethylene (TCE), trans-1,2-dichloroethylene (1,2-tDCE), and vinyl chloride (VC) at water-supply well HP-651 using numerical (MT3DMS) and linear control methodology (LCM; TechControl) models, Hadnot Point study area (Guan and Aral 2013, Maslia et al. 2013).

Figure 7.25. Reconstructed (simulated) finished-water concentrations of tetrachloroethylene (PCE), trichloroethylene (TCE), *trans*-1,2-dichloroethylene (1,2-tDCE), vinyl chloride (VC), and benzene, and measured concentrations (Faye et al. 2010), Hadnot Point water treatment plant, Hadnot Point–Holcomb Boulevard study

List of Tables

Table 7.9. Summary of reconstructed (simulated) values and observed data of tetrachloroethylene (PCE) at water-supply wells, Tarawa Terrace (Maslia et al. 2007).

Table 7.10. Summary of reconstructed (simulated) values and observed data of tetrachloroethylene (PCE) at the water treatment plant, Tarawa Terrace (Maslia et al. 2007).

Table 7.11. Summary statistics for reconstructed (simulated) tetrachloroethylene (PCE) contamination of selected water-supply wells and the water treatment plant based on calibrated model simulations, Tarawa Terrace (Maslia et al. 2007).

Table 7.12. Computed and observed tetrachloroethylene (PCE) concentrations in water samples collected at the Tarawa Terrace water treatment plant and calibration target range, Tarawa Terrace (Fay 2008).

Table 7.13. Identification of documented source areas, primary contaminants, and location of major dissolved-phase sources, Hadnot Point area, U.S. Marine Corps Base Camp Lejeune, North Carolina (Figure references are to the Chapter A report [Maslia et al. 2013]).

Table 7.14. Calibrated model parameter values used to simulate groundwater flow and contaminant fate and transport, Hadnot Point–Holcomb Boulevard study area, U.S. Marine Corps Base Camp Lejeune, North Carolina.

Table 7.15. Selected measured and reconstructed (simulated) concentrations of tetrachloroethylene (PCE), trichloroethylene (TCE), *trans*-1,2-dichloroethylene (1,2-tDCE), vinyl chloride (VC), and benzene at the Hadnot Point water treatment plant, Hadnot Point study area (Maslia et al. 2013).

Table 7.16. Summary statistics for reconstructed contaminant concentrations at selected water-supply wells and the Hadnot Point water treatment plant, Hadnot Point study area (Maslia et al. 2013).

Table 7.17. Reconstructed (simulated) mean concentrations of tetrachloroethylene, trichloroethylene, *trans*-1,2-dichloroethylene, vinyl chloride, and benzene in finished water distributed to Holcomb Boulevard family housing areas for selected months, Hadnot Point– Holcomb Boulevard study area (Maslia et al. 2013, Sautner et al. 2013b).

1.0 Introduction

I am Morris L. Maslia, P.E. (a licensed professional engineer in the State of Georgia), and I have conducted consulting engineering, research, and scientific studies in the areas of environmental fate and transport, water resources (including water-distribution systems), hazardous waste remediation, environmental health, exposure assessment, and public health. I have worked with international organizations, non-profit organizations, U.S. federal agencies, state government agencies, engineering consulting firms, and private industry. I have developed and presented workshops, lectures, and training courses for international, government, and academic institutions (*e.g.*, University of San Luis Potosi, Mexico, Emory University, and Georgia Tech, Atlanta, Georgia). My areas of experience, expertise, and continued interests include public health, water resources and sanitation, global impacts of contamination of water resources, environmental analyses, epidemiological studies, exposure assessment, water-distribution system analysis, engineering and research report review, and volunteering and working with non-profit organizations.

2.0 Details of Experience

A summary and overview of my professional experiences and professional registrations are listed below. Specific details of my professional experiences are provided in my current curriculum vitae (CV), that is in **Appendix A** of this report.

My professional work experience and history are listed below in chronological order, beginning with the most recent professional experiences.

- **M. L. Maslia Consulting Engineer, Peachtree Corners, Georgia**
  Owner, 2018–Present
- **Agency for Toxic Substances and Disease Registry, Atlanta, Georgia**
  Research Environmental Engineer and Project Officer, 1992–2017 (December 31)
- **Rollins School of Public Health, Emory University, Atlanta, Georgia**
  Adjunct Faculty, Department of Environmental Health, 2000–2015
- **Geosyntec Consulting Engineers, Norcross, Georgia**
  Water Resources Group Manager and Hydrologist, 1989–1992
- **U.S. Geological Survey, Water Resources Division, Doraville, Georgia**
  Research Hydrologist, 1980–1989
- **Federal Energy Regulatory Commission, Washington, DC/Atlanta, Georgia**
  (f/k/a, Federal Power Commission)
  Civil / Hydraulic Engineer, 1976–1980

Throughout my professional career, I have participated in, contributed to, and directed several high-profile, public water resources, environmental and public health projects. A complete list is found in my CV (**Appendix A**). Below are summaries of sentinel projects and experiences.

One of the high-profile, public sites that I was the Technical/Scientific Project Officer for was the project for water-modeling of volatile organic compound (VOC) contamination of drinking water supplies at U.S. Marine Corps Base Camp (USMCB) Camp Lejeune, Noth Carolina. In terms of overseeing and managing this project, I was responsible for putting together a multidisciplinary team of scientists, engineers, and data analysts consisting of available staff from the Agency for Toxic Substances and Disease Registry (ATSDR); coordinating with a cooperative agreement University Partner (the Multimedia Environmental Simulations Laboratory in the School of Civil and Environmental Engineering at the Georgia Institute of Technology); hiring outside consulting experts for task-specific assignments; coordinating with an ATSDR contractor (Eastern Research Group) to provide engineering and hydrologic science sub-contractor support and project logistical and administrative support; and requesting and executing cooperative agreements with other federal agencies (U.S. Geological Survey [USGS]) to provide modeling and cartographic support personnel. In total, there were 21 people that I supervised and 3 outside organizations that I coordinated with (Eastern Research Group, a university partner, and the USGS) from 2003–2013 for this project. Table 2.1 lists the partners and team members by organization. **Appendix B** lists team members, their occupation, organization, and their respective technical and scientific expertise provided to the project.

Table 2.1. Partners and Team Members Supporting the Agency for Toxic Substances and Disease Registry's (ATSDR's) Water-Modeling Activities for the Camp Lejeune Drinking-Water Health Studies.

ATSDR	**Consultants**	**University Partner**[1]	**Other Federal Agency**
B.A. Anderson	Eastern Research Group[2]	M.M. Aral	U. S. Geological Survey (USGS)
F.J. Bove	J. Doherty[3]	B. Chang	L.E. Jones[7]
M.L. Maslia	R.E. Faye[4]	J. Guan	S. J. Lawrence[7]
S.M. Moore	W.M. Grayman[5]	W. Jang	K.A. Waltenbaugh[8]
P.Z. Ruckart	I.T. Telci[6]	I,T. Telci	C.J. Wipperfurth[8]
J.B. Sautner	J.W. Green, Jr.		
R.J. Suárez-Soto	C. Valenzuela		

[1]Multimedia Environmental Simulations Laboratory, School of Civil and Environmental Engineering, Georgia Institute of Technology
[2]Under contract to ATSDR for multi-site assistance and logistic support
[3]Watermark Numerical Computing
[4]R.E. Faye and Associates, sub-contractor to Eastern Research Group
[5]W.M. Grayman Consulting Engineer
[6]Sub-contractor to Oak Ridge Institute for Science and Education (ORISE)
[7]Georgia Water Science Center, USGS
[8]Science Publishing Network, USGS

2.1 U.S. Geological Survey (USGS), 1980–1989

Regional Aquifer Systems Analysis (RASA)

The major groundwater systems of the United States were investigated by the U.S. Geological Survey (USGS) through its Regional Aquifer-System Analysis (RASA) Program. During the first 15 years of the program (1978-92), 25 regional aquifer systems, including the most heavily pumped aquifers in the Nation, were intensively studied. One of the aquifer systems, the Floridan Aquifer

System, is located in southwest Georgia, southernmost Alabama, and all of Florida. I had the opportunity to develop and calibrate two-dimensional groundwater-flow models for southwest Georgia (an area of extensive agricultural pumpage) and northwest Florida (an area of extensive agricultural and water-supply pumpage). The results of the RASA studies are detailed in the series of USGS Professional Papers publications (1403 series for the Floridan Aquifer System). Two sentinel publications that I co-authored are Hayes et al. (1983) and Maslia and Hayes (1988). A peer-reviewed journal article that I co-authored was published in the journal *Ground Water* and was a result of research efforts conducted on the Floridan RASA program (Randolph et al. 1985).

Investigation of Groundwater Flow, Hyde Park Landfill, New York

Early in my tenure with the USGS Water Resources Division, I and a colleague were asked by the U.S. Environmental Protection Agency (USEPA) to assist them with evaluating and understanding the hydrogeologic controls on groundwater flow in a fractured rock aquifer at Niagara Falls, New York. The Hyde Park landfill, owned and operated by Hooker Chemical Company and located in the vicinity of Love Canal and the S-Area, had buried, toxic wastes underlain by a fractured rock aquifer. We applied a saturated-unsaturated finite element groundwater-flow model that I had developed as part of my Master's Degree dissertation (Maslia 1980) to conduct the analysis. The results of the analyses were used by the USEPA to determine the direction and travel time for groundwater (and hence groundwater contaminated with chemicals) from the Hyde Park landfill to the Niagara River Gorge. This research effort resulted in two publications (a USGS Open-File Report and a peer-reviewed journal article) that are described in Maslia and Johnston (1982, 1984). The resulting calibrated hydrogeologic and aquifer parameter values have stood the test of time and have been used by other researchers conducting groundwater-flow modeling in this area over the years. *Noteworthy of this research is that the results were used by the USEPA to support its first legal proceedings under the newly enacted CERCLA (Superfund) legislation*.

Determining Anisotropic Transmissivity Tensor Components of Two-Dimensional Groundwater Flow

The equations that represent the movement of water in an aquifer when water is being withdrawn from a well form the basis of methods used to analyze aquifer-test data. These equations were derived under the assumption of aquifer isotropy and are not valid for analysis of anisotropic aquifers that include, for example, flow in some secondary permeability terrains and fractured rocks. Thus, in conjunction with aquifer-test data, the anisotropic equations can be used to determine aquifer anisotropy and the components of the anisotropic transmissivity tensor. In this research, the method originally described by Papadopulos (1965) was applied to aquifer hydraulic data to determine the components of the anisotropic transmissivity tensor. In addition, this research described the development, codification, and use of the computer program TENSOR2D, which automates the solution of hydraulic parameters and tensor components of the anisotropic transmissivity tensor. This research resulted in two USGS publications (Maslia and Randolph, 1986, 1987) and has been incorporated into several public and proprietary desktop aquifer analysis programs used today by consulting engineers. An updated version of the TENSOR2D program was described in a note to the journal *Ground Water* (Maslia 1994).

Effects of Faults on Groundwater Flow and Chloride Contamination in the Upper Floridan Aquifer, Brunswick, Glynn County, Georgia

This research focused on the effects of inferred faults based on geophysical, hydrogeologic, and water-quality data within the Upper Floridan aquifer underlying Brunswick, Glynn County, Georgia.

This area has historically withdrawn large quantities of groundwater to support the chemical and pulp industries in Georgia, and in addition, provide drinking water to local municipalities. The research developed a unified, multidiscipline hypothesis to explain the anomalous pattern by which chloride has been found in water of the Upper Floridan aquifer. Analysis of geophysical, hydraulic, water chemistry, and aquifer-test data using the equivalent porous medium (EPM) approach were used to support the hypothesis and to improve further understanding of the fracture-flow system in this area. Results are described in a peer-reviewed journal article (Maslia and Prowell 1990) and two USGS publications (Jones and Maslia 1994; Jones et al. 2002).

2.2 Geosyntec Consultants, 1990–1992

Evaluation of Groundwater Flow Regime at a Landfill in New York
The High Acres Landfill is located southeast of Rochester, New York, in Monroe County, on the eastern border of the town of Perinton. The design, construction, and operation of a waste disposal facility requires owners and operators to comply with applicable state and federal regulations. These regulations require the owner/operator to demonstrate that a minimum distance can be maintained between waste and groundwater to assure that the waste is not placed in the saturated zone (zone at and below the water table). For this site, the owner/operator had to demonstrate that the seasonal-high water table could be maintained 5 feet below the liner system. A multilayer finite-element aquifer model was applied to the site to (1) simulate the mechanism by which groundwater moves through the landfill at the site, and (2) evaluate the average and seasonal high water-table conditions at the site with and without the liner system. Based on the simulations, critical design aspects of the landfill liner system and its effect on local groundwater flow regime were evaluated throughout the entire site. Details of the analyses are provided in a peer-reviewed journal article (Maslia et al.1992).

2.3 Agency for Toxic Substances and Disease Registry (ATSDR),1992–2017

Exposure-Dose Reconstruction Program
In 1980, Congress created the Agency for Toxic Substances and Disease Registry (ATSDR) to implement the health-related sections of laws that protect the public from hazardous wastes and environmental spills of hazardous substances. ATSDR was created under the Comprehensive Environmental Response, Compensation, and Liability Act (CERCLA)—also known as Superfund. A critical activity in achieving ATSDR's mission is characterizing past and current human exposures to, and doses received from, hazardous substances. Because direct measures of exposure and dose are often unavailable to agency health assessors and health scientists, sensitive, integrated, science-based methods for exposure-dose characterization needed to be developed. On December 23, 1992, Dr. Barry L. Johnson, Assistant Administrator, ATSDR, requested that a coordinated, comprehensive plan be developed that would serve as the agency's strategy for exposure-dose reconstruction activities. That plan, which I co-authored for ATSDR, is presented in **Appendix C**.

The overall goal of the Exposure-Dose Reconstruction Program (EDRP) was to enhance the agency's capacity to characterize exposure and dose to better support health assessments and consultations, health studies, and exposure registries. As agency and division needs and requirements were identified, specific projects under the auspices of the EDRP were proposed and developed. The EDRP workplan (**Appendix C**), therefore, sets forth ATSDR's program objectives and priorities for conducting exposure-dose reconstruction activities. Listed below are examples of projects, analyses and methods development conducted under the auspices and funding of the EDRP (1993–2013) that are described in agency reports and peer-reviewed literature.

Two very high-profile sites where the EDRP was requested to provide scientific and technical expertise were: (1) the Dover Township (Toms River), New Jersey childhood cancer cluster investigation (1998–2001) and (2) exposure to volatile organic compound-contamination of drinking water supplies at U.S. Marine Corps Base (USMCB) Camp Lejeune, North Carolina (2003–2015). The Dover Township analysis, which applied a water-distribution system model and developed the novel concept of proportional contribution for an epidemiological study is described in detail in **Appendix D**. The Camp Lejeune analysis, which applied groundwater flow, contaminant fate and transport, and water-distribution system models (in addition to other specialized analysis methods) is described in detail in Section 7.0 of this report. Supporting documentation, including all materials referenced therein, for the Camp Lejeune analysis are provided in **Appendixes E–O** of this report. Listed below are selected sites where the EDRP applied analysis tools to reconstruct (or predict) contaminant concentrations.

- **The Analytical Contaminant Transport Analysis System (ACTS)—Multimedia Environmental Fate and Transport**
  The analytical contaminant transport analysis system (ACTS) is a computational platform designed to assist environmental engineers and health scientists with assessing and quantifying environmental multimedia fate and transport of contaminants within four environmental transport pathways—air, soil, surface water, and groundwater. ACTS was developed by the ATSDR Cooperative Agreement University partner, the Multimedia Environmental Simulations Laboratory (MESL) at the Georgia Institute of Technology (Ga. Tech, Atlanta, GA), and was applied by ATSDR engineers and health scientists to several sites ATSDR was investigating. ACTS contains more than 100 models and associated analytical solutions that are available in the public domain. Analyses can be conducted using a deterministic (single-point) and a probabilistic analysis (two-stage Monte Carlo simulation) to assess the fate and transport of contaminants in multi-pathway environmental assessments. ACTS is a user-friendly computational platform that was released publicly (Aral 1998), described in detail and applied to specific case studies in Maslia and Aral (2004), including: (1) deterministic fate and transport of tetrachloroethylene (PCE) at the North Railroad Avenue Plume site (Española, New Mexico), (2) probabilistic fate and transport of tetrachloroethylene (PCE) in groundwater using two-stage Monte Carlo simulation, and (3) probabilistic multi-pathway environmental fate and transport analysis of ethylene dibromide (EDB) using two-stage Monte Carlo simulation at the Massachusetts Military Reservation, Otis Air Force Base, near Hatchville, Massachusetts.

- **Use of Computational Models to Reconstruct and Predict Trichlorethylene (TCE) Exposure**
  ATSDR evaluates the public threat of hazardous waste sites using environmental and health outcome data and community concerns. For the Gratuity Road Site, located in the town of Groton, Massachusetts, the health assessment indicated onsite and off-site residential contamination of groundwater wells with TCE. Because direct measures of historical TCE were unavailable for the site, computational models were used to reconstruct and predict exposure to TCE. Groundwater flow and contaminant fate and transport models were applied to the site. Using output from these models, inhalation exposure to TCE during showering was estimated using empirical formulas developed from the results of laboratory studies, and these results

were compared with results of estimates of exposure by ingestion. The analyses are described in detail in a peer-reviewed article in the *Journal of Toxicology and Industrial Health* (Maslia et al. 1996).

- **Estimating Exposure to Volatile Organic Compounds (VOCs) using Water-Distribution System Modeling**
  In the 1970s, the groundwater aquifer supplying water to the town of Southington, Connecticut, was contaminated with VOCs thereby potentially exposing the town's residents to VOCs in their drinking water. The Southington water-supply system was characterized by a distribution network that contained more than 1,700 pipeline segments of varying diameters and construction materials, more than 186 miles of pipe, 9 groundwater extraction wells capable of pumping more than 4,700 gallons per minute and 3 municipal reservoirs. For this analysis, we applied a computational model (EPANET) to the water-distribution system to characterize and quantify the distribution of VOCs in the pipelines, from which we estimated the demographic distribution of potential exposure to the town's residents. Results were used to demonstrate that the use of a computational model, such as EPANET (Rossman 1994), allows for a more refined and rigorous methodology with which to estimate census-block-level contamination for exposure assessment and epidemiologic investigations. Details of the analyses are presented in the journal *Archives of Environmental Health* (Aral et al. 1996).

- **Exposure Assessment of Tetrachloroethylene (PCE) Groundwater Contamination Using Analytical and Numerical Models**
  At the Osborn Connecticut Correctional Institution (OCCI), near Somers, Connecticut, PCE from the OCCI dry-cleaning facility contaminated groundwater supplies under the prison and impacted domestic wells in the adjacent Rye Hill Circle neighborhood. Based on water-quality samples on the OCCI property, PCE concentrations ranged from 2,553 μg/L in the glacial till aquifer to 1,860 μg/L in the underlying bedrock aquifer. In residential wells tapping the same bedrock aquifer, PCE concentrations ranged from 545 μg/L to below detection limits (<1 μg/L). Analysis of the site by ATSDR included the use and application of simplified analytical and more complex numerical groundwater flow and contaminate fate and transport models, including parameter uncertainty analysis. The analysis indicated that the wells supplying drinking water to the Rye Hill Circle community were most likely contaminated since their installation, which occurred from 1978 through 1981. Thus, based on the ATSDR historical reconstruction, the citizens of the Rye Hill Circle community were most likely exposed to PCE-contaminated groundwater for 16 years—1978 through 1993, when carbon activated filters were installed on each well. The important lesson that was derived from this study was that the use of simplified one- and two-dimensional fate and transport models in an appropriately simplified hydrogeologic setting yielded meaningful and useful results for the community and state public health officials. Details of the analyses and results are available in the peer-reviewed *Practice Periodical of Hazardous, Toxic, and Radioactive Waste Management* (Maslia et al. 1997), published by the American Society of Civil Engineers.

- **Groundwater Modeling and GIS to Determine Exposure to TCE at Tucson, Arizona**
  ATSDR determined what portion of the city of Tucson, Arizona, received trichloroethylene (TCE)-contaminated drinking water from the Tucson International Airport Area National Priorities List (NPL) site. This study was accomplished by using analytical solutions for two-dimensional contaminant fate and transport in the underlying groundwater systems to

estimate the historical movement of groundwater contamination. The results of the groundwater analysis, the location of the municipal water-supply wells and distribution system, and the U.S. census tract locations were integrated using a geographic information system (GIS). By integrating these disparate databases and information sources using a GIS, ATSDR was able to estimate what portions of the Tucson population were exposed to site-related TCE, how long those people were exposed, and what the range of human exposure may have been. Details of this analysis are presented in American Society of Civil Engineers peer-reviewed *Practice Periodical of Hazardous, Toxic, and Radioactive Waste Management* (Rodenbeck and Maslia 1998).

- **Probabilistic Analysis of Pesticide Transport in Shallow Groundwater at the Oatland Island Education Center, Oatland Island, Georgia**
  The Oatland Island Education Center is located immediately east of Savannah, Georgia. The Center is owned and operated by the Savannah-Chatham County Public Schools as an environmental education facility. The 173-acre facility contains several buildings, wildlife enclosures, and trails. The Communicable Disease Center (now known as the Centers for Disease Control and Prevention [CDC]) and its predecessor agency, the Office of Malaria Control on War Areas, operated the Technical Development Laboratories (TDL) on the site during 1943–1973. In 1974, the U.S. Government deeded the property to the Savannah-Chatham Board of Public Education with the stipulation that the property be used for educational purposes for a period of 30 years. In 1998, school officials discovered a map from 1973 that indicated the location of two onsite disposal areas labeled "Insecticide Burial Area" and "Radioactive Burial Area". ATSDR became involved with the Oatland Island site at the request of the CDC Office of Health and Safety (OHS) to evaluate potential public health impacts associated with pesticide contamination at the site. The Insecticide Burial Area, designated as Area A, was the focus of the analysis by ATSDR's Exposure-Dose Reconstruction Program.

  ATSDR applied the analytical contaminant transport analysis system (ACTS, Maslia and Aral, 2004), to examine the fate and transport of organochlorine pesticides in shallow groundwater at the Oatland Island Education Center, Oatland Island, Georgia. Specific objectives included: (1) estimating the probability of affecting coastal wetlands located 800 feet (ft) downgradient of the pesticide source area, and (2) developing reference tools (probabilistic type curves) for evaluating future groundwater monitoring results at key site monitoring wells.

  Deterministic (single-point) modeling results were in good agreement with measured data from the Oatland Island site. Deterministic simulations using calibrated, single-value input parameters indicate the contaminant plume will not affect the wetlands. Probabilistic results derived by conducting a two-stage Monte Carlo analysis using 10,000 realizations for eight different input parameters indicated that the probability of exceeding the detection limit of 0.044 μg/L total benzene hexachloride (BHC, also known as HCH, hexachlorocyclohexane) in groundwater at the wetlands boundary increases from 1% during 2000 to a maximum of 13% during 2065. This represents an 87% confidence level that the wetlands will not be affected in the future by pesticide migration from Area A. Details of the ATSDR analysis are presented in a peer-reviewed ATSDR report available on the ATSDR websites (Anderson et al. 2007).

- **Modeling Indoor Air Quality from Formaldehyde Emissions of Chinese-Manufactured Laminate Flooring Products**
  In a letter dated March 4, 2015, Senator Bill Nelson (Florida) requested that the Consumer Product Safety Commission (CPSC) determine if Chinese-manufactured laminate flooring products— specifically products from Lumber Liquidators® as seen on the television program 60 Minutes—present an unreasonable risk to consumers. In response to Senator Nelson's letter, the CPSC requested ATSDR's assistance in estimating indoor air formaldehyde (HCOH) concentrations in homes containing the Chinese-manufactured laminate flooring products sold by Lumber Liquidators®. The EDRP conducted data analyses and modeled (simulated) indoor air HCOH. To accomplish this, the EDRP used an analytical model coupled with probabilistic analyses (Monte Carlo simulation) to estimate the range of possible indoor air HCOH concentrations in a residential setting. In this analysis, the mathematical model for a room is referred to as a "*well-mixed room model with a constant emission rate*" (IHMod 2015). Details of ATSDR's EDRP analyses are described in a Centers for Disease Control and Prevention (CDC)/National Centers for Environmental Health (NCEH)/ATSDR report (CDC/NECH/ATSDR 2016).

3.0 Awards

Throughout my career, I have been honored by my peers and professional organizations with awards recognizing the high level of research that I have conducted. A complete list of awards is provided in my CV (**Appendix A**). Listed below are the most notable.

- **American Academy of Environmental Engineers and Scientists (AAEES)**, 2015 Excellence in Environmental Engineering Award, Grand Prize, Research Category, April 2015: "*Using Environmental Engineering Tools, Scientific Analyses and Epidemiological Studies to quantify Human Exposure to Contaminated Drinking Water and to Benefit Public Health*."
- **American Society of Civil Engineers (ASCE)**, 2011 James R. Croes Medal, for the paper, "*Optimal Design of Sensor Placement in Water Distribution Networks*," Journal of Water Resources Planning and Management, January-February 2010.
- **U.S. Public Health Service Engineering Literary Award (Publications Category)**, 2005, for the publication, "*Analytical Contaminant Transport Analysis System (ACTS)—Multimedia Environmental Fate and Transport*".
- **American Academy of Environmental Engineers (AAEE),** 2003 Excellence in Environmental Engineering Award, Grand Prize, Research Category, April 2003: "*Enhancing Environmental Engineering Science to Benefit Public Health, Dover Township, Ocean County, New Jersey*"
- **Cumming Award, American Society of Military Engineers**, 2000, to the Dover Township Water-Distribution System Modeling Team.
- **American Society of Civil Engineers (ASCE)**, 2001, Best Practice-Oriented Paper of 2000 for the paper, *"Using Water-Distribution System Modeling to Assist Epidemiologic Investigations,"* ASCE Journal of Water Resources Planning and Management, Vol. 126, July/August 2000.

4.0 Professional Registration and Certifications

- Registered Professional Engineer (GA), #PE012689 (active)
- Certified Ground Water Professional, National Ground Water Association #115205
- Diplomate, American Academy of Water Resources Engineers, D.WRE #00066
- Diplomate, American Academy of Environmental Engineers & Scientists, DEE #00-20013

5.0 Scope of Work

I was retained by the Bell Legal Group in July 2022 on behalf of the *Camp Lejeune Water Litigation* Plaintiffs to consult and testify regarding the methodology and results of ATSDR's historical reconstruction study at USMCB Camp Lejeune and other associated facts, which estimated the locations and concentrations of contaminants in finished water[2] at the Base from 1953 to 1987. Specifically, I was tasked with the following:

1. Provide a high-level explanation of the ATSDR's historical reconstruction process for the Tarawa Terrace (TT), Hadnot Point (HP), and Holcomb Boulevard (HB) study sites, including my and other team members involvement in same for which I supervised.
2. Provide an explanation of measured and reconstructed (simulated) concentrations of contaminants in finished water at Camp Lejeune for the periods of 1951–1987 for TT, 1942–2008 for HP, and 1972–1985 for HB.
3. Provide an explanation of the calibration, sensitivity analysis, and probabilistic uncertainty analysis techniques for each of the models.
4. Summarize the conclusions and opinions included in the published ATSDR Reports for the study areas, as well as review, analysis and conclusions of the National Academy of Sciences 2009 NRC Report and its evolvement and committee activities for which I have knowledge and opinions.
5. Provide additional opinions beyond those already included in the ATSDR published works.

I am being compensated at an hourly rate of $400 for my work preparing this report. My rate for depositions and trial testimony is $2,000 per day.

6.0 Summary of Opinions

Based on the analysis presented in this report, my decades of expertise in environmental analysis and water modeling, and the 11 years I spent working on and overseeing ATSDR's historical reconstruction of contamination at Camp Lejeune, I have reached the following opinions within reasonable scientific and engineering certainty:

1. The models and techniques used by the ATSDR to determine the mean monthly concentrations of contaminants in finished water at Camp Lejeune were state of the art, consistent with standard practices in the field, and subject to peer review.

[2] For the ATSDR study and in this report, finished water is groundwater that has undergone treatment at a water treatment plant and subsequently is delivered to a family housing unit or other facility—also referred to as drinking water, finished drinking water, potable water, or tap water.

2. The model results show reconstructed finished water at Camp Lejeune was contaminated with varying levels of tetrachloroethylene (PCE), trichloroethylene (TCE), *trans*-1,2-dichloroethylene (1,2-tDCE), vinyl chloride (VC), and benzene. For TT, finished water was primarily contaminated with PCE and its degradation by-products TCE, 1,2-tDCE, and VC for the period 1953–1987. For HP, finished water was primarily contaminated with TCE, PCE and is by-degradation products, and benzene for the period 1953–1996. For HB, finished water was primarily contaminated with TCE from the HP water-distribution system for the period 1972–1985.

3. The reconstructed (simulated) monthly mean concentrations of PCE, TCE, 1,2-tDCE, VC, and benzene at TT, HP and HB are contained in ATSDR report appendices A2 for TT[3], A3 and A7 for HP[4], and A8 for HB[5]. These reconstructed monthly mean concentrations are also included in this report in **Appendixes H, I, J and K**, are reliable, and represent, within reasonable scientific and engineering certainty, the contaminant levels in selected water-supply wells and in finished water at Camp Lejeune from 1953 to 1996.

4. A water-modeling approach is a reliable and generally accepted method of reconstructing historical contamination in groundwater and water-distribution systems.

5. The analyses published in all ATSDR chapter reports, supplemental reports, supplemental information and scientific journal publications regarding Camp Lejeune, including the conclusions and monthly concentration data, were all done applying proper scientific methodologies that are generally accepted and remain to this day to be reliable, true and correct.

6. Any concerns or criticisms about whether the ATSDR Tarawa Terrace and Handot Point-Holcomb Boulevard models have been "validated" (e.g., August 6, 2024, deposition of D. Waddill; June 19, 2008, Department of the Navy (DON) letter to ATSDR on assessment of ATSDR water-modeling at Tarwa Terrace (**Appendix L**) are misplaced, inappropriate, and scientifically indefensible.

7. The opinions and conclusions expressed in the National Research Council's report on contaminated water-supplies at Camp Lejeune (NRC 2009) cannot be considered an authoritative interpretation or guidance document related to the historical exposure assessment of contaminated drinking water at Camp Lejeune because: (1) they are based on incomplete and missing information (even though ATSDR offered to provide such information to the NRC Committee Executive Secretary), (2) contains many errors and misrepresentations with respect to the findings of the ATSDR water-modeling analyses and (3) conclusions and recommendations contained in the NRC report are at such odds with recommendations rendered by several review panels consisting of national and international experts in water modeling and epidemiology (see **Appendix M** for ATSDR's response to NRC report).

[3] ATSDR's Tarawa Terrace Chapter A report, Appendix A2 (Maslia et al. 2007).
[4] ATSDR's Hadnot Point-Holcomb Boulevard Chapter A report, Appendixes A3 and A7 (Maslia et al. 2013).
[5] ATSDR's Hadnot Point-Holcomb Boulevard Chapter A report, Appendix A8 (Maslia et al. 2013).

8. The opinions discussed in issue number 5 (September-October) of the 2010 *Ground Water* journal published article, "*Complexities in Hindcasting Models-When Should We Say Enough is Enough?*" by author T. P. Clement (2010), are lacking in detail on several key issues with respect to ATSDR's modeling approaches and methods, the physics of contaminant transport in the subsurface, and ATSDR policies for the review and dissemination of data and reports. I submitted an editorial response to the article , which was published in issue number 1 (January-February) of the 2012 *Ground Water* journal. A copy of my editorial response (Maslia et al. 2012) is provided in **Appendix N** of this report.

9. I have read and reviewed the report, "Tarawa Terrace Flow and Transport Model Post-Audit," by N.L. Jones and R.J. Davis (2024, **Appendix O**). They applied acceptable scientific principles, groundwater-flow and contaminant fate and transport methods.

I have reviewed and relied on published literature, data and documents made available to me while consulting on this case and during my work on the Camp Lejeune studies as an employee of ATSDR. The materials I have considered include the literature identified in the references section of this report, as well as the documents listed in **Appendix P** of this report. Most of these materials, documents, and data are also listed in the publicly available ATSDR HP-HB Chapter A report, Appendix A2 (Maslia et al. 2013).

7.0 U.S. Marine Corps Base Camp Lejeune, North Carolina: Reconstructing Volatile Organic Compound Contamination of Drinking-Water Supplies[6]

The Agency for Toxic Substances and Disease Registry (ATSDR), a U.S. government health agency, conducted epidemiological studies to evaluate whether exposures to drinking water contaminated with volatile organic compounds (VOC) at USMCB Camp Lejeune, North Carolina, were associated with increased health risks to children and adults. These health studies required knowledge of contaminant concentrations in finished water—*at monthly intervals*—delivered to family housing, barracks, and other facilities within the study area. Because concentration data were limited or unavailable during much of the period of contamination (1950s–1987), the historical reconstruction process, which included substantial efforts in information gathering and data mining, water-modeling methods, and sensitivity and probabilistic uncertainty analyses, was used to estimate mean monthly contaminant-specific concentrations. These methods and analyses included *linking materials mass balance (mixing) and water-distribution system models to groundwater-flow and contaminant fate and transport models* to derive and quantify monthly mean concentrations and ranges of concentrations of contaminants of interest to the ATSDR epidemiological studies (PCE, TCE, *1,2*-tDCE, VC, and benzene).

[6] This section of the expert report refers to figures and tables contained within this report and figures and tables contained in ATSDR reports (e.g., Maslia et al. 2007, 2013, Faye 2008). Figures and tables in this report section begin with the number **7** and are numbered sequentially (e.g., Figure 7.1, Figure 7.2; Table 7.1, Table 7.2). Figures and tables that begin with the letter "**A**" (e.g., Figure A12, Table A4), refer to the ATSDR Chapter A reports (Maslia et al. 2007, 2013).

7.1 Introduction

As project manager I utilized both internal expertise at the ATSDR and brought in outside experts to create a multidisciplinary team with the required skill set to conduct the historical reconstruction analysis for the TT and HP-HB study areas. This team consisted of over 20 individuals that encompassed expertise in a variety of scientific and engineering disciplines, and spans every area and specialty involved in water modeling. Table 2.1 (previously discussed in Section 2.0 above) lists team members and organizations; **Appendix B** provides detailed information on each team member, including their organization and technical/scientific areas of expertise for the ATSDR Water Modeling Team.

Many years of effort have gone into ATSDR's drinking-water exposure and health studies at USMCB Camp Lejeune resulting in numerous agency reports and published papers. Owing to brevity, this section summarizes these efforts, reports, and papers into a synthesis of the overall approach to, and results from, the historical contaminant reconstruction study.

With respect to the three housing areas, barracks, and workplaces of interest to the ATSDR drinking-water exposure and health studies—Tarawa Terrace (TT), Hadnot Point (HP), and Holcomb Boulevard (HB) (Figure 7.1)—TT results are published as a series of externally peer-reviewed ATSDR reports that are summarized in the Tarawa Terrace Chapter A Report (Summary of Findings) by Maslia et al. (2007). TT results are also published in a peer-reviewed journal article (Maslia et al. 2009a). Approaches, methods, and results for the HP-HB areas are published as a series of externally peer reviewed ATSDR reports that are summarized in the HP-HB Chapter A Report (Summary of Findings) by Maslia et al. (2013). HP-HB results are also published in a peer-reviewed journal article (Maslia et al. 2016). The ATSDR reports contain very specific details for the TT, HP, and HB drinking-water analyses. Each summary report (Maslia et al. 2007, 2013) provides references to and descriptions of additional detailed ATSDR reports on the application of the historical reconstruction process to quantify historical drinking-water contamination from VOCs at USMCB Camp Lejeune, North Carolina.

Results show that at the TT water treatment plant (TTWTP) reconstructed (simulated) PCE concentrations reached a maximum monthly average value of 183 micrograms per liter (µg/L) compared to a one-time maximum measured value of 215 µg/L and exceeded USEPA's current maximum contaminant level (MCL) of 5 µg/L during the period November 1957–February 1987. At the HP water treatment plant (HPWTP), reconstructed TCE concentrations reached a maximum monthly average value of 783 µg/L compared to a one-time maximum measured value of 1,400 µg/L during the period August 1953–December 1984. The HPWTP also provided contaminated drinking water to the HB housing area continuously prior to June 1972, when the HB water treatment plant (HBWTP) came online (maximum reconstructed TCE concentration of 32 µg/L) and then intermittently during the period June 1972–February 1985 (maximum reconstructed TCE concentration of 66 µg/L). Drinking-water concentrations at the TTWTP and HPWTP for PCE, TCE, 1,2-tDCE, and VC and benzene were also reconstructed. **Appendixes H, J, and K** contain TT, HP, and HB, respectively, reconstructed mean monthly contaminant-specific concentration data in tabular form. **Appendix I** contains reconstructed monthly mean concentrations for selected HP-HB water-supply wells.

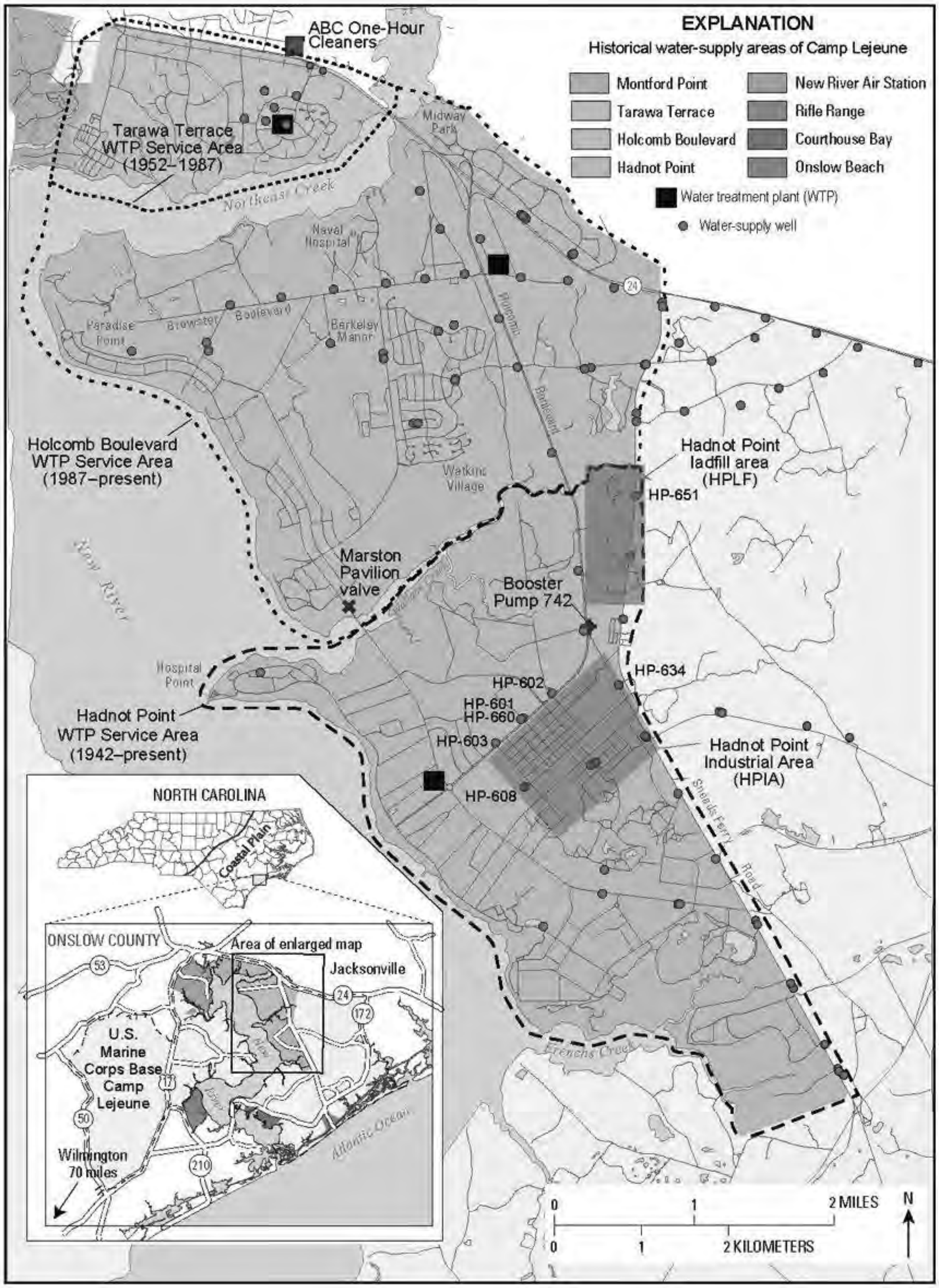


Figure 7.1. Water-supply areas with focus on housing areas, barracks, and workplaces included in the Agency for Toxic Substances and Disease Registry (ATSDR) drinking-water exposure and health studies, U.S. Marine Corps Base Camp Lejeune, North Carolina (Maslia et al. 2013, 2016).

7.2 Water Supply and Contamination at Camp Lejeune

USMCB Camp Lejeune is in the Coastal Plain of North Carolina, in Onslow County, southeast of the City of Jacksonville and about 70 miles northeast of the City of Wilmington, North Carolina. In general, the study area is bounded to the north by North Carolina Highway 24 (SR 24), to the west by New River, to the south by Frenchs Creek, and generally to the east by the drainage divides of upstream tributaries of Wallace and Frenchs Creeks. Northeast Creek separates the TT base housing area from the HP and HB base housing areas (Figure 7.1).

Groundwater is the sole source of water supply for USMCB Camp Lejeune. Eight water-distribution systems have supplied or currently (2024) supply drinking water to family housing, barracks, workplaces, and other facilities at USMCB Camp Lejeune. The three water-distribution systems of interest to the ATSDR health studies–TT, HP, and HB (Figure 7.1)–have historically supplied finished water to most family housing units, enlisted personnel barracks, and workplaces at the base. ATSDR documented information and aggregated data related to water-supply chronology within the study areas of Camp Lejeune. Details pertinent to water-supply well operations (e.g., construction, in-service, and out-of-service dates) and WTP operations are provided in Maslia et al. (2007, 2013).

HP was the original water-distribution system, serving the entire base with drinking water beginning in the early 1940s. The HPWTP was constructed and began operations likely during 1941–1942. The TTWTP began delivering drinking water during 1952–1953, and the HBWTP began delivering drinking water during June 1972 (Table 7.1). Currently (2024), the HPWTP services the HP area, and the HBWTP services the HB and TT base housing areas because the TTWTP was shut down during 1987 due to contamination of several supply wells (Table 7.1).

The HB water-distribution system is connected to the HP water-distribution system at the Marston Pavilion valve and at booster pump 742 (Figure 7.1). Booster pump 742 was removed during 2007, but the two systems can still be interconnected by opening a valve at the same location. For operational reasons, the two water-distribution systems are rarely connected—exceptions being some documented (and undocumented) intermittent connections that occurred during late spring and summer months of 1972–1986 and a continuous 8-day period of 28 January–4 February 1985 (Maslia et al. 2013, 2016) (refer to Camp Lejeune Water documents [CLW] 6774–8761, 8109, and 8117 [CLW, 2007]).

Operational chronologies for water-supply wells in the TT, HP, and HB study areas during the period 1942–2008 are provided in Figures 7.2 and 7.3. These graphs show dates of operation for each well that supplied raw water to the TTWTP, HPWTP, and HBWTP, the dates when some of the wells were permanently taken out of service, and wells with documented contamination. The water-supply well historical operations graph and chronology table for TT are shown below as Figure 7.2. For HP-HB, Figure 7.3 shows water-supply well operations and chronologies graphically. Note, TT had a total of 16 water-supply wells whereas HP-HB had nearly 100 water-supply wells.

Table 7.1. Chronology of selected events related to water supply and environmental contamination at U.S. Marine Corps Base Camp Lejeune, North Carolina, and vicinity. [#, *]

Event	Date or approximate date
Hadnot Point water treatment plant (WTP) comes online	1941–42
Tarawa Terrace WTP comes online	1952–53
Holcomb Boulevard WTP comes online	June 1972
Several Tarawa Terrace and Hadnot Point water-supply wells shut down due to documented volatile organic compound (VOC) contamination	November 1984–February 1985
Marston Pavilion interconnection valve opened and booster pump 742 continuously operated for eight days (because of shut down of Holcomb Boulevard WTP) to augment Holcomb Boulevard drinking-water supply with contaminated Hadnot Point drinking water	January 27–February 4, 1985
Holcomb Boulevard WTP expanded to provide water to Tarawa Terrace and Camp Johnson water-distribution system areas	1987
Tarawa Terrace WTP and remaining operating supply wells shut down and taken out of service	March 1987
ABC One-Hour Cleaners placed on the USEPA's National Priorities List (NPL) of contaminated sites	March 1989
USMCB Camp Lejeune placed on the USEPA's NPL of contaminated sites	October 1989

[#]Refer to Maslia et al. (2007, 2009a, 2013, and 2016) for details
[*]See Figure 7.1 for location of water-supply areas.

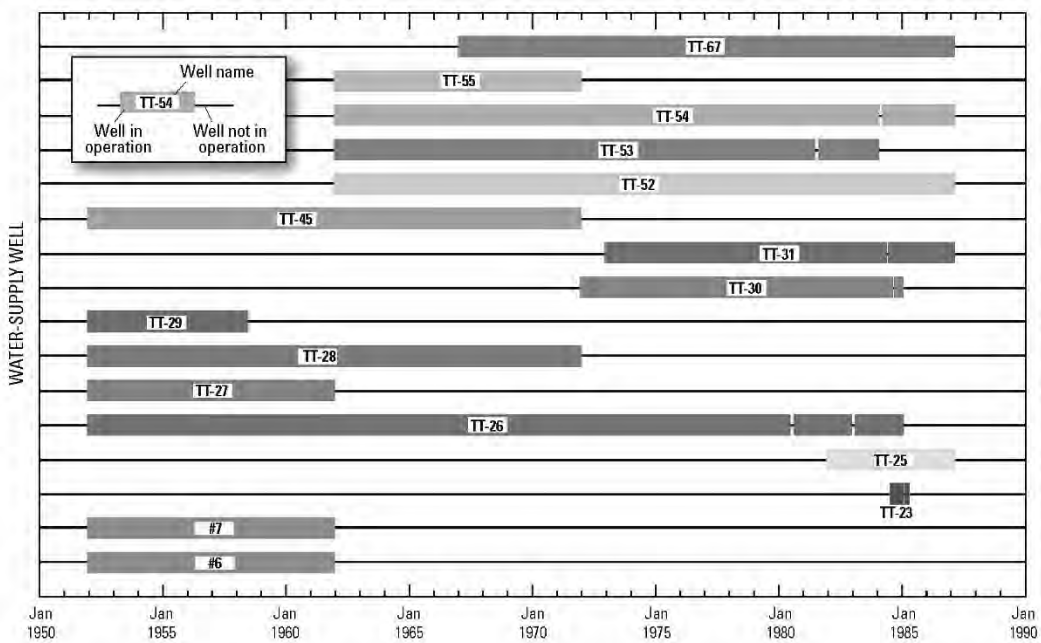


Figure A5. Historical operations of water-supply wells, 1952–87, Tarawa Terrace and vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina.

Table A6. Historical operations for water-supply wells, 1952–1987, Tarawa Terrace and vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina.[1]

[—, not applicable]

Well identification	In service	Off-line	Service terminated
#6	January 1952	—	January 1962
#7	January 1952	—	January 1962
TT-23	August 1984	February 1985	May 1985
TT-25	January 1982	—	March 1987
TT-26	January 1952	July–August 1980; January–February 1983	February 1985
TT-27	January 1952	—	January 1962
TT-28	January 1952	—	January 1972
TT-29	January 1952	—	July 1958
TT-30	January 1972	September 1984	February 1985
TT-31	January 1973	June 1984	March 1987
TT-45	January 1952	—	January 1972
TT-52	January 1962	March 1986	March 1987
TT-53	January 1962	July–August 1981	February 1984
TT-54	January 1962	February–March 1984	March 1987
TT-55	January 1962	—	January 1972
TT-67	January 1967	—	March 1987

[1]Refer to the Chapter C report (Faye and Valenzuela In press 2007) for additional details

Figure 7.2. Operational chronologies of Tarawa Terrace water-supply wells, Tarawa Terrace study area, 1952–1987 (Maslia et al. 2007).

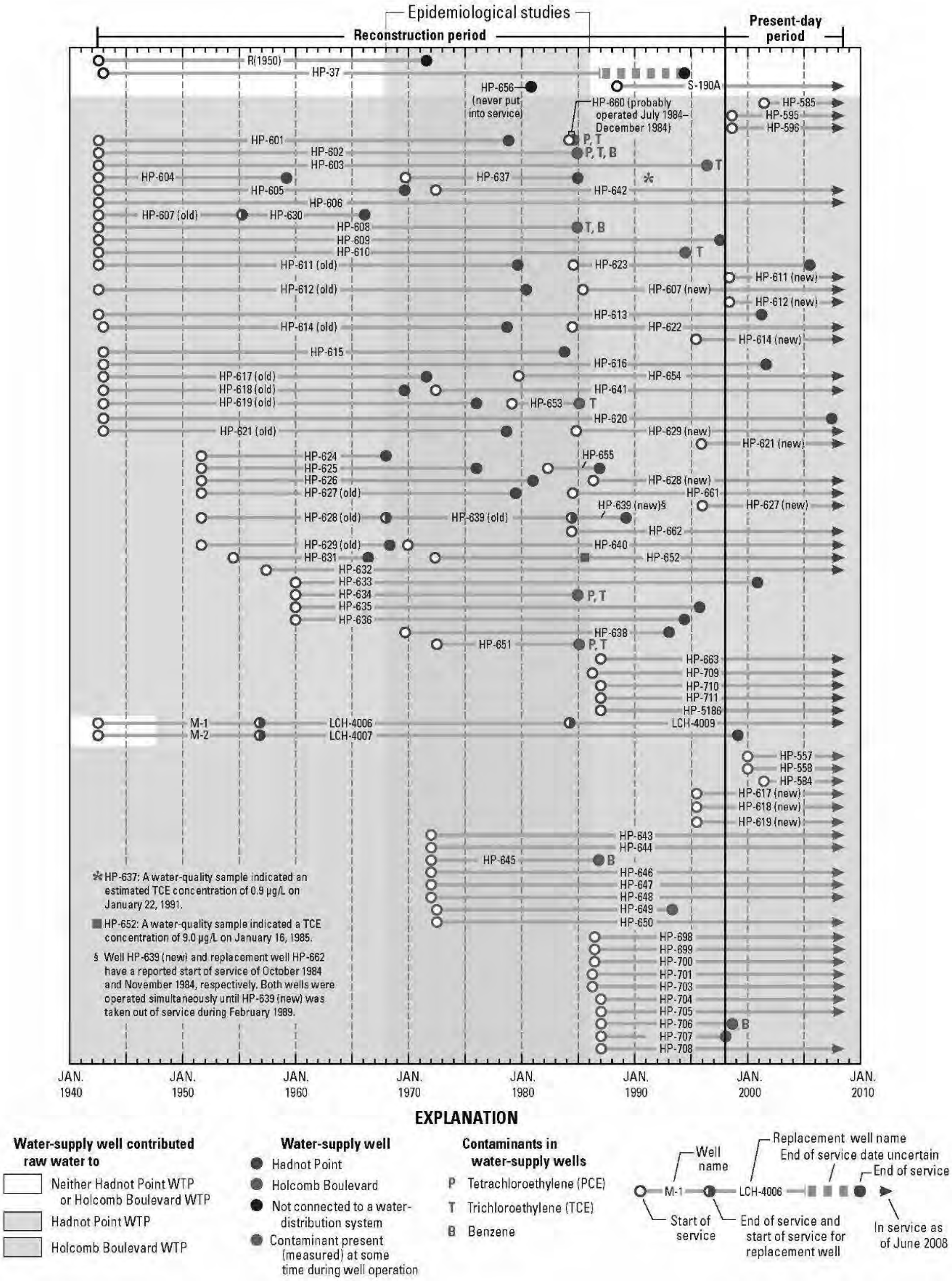


Figure 7.3. Operational chronology of Hadnot Point and Holcomb Boulevard water-supply wells, Hadnot Point-Holcomb Boulevard study area (Maslia et al. 2013).

During the early 1980s, high concentrations of VOCs were discovered in groundwater and drinking water serving some areas at Camp Lejeune. Within the TTWTP service area, groundwater was contaminated mostly with PCE and its degradation products. An off-base dry-cleaning facility (ABC One-Hour Dry Cleaners—Figure 7.1) was identified as being responsible for contaminating several on-base water-supply wells at Tarawa Terrace (Maslia et al. 2007, 2009a). Within the HPWTP service area, groundwater was contaminated mostly with TCE, as well as PCE and refined petroleum products, such as BTEX compounds. Historical base operations and lack of environmentally protective disposal practices at Camp Lejeune have been identified as being responsible for contamination of groundwater and drinking-water supplies within the HPWTP service area (Faye et al. 2010, 2012). Within the HBWTP service area, drinking water remained predominantly uncontaminated except for intermittent supply during spring and summer months of contaminated HP water during years 1972–1985. Maximum measured concentrations of selected contaminants within the study areas have been documented as follows (CLW 2007, Maslia et al. 2007, 2013, Faye et al. 2010, 2012):

- 18,900 μg/L of TCE in an HPWTP supply well (May 1985),
- 1,400 μg/L of TCE in finished water at the HPWTP (May 1982),
- 380 μg/L and 720 μg/L of benzene in a HPWTP supply well (July and December 1984, respectively),
- 215 μg/L of PCE in finished water at the TTWTP (February 1985), and
- 1,580 μg/L of PCE in a TTWTP supply well (January 1985).

In 1989, USMCB Camp Lejeune and ABC One-Hour Cleaners (an offsite dry-cleaning facility, Figure 7.1) were placed on the USEPA's National Priorities List (NPL) of hazardous waste sites. ATSDR is required to gather information and data to assess human health impacts from exposures at NPL sites. Because of the potential exposures to high VOC concentrations, ATSDR began health studies in 1995 to evaluate effects of exposure to contaminated drinking water.

7.3 Water-Modeling and Study Objectives

When ATSDR health study epidemiologists requested scientific and technical support from the Exposure-Dose Reconstruction Program, they presented a list of five objectives and questions that they wanted to achieve and to answer. These five objectives and questions were originally presented at a meeting held on October 8, 2003, at ATSDR Headquarters in Chamblee, Georgia, with attendance by ATSDR (staff, Management, and Leadership), U.S. Marine Corps (Camp Lejeune and Headquarters staff), DON, Naval Facilities Engineering Command (NAVFAC) staff, the ATSDR University Partner, and contractors. The five study objectives and questions are listed below.

- **Objective 1:** What chemical compounds contaminated the drinking water and where did they come from (*determine sources of contaminants*)?
- **Objective 2:** When did contaminated groundwater reach water-supply wells and what was the duration of the contamination (*determine arrival dates*)?
- **Objective 3:** What were the *mean monthly* drinking-water *concentrations*?

- **Objective 4:** How was contaminated water distributed to housing areas (*quantify and identify water transfers*)?
- **Objective 5:** What were the ranges of concentration values (based on modeling results) for a specific month (*conduct sensitivity and uncertainty analysis*)?

These objectives and questions were successfully achieved and answered for the TT, HP, and HB study areas based on applying the historical reconstruction process for water-modeling analyses. They are described in detail in externally peer-reviewed ATSDR reports (Maslia et al. 2007, 2013) and peer-reviewed scientific journals (Maslia et al. 2009a, 2016).

The ATSDR water-modeling analyses and epidemiological studies were guided by recommendations contained in the 1990 ABC One-Hour Dry Cleaner and 1997 USMCB Camp Lejeune Public Health Assessments. Therefore, only VOCs (PCE, TCE, 1,2-tDCE, VC, and BTEX compounds) and VOC contamination of finished water supplies at the three housing areas (TT, HP, and HB), barracks, and workplaces of interest to the ATSDR drinking-water exposure and health studies at Camp Lejeune were studied.

7.4 Historical Reconstruction Methods

When direct, past knowledge of contaminant concentrations in drinking water is limited or data are unavailable, historical reconstruction methods can be used to provide estimates of contaminant concentrations. The process of historical reconstruction is an accepted methodology. Sahmel et al. (2010) provide a review of more than 400 papers in exposure reconstruction for substances of interest to human health. Water modeling (e.g., contaminant fate and transport and water-distribution systems analysis) is an accepted method to reconstruct (or predict) contaminants delivered through water systems. Examples of historical reconstruction applied to different sites are found in Grayman et al. (2004, Chapter 10). They provide summaries of successful and accepted historical reconstruction applied to Gideon, Missouri; Walkerton, Ontario; Dover Township (Toms River), New Jersey; and Redlands, California. Historical reconstruction includes information gathering and data mining activities and the application of simulation tools, such as models, to re-create or represent past conditions There are numerous examples demonstrating this including Costas et al. (2002), Grayman et al. (2004), Kopecky et al. (2004), McLaren/Hart-ChemRisk (2000), Maslia et al. (2000b, 2001, 2005, 2007, 2009a, 2013, 2016), Reif et al. (2003), Rodenbeck and Maslia (1998), and Samhel et al. (2010). For ATSDR's drinking-water exposure analyses at Camp Lejeune, methods included linking materials mass balance (mixing) and water-distribution system models to groundwater-flow and contaminant fate and transport models.

7.4.1 Overview

The generalized five-step process used to identify information sources, extract usable model-specific data, and develop, apply, and calibrate models to reconstruct historical contaminant-specific concentrations in drinking water at USMCB Camp Lejeune is shown in Figure 7.4. By its very nature, historical reconstruction is an *iterative* process. The five-steps of the process are:

(1) review information sources,

(2) extract information and data and develop databases,

(3) develop, simulate, and calibrate models,

(4) determine if model conceptualization or calibration issues exist, and if they do, use subject matter experts to iteratively refine model databases and search for additional information sources, and

(5) assess when sufficient agreement exists between water-level, groundwater contaminant concentration, and water treatment plant concentration data (historical and present-day) and model results.

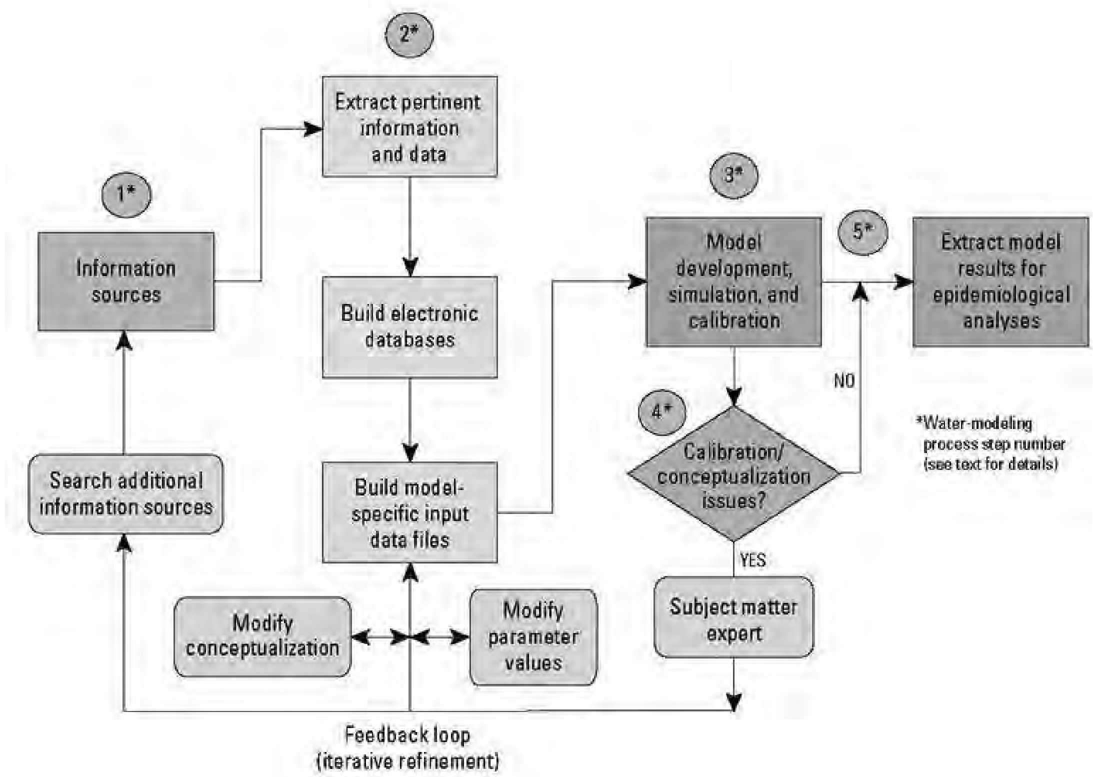


Figure 7.4. A generalized process of identifying information, extracting usable model-specific data, and applying models to reconstruct historical drinking-water contaminant-specific concentrations (Maslia et al. 2013, 2016).

After satisfactory completion of these five steps, historical contaminant concentration simulation results were extracted from model-output databases and provided to ATSDR epidemiologists for use in the Camp Lejeune epidemiological analyses (Bove et al. 2014a, b; Ruckart et al. 2013, 2014, 2015). It is important to note that throughout the historical reconstruction process, **data analysts and water modelers were blinded to the health outcome status** of individuals included in the epidemiological studies.

7.4.2 Information and Data Discovery

Substantial effort and resources were dedicated to the task of identifying information sources and extracting data because of the voluminous and disparate sources of information and data pertinent to the study area (**Appendix E** of this report and in Maslia et al. 2013, Appendix A2). The purpose was to obtain information and data that could be extracted and transformed into digital databases to conduct historical reconstruction analyses using a modeling approach. By its very nature, information discovery and data mining are not an exact process that can be used or relied upon to identify a single, specific piece of information or data point. Numerous information sources were identified, located, and assessed prior to extracting usable model-specific data. Once pertinent model-specific data were identified and extracted, they had to be entered into digital databases. Computer model-specific input databases were then developed from these digital databases. A list of information and data sources used to develop model-input databases for the TT, HP, and HB study areas is provided in **Appendix E**.

Information and data discovery is an iterative process with ATSDR requesting information and data from Camp Lejeune and DON. At times, this process became a contentious issue but was eventually resolved. However, the consequences and impacts on project timelines and completion dates were delays and needs for increased resources for data extraction and processing required for model calibration and completing the water-modeling analyses. Three examples are noteworthy:

1. Based on discussions of the 2005 ATSDR Expert Peer Review Panel evaluating ATSDR's water-modeling activities at Camp Lejeune (Maslia 2005), panel members recommended that ATSDR put additional effort and resources into conducting more rigorous data discovery activities. DON brought in a contractor, Booz-Allen-Hamilton (BAH), to search for information and documents in buildings throughout Camp Lejeune. This activity began with a "kick-off" meeting during November 2005. The results of the BAH effort provided the USMC and DON with a document referred to as the "Marine Corps Base Camp Lejeune Consolidated Repository Index (4-27-2009)," which was approximately 514 pages long, that ATSDR staff, contractors, and subject matter experts searched in April 2009 and thereafter.

2. During March 2009, an ATSDR subcontractor discovered through a series of email exchanges with Camp Lejeune staff, a password protected portal containing more than 1,530 folders and files pertinent to underground storage tank (UST) information (**Appendix E**). Identifying the existence of this portal (containing pertinent information needed by ATSDR), although known to Camp Lejeune beginning July 2003, was not communicated to ATSDR until March 2009. The consequences of finding out about the UST portal resulted in ATSDR devoting additional time and resources to developing an additional chapter report for the HP-HB study area on above ground and underground storage tank information and data (Chapter D of the HP-HB report series [Faye et al. 2012];).

3. As a result of ongoing information and data needs for ATSDR's water-modeling activities, Camp Lejeune leadership (civilian and military) recognized the need to document and provide ATSDR with a comprehensive catalogue of all information and data sources known

or unknown to USMC, NAVFAC, DON and DON contractors. Therefore, on June 30, 2010, an initial meeting of the "DON-ATSDR Camp Lejeune Data Mining Technical Workgroup" was held in Washington, DC. The charge of the workgroup was:

a. Develop a plan to ensure that ATSDR possesses all relevant data and information needed for their health activities. This includes information and data possessed by current DON contractors. All reasonable efforts will be made to ensure that ATSDR possesses all relevant data and information possessed by former contractors and other federal and state agencies.

b. Implement the plan to ensure ATSDR possesses all relevant data and information needed for their health activities.

c. Complete the data mining phase that must be done prior to the historical dose reconstruction modeling and epidemiological phases of the health activities.

The DON-ATSDR Camp Lejeune Data Mining Technical Workgroup completed its task and issued a final report on November 27, 2012. Much of the information and information sources listed in **Appendix E** of this report is a result of the effort of the DON-ATSDR Camp Lejeune Data Mining Technical Workgroup.

Most of the information sources listed in **Appendix E** were not in readily usable digital format that could be directly used for developing input databases for modeling. Rather, a time-consuming process was required to extract pertinent and usable information. This process consisted of determining potentially pertinent documents and information, reviewing pertinent documents, manually extracting data (in most cases), and then entering these data into digital databases. A generalized three-stage process was developed for reviewing, assessing, and extracting information and data. This process is shown in Figure 7.5 and is described below.

- *Stage 1*: A cursory review was conducted to determine if a particular source of information or data referred to the TT, HP, or HB study areas; if not, the information source or data was noted and not reviewed,

- *Stage 2*: Information sources and data pertinent to the study areas were filtered by content and subject matter (e.g., remedial investigation, lab analysis). Depending on the content and subject matter, certain files were not reviewed in detail (e.g., meeting notes), whereas other files were promoted to a stage 3 review (e.g., site characterization data, laboratory analyses, groundwater-level data), and

- *Stage 3*: If a file contained certain key words or dates (e.g., water supply, VOC, benzene, underground storage tank, TT-26, HP-651, WTP), it was reviewed in detail by subject matter experts. Pertinent information and data were identified, and contract staff extracted the information and data and entered it into digital databases. Then, data were extracted from the digital databases and appropriate model-input databases were prepared. It is important to note, however, that even with the three-stage review process, because of the volume of information, not every document was reviewed, nor was every page of every document reviewed unless such a review was determined to be critical to extracting information and data pertinent to the historical reconstruction process and specifically to computer model-specific input database development. For example, daily water-supply well operational data available during 1999–2008 consisted of 10,000 pages of pertinent information, all of which were reviewed, evaluated, and transcribed to digital data (**Appendix E**).

7.4.3 Water-Modeling Approach and Simulation Tools

The water-modeling approach used to reconstruct historical drinking-water concentrations at the TTWTP and HPWTP and within the HB water-distribution system is shown as a flowchart (Figure 7.6). The modeling required four steps: characterizing (1) the subsurface contamination sources, (2) the groundwater flow under natural (pre-development) and pumping conditions, (3) contaminant migration influenced by the groundwater flow as well as other transformation processes (e.g., adsorption, degradation), and (4) the mixing of contaminants from pumping wells at the WTP and within the distribution system and delivery to the housing areas, barracks, and other buildings. The analyses and simulation tools used as part of the historical reconstruction process for TT, HP and HB included: (1) geohydrologic analyses; (2) water-distribution system field testing; (3) water-level data to characterize groundwater flow; (4) groundwater-flow and contaminant fate and transport models (for dissolved and light nonaqueous-phase liquid [LNAPL] constituents); (5) parameter sensitivity and uncertainty analyses; (6) probabilistic Markov analyses; and (7) water-distribution system modeling. Detailed descriptions of each analysis and simulation tool, the type of analysis (e.g., data, interpretation, or simulation) and supporting references are provided in Maslia et al. (2007, 2013). Details of the groundwater-flow and contaminant fate and transport models are provided in Maslia et al. (2007, 2009a, 2013, 2016) and associated reports.

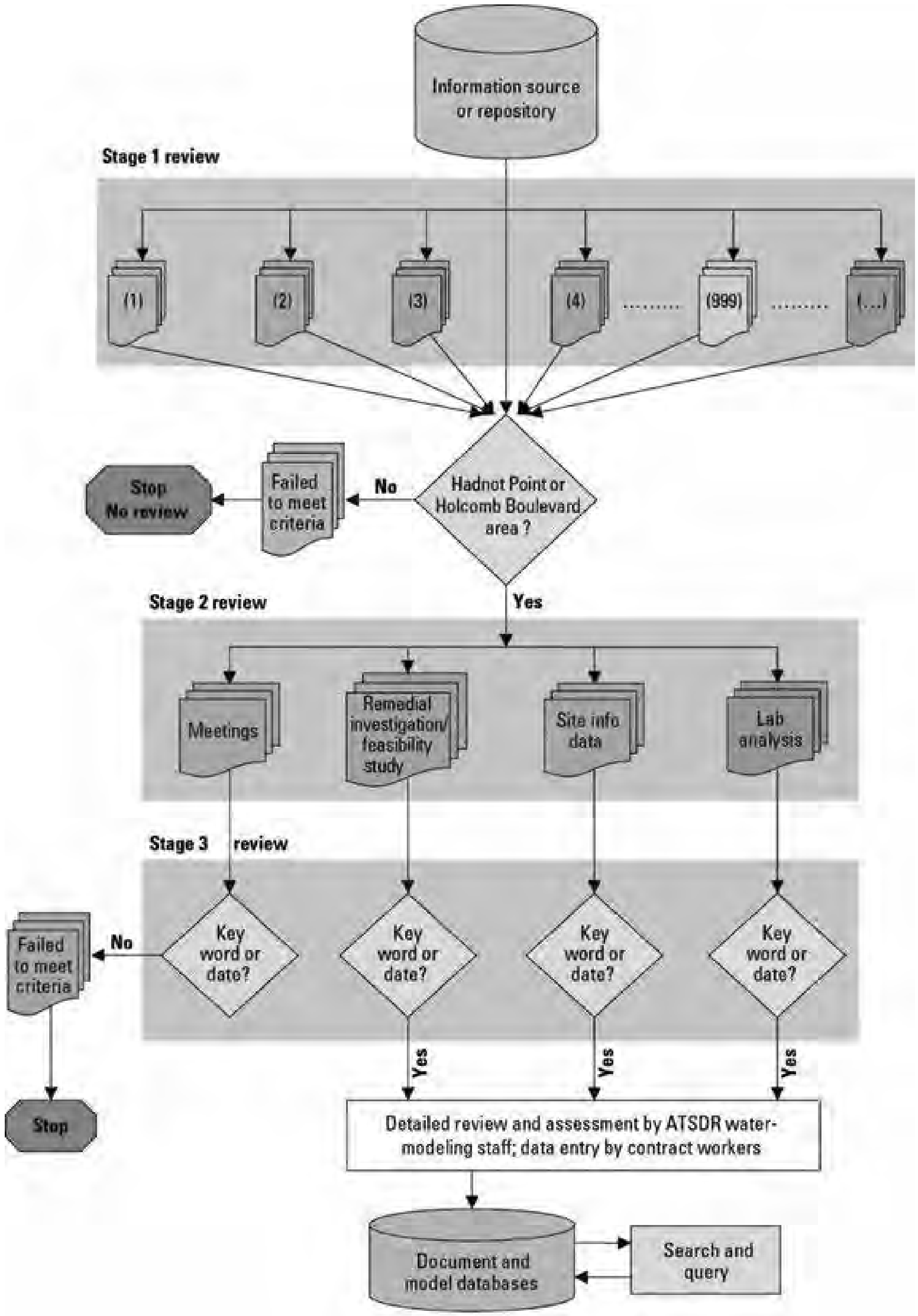


Figure 7.5. Three-stage process used for identifying relevant information and extracting data for databases and model development, Tarawa Terrace, Hadnot Point, and Holcomb Boulevard study areas (Maslia et al. 2013).

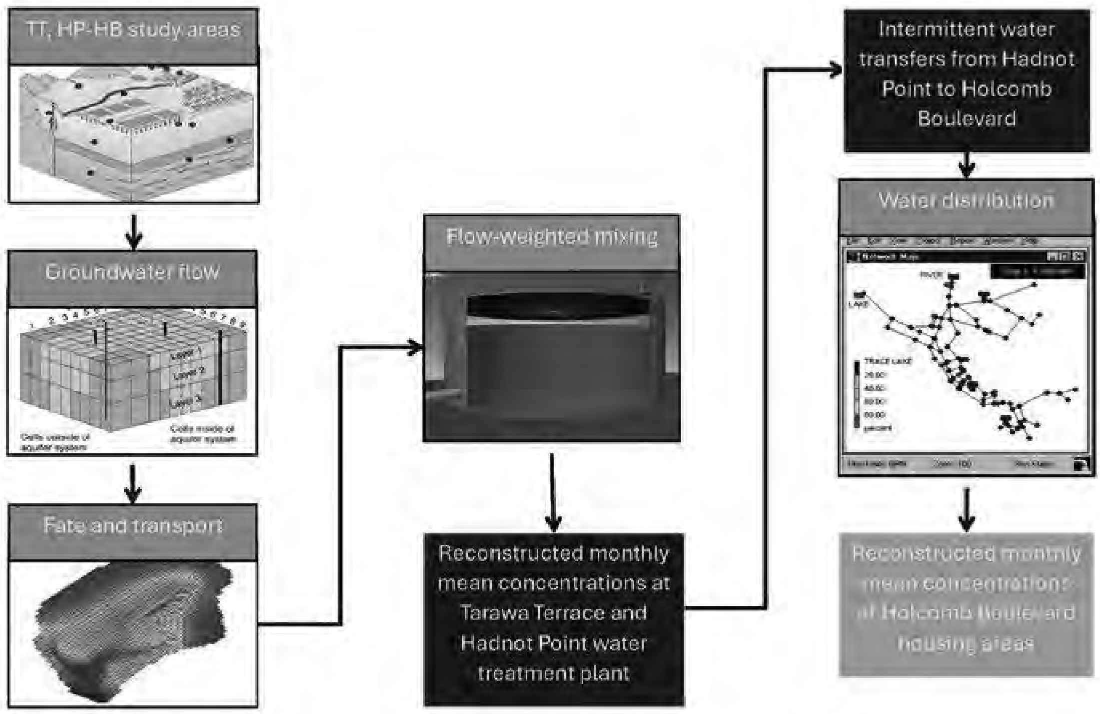


Figure 7.6. Water-modeling approach used for reconstructing historical drinking-water contaminant concentrations at Tarawa Terrace (TT), Hadnot Point (HP), and Holcomb Boulevard (HB). (Details of the groundwater-flow and contaminant fate and transport models are provided in Maslia et al. [2007, 2009a, 2013, 2016] and associated reports.)

To reconstruct groundwater levels, three-dimensional steady-state (pre-development, i.e., before pumping began) and transient groundwater-flow models were used and were calibrated using available geohydrologic field data, hydrogeologic and aquifer property data, and water-supply well monthly pumping and on-off cycling. Upon achieving an acceptable calibration for predevelopment (steady state) conditions and transient conditions (water-supply well pumping), the calibrated groundwater-flow velocity field and required fate and transport parameters (e.g., dispersity, retardation, source concentration variation) were input to a three-dimensional contaminant fate and transport model to simulate and calibrate the fate and transport of contaminants such as PCE.

Several custom methods and models were developed as part of the historical reconstruction process owing to the complex character of the study area, the complex historical water-supply well operations, and the need to reconstruct mean monthly contaminant-specific concentrations. Summarized below are some of these methods:

- Effective and efficient (with respect to published methods) fire-flow test method for water-distribution system model calibration (Grayman et al. 2006),
- Historical monthly operations and pumped groundwater volumes reconstructed for nearly 100 supply wells (Telci et al. 2013),

- Linear state-space representation of a contaminated aquifer developed to reconstruct historical concentrations in supply wells without the need to use traditional numerical fate and transport modeling (Guan et al. 2013),
- Volume estimates of lost benzene and LNAPL fate and transport in groundwater (Jang et al. 2013), and
- Probabilistic Markov process to estimate the number of intermittent transfers of drinking water between a contaminated and uncontaminated drinking-water system (Sautner et al. 2013b).

Specific details and descriptions for each type of analysis and each type of model or computational tool used are provided in Maslia et al. (2007, 2013) and set out below. Use of custom methods such as proprietary models is consistent with EPA guidance to produce the most reliable results for specific sites. (USEPA 2009). Further details regarding the proprietary models used by ATSDR are set forth in the expert report of Dr. Mustafa M. Aral.

Tarawa Terrace

Table 7.2 lists the analyses and simulation tools (models) used to reconstruct historical contamination events at Tarawa Terrace and vicinity. The primary focus for the investigation of the Tarawa Terrace historical reconstruction analyses was the fate and transport of, and concentration levels of a single constituent—PCE.

For Tarawa Terrace the information and data in Table 7.2 were applied to the models in the following sequence:

1. Geohydrologic framework information, aquifer and confining unit hydraulic data, and climatic data were used to determine predevelopment (prior to 1951) groundwater-flow characteristics. To simulate predevelopment groundwater-flow conditions, the public-domain code **MODFLOW-96** (Harbaugh and McDonald 1996)—a three-dimensional groundwater-flow model code—was used.
2. Transient groundwater conditions occurring primarily because of the initiation and continued operation of water-supply wells at Tarawa Terrace also were simulated using the three-dimensional model code **MODFLOW-96**; well operations were accounted for and could vary on a monthly basis.
3. Groundwater velocities or specific discharges derived from the transient groundwater-flow model were used in conjunction with PCE source, fate, and transport data to develop a fate and transport model. To simulate the fate and transport of PCE as a single species from its source at ABC One-Hour Cleaners to Tarawa Terrace water-supply wells, the public domain code **MT3DMS** (Zheng and Wang 1999) was used. **MT3DMS** is a model capable of simulating three-dimensional fate and transport. Simulations describe PCE concentrations on a monthly basis during January 1951–December 1994.[7]

[7] The contaminant fate and transport model, MT3DMS, has several options for solving the transport equation. These solvers include Finite-Difference (F-D), Method of Characteristics (MOC), and Total Variation Diminishing (TVD). The F-D solver produces more numerical dispersion whereas the TVD solver minimizes numerical dispersion at the expense of

4. The monthly concentrations of PCE assigned to finished water at the Tarawa Terrace WTP were determined using a materials mass balance model (simple mixing) to compute the flow-weighted average concentration of PCE. The model is based on the principles of continuity and conservation of mass (Masters 1998).
5. To analyze the degradation of PCE into degradation by-products (TCE, 1,2-tDCE, and VC) and to simulate the fate and transport of these contaminants in the unsaturated zone (zone above the water table), a three-dimensional, multispecies, and multiphase mass transport model (**TechFlowMP**) was developed by the Multimedia Simulations Laboratory (MESL) at the Georgia Institute of Technology (Jang and Aral 2005, 2007).
6. To analyze and understand the impacts of unknown and uncertain historical pumping schedule variations of water-supply wells on arrival of PCE at the Tarawa Terrace water-supply wells and WTP, a pumping and schedule optimization system tool (**PSOpS**) was used. This model was also developed by the MESL (Wang and Aral 2007).
7. To assess parameter sensitivity, uncertainty, and variability associated with model simulations of flow, fate and transport, and computed PCE concentrations in finished water at the Tarawa Terrace WTP, sensitivity and probabilistic analyses were conducted. Sensitivity analyses were conducted using a one-at-a-time approach; the probabilistic analyses applied Monte Carlo simulation (MCS) and sequential Gaussian simulation (SGS) methods to results previously obtained using **MODFLOW-96, MT3DMS**, and the drinking-water mixing model.
8. The initial approach for estimating the concentration of PCE delivered to residences of Tarawa Terrace used the public domain model, **EPANET 2** (Rossman 2000)—a water-distribution system model used to simulate street-by-street PCE concentrations (Sautner et al. 2005, 2013b).

introducing oscillations. For both the TT and HP models, the F-D solver was used. A sensitivity analysis was conducted to assess the different solution methods for the HP models (Jones et al. 2013, Figure S6.21, p. S6.41).

Table 7.2. Analyses and simulation tools (models) used to reconstruct historical contamination events at Tarawa Terrace and vicinity (Maslia et al. 2007)

[VOC, volatile organic compound; PCE, tetrachloroethylene; GIS, geographic information system; WTP, water treatment plant; TCE, trichloroethylene; 1,2-tDCE, *trans*-1,2-dichloroethylene; VC, vinyl chloride]

Analysis	Description	Analysis or simulation tool and type	Reference
Geohydrologic framework	Detailed analyses of well and geohydrologic data used to develop framework of the Castle Hayne aquifer system at Tarawa Terrace and vicinity	Data analysis	Faye (In press 2007a)
Predevelopment groundwater flow	Steady-state groundwater flow, occurring prior to initiation of water-supply well activities (1951) or after recovery of water levels from cessation of pumping activities (1994)	MODFLOW-96—numerical model	Harbaugh and McDonald (1996); Faye and Valenzuela (In press 2007)
Transient groundwater flow	Unsteady-state groundwater flow occurring primarily because of the initiation and continued operation of water-supply wells (January 1951–December 1994)	MODFLOW-96—numerical model	Harbaugh and McDonald (1996); Faye and Valenzuela (In press 2007)
Properties of VOCs in groundwater	Properties of degradation pathways of common organic compounds in groundwater	Literature survey	Lawrence (2006, In press 2007)
Computation of PCE mass	Estimates of mass (volume) of PCE; (a) unsaturated zone (above water table) in vicinity of ABC One-Hour Cleaners based on 1987–1993 data; (b) within Tarawa Terrace and Upper Castle Hayne aquifers based on 1991–1993 data	Site investigation data, GIS, and spatial analyses	Roy F. Weston, Inc. (1992, 1994); Pankow and Cherry (1996); Faye and Green (In press 2007)
Fate and transport of PCE	Simulation of the fate and migration of PCE from its source (ABC One-Hour Cleaners) to Tarawa Terrace water-supply wells (January 1951–December 1994)	MT3DMS—numerical model	Zheng and Wang (1999); Faye (In press 2007b)
PCE concentration in WTP finished water	Computation of concentration of PCE in drinking water from the Tarawa Terrace WTP using results from fate and transport modeling	Materials mass balance model using principles of conservation of mass and continuity—algebraic	Masters (1998); Faye (In press 2007b)
Fate and transport of PCE and degradation by-products in groundwater and vapor phase	Three-dimensional, multiphase simulation of the fate, degradation, and transport of PCE degradation by-products: TCE, 1,2-tDCE, and VC	TechFlowMP—numerical	Jang and Aral (2005, 2007, In press 2007)
Early and late arrival of PCE at WTP	Analysis to assess impact of schedule variation of water-supply well operations on arrival of PCE at wells and the Tarawa Terrace WTP	PSOpS—numerical; optimization	Wang and Aral (2007, In press 2007)
Parameter uncertainty and variability	Assessment of parameter sensitivity, uncertainty, and variability associated with model simulations of ground-water flow, fate and transport, and water distribution	PEST; Monte Carlo simulation—probabilistic	Doherty (2005); Maslia et al. (In press 2007b)
Distribution of PCE in drinking water	Simulation of hydraulics and water quality in water-distribution system serving Tarawa Terrace based on present-day (2004) conditions	EPANET 2—numerical	Rossman (2000); Sautner et al. (In press 2007)

Hadnot Point – Holcomb Boulevard

Table 7.3 lists the analyses and simulation tools (models) used to reconstruct historical contamination events at Hadnot Point and Holcomb Boulevard.

For the Hadnot Point-Holcomb Boulevard (HP-HB) study area the information and data in Table 7.3 were applied to the models in the following sequence:

1. Geohydrologic framework information, aquifer and confining unit hydraulic data, and climatic data were used to determine predevelopment (prior to 1942) groundwater-flow characteristics. Detailed analyses of well and geohydrologic data used to develop the framework of the Brewster Boulevard and Castle Hayne aquifer systems and Tarawa Terrace aquifer are described in Faye (2012).

2. Water-level data were used to characterize groundwater flow in the study area. Detailed water-level data and analyses are presented in Faye et al. (2013).

3. To simulate predevelopment groundwater-flow conditions, the code MODFLOW-2005 (Harbaugh 2005)—a three-dimensional groundwater-flow model code—was used. Estimates of model parameter values also were obtained using the objective parameter estimation code PEST-12 (Doherty 2003, 2010).

4. To simulate the transient (unsteady) effects caused primarily by the onset and continued operation of water-supply wells in the study area, historical water-supply well operating schedules were developed. This was accomplished by documenting water-supply well capacities and histories (Sautner et al. 2013a) and reconstructing operating schedules on a monthly basis for the period 1942–2008 (Telci et al. 2013); operational chronologies for all water-supply wells in the study area are shown in Figure 7.3.

5. Transient groundwater conditions primarily caused by the onset and continued operation of water-supply wells within the HP-HB study area (and the onset of remediation pumping during the late 1990s and 2000s) also were simulated using the MODFLOW three-dimensional groundwater-flow model code; water-supply well operations were accounted for. To address historical water-supply well operations and the absence of nearby hydrologic boundaries, the active model domain (Figure 7.7) was further discretized into two individual variably spaced grid models, one for the Hadnot Point Industrial Area (HPIA) and one for the Hadnot Point Landfill (HPLF). Descriptions and characterizations of the groundwater-flow model discretization properties used to simulate three-dimensional groundwater flow and contaminant fate and transport in the HP-HB study area and comparison with the model used in the TT study area are listed in Table 7.4. A map of the active model domain for groundwater flow and the HPIA and HPLF area subdomain model areas selected for transient groundwater flow and contaminant fate and transport is shown in Figure 7.7.

6. Groundwater velocities or specific discharges derived from the calibrated transient groundwater-flow model were used in conjunction with contaminant source, fate, and property data in the HPIA to simulate the fate and transport of TCE and benzene (as single species) dissolved in groundwater using the model code MT3DMS-5.3 (Zheng and Wang 1999; Zheng 2010). In addition, the fate and transport of PCE and TCE from source areas in the HPLF area to water-supply well HP-651 was simulated using the MT3DMS code. Details pertaining to the fate and transport model calibration and reconstruction of PCE, TCE, and

benzene dissolved in groundwater are provided in Jones et al. (2013). The HPIA and HPLF contaminant fate and transport model subdomain areas, contaminant sources, and nearby historically operated water-supply wells are shown in Figure 7.7 Larger scale maps are shown in Maslia et al. (2013, Figures A13 and A14).

7. The occurrence of benzene as an LNAPL in the subsurface in the vicinity of the HPFF and HPIA is described in Faye et al. (2010 and 2012). Estimates of subsurface LNAPL volume were developed using historical measurements of LNAPL thickness over time—monitor well data—in the HPIA combined with the TechNAPLVol code that uses semi-analytical and numerical methods in a three-dimensional domain (Jang et al. 2013). The resulting saturation profile from the LNAPL volume analysis was used within the TechFlowMP model code (Jang and Aral 2007 2013) to simulate the dissolution of LNAPL constituents and the fate and transport of dissolved-phase benzene. Details pertinent to the application of TechFlowMP to the HPIA subdomain area and historical reconstruction results for the fate and transport of benzene are described in detail by Jang et al. (2013). The historical area of free product (fuel) and location of former fuel lines from the HPFF to other sites within the HPIA are shown in Figure A13 of Maslia et al. (2013).

8. An alternative method, a linear state-space representation of a contaminated aquifer system designated as the linear control model (LCM) methodology, was developed to reconstruct contaminant concentrations in water-supply wells (Guan et al. 2013). Using the model code TechControl, this simplified approach was used to reconstruct historical contaminant concentrations, including PCE, TCE, 1,2-tDCE, and VC, in water-supply well HP-651 in the HPLF area (Figure 7.7). Details pertinent to the development, testing, and application of the LCM methodology are presented in Guan et al. (2013). Results from the LCM application at water-supply well HP-651 are compared to simulated PCE and TCE concentrations obtained using the MT3DMS numerical fate and transport code (item 6, above) later in this report.

9. Reconstructed (simulated) monthly mean concentrations of PCE, TCE, 1,2-tDCE, VC, and benzene for finished water at the HPWTP were determined by using a materials mass balance model (simple mixing) to compute the flow-weighted average concentration of the aforementioned contaminants. This computational method is based on the principles of continuity and conservation of mass (Masters 1998). The use of the materials mass-balance method is justified because all raw water from water-supply wells within the HPWTP service area was mixed at the HPWTP prior to treatment and distribution. Details of this method are described in a subsequent section of this report.

10. Intermittent operations of booster pump 742 and the opening of the Marston Pavilion valve transferred contaminated Hadnot Point finished water to Holcomb Boulevard family housing areas and other facilities (Figure 7.1). Owing to missing data related to pump and valve operations, probabilistic analyses of the intermittent water transfers during the period 1972–1985 were conducted using a Markov analysis (Ross 1977) and the code TechMarkovChain. Results provided probabilistic estimates of the intermittent transfer of contaminated Hadnot Point finished water to the Holcomb Boulevard family housing areas. Details of the application of the TechMarkovChain code to the Hadnot Point-Holcomb Boulevard study area are described in Sautner et al. (2013b).

Table 7.3. Analyses and simulation tools (models) used to reconstruct historical contamination events at Handot Point-Holcomb Boulevard and vicinity (Maslia et al. 2013).

[ft, foot; HPIA, Hadnot Point Industrial Area; HPLF, Hadnot Point landfill; VOC, volatile organic compound; BTEX, benzene, toluene, ethylbenzene, and xylenes; IRP, Installation Restoration Program; AST/UST, above-ground storage tank/underground storage tank; TCE, trichloroethylene; PCE, tetrachloroethylene; GIS, geographic information system; LNAPL, light nonaqueous phase liquid; 1,2-tDCE, *trans*-1,2-dichloroethylene; VC, vinyl chloride; WTP, water treatment plant]

Analysis	Description	Analysis type and simulation tool	[1]Reference
Geohydrologic framework	Detailed analyses of well and geohydrologic data used to develop framework of the Brewster Boulevard and Castle Hayne aquifer systems and Tarawa Terrace aquifer	Data analysis and interpretation	Faye (2012)
Water-level analyses and groundwater flow	Characterizations of water-level data and groundwater flow	Data analysis and interpretation	Faye et al. (2013)
Predevelopment groundwater flow	Steady-state, three-dimensional groundwater flow, occurring prior to initiation of water-supply well activities (1942) using a grid of uniform cells of 300 ft × 300 ft	Simulation using MODFLOW-2005	Harbaugh (2005); Suárez-Soto et al. (2013)
Historical water-supply well operations	Documenting water-supply well capacities, histories, and reconstructing operating schedules on a monthly basis for the period 1942–2008	Data analysis, interpretation, and simulation using TechWellOp	Sautner et al. (2013a); Telci et al. (2013)
Transient groundwater flow	Unsteady-state, three-dimensional groundwater flow occurring primarily because of the initiation and continued operation of water-supply wells (July 1942–June 2008), using a variably spaced grid ranging in area from 300 ft × 300 ft to 50 ft × 50 ft in the HPIA and HPLF model subdomain areas	Simulation using MODFLOW-2005	Harbaugh (2005); Suárez-Soto et al. (2013)
Properties of VOCs in groundwater	Properties of degradation pathways of common organic compounds in groundwater	Literature survey	Lawrence (2007)
Occurrence of selected contaminants in groundwater	Description and summaries of groundwater contaminants of selected VOCs and BTEX components at IRP and AST/UST sites; listing of water-supply and monitor well location and construction data	Data analysis	Faye et al. (2010, 2012)
Computation of mass for PCE, TCE, and benzene	Estimates of mass (volume) of TCE, PCE, and benzene in groundwater using field data and a variety of analytical and numerical techniques (Tables A6, A15, and A16)	Site investigation data, GIS spatial analyses, LNAPL volume analyses (TechNAPLVol)	Ricker (2008); Faye et al. (2010, 2012); Jones et al. (2013); Jang et al. (2013)
Fate and transport of TCE, PCE, and benzene	Simulation of the fate and migration of TCE and benzene from sources in the HPIA; simulation of the fate and migration of PCE from the HPLF	Simulation using MT3DMS-5.3	Zheng and Wang (1999); Zheng (2010); Jones et al. (2013)
Fate and transport of benzene (LNAPL)	Simulation of the fate and migration of benzene as an LNAPL from sources at the Hadnot Point fuel farm in the HPIA	Simulation using TechFlowMP	Jang and Aral (2007, 2008a, b); Jang et al. (2013)
Concentrations of PCE, TCE, 1,2-tDCE, and VC in a water-supply well	Reconstructing concentrations of PCE, TCE, 1,2-tDCE, and VC in water-supply well HP-651 (HPLF) using a linear control model (LCM) methodology	Simulation using TechControl	Guan et al. (2009, 2010, 2013)
TCE, PCE, 1,2-tDCE, VC, and benzene in WTP finished water	Computations of concentrations of TCE, PCE, 1,2-tDCE, VC, and benzene in drinking water from the Hadnot Point WTP using results from fate and transport and linear control model simulations	Materials mass balance model using principles of conservation of mass and continuity—algebraic	Masters (1998); Jones et al. (2013)
Parameter sensitivity and uncertainty	Assessment of parameter sensitivity and uncertainty associated with model simulations of groundwater flow, fate and transport, and water distribution	One-at-a-time sensitivity analysis (OAT), Monte Carlo (MC) simulation using Latin hypercube sampling (LHS), and MC simulation	Saltelli et al. (2000); Suárez-Soto et al. (2013); Jones et al. (2013); Sautner et al. (2013b)
Intermittent pump operation for transfer of finished water	Probabilistic analysis of the occurrence of pumping operations during the period 1972–1985 for transferring Hadnot Point finished water to Holcomb Boulevard housing areas	Probabilistic Markov analysis using TechMarkovChain	Ross (1977); Sautner et al. (2013b)
Distribution of TCE, PCE, 1,2-tDCE, VC, and benzene throughout the Holcomb Boulevard housing areas	Simulation of hydraulics and water quality in the water-distribution system serving the Holcomb Boulevard housing areas, 1972–1985; intermittent pumping operations estimated by using data and Markov analysis	Simulation using EPANET 2	Rossman (2000); Sautner et al. (2013b)

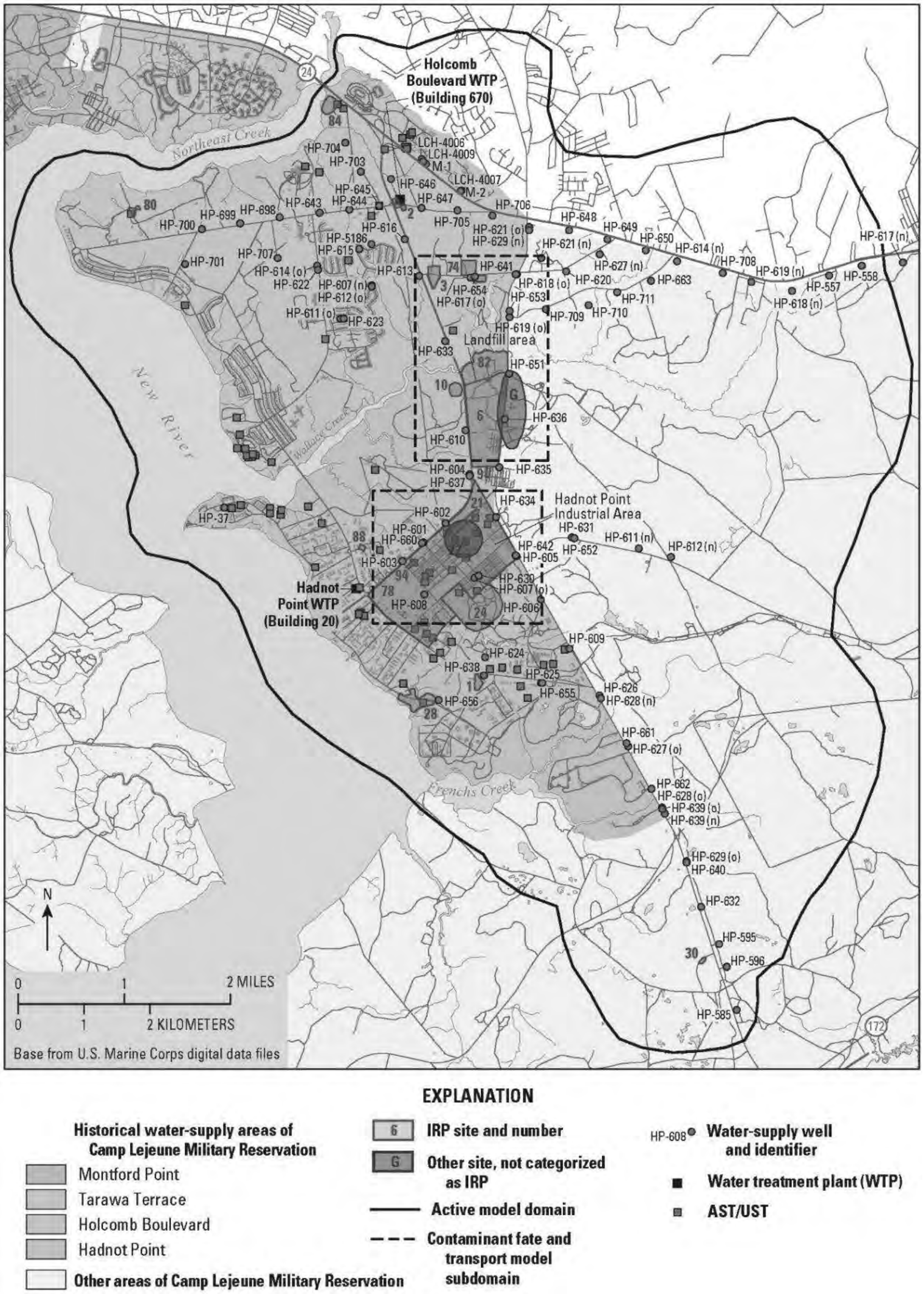


Figure 7.7. Groundwater-flow model domain and contaminate fate and transport model subdomains for the Hadnot Point Industrial Area (HPIA) and Hadnot Point landfill (HPLF). (Maslia et al. 2013).

Table 7.4. Description and characteristics of model properties used to simulate three-dimensional groundwater flow and contaminant fate and transport, Hadnot Point- Holcomb Boulevard and Tarawa Terrace study areas (Maslia et al. 2013).

[ft, foot; mi², square mile; TCE, trichloroethylene; PCE, tetrachloroethylene; —, not applicable]

Model feature	[1]Hadnot Point–Holcomb Boulevard study area					[4]Tarawa Terrace study area
	[2]Uniform grid	[3]Variably spaced grid		Fate and transport model subdomain		
		Hadnot Point Industrial Area	Hadnot Point landfill area	Hadnot Point Industrial Area	Hadnot Point landfill area	
Number of rows	152	288	348	132	204	200
Number of columns	172	298	268	168	132	270
Number of layers	7	7	7	7	7	7
Total number of finite-difference cells	183,008	600,768	652,848	155,232	188,496	378,000
Number of active domain or subdomain cells	108,695	453,654	532,287	155,232	188,496	191,927
Finite-difference cell size (ft×ft)	300×300	300×300–50×50	300×300–50×50	50×50	50×50	50×50
Total model or subdomain area (mi²)	84	84	84	2.0	2.4	4.8
Active domain area (mi²)	50	50	50	2.0	2.4	2.5
Contaminant-source areas (contaminants)	—	—	—	Building 900 (TCE); Building 1115 (TCE); Building 1401 (TCE); Building 1601 (TCE, benzene)[5]	Hadnot Point landfill (PCE, TCE)	ABC One-Hour Cleaners (PCE)

[1] Groundwater-flow simulation using MODFLOW-2005 (Harbaugh 2005); fate and transport simulation using MT3DMS (Zheng and Wang 1999); see Figure A12 for locations of active model boundaries and contaminant fate and transport model subdomains

[2] Uniform grid of 300-ft×300-ft cells used for simulating and calibrating predevelopment (steady-state) groundwater flow

[3] Variably spaced grid used for simulating and calibrating transient groundwater flow and contaminant fate and transport

[4] Groundwater-flow simulation using MODFLOW-96 (Harbaugh and McDonald 1996); fate and transport simulation using MT3DMS (Zheng and Wang 1999); uniform and coincident grids used for groundwater-flow and fate and transport simulations, refer to Maslia et al. (2007), Faye and Valenzuela (2007), and Faye (2008)

[5] Benzene occurs as a light nonaqueous phase liquid (LNAPL) at Building 1115 and at the Hadnot Point fuel farm (HPFF); see Jang et al. (2013) for modeling details.

11. Using the reconstructed monthly mean concentrations of PCE, TCE, 1,2-tDCE, VC, and benzene in finished water from the HPWTP and the Markov analysis to estimate the occurrence of intermittent water transfers, extended period simulations (EPS) of hydraulics and water quality for the water-distribution system serving the HB housing areas and other facilities during the period 1972–1985 were conducted using the model code EPANET 2 (Rossman 2000). Details pertaining to these analyses are presented in Sautner et al. (2013b) and are summarized in a subsequent section of this report.

Assessment of parameter sensitivity, variability, and uncertainty associated with model simulations of groundwater flow, contaminant fate and transport, and water-distribution system analyses were conducted using (1) one-at-a-time (and a variation of the one-at-a-time) sensitivity analysis (Saltelli et al. 2000),(2) Monte Carlo simulation (Tung and Yen 2005), and (3) the parameter estimation code PEST (Doherty 2003, 2010). Details relevant to the application of parameter estimation and sensitivity and uncertainty analyses for the HP-HB study area models are provided in Guan et al.

(2013), Jang et al. (2013), Jones et al. (2013), Sautner et al. (2013b), and Suárez-Soto et al. (2013), and are summarized in subsequent sections of this report.

Because all water-supply wells for TT mixed at the TTWTP before finished water was distributed throughout the water-distribution system network and all water-supply wells for HP were mixed at the HPWTP before finished water was distributed throughout the water-distribution system network, ATSDR determined that a simple-mixing model approach using flow-weighted mixing consisting of equations for continuity and conservation of mass (Masters 1998; Maslia et al. 2007) could be used to reconstruct contaminant concentrations within the water-distribution systems. Using the simple mixing-model approach, for any given month during the historical reconstruction period, PCE and TCE concentrations of finished water at the TTWTP and HPWTP, respectively, were computed using the following equations:

$$Q_T = \sum_{i=1}^{NWP} Q_i \qquad (7.1)$$

and

$$C_{WTP} = \frac{\sum_{i=1}^{NWP} C_i Q_i}{Q_T} \qquad (7.2)$$

where:

NWP is the number of water-supply wells simulated as operating (pumping) during the month of interest,

Q_i is the simulated groundwater pumping rate of water-supply well i,

Q_T is the total simulated groundwater pumping rate from all operating water-supply wells during the month of interest,

C_i is the simulated concentration for water-supply well i, and

C_{WTP} is the concentration of finished water delivered from the TTWTP or HPWTP to the respective distribution systems for the month of interest.

Equation (7.1) is known as the continuity equation and Equation (7.2) describes the conservation of mass (Masters 1998). The assumptions for using the simple mixing model approach are: (1) mixing is instantaneous and uniform, (2) average steady-state conditions during each particular month, and (3) contaminants are conservative (no degradation or decay within the WTP and water-distribution system). A schematic representation comparing the simple-mixing model approach with the more complex network representation used by EPANET is shown in Figure 7.8A and 7.8B, respectively.

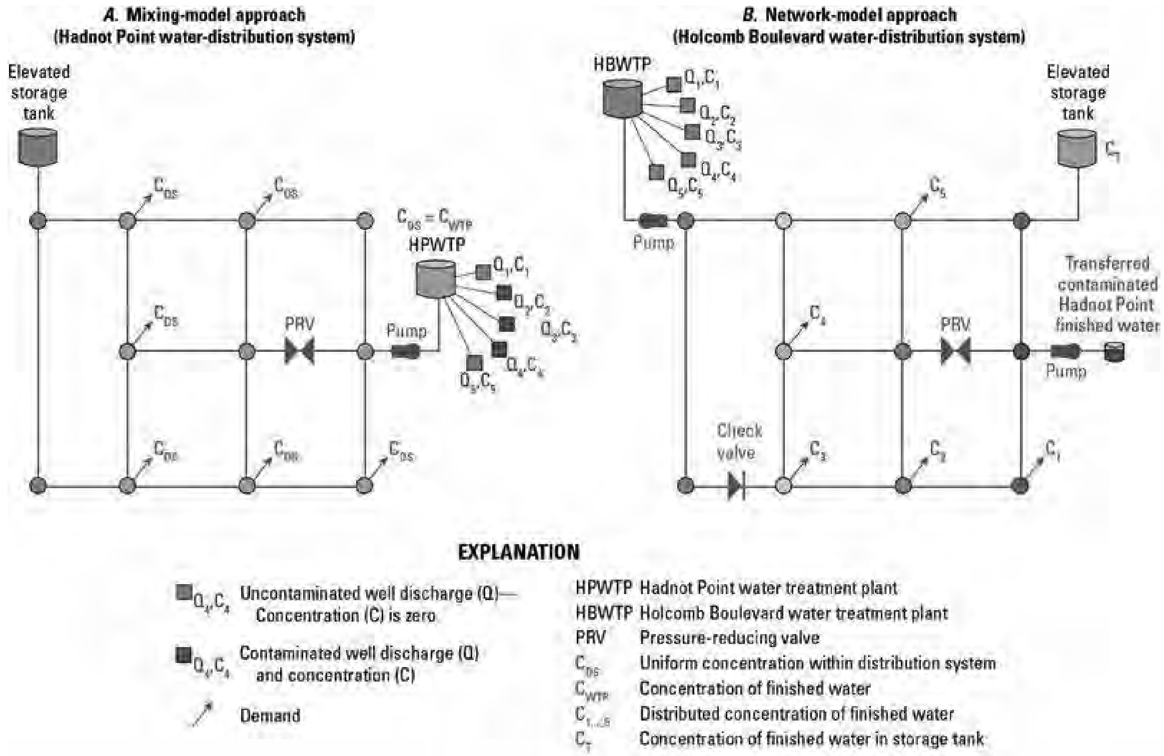


Figure 7.8. Schematic node-link representations for water-distribution systems: *(A)* mixing-model approach used for the Tarawa Terrace and Hadnot Point water treatment plant analyses and *(B)* network-model approach used for the Hadnot Point and Holcomb Boulevard interconnection analyses (Maslia et al. 2013).

To test the appropriateness of this assumption (simple mixing at the WTPs), results of a simulation for December 1984 conditions based on using the mixing model and the water-distribution system model approaches are described in Maslia et al (2009b, Table I4). These results demonstrated that after 7 days, the mixing model and the spatially derived EPANET (Rossman 1994) concentrations of PCE for TT were equivalent—even at the furthest extent of the water-distribution system (Montford Point area, Maslia et al. 2009b, Figure I3). These results confirmed the appropriateness of the decision to use the simple mixing model approach for estimating (reconstructing) PCE and TCE concentrations in finished water delivered to the Tarawa Terrace and Hadnot Point areas from the TTWTP and HPWTP, respectively.

Because of the interconnection of the HP and HB water-distribution systems, a more complex analysis was necessary compared to the simple mixing-model approach (Figure 7.8) described by Equations (7.1) and (7.2). This more complex numerical analysis was used to determine the concentration of finished water in the HB water-distribution system during periods of interconnection. This required the application of the EPANET (version 2 or EPANET 2) water-distribution system model (Rossman 2000) and extended period simulation (EPS). The EPANET water-distribution system model was calibrated for the HB water-distribution system using field data collected by the ATSDR water-modeling team; field data represented operational conditions during 2004 (Sautner et al. 2013b). EPSs were used to reconstruct water-distribution system flow and mass transport patterns during discrete interconnection events (Maslia et al. 2013, Figure A28) when booster pump 742 (Figure 7.1) was intermittently operated, resulting in the transfer of contaminated finished water from the HP water-distribution system to the "uncontaminated" HB water-distribution system. Pipelines represented in the water-distribution system network model coincide with locations of streets within the HP-HB study area (Maslia et al. 2009b, Figure I3; Sautner et al. 2013b).

7.4.4 Model Calibration, Sensitivity, and Uncertainty

ATSDR utilized a stepwise or hierarchical, four-level calibration process (Maslia et al. 2007, Faye and Valenzuela, 2007; Faye, 2008; Maslia et al. 2013) whereby groundwater-flow and contaminant fate and transport models of TT and HP-HB were calibrated to available historical field data. Level 1 of the calibration was for a steady-state (pre-development) groundwater-flow model. Level 2 calibration was for the transient (pumping conditions), and Level 3 of the calibration was for the fate and transport of PCE and/or TCE from contaminant sources (ABC One-Hour Cleaners, HPIA, and HPLF) to water-supply wells at USMCB Camp Lejeune supplying water to the TTWTP and the HPTWP. The Level 4 calibration was essentially a confirmation of or testing a "goodness of fit" of the previous three levels of calibration because in Level 4, measured PCE and TCE concentrations at the WTPs were compared to the flow-weighted mixing model used to compute the monthly mean concentrations at the TTWTP and the HPWTP (refer to section 7.4.3 of this report and Equations 7.1 and 7.2). That is, the measured WTP water-quality samples of PCE and TCE were **never used** to adjust **any model parameters**, but rather, to **test the adequacy** of the groundwater-flow, contaminant fate and transport, and flow-weight mixing models. Discussion of the results of the calibration process is contained in section 7.5 below.

Best modeling practice requires that evaluations be conducted to ascertain confidence in models and model results by assessing parameter sensitivity, variability, and uncertainty associated with the modeling process and with the outcomes attributed to models (ASTM International 1994; Saltelli et al. 2000). There are numerous methods for characterizing a model's sensitivity and uncertainty based on variations of calibrated parameter values (ASTM International 1994, Cullen and Frey 1999, Saltelli et al. 200, Tung and Yen 2005, Hill and Tiedeman 2007). These methods are generally classified into two groups: (1) sensitivity analysis, wherein calibrated model parameter values are varied either manually or through some automated method and (2) probabilistic uncertainty analysis, wherein probabilistic methods are used to characterize and quantify the input and output parameter variation and uncertainty. Substantial numbers of sensitivity analyses (using a one-at-a-time method) and uncertainty analyses (using Monte Carlo simulation (MCS)) were conducted as part of the Camp Lejeune historical reconstruction analysis. These analyses and results are presented below; readers are referred to Maslia et al. (2007; 2013) for additional specific details and results. An example of a probabilistic uncertainty analysis for the finished-water concentrations at the TTWTP is shown in Figure A26 (Maslia et al. 2007, p. A60). Based on these analyses, for the TT study area, reconstructed drinking-water concentrations of PCE varied within a range of about 3 or less for all the MCS relative to the calibrated single values (Figure A26). For the HP-HB study areas, reconstructed drinking-water concentrations of TCE ranged by a factor of about 10 or less (Maslia et al. 2013, Figure A41).

7.5 Historical Reconstruction Analyses and Results

Details of historical reconstruction analyses and results are described in substantial detail in peer-reviewed ATSDR reports for the TT, HP, and HB areas. Reports describing geohydrologic data, hydrogeologic data, water supply data, analyses and results are presented Tables 7.5 and 7.6 for the TT and HP-HB study areas, respectively.

- **Tarawa Terrace and Vicinity**

Table 7.5. Reports describing geohydrologic data, hydrogeologic data, water-supply data, analyses and results for the Tarawa Terrace study area.

Year of Publication	ATSDR Report (Publication)	Reference Citation
2007	Chapter A: Summary of Findings	Maslia et al. (2007)
2007	Chapter B: Geohydrologic Framework of the Castle Hayne Aquifer System	Faye (2007)
2007	Chapter C: Simulation of Three-Dimensional Groundwater Flow	Faye and Valenzuela (2007)
2007	Chapter D: Properties of Degradation Pathways of Common Organic Compounds in Groundwater	Lawrence (2007)
2007	Chapter E: Occurrence of Contaminants in Groundwater	Faye and Green, Jr. 2007)
2008	Chapter F: Simulation of the Fate and Transport of Tetrachloroethylene (PCE)	Faye (2008)
2008	Chapter G: Simulation of Three-Dimensional, Multispecies Mass Transport of Tetrachloroethylene (PCE) and Associated Degradation By-Products	Jang and Aral (2008)
2008	Chapter H: Effect of Groundwater Pumping Schedule Variation on Arrival of Tetrachloroethylene (PCE) at Water-Supply Wells and the Water Treatment Plant	Wang and Aral (2008)
2009	Parameter Sensitivity, Uncertainty, and Variability Associated with Model Simulations of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water	Maslia et al. (2009b)

- **Hadnot Point, Holcomb Boulevard and Vicinity**

Table 7.6. Reports describing geohydrologic data, hydrogeologic data, water-supply data, analyses and results for the Hadnot Point-Holcomb Boulevard study area.

Year of Publication	ATSDR Report (Publication)	Reference Citation
2013	Chapter A: Summary of Findings	Maslia et al. (2013)
2013	Chapter A–Supplement 1: Descriptions and Characterizations of Data Pertinent to Water Supply, Well Capacities, Histories, and Operations	Sautner et al. (2013a)
2013	Chapter A–Supplement 2: Development and Application of a Methodology to Characterize Present-Day and Historical Water-Supply Well Operations	Telci et al. (2013)
2013	Chapter A–Supplement 3: Descriptions and Characterization of Water-Level Data and Groundwater Flow for the Brewster Boulevard and Castle Haye Aquifer Systems and the Tarawa Terrace Aquifer	Faye et al. (2013)
2013	Chapter A–Supplement 4: Simulation of Three-Dimensional Groundwater Flow	Suárez-Soto et al. (2013)
2013	Chapter A–Supplement 5: Linear Control Methodology to Reconstruct Contaminant Concentrations at Selected Water-Supply Wells	Guan et al. (2013)
2013	Chapter A–Supplement 6: Simulation of Fate and Transport of Selected Volatile Organic Compounds in the Vicinities of the Handot Point Industrial Area and Landfill	Jones et al. (2013)
2013	Chapter A–Supplement 7: Source Characterization and Simulation of the Migration of Light Nonaqueous Phase Liquids (LNAPLs) in the Vicinity of eh Hadnot Point Industrial Area	Jang et al. (2013)
2013	Chapter A–Supplement 8: Field Tests, Data Analyses, and Simulation of the Distribution of Drinking Water with Emphasis on intermittent Transfers of Drinking Water between the Handot Point and Holcomb Boulevard Water-Distribution Systems	Sautner et al. (2013b)
2012	Chapter B: Geohydrologic Framework of the Brewster Boulevard and Castle Hayne Aquifer System and Tarawa Terrace Aquifer	Faye (2012)[8]
2010	Chapter C: Occurrence of Selected Contaminants in Groundwater at Installation Restoration Sites	Faye et al. (2010)
2012	Chapter D: Occurrence of Selected Contaminants in Groundwater at Above Ground and Underground Storage Tank Sites	Faye et al. (2012)

Historical reconstruction results for TT, HP, and HB are summarized below. Specific details can be found in the peer-reviewed ATSDR reports listed above and available online at the ATSDR website: https://www.atsdr.cdc.gov/sites/lejeune/Water-Modeling.html.

[8] In December 2011, ATSDR released the HP-HB Chapter B report (Geohydrologic Framework of the Brewster Boulevard and Castle Hayne Aquifer Systems and the Tarwa Terrace Aquifer). On January 5, 2012, ATSDR received a letter from the USMC (written communication from Major General J. A. Kessler, USMC to Dr. Thomas Sinks, Deputy Director, ATSDR) requesting ATSDR to address security concerns related to identification of coordinate locations of active drinking water-supply wells (based on 18 U.S.C. 795(a)). In January 2012, ATSDR publicly released a **redacted** version of the HP-HB Chapter B report (Faye 2012). The unredacted version of the Chapter B report was externally peer reviewed like all ATSDR Camp Lejeune reports. References in this expert report to Faye (2012) are to the **redacted** HP-HB Chapter B report.

7.5.1 Tarawa Terrace (TT)

As discussed in Section 7.4.4 (Calibration, Sensitivity, and Uncertainty) above, ATSDR utilized a four-level calibration process (Maslia et al. 2007, Faye and Valenzuela, 2007; Faye, 2008) whereby groundwater-flow and contaminant fate and transport models for Tarawa Terrace were calibrated in a hierarchical, stepwise approach to available historical field data (Maslia et al. 2007, Figure A9). At each hierarchical level, an initial calibration target or "goodness of fit" criterion was selected based on the availability, method of measurement or observation, and overall reliability of field data and related information. Once model-specific parameters were calibrated, statistical and graphical analyses were conducted to determine if selected parameters met calibration criteria targets. Summaries of calibration targets and resulting calibration statistics for each of the four hierarchical levels are listed in Table 7.7.

Table 7.7. Summary of calibration targets and resulting calibration statistics for models used to reconstruct historical contamination events at Tarawa Terrace and vicinity (Maslia et al. 2007).

Calibration level[1, 2]	Analysis type	Calibration target[3]	Resulting calibration statistics[4]	[5]Number of paired data points (N)
1	Predevelopment (no pumping) groundwater flow	Magnitude of head difference: 3 feet	$\lvert\overline{\Delta h}\rvert = 1.9$ ft $\sigma = 1.5$ ft $RMS = 2.1$ ft	59
2	Transient groundwater flow—monitor wells	Magnitude of head difference: 3 feet	$\lvert\overline{\Delta h}\rvert = 1.4$ ft $\sigma = 0.9$ ft $RMS = 1.7$ ft	263
	Transient groundwater flow—supply wells	Magnitude of head difference: 12 feet	$\lvert\overline{\Delta h}\rvert = 7.1$ ft $\sigma = 4.6$ ft $RMS = 8.5$ ft	526
3	Contaminant fate and transport—supply wells	Concentration difference: ± one-half order of magnitude or model bias (B_m) ranging from 0.3 to 3	Geometric bias [6]$B_g = 5.8/3.9$	[7]36
4	Mixing model—treated water at water treatment plant	Concentration difference: ± one-half order of magnitude or model bias (B_m) ranging from 0.3 to 3	Geometric bias $B_g = 1.5$	[8]25

[1]Refer to the Chapter C report (Faye and Valenzuela In press 2007) for calibration procedures and details on levels 1 and 2

[2]Refer to the Chapter F report (Faye In press 2007b) for calibration procedures and details on levels 3 and 4

[3]Head difference is defined as observed water level (h_{obs}) minus simulated water level (h_{sim}); Magnitude of head difference is defined as: $|\Delta h| = |h_{obs} - h_{sim}|$; a concentration difference of ± one-half order of magnitude equates to a model bias of 0.3 to 3, where, B_m = model bias and is defined as: $B_m = C_{sim}/C_{obs}$, where C_{sim} is the simulated concentration and C_{obs} is the observed concentration; when $B_m = 1$, the model exactly predicts the observed concentration, when $B_m > 1$, the model overpredicts the concentration, and when $B_m < 1$, the model underpredicts the concentration

[4]Average magnitude of head difference is defined as: $\left|\overline{\Delta h}\right| = \frac{1}{N}\sum_{i=1}^{N}\left|\Delta h_i\right|$; standard deviation of head difference is defined as: $\sigma = \sqrt{\frac{\sum_{i=1}^{N}\left(\Delta h_i - \overline{\Delta h}\right)^2}{N-1}}$, where $\overline{\Delta h}$ is the mean or average of head difference; root-mean-square of head difference is defined as: $RMS = \left[\frac{1}{N}\sum_{i=1}^{N}\Delta h_i^2\right]^{\frac{1}{2}}$; geometric bias, B_g, is defined as: $B_g = \exp\left[\frac{\sum_{i=1}^{N}\ln\left(B_{m,i}\right)}{N}\right]$, where ln ( ) is the Naperian logarithm

[5]A paired data point is defined as any location with observed data that is associated with a model location for the purpose of comparing observed data with model results for water level or concentration

[6]$B_g = 5.8$ computed using all water-supply wells listed in table A9; $B_g = 3.9$ computed without considering water-supply well TT-23—See text for explanation

[7]Observed concentration of 17 samples recorded as nondetect (see Table A9) and are not used in computation of geometric bias

[8]Observed concentration of 15 samples recorded as nondetect (see Table A10) and are not used in computation of geometric bias

Level 1 Calibration (Predevelopment Conditions)

Level 1 calibration of the Tarawa Terrace groundwater-flow model (details provided in Maslia et al. 2007, p.A24–A31) was accomplished by successfully simulating estimated predevelopment conditions; that is, flow and water-level conditions prior to development of the underlying aquifers by wells. Predevelopment conditions are considered representative of long-term, average annual flow and water-level conditions within the Tarawa Terrace aquifer and the Upper Castle Hayne aquifer system at Tarawa Terrace and vicinity. Criteria used to determine a satisfactory predevelopment calibration were: (1) conformance of simulated conditions to the conceptual groundwater-flow model and (2) a satisfactory comparison of simulated and observed (measured) water levels within the active model domain. A scatter diagram showing the agreement between simulated and observed water levels for simulated predevelopment conditions is shown in Figure 7.9. The flow model (MODFLOW-96) spatially interpolates simulated results from cell centers to the location coordinates assigned to various observation points, such as well locations, to facilitate direct comparisons of simulated and observed conditions. All Tarawa Terrace water-supply wells and several monitor wells are open to multiple aquifers. At these sites, simulated water levels were processed post-calibration by proportioning simulated water levels in several aquifers at multiaquifer wells to compute a composite water level. This composite water level was then compared to the observed water level to evaluate calibration "goodness of fit."

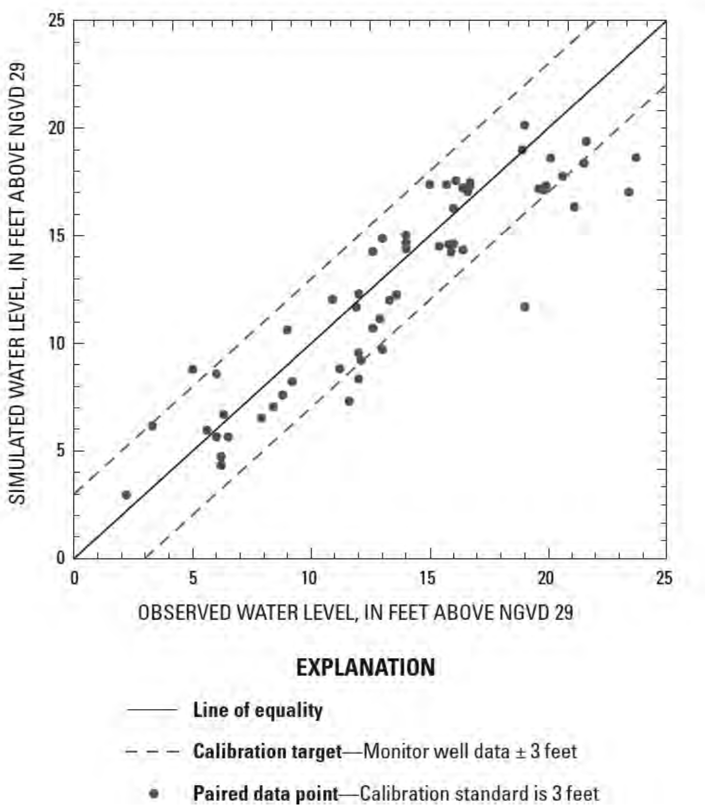


Figure 7.9. Simulated and observed predevelopment water levels, Tarawa Terrace and vicinity (Faye and Valenzuela 2007).

When the data points plot near or on the solid diagonal "line of equality," the simulated and measured water levels are the same. When the data points plot above the solid line, the simulated values are higher than the measured values, and when the data points plot below the solid line, the simulated values are lower than the measured values. The dashed lines correspond to the desired range (calibration goal) of values about the equality line. The input parameter values are systematically varied to minimize the deviation about the line of equality while maximizing the data points within the target range about the line of equality.

Level 2 Calibration (Transient Conditions)

Details of the Level 2 calibration are described in the ATSDR TT Chapter C report by Faye and Valenzuela (2007). Calibration of the transient flow model was achieved using pumpage (Tables C8 and C9), water-level (Appendix C1, Tables C1.1– C1.11), and well capacity (Appendix C3, Tables C3.1– C3.10) data collected at Tarawa Terrace and vicinity (Faye and Valenzuela 2007). An indication of gross model calibration is shown in the scatter diagram of Figure 7.10. Paired data shown within the bottom half of the diagram generally correspond to water-supply well data. Paired data within the upper part of the diagram generally correspond to data listed. The average absolute difference between simulated and observed water levels for 789 paired water levels shown in Figure 7.10 is 5.2 ft. The root-mean-square error of the absolute differences is 7.0 ft.

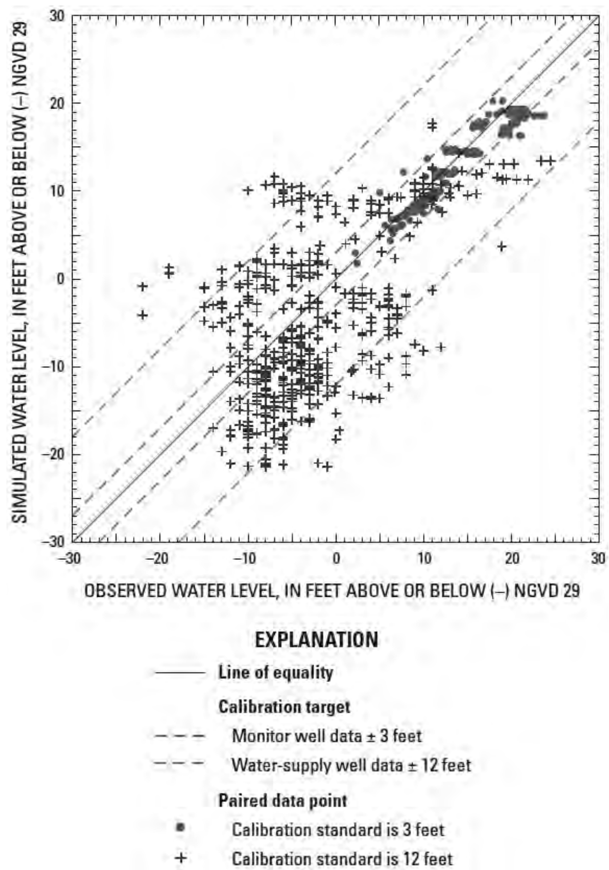


Figure 7.10. Simulated and observed transient water levels, Tarawa Terrace and vicinity (Faye and Valenzuela 2007).

Input parameters are calibrated to minimize deviations between simulated and observed elevations. It should be noted that four decades of data were available for this calibration (1951-1994). Figure 7.10 demonstrates that the groundwater flow model (calibration Levels 1 and 2) has been successfully calibrated to produce reconstructed values in close agreement with measured values. Table 7.8 lists the calibrated model parameter values used for simulating groundwater flow at TYT and vicinity.

Table **7.8**. Calibrated model parameter values used for simulating groundwater flow and contaminant fate and transport, Tarawa Terrace and vicinity (Faye 2008).

[ft/d, foot per day; ft^3/d, cubic foot per day; ft^3/g, cubic foot per gram; g/ft^3, gram per cubic foot; d^{-1}, 1/day; g/d, gram per day; ft, foot; ft^2/d, square foot per day; —, not applicable]

Model parameter[1]	Model layer number[2]						
	1	2	3	4	5	6	7
Predevelopment groundwater-flow model (conditions prior to 1951)							
Horizontal hydraulic conductivity, K_H (ft/d)	12.2–53.4	1.0	4.3–20.0	1.0	6.4–9.0	1.0	5.0
Ratio of vertical to horizontal hydraulic conductivity, K_V/K_H[3]	1:7.3	1:10	1:8.3	1:10	1:10	1:10	1:10
Infiltration (recharge), I_R (inches per year)	13.2	—	—	—	—	—	—
Transient groundwater-flow model, January 1951–December 1994							
Specific yield, S_y	0.05	—	—	—	—	—	—
Storage coefficient, S	—	4.0×10^{-4}	4.0×10^{-4}	4.0×10^{-4}	4.0×10^{-4}	4.0×10^{-4}	4.0×10^{-4}
Infiltration (recharge), I_R (inches per year)	6.6–19.3	—	—	—	—	—	—
Pumpage, Q_k (ft^3/d)	See footnote[4]	—	See footnote[4]	—	0	—	0
Fate and transport of tetrachloroethylene (PCE) model, January 1951–December 1994							
Distribution coefficient, K_d (ft^3/g)	5.0×10^{-6}	5.0×10^{-6}	5.0×10^{-6}	5.0×10^{-6}	5.0×10^{-6}	5.0×10^{-6}	5.0×10^{-6}
Bulk density, ρ_b (g/ft^3)	77,112	77,112	77,112	77,112	77,112	77,112	77,112
Effective porosity, n_E	0.2	0.2	0.2	0.2	0.2	0.2	0.2
Reaction rate, r (d^{-1})	5.0×10^{-4}	5.0×10^{-4}	5.0×10^{-4}	5.0×10^{-4}	5.0×10^{-4}	5.0×10^{-4}	5.0×10^{-4}
Mass-loading rate[5], $q_S C_S$ (g/d)	1,200	—	—	—	—	—	—
Longitudinal dispersivity, α_L (ft)	25	25	25	25	25	25	25
Transverse dispersivity, α_T (ft)	2.5	2.5	2.5	2.5	2.5	2.5	2.5
Vertical dispersivity, α_V (ft)	0.25	0.25	0.25	0.25	0.25	0.25	0.25
Molecular diffusion coefficient, D* (ft^2/d)	8.5×10^{-4}	8.5×10^{-4}	8.5×10^{-4}	8.5×10^{-4}	8.5×10^{-4}	8.5×10^{-4}	8.5×10^{-4}

[1] Symbolic notation used to describe model parameters obtained from Chiang and Kinzelbach (2001)

[2] Refer to Chapter B (Faye 2007) and Chapter C (Faye and Valenzuela 2007) reports for geohydrologic framework corresponding to appropriate model layers; aquifers are model layers 1, 3, 5, and 7; confining units are model layers 2, 4, and 6

[3] For model cells simulating water-supply wells, vertical hydraulic conductivity (K_V) equals 100 feet per day to approximate the gravel pack around the well

[4] Pumpage varies by month, year, and model layer; refer to Chapter K report (Maslia et al. In press 2008) for specific pumpage data

[5] Introduction of contaminant mass began January 1953 and terminated December 1984

Level 3 Calibration (Contaminant Fate and Transport)

The hydraulic characteristic and recharge arrays of the MODFLOW-96 flow model assigned following the Level 2 calibration were not adjusted during Level 3 calibration. Initial values of several transport parameters were modified during trial-and-error calibration and are described in the TT Chapter F report (Faye 2008). Final calibrated parameter values are listed in Table 7.8. Level 3 model calibration was achieved by comparing simulated PCE concentrations at TT water-supply wells to corresponding observed concentrations. Simulated PCE concentrations were computed at the end of each stress period and were considered representative of an average (mean) concentration for the respective month. Field data (observed PCE concentrations) were compared to the simulated concentration closest in time (days) to the simulated day.

Figure 7.11 shows a plot for simulated and observed PCE concentrations in TT water-supply wells (Level 3 calibration), demonstrating the ability of the contaminant migration (fate and transport) modeling to reproduce contaminant concentrations in the individual water-supply wells. In this graph, points plotting above the line of equality correspond to simulated values higher than measured values. In contrast, values plotting below the line represent simulated values lower than measured values. It is observed that the simulated concentrations tended to overestimate lower measured concentrations while underestimating the highest observed concentrations. Although model calibration could have resulted in a line of equality with more data points closer to equality, doing so would have meant that the highest simulated concentrations would have been underestimated even more. Thus, the Level 3 calibration minimized the overall deviations between measured and observed values.

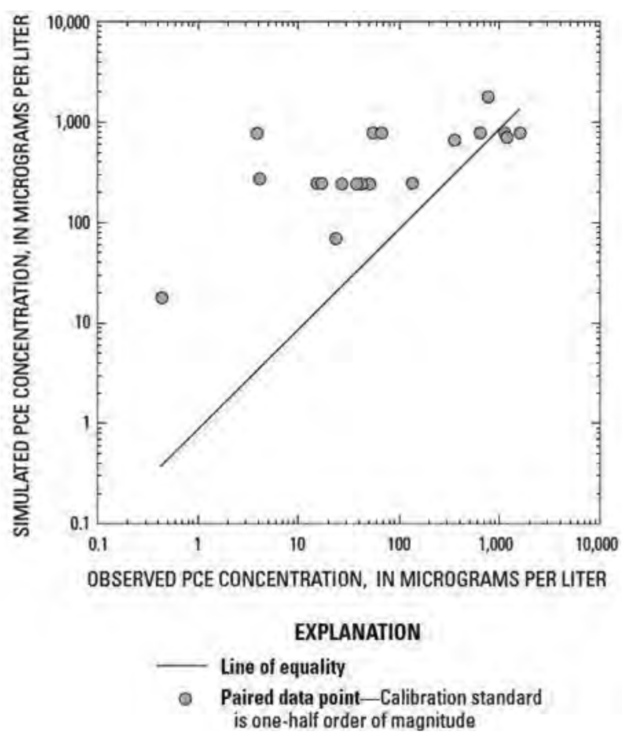


Figure 7.11. Simulated and observed tetrachloroethylene (PCE) concentrations at selected water-supply wells, Tarawa Terrace and vicinity (Faye 2008).

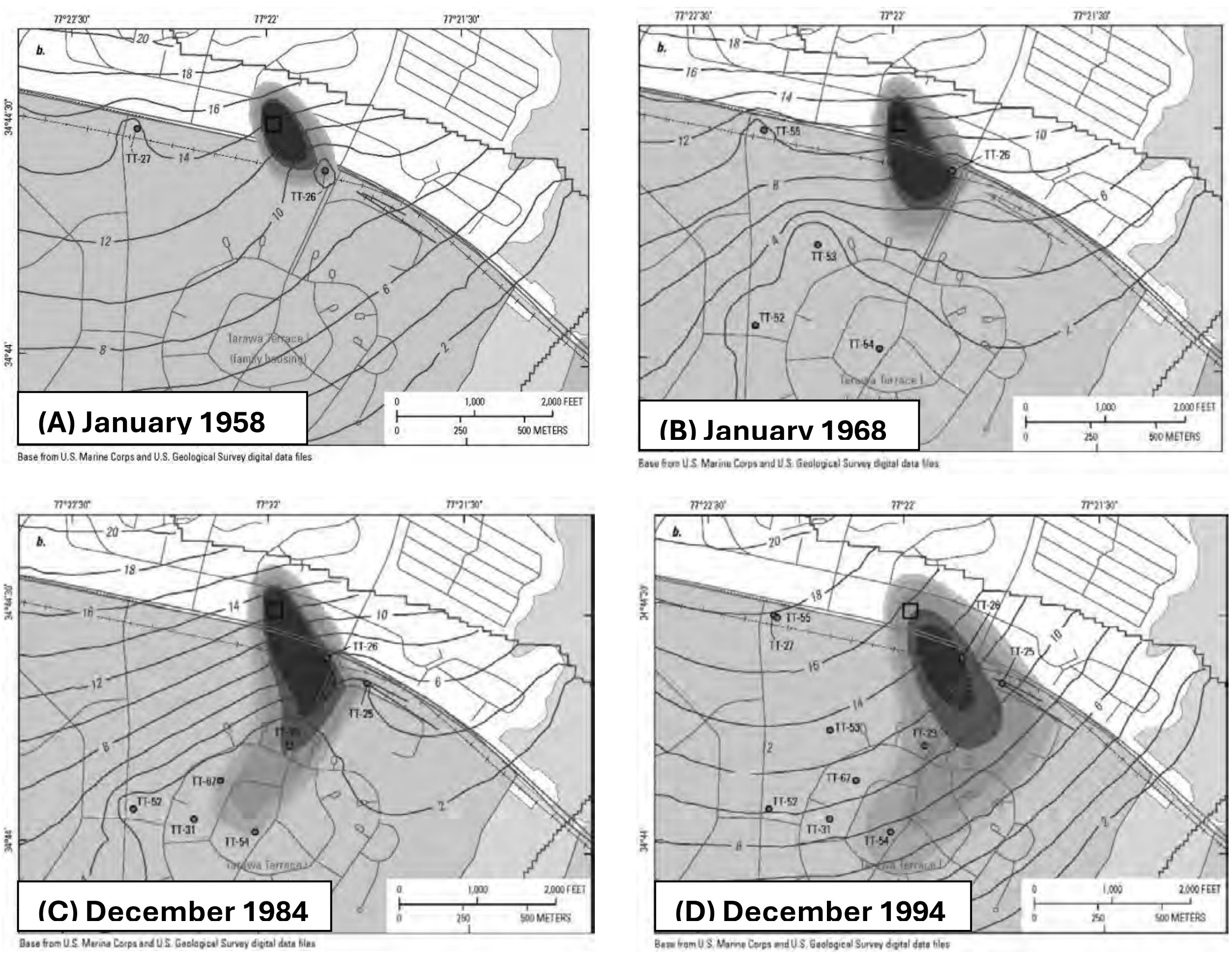
Table 7.9. Summary of reconstructed (simulated) values and observed data of tetrachloroethylene (PCE) at water-supply wells, Tarawa Terrace (Maslia et al. 2007).

[PCE, tetrachloroethylene; μg/L, microgram per liter; J, estimated; ND, nondetect]

Model-derived value		Observed data				
Month and year	PCE concentration, in μg/L	Sample date	PCE concentration, in μg/L	Detection limit, in μg/L	Calibration targets[2], in μg/L	Sample number[1]
		Supply well TT-23				
January 1985	254	1/16/1985	132	10	41.7–417	1
February 1985	253	2/12/1985	37	10	11.7–117	2
February 1985	253	2/19/1985	26.2	2	8.3–82.9	3
February 1985	253	2/19/1985	ND	10	1–10	4
March 1985	265	3/11/1985	14.9	10	4.7–47.1	5
March 1985	265	3/11/1985	16.6	2	5.2–52.5	6
March 1985	265	3/12/1985	40.6	10	12.8–128	7
March 1985	265	3/12/1985	48.8	10	15.4–154	8
April 1985	274	4/9/1985	ND	10	1–10	9
September 1985	279	9/25/1985	4J	2	1.3–12.6	10
July 1991	191	7/11/1991	ND	10	1–10	11
		Supply well TT-25				
February 1985	7.3	2/5/1985	ND	10	1–10	12
April 1985	9.6	4/9/1985	ND	10	1–10	13
September 1985	18.1	9/25/1985	0.43J	10	0.14–1.4	14
October 1985	20.4	10/29/1985	ND	10	1–10	15
November 1985	22.8	11/4/1985	ND	10	1–10	16
November 1985	22.8	11/12/1985	ND	10	1–10	17
December 1985	25.5	12/3/1985	ND	10	1–10	18
July 1991	72.7	7/11/1991	23	10	7.3–72.7	19
		Supply well TT-26				
January 1985	804	1/16/1985	1,580.0	10	500–4,996	20
January 1985	804	2/12/1985	3.8	10	1.2–12	21
February 1985	798	2/19/1985	64.0	10	20.2–202	22
February 1985	798	2/19/1985	55.2	10	17.5–175	23
April 1985	801	4/9/1985	630.0	10	199–1,992	24
June 1985	799	6/24/1985	1,160.0	10	367–3,668	25
September 1985	788	9/25/1985	1,100.0	10	348–3,478	26
July 1991	670	7/11/1991	350.0	10	111–1,107	27
		Supply well TT-30				
February 1985	0.0	2/6/1985	ND	10	1–10	28
		Supply well TT-31				
February 1985	0.17	2/6/1985	ND	10	1–10	29
		Supply well TT-52				
February 1985	0.0	2/6/1985	ND	10	1–10	30
		Supply well TT-54				
February 1985	6.0	2/6/1985	ND	10	1–10	31
July 1991	30.4	7/11/1991	ND	5	1–5	32
		Supply well TT-67				
February 1985	4.1	2/6/1985	ND	10	1–10	33
		Supply well RW1				
July 1991	0.0	7/12/1991	ND	2	1–2	34
		Supply well RW2				
July 1991	879	7/12/1991	760	2	240–2,403	35
		Supply well RW3				
July 1991	0.0	7/12/1991	ND	2	1–2	36

Selected Simulation Results: Tarawa Terrace

Examples of simulated results (reconstructed PCE concentrations) in groundwater for model layer 1 are shown as a series of maps (Figure 7.12 A–D) for January 1958, January 1968, December 1984, and December 1994, respectively. These maps show the areal spread of PCE within model layer 1 under the influence of pumping wells (Figure 7.12 A–C) and under no-pumping conditions (Figure 7.12D) once all water-supply wells were removed from service by March 1987. Table 7.9 lists a summary of reconstructed (simulated) values and observed data of PCE at TT water-supply wells.



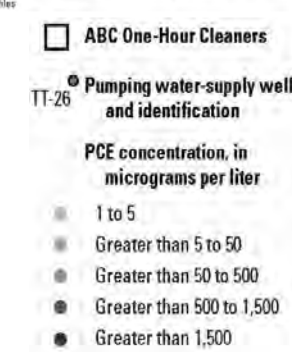


Figure 7.12. Reconstructed (simulated) distribution of tetrachloroethylene (PCE), model layer 1: (A) January 1958, (B) January 1968, (C) December 1984, and (D) December 1994 (Faye 2008).

January 1958

With the onset of simulated pumping at water-supply well TT-26 during January 1952, local cones of depression developed around all active supply wells (Figure 7.12A). In general, however, the flow is toward Northeast Creek and Frenchmans Creek. Under these flow conditions, PCE migrated southeast from its source at the site of ABC One-Hour Cleaners in the direction of water-supply well TT-26 (Figure 7.12A). The simulated PCE concentration at water-supply well TT-26 during January 1958 was about 29 µg/L.

January 1968

During January 1968 (Figure 7.12B), the designated start date of the epidemiological case-control study, groundwater flow in the northern half of the model domain was little changed from January 1958 conditions. In the immediate vicinity of the Tarawa Terrace I housing area, groundwater flow and water levels are affected by pumpage from water-supply wells TT-52, TT-53 and TT-54. Groundwater flow from the vicinity of TT-26 toward well TT-54 is particularly evident (Maslia et al. 2007, Figure A14). Under these flow conditions, PCE has migrated in a more southwardly direction from its source at the site of ABC One-Hour Cleaners toward water-supply well TT-54 (Figure 7.12B) and covers a greater spatial extent than during January 1958. By January 1968, the simulated concentration of PCE in water-supply well TT-26 was 402 µg/L.

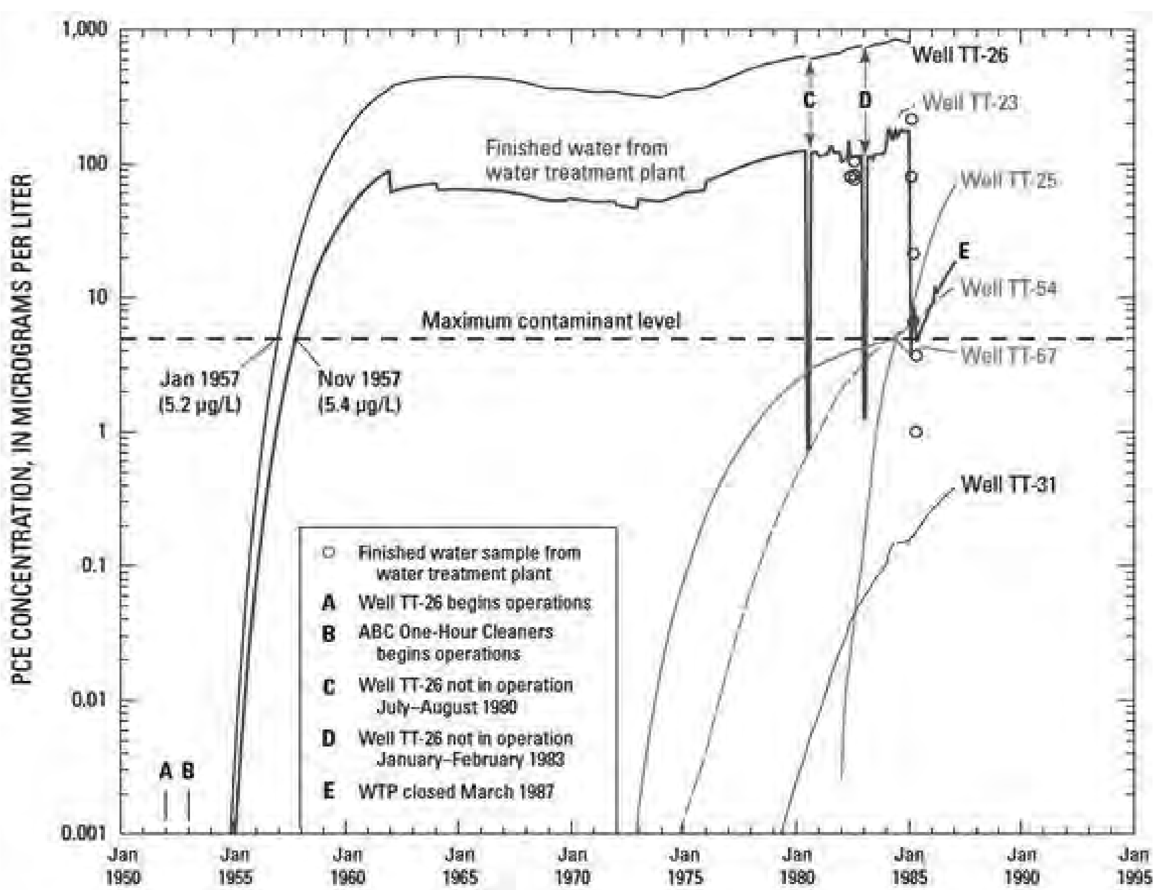
December 1984

Groundwater pumpage increased water-level declines during December 1984 (Figure 7.12C) in the vicinity of the Tarawa Terrace I housing area and probably accelerated the migration of PCE toward the vicinity of well TT-54. Between January 1968 and December 1984, the center of mass of PCE migrated generally southeastward from its source at the site of ABC One-Hour Cleaners, and the arm of the PCE plume migrated southwestward toward water-supply wells TT-23, TT-67, and TT-54 (Figure 7.12C). The areal extent of simulated PCE contamination has increased significantly from the areal extent of January 1958 and January 1968 (Figures 7.13A and 7.13B, respectively). By December 1984, the simulated concentration of PCE in water-supply wells TT-23, TT-25, and TT-26 was 255 µg/L, 6 µg/L, and 805 µg/L, respectively.

December 1994

Owing to documented PCE contamination in water samples obtained from the TT water-supply wells and the TTWTP (Tables 7.9 and 7.10), wells TT-23 and TT-26 were taken off-line during February 1985. The TTWTP was closed and pumping at all Tarawa Terrace water-supply wells was discontinued during March 1987 (Table 7.1 and Figure 7.2). As a result, potentiometric levels began to recover. By December 1994 (Figure 7.12D), the simulated potentiometric levels were nearly identical to predevelopment conditions of 1951 (Faye and Valenzuela 2007). Groundwater flow was from the north and northwest to the south and east, discharging to Northeast Creek. Groundwater discharge also occurs to Frenchmans Creek in the westernmost area of the model domain. TT water-supply wells shown in Figure 7.12D were not operating during December 1994 but are shown on this illustration for reference purposes.

A graph showing simulated concentrations of PCE at TT water-supply wells from the beginning of operations at ABC One-Hour Cleaners through the closure of the wells and the TTWTP is shown in Figure 7.13. Simulated PCE concentrations in water-supply well TT-26 exceeded the current MCL of 5 µg/L for PCE during January 1957 (simulated value is 5.2 µg/L) and reached a maximum simulated value of 851 µg/L during July 1984. The mean simulated PCE concentration in water-supply well TT-26 for its entire period of operation was 351 µg/L. The mean simulated PCE concentration for the period exceeding the current MCL of 5 µg/L—January 1957 to January 1985—was 414 µg/L (Table 7.11). This represents a duration of 333 months (27.7 years). These results are summarized in Table 7.11 along with simulated results for water-supply wells TT-23 and TT-25. It should be noted that although simulation results indicate several water-supply wells were contaminated with PCE (wells TT-23, TT-25, TT-31, TT-54, and TT-67–Table 7.9), by far, the highest concentration of PCE and the longest duration of contamination occurred in water-supply well TT-26 (Figure 7.13).



7.13. Concentration of tetrachloroethylene (PCE): (1) simulated at selected water-supply wells and in finished water at the water treatment plant and (2) measured in finished water at the water treatment plant, Tarawa Terrace (Maslia et al. 2007).

Table 7.10. Summary of reconstructed (simulated) values and observed data of tetrachloroethylene (PCE) at the water treatment plant, Tarawa Terrace (Maslia et al. 2007).

[PCE, tetrachloroethylene; µg/L, microgram per liter; J, estimated; ND, nondetect]

Model-derived value		Observed data				
Month and year	PCE concentration, in µg/L	Sample date	PCE concentration, in µg/L	Detection limit, in µg/L	Calibration targets, in µg/L[2]	Sample number[3]
May 1982	148	5/27/1982	80	10	25–253	1
July 1982	112	7/28/1982	104	10	33–329	2
July 1982	112	7/28/1982	76	10	24–240	3
July 1982	112	7/28/1982	82	10	26–259	4
January 1985	176	2/5/1985	80	10	25–253	5
January 1985	176	2/11/1985	215	10	68–680	6
February 1985	3.6	2/13/1985	ND	10	1–10	7
February 1985	3.6	2/19/1985	ND	2	1–2	8
February 1985	3.6	2/22/1985	ND	10	1–10	9
March 1985	8.7	3/11/1985	ND	2	1–2	10
March 1985	8.7	3/12/1985	6.6	10	2.1–21	11
March 1985	8.7	3/12/1985	21.3	10	6.7–67	12
April 1985	8.1	4/22/1985	1	10	0.3–3.2	13
April 1985	8.1	4/23/1985	ND	10	1–10	14
April 1985	8.1	4/29/1985	3.7	10	1.2–11.7	15
May 1985	4.8	5/15/1985	ND	10	1–10	16
July 1985	5.5	7/1/1985	ND	10	1–10	17
July 1985	5.5	7/8/1985	ND	10	1–10	18
July1985	5.5	7/23/1985	ND	10	1–10	19
July 1985	5.5	7/31/1985	ND	10	1–10	20
August 1985	6.0	8/19/1985	ND	10	1–10	21
September 1985	6.5	9/11/1985	ND	10	1–10	22
September 1985	6.5	9/17/1985	ND	10	1–10	23
September 1985	6.5	9/24/1985	ND	10	1–10	24
October 1985	7.1	10/29/1985	ND	10	1–10	25

Table 7.11. Summary statistics for reconstructed (simulated) tetrachloroethylene (PCE) contamination of selected water-supply wells and the water treatment plant based on calibrated

[MCL, maximum contaminant level; µg/L, microgram per liter; WTP, water treatment plant; PCE, tetrachloroethylene]

Water supply	Month and year and duration exceeding MCL[1]	Month and year of maximum value and maximum concentration, in µg/L	Average concentration,[2] in µg/L
TT-23	August 1984–April 1985 8 months[3]	April 1985 274	252
TT-25	July 1984–February 1987 32 months	February 1987 69	27
TT-26	January 1957–January 1985 333 months[4]	July 1984 851	414
WTP	November 1957–February 1987 346 months	March 1984 183	70

[1] Current MCL for PCE is 5 µg/L, effective date July 6, 1992 (40 CFR, Section 141.60, Effective Dates, July 1, 2002, ed.)

[2] For periods exceeding 5 µg/L when water-supply well was operating

[3] Water-supply well TT-23 was not operating during February 1985

[4] Water-supply well TT-26 was not operating July–August 1980 and January–February 1983

It is clear from the graph in Figure 7.13 that the Tarawa Terrace finished water (blue trace) mimicked the concentration of PCE at well TT-26 but at a lower level. The finished water trace indicated the concentration of PCE after all supply wells have been mixed at the TTWTP. TT-26's mixing with the uncontaminated wells in the supply field resulted in a reduction in concentration. See Tables 7.9 and 7.10 for comparisons of model-derived values and observed data of PCE at selected water-supply wells and the TTWTP, respectively.

Well TT-26

Based on calibrated model simulations, water- supply well TT-26 had the highest concentration of PCE- contaminated groundwater and the longest duration of PCE-contaminated groundwater with respect to any other Tarawa Terrace water-supply well (Figure 7.13). This is due to two reasons (1) its proximity to ABC One-Hour Cleaners source and (2) its total run time over the 1953 to 1987 time period.

Assessing Level 3 calibration results using MT3DMS discussed above, water-modeling staff relied on the measured water-quality sample data to compare with reconstructed (simulated) concentrations (Figure 7.14, Table 7.9). An additional assessment of the Level 3 calibration is to compare PCE mass remaining in the Tarawa Terrace and Upper Castle Haye aquifers calculated from field observations (Fay 2008, Table F11, p. F30) with MT3DMS calibrated mass computations, which represents PCE mass in all model layers for each pumping period. Most of the data used to calculate the quantity of PCE mass in solution summarized in Faye (2008, Table F11, p. F30), were collected between December 1991-April 1992 (Roy F. Weston, Inc. 1992, 1994). Algebraic manipulation of mass balance data computed for February 1992 indicates the remaining PCE mass in solution at that time equals 1.0 X 10^6 g. This simulated quantity of remaining PCE mass compares very favorably to the calculated quantity of PCE mass remaining in the Tarawa Terrace and Upper Castle Hayne aquifers of 1.5×10^6 g tabulated in Faye (2008, Table F11, p,. F30) using observed PCE concentrations (Roy F. Weston, Inc. 1992, 1994). It is quite remarkable that both numbers compare so favorably and is a confirmation of the concordance of model results (MT3DMS) with observed data. This is another indicator that reconstructed PCE concentrations (using the Level 3 calibration of MT3DMS) at Tarawa Terrace represent real-world conditions.

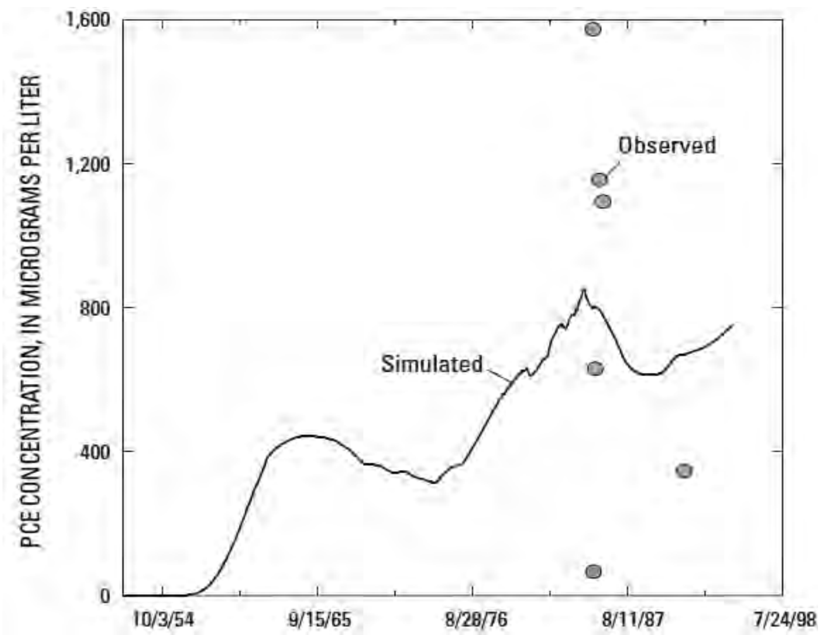


Figure 7.14. Reconstructed (simulated) and observed tetrachloroethylene (PCE) concentrations at water-supply well TT-26, Tarawa Terrace (Faye 2008).

Level 4 Calibration (Mixing Model)

The final level of model calibration employed a simple mixing (flow-weighted average) model to compute PCE concentrations delivered to the TTWTP from all operating water-supply wells and subsequently to the Tarawa Terrace water-supply distribution network. The model is based on the principles of continuity and conservation of mass (Masters 1998) and is used to compute the flow-weighted average concentration of PCE. For each stress period (month) of the simulation period (from January 1951 to December 1994), the PCE concentration simulated at each operating water-supply well is weighted by the respective well discharge to compute a weighted-mean PCE concentration. This weighted-mean concentration was considered the monthly mean PCE concentration delivered to the TTWTP. The results of these computations compared to an analysis of a water sample collected at a point in time, either at the TTWTP or at a location within the TT water-distribution system such as an outdoor or indoor faucet, are summarized in Table 7.12. The computed PCE concentration is compared to the observed PCE concentration on a same-month basis; that is, if a sample date was reported as May 1, 1982, then the corresponding computed PCE concentration was the weighted-mean concentration for the month of May 1982. Results of the reconstructed mean monthly PCE concentrations at the TTWTP are listed in **Appendix H1** (Column 3) for each stress period, January 1951–March 1987. Data listed in **Appendix H1** are from Maslia et a. (2007, Appendix A2).

Computations were accomplished for simulated pumpage and PCE concentrations for all 528 stress periods and are plotted in Figure 7.13 (the blue line representing the reconstructed mean monthly PCE concentrations at the TTWTP). Computed breakthrough of PCE at the MCL concentration of 5 µg/L occurs at the TTWTP about October or November 1957 and, except when water-supply well TT-26 was temporarily removed from service, continues above 40 µg/L from about December 1959 until the termination of operations at well TT-26 during February 1985. The precipitous declines in PCE concentration noted in Figure 7.13 represent periods when well TT-26 was temporarily removed from service during July and August 1980 and January and February 1983. The last decline in PCE concentration corresponds to the final removal of well TT-26 from service. The points indicating "observed" PCE concentrations on Figure 7.13 correspond to the numerical concentrations listed in Table 7.10.

Table 7.12 summarizes simulated and observed PCE water treatment plant concentrations at the TTWTP. In Table 7.12, the measured PCE concentrations ranged from 215 µg/L to non-detect (detection limits of 2-10 µg/L). For the same period, model predictions of PCE concentrations at the TTWTP ranged from 176 µg/L to 3.6 µg/L (Table 7.12). This close agreement between simulated and measured values supports the collective ability of the four-stage modeling and calibration process to capture the Tarawa Terrace water-distribution system behavior accurately.

The results shown in Figure 7.13 and Table 7.12 represent the calibrated model being compared to a separate dataset than that used for the calibration of the model (Figure 7.14). The observed data used for calibration included all available geologic data, supply well characteristics and observed well contaminate values. The observed values in Figure 7.13 represent the measured concentrations taken at both the TTWTP and at other locations in the TT water-distribution system. It is important to note these **observed values were not used in the calibration process** and therefore represent an additional set of observed (field) data by which to assess the "goodness of fit" of the four-level, hierarchical calibration process.

Table 7.12. Computed and observed tetrachloroethylene (PCE) concentrations in water samples collected at the Tarawa Terrace water treatment plant and calibration target range, Tarawa Terrace (from Fay 2008).

[µg/L, microgram per liter; TTWTP, Tarawa Terrace water treatment plant; ND, not detected]

Date	PCE concentration, in µg/L		Calibration target range, in µg/L
	Computed[1]	Observed	
[2]TTWTP Building TT-38			
5/27/1982	148	180	25–253
7/28/1982	112	[3]104	33–329
7/28/1982	112	[3]76	24–240
7/28/1982	112	[3]82	26–259
2/5/1985	176	[3,4]80	25–253
2/13/1985	3.6	[5]ND	0–10
2/19/1985	3.6	[6]ND	0–2
2/22/1985	3.6	[5]ND	0–10
3/11/1985	8.7	[6]ND	0–2
3/12/1985	8.7	[6,7]6.6	2.1–21
3/12/1985	8.7	[6,8]21.3	6.7–67
4/22/1985	8.1	[5]1	0.3–3.2
4/23/1985	8.1	[5]ND	0–10
4/29/1985	8.1	[3]3.7	1.2–11.7
5/15/1985	4.8	[5]ND	0–10
7/1/1985	5.5	[5]ND	0–10
7/8/1985	5.5	[5]ND	0–10
7/23/1985	5.5	[5]ND	0–10
7/31/1985	5.5	[5]ND	0–10
8/19/1985	6.0	[5]ND	0–10
9/11/1985	6.0	[5]ND	0–10
9/17/1985	6.0	[5]ND	0–10
9/24/1985	6.0	[5]ND	0–10
10/29/1985	6.0	[5]ND	0–10
[2]TTWTP Tank STT-39			
2/11/1985	176	[5]215	0–10

[1]Weighted-average computation
[2]See Plate 1, Chapter A report, for location (Maslia et al. 2007)
[3]Detection limit is unknown
[4]Analysis of tap water sample for Tarawa Terrace, address unknown
[5]Detection limit = 10 µg/L
[6]Detection limit = 2 µg/L
[7]Sample collected downstream of TTWTP reservoir after operating well TT-23 for 24 hours
[8]Sample collected upstream of TTWTP reservoir after operating well TT-23 for 22 hours

To build further confidence in the four-level calibration for TT and to assess model uncertainty, a multiphase, multispecies finite-element model, TechFlowMP (Jang and Aral 2005, 2008), developed by ATSDR's University Partner, MESL, was run using the calibrated parameter values from MODFLOW-96 and MT3DMS (Table 7.8). Unlike MT3DMS that simulated contaminant fate and transport in the saturated zone for a single contaminant that does not undergo degradation, TechFlowMP can simulate flow in the unsaturated zone (above the water table), in the saturated zone (below the water table), the degradation of PCE (into TCE, 1,2-tDCE, and VC), and the loss of PCE by accounting for volatilization. Reconstructed (simulated) concentrations of PCE and its degradation products (TCE, 1,2-tDCE, and VC) for each stress period (month), January 1951–March 1987 are listed **Appendix H1** (Columns 4–7) alongside the reconstructed PCE concentrations simulated by MT3DMS for PCE that is not degraded or volatilized (**Appendix H1**, Column 3). Results of the two modeling approaches are also compared in graphs in Maslia et al. (2007, Figure A19, p. A43). As would be expected, the reconstructed PCE concentrations simulated using TechFlowMP are slightly lower than those simulated by MT3DMS because PCE mass is degraded to TCE, 1,2-tDCE, and VC by TechflowMP. In addition, PCE mass is lost (destroyed) in TechflowMP because it simulates volatilization within the unsaturated zone. If one sums the concentrations of PCE, TCE, 1,2-tDCE, and VC for a given month from TechFlowMP (**Appendix H1**, Columns 4–7), they should be approximately near the PCE concentrations reconstructed using MT3DMS (**Appendix H1**, Column3). This very close agreement between two different contaminant fate and transport models, solving two different transport equations (to assess model uncertainty) provides additional evidence and confidence that the reconstructed concentrations at the TTWTP represent "real world" conditions.

Post-Audit of the Tarawa Terrace Models

Additional confidence in groundwater-flow and contaminant fate and transport models can be assessed by conducting a "**post-audit**." A post-audit uses calibrated model parameter values (e.g., Table 7.8) and extends the model out to another time wherein additional and sufficient observation data are available. Jones and Davis (2024) conducted a post-audit with the TT groundwater-flow and contaminant fate and transport models by extending the TT simulations for the time 1995–2008, where ample PCE remediation data for ABC One-Hour Cleaners was available. Their conclusions were, "*In summary, the extended model demonstrates that the original model was developed using sound methods, and the model remains a reliable tool for understanding the general trends of contaminant migration in the Tarawa Terrace region. Based on this post-audit, we can find no significant evidence that would invalidate the analyses performed by ATSDR with the original model*." Details and results of the post-audit (Jones and Davis 2024) are provided **in Appendix O**.

Uncertainty

Models and associated calibrated parameters described previously are inherently uncertain because they are based on limited data. Under such circumstances, good modeling practice requires that evaluations be conducted to ascertain the confidence in models by assessing uncertainties associated with the modeling process and with the outcomes attributed to models (Saltelli et al. 2000). With respect to model simulations at TT, the availability of data to thoroughly characterize and describe model parameters and operations of water-supply wells was considerably limited, which gave rise to the following questions:

1. Could alternative water-supply well operating schedules or combinations of model parameter values provide acceptable simulation results when compared to observed data and previously established calibration targets?

2. What is the reliability of the historically reconstructed estimates of PCE concentration determined using the calibrated models (for example, results shown in Figure 7.13 and Table 7.10)?

To answer these questions and address the over-arching issues of model and parameter variability and uncertainty, three analyses were conducted using the calibrated groundwater-flow and contaminant fate and transport models described in Faye and Valenzuela (2007) and Faye (2008), respectively. These analyses were: (1) an assessment of pumping schedule variation at TT water-supply wells with respect to contaminant arrival times and concentrations, (2) sensitivity analysis, and (3) probabilistic analysis.

Water-Supply Well Scheduling Analysis

The scheduling and operation histories of TT water-supply wells directly affected times and concentrations of PCE in groundwater at wells and at the WTP during 1952–1987. Thus, simulated water-supply well operations could be a major cause and contributor to uncertainty and variability with respect to PCE arrival and PCE concentrations at water-supply wells and in finished water at the TTWTP. To assess the impact of pumping schedule variability and uncertainty on groundwater-flow, contaminant fate and transport, and WTP mixing models, a procedure was developed that combined groundwater simulation models and optimization methods.

The simulation tool developed for this analysis—PSOpS (Table 7.2)—combines the MODFLOW-96 and MT3DMS groundwater simulators with a rank-and-assign optimization method developed specifically for the TT analysis. This tool optimizes pumping (operational) schedules to minimize or maximize the arrival time of contaminants at water-supply wells. Based on the optimized operational schedules, the concentration of a contaminant is recalculated, and the effect of pumping schedule variation on contaminant concentration and the arrival time of groundwater exceeding the current MCL of PCE (5 µg/L) are evaluated. Details of the water-supply well analysis are provided in Wang and Aral (2008) and are summarized in Maslia et al. (2007, p. A47). PSOpS simulations demonstrated that the current MCL for PCE (5 µg/L) would have been exceeded in finished drinking water from the Tarawa Terrace WTP as early as December 1956 and no later than June 1960 (Maslia et al. 2007, Figure A21, p. A48)

Sensitivity Analysis

Sensitivity analysis is a method used to ascertain the dependency of a given model output (for example, water level or concentration) upon model input parameters (for example, hydraulic conductivity, pumping rate, and mass loading rate). Sensitivity analysis is important for checking the quality of the calibration of a given model, as well as a powerful tool for checking the robustness and reliability of model simulations. Thus, sensitivity analysis provides a method for assessing relations between information provided as input to a model—in the form of model input parameters—and information produced as output from the model. Maslia et al. (2007, p. A50) describe and discuss details of varying 7 groundwater-flow model parameter values and 7 contaminant fate and transport model parameter values and list the results in Table A14 (Maslia et al. 2007, p. A51).

Probabilistic Analysis

A probabilistic analysis is used to generate uncertainties in model inputs (e.g., hydraulic conductivity or contaminant source mass loading rate) so that estimates of uncertainties in model outputs (e.g., water level or PCE concentration in groundwater) can be made. Although the sensitivity analysis provided some insight into the relative importance of selected model parameters, a probabilistic analysis provides quantitative insight about the range and likelihood (probability) of model outputs. Thus, one purpose of a probabilistic analysis is to assist with understanding and characterizing variability and uncertainty of model output (Cullen and Frey 1999). Several methods are available for conducting a probabilistic analysis. These methods can be grouped as follows: (1) analytical solutions for moments, (2) analytical solutions for distributions, (3) approximation methods for moments, and (4) numerical methods. The probabilistic analysis conducted on the TT models used numerical methods—Monte Carlo simulation (MCS) and sequential Gaussian simulation (SGS)—to assess model uncertainty and parameter variability.

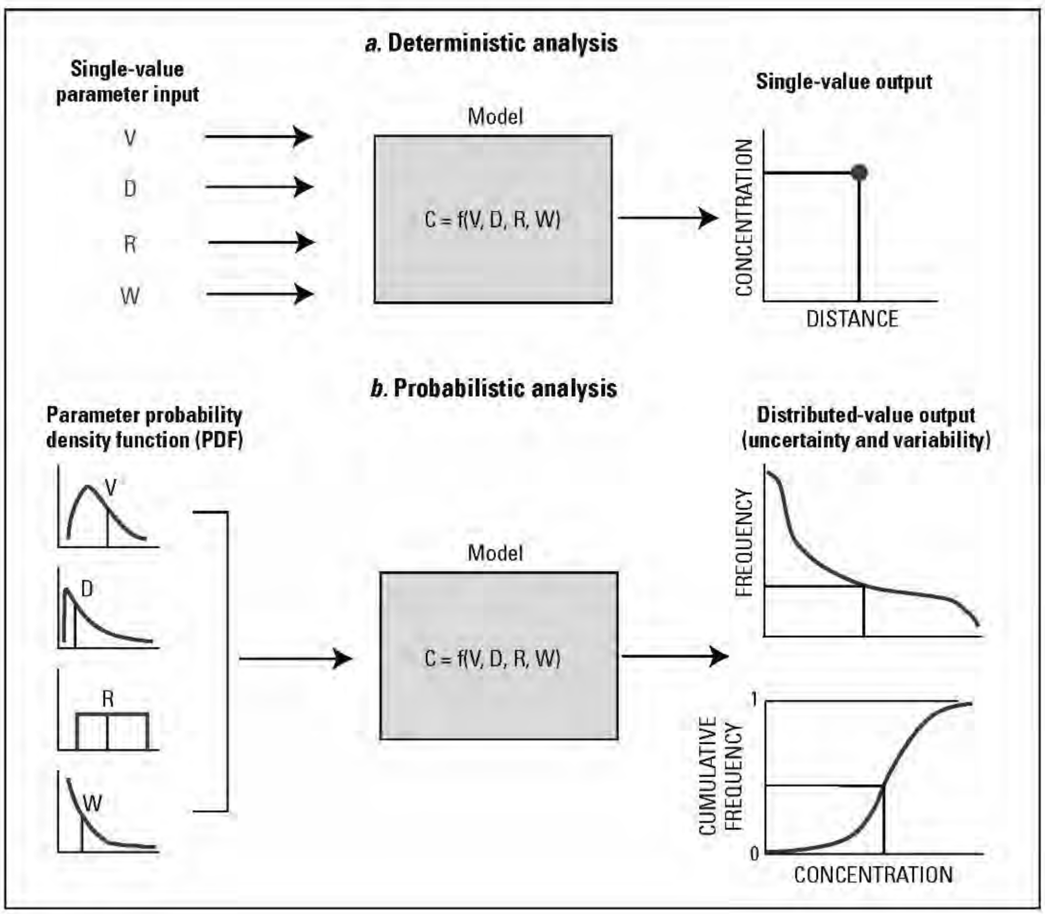


Figure 7.15. Conceptual framework for (a) a deterministic analysis and (b) a probabilistic analysis (from Maslia and Aral 2004).

Before proceeding with the probabilistic analysis applied to the TT models, it is important to understand the conceptual difference between the deterministic modeling analysis approach used to calibrate groundwater-flow (Faye and Valenzuela 2007) and fate and transport (Faye 2008) model parameter values and a probabilistic analysis. As described in Maslia and Aral (2004), with respect to the approach referred to as a deterministic modeling analysis, **single-point values** are specified for model input parameters and results are obtained in terms of **single-valued output**, for example, the concentration of PCE. This approach is shown conceptually in Figure 7.15*a*. In a probabilistic analysis, input parameters (all or a selected subset) of a particular model (for example, contaminant fate and transport) may be characterized in terms of **statistical distributions** that can be generated using the MCS method (USEPA 1997, Tung and Yen 2005) or the SGS method (Deutsch and Journel 1998, Doherty 2005). Results are obtained in terms of **distributed-value output** that can be used to assess model uncertainty and parameter variability as part of the probabilistic analysis (Figure 7.15*b*). MCS is a computer-based (numerical) method of analysis that uses statistical sampling techniques to obtain a probabilistic approximation to the solution of a mathematical equation or model (USEPA 1997). The MCS method is used to simulate probability density functions (PDFs). PDFs are mathematical functions that express the probability of a random variable (or model input) falling within some interval. SGS is a process in which a field of values (such as horizontal hydraulic conductivity) is obtained multiple times assuming the spatially interpolated values follow a Gaussian (normal) distribution. Additional details pertaining to the SGS methodology are provided in Deutsch and Journel (1998) and Doherty (2005).

The probabilistic analysis conducted using MCS was applied to the entire period of operation of the TTWTP (January 1953–February 1987). The PCE concentration in finished water determined using the deterministic analysis (single-value parameter input and output; Figure 7.13, **Appendix H2**-Column 3) also can be expressed and presented in terms of a range of probabilities for the entire duration of WTP operations. Water-supply well pumping variation and uncertainty could have a significant impact on contaminated groundwater delivered to the TTWTP. For example, Figure 7.16a shows a comparison of the calibrated pumping schedule for well TT-26 (Faye and Valenzuela 2007) with a pumping schedule generated using a Gaussian pseudo-random number generator (PRNG) and MCS.[9] (See Maslia et al. 2009b for specific details).

To assess pumping schedule uncertainty (like that shown in Figure 7.16a for well TT-26), two MCSs were conducted. In scenario 1, pumping uncertainty was excluded (i.e., the calibrated pumping schedules were used [red line in Figure 7.16a]); in scenario 2, pumping uncertainty was included (a randomly generated pumping schedule for well TT-26 shown by the blue lines in Figure 7.16a).

[9] A pseudo-random number generator (PRNG) is an algorithm for generating a sequence of numbers that approximates the properties of random numbers. These approximate random numbers can be used in MCS to generate a probability density function, such as a normal or log-normal distribution.

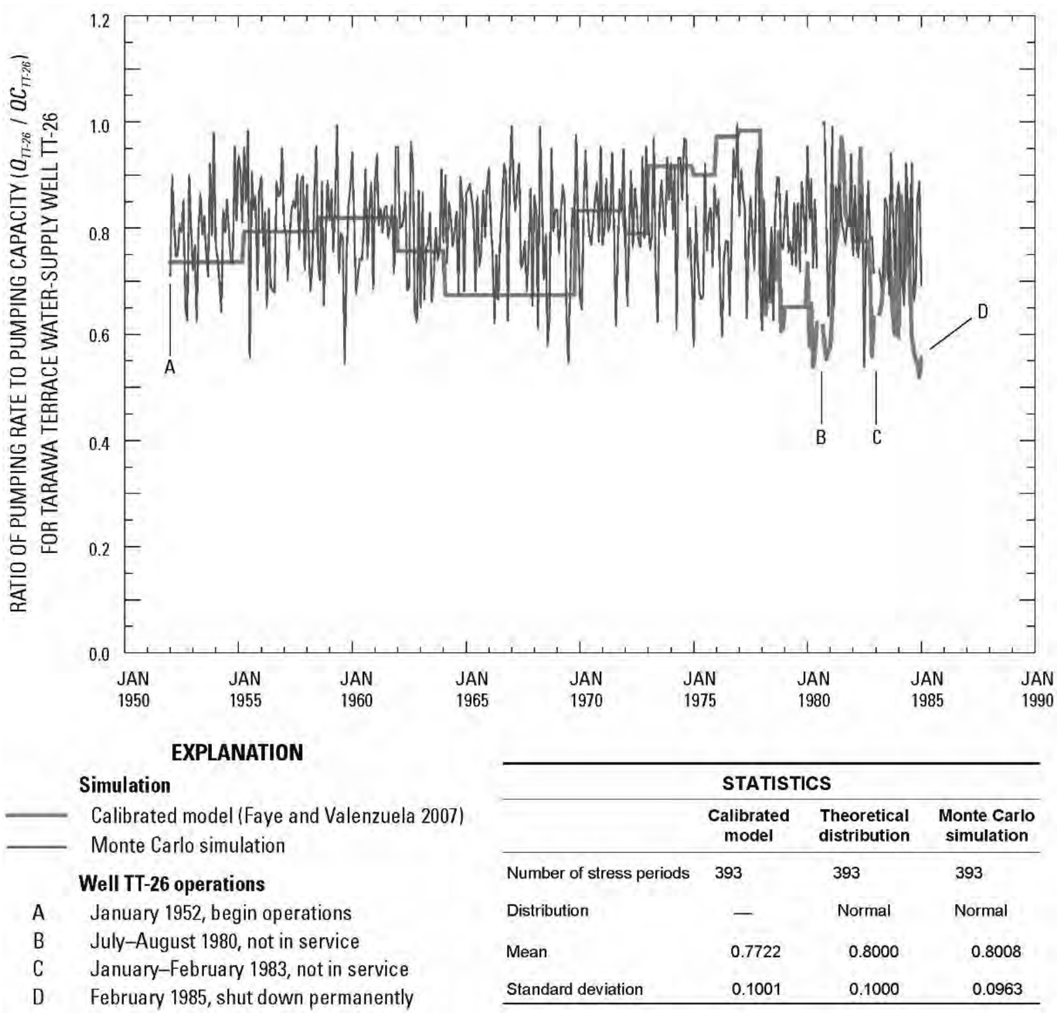


Figure 7.16a. Ratio of pumping rate to pumping capacity ($Q_{TT\text{-}26}$ / $QC_{TT\text{-}26}$) for water-supply well TT-26 for calibrated model and Monte Carlo simulation, Tarawa Terrace (Maslia et al. 2009b).

The concentration of PCE in finished water at the TTWTP is shown in Figure 7.16b, considering the following conditions:

(a) calibrated (reconstructed) PCE concentrations simulated using MT3DMS (blue line in Figure F.16b; **Appendix H2**–Column 3),
(b) pumping uncertainty excluded (scenario 1, yellow band in Figure 7.16b (**Appendix H2**-Scenario 1, Columns 4–6), and
(c) pumping uncertainty included (scenario 2, red lines in Figure 7.16b (**Appendix H2**-Scenario 2, Columns 7–9).

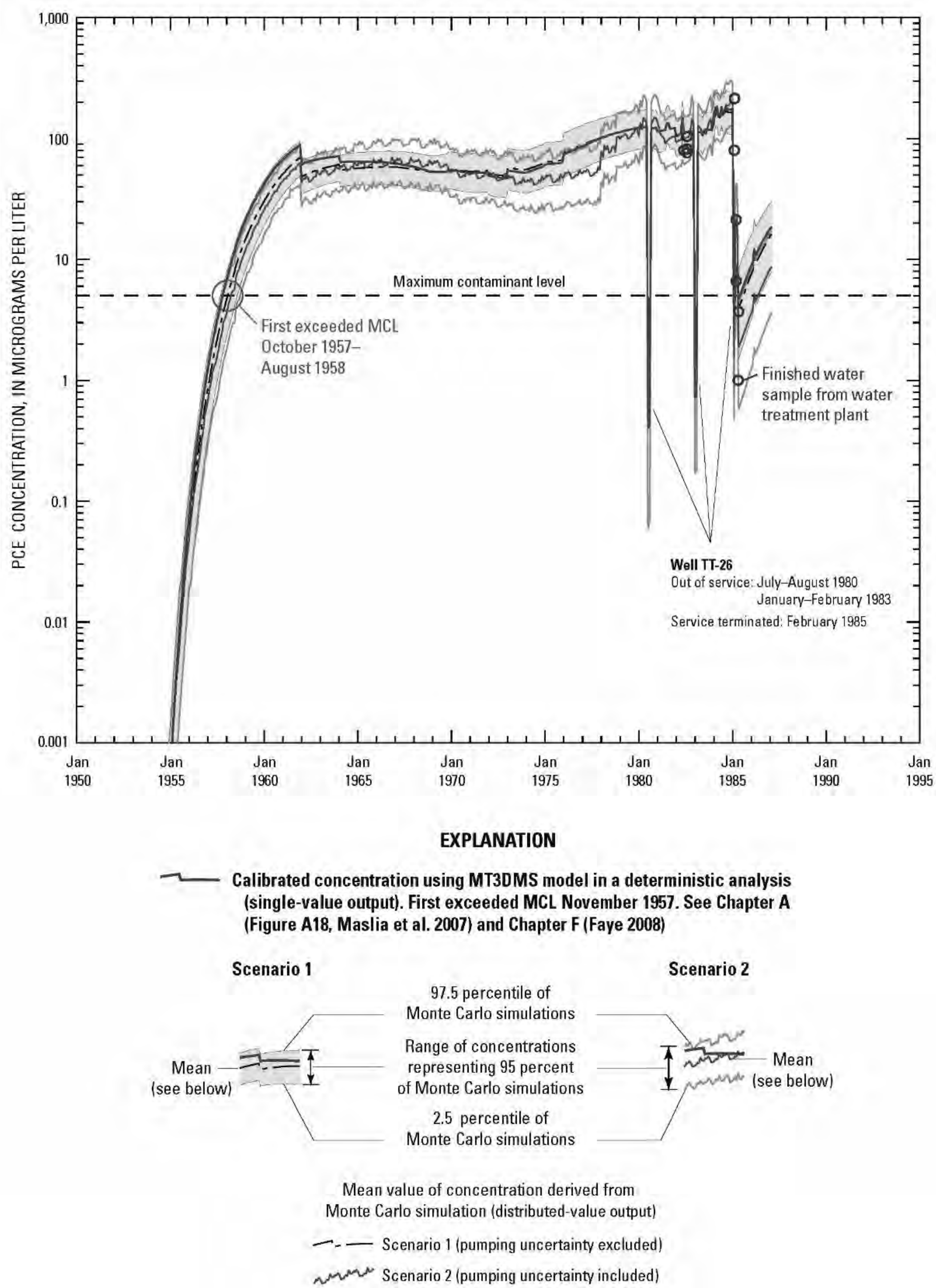


Figure 7.16b. Concentrations of tetrachloroethylene (PCE) in finished water at the water treatment plant derived from the calibrated MT3DMS model, probabilistic analysis using Monte Carlo simulation for scenario 1 (pumping uncertainty excluded) and scenario 2 (pumping uncertainty included), Tarwa Terrace study area (Maslia et al. 2009b).

The probabilistic results shown in Figure 7.16b (derived from MCS and MT3DMS) represent a range of concentrations representing 95% percent of Monte Carlo simulations. Therefore, we now have established a lower confidence level (LCL) and an upper confidence level (UCL), which are represented by the 2.5 percentile and 97.5 percentile, respectively, of Monte Carlo simulations. Two examples, in reference to **Appendix H2** (digital output used to construct Figure 7.16b) are now looked at in detail.

- **January 1968 (stress period 205)**: the calibrated (reconstructed) PCE concentration in finished water at the TTWTP is 58 μg/L (**Appendix H2**-Column 3). Under scenario 1 (pumping uncertainty excluded, the LCL ($P_{2.5}$) concentration is 39 μg/L and the UCL ($P_{97.5}$) is 76 μg/L. Under scenario 2 (pumping uncertainty included), the LCL ($P_{2.5}$) concentration is 41 μg/L and the UCL ($P_{97.5}$) is 98 μg/L. The range of concentrations between the LCL ($P_{2.5}$) and UCL ($P_{97.5}$) represent 95% of the MCSs, or a 95% confidence that for January 1968, PCE concentration in finished water at the TTWTP would lie between the LCL and UCL range.

- **December 1984 (stress period 408)**: the calibrated (reconstructed) PCE concentration in finished water at the TTWTP is 173 μg/L (**Appendix H2**-Column 3). Under scenario 1 (pumping uncertainty excluded, the LCL ($P_{2.5}$) concentration is 108 μg/L and the UCL ($P_{97.5}$) is 246 μg/L. Under scenario 2 (pumping uncertainty included), the LCL ($P_{2.5}$) concentration is 128 μg/L and the UCL ($P_{97.5}$) is 301 μg/L. The range of concentrations between the LCL ($P_{2.5}$) and UCL ($P_{97.5}$) represent 95% of the MCSs, or a 95% confidence that for December 1984, PCE concentration in finished water at the TTWTP would lie between the LCL and UCL range.

Four points are worth noting about the probabilistic uncertainty analysis results:

1. In a world without any uncertainty, the calibrated mean monthly finished water PCE concentrations (**Appendix H2**-Column 3) would equal the P_{50} values, or 50 percentile MCSs (**Appendix H2**-Columns 5 and 8). Because there is uncertainty, the calibrated mean monthly PCE concentrations values at the TTWTP are close to the P_{50} values obtained from MCS, but not necessarily equal in value.
2. The bands in Figure 7.16b (and tabular values in **Appendix H2**), demonstrate that uncertainty ranges within a factor of about 3 for any given month, providing additional confidence in the reconstructed mean monthly PCE concentrations at the TTWTP.
3. In Figure 7.16b, every observed data point falls within the banded regions of the MCSs. This is quite remarkable that calibrated and MCS-derived monthly PCE values compare so favorably with observed (measured) PCE values at the TTWTP and is a confirmation of the concordance of model results with observed data (even under uncertainty). This is another indicator that reconstructed PCE concentrations represent real-world conditions at Tarawa Terrace.
4. The PCE concentration in TTWTP finished water during January 1985, simulated using the probabilistic analysis, ranges from 110–251 µg/L (pumping uncertainty excluded, 95 percent of Monte Carlo simulations) and 123–293 µg/L (pumping uncertainty included) . These ranges include the maximum calibrated value of 183 µg/L (derived without considering uncertainty and variability using MT3DMS [Faye 2008]) and the maximum measured value of 215 µg/L (Table 7.8).

Therefore, these probabilistic analysis results—obtained by using MCS—instill confidence in the historically reconstructed PCE concentrations that were delivered to residents of Tarawa Terrace in finished water from the TTWTP.

In summary, effects of parameter uncertainty and variability were analyzed using three approaches—water-supply well scheduling analysis, sensitivity analysis, and probabilistic analysis. Individually and combined, these analyses demonstrate the high reliability of and confidence in results determined using the calibrated MODFLOW-96 and MT3DMS models. The probabilistic analysis conducted using the combination of MODFLOW-2K, MT3DMS, MCS, SGS and PRNG, provides a tool to address issues of parameter uncertainty and variability with respect to the concentration of PCE in finished water delivered from the TTWTP to residents of family housing at Tarawa Terrace and vicinity.

Conclusions Regarding Tarawa Terrace

Based on field data, modeling results, and the historical reconstruction process, the following conclusions are made with respect to drinking-water contamination at Tarawa Terrace:

- Simulated PCE concentrations exceeded the current MCL of 5 µg/L at water-supply well TT-26 for 333 months—January 1957–January 1985; the maximum simulated PCE concentration was 851 µg/L; the maximum measured PCE concentration was 1,580 µg/L during January 1985.
- Simulated PCE concentrations exceeded the current MCL of 5 µg/L in finished water at the TTWTP for 346 months—November 1957–February 1987; the maximum simulated PCE concentration in finished water was 183 µg/L; the maximum measured PCE concentration in finished water was 215 µg/L during February 1985.
- Simulation of PCE degradation by-products—TCE, 1,2-tDCE, and VC—indicated that maximum concentrations of the degradation by-products generally were in the range of 10 –100 µg/L at water-supply well TT-26; measured concentrations of TCE and 1,2-tDCE on January 16, 1985, were 57 and 92 µg/L, respectively.
- Maximum concentrations of the degradation by-products in finished water at the TTWTP generally were in the range of 2–15 µg/L; measured concentrations of TCE and 1,2-tDCE on February 11, 1985, were 8 and 12 µg/L, respectively.
- Monthly mean reconstructed concentrations at the TTWTP for the entire historical period included with this report as **Appendix H1** (single-specie and multi-species PCE) and **Appendix H2** (probabilistic analysis using MCS) represent, within reasonable scientific and engineering certainty, the contaminant levels in finished water from 1953 to 1987.
- In addition to assurances in model reliability afforded by ATSDR's probabilistic and uncertainty analysis, the results of a post-audit using remediation data for ABC One-Hour Cleaners (1995–2008) instill further confidence in the TT models. (See report of Dr. Norman Jones and Jeff Davis in **Appendix O)**.

PCE concentrations in finished water at the TTWTP exceeding the current MCL of 5 µg/L could have been delivered as early as December 1956 and no later than December 1960. Concentrations of PCE in finished water at the TTWTP were also reconstructed under a probabilistic uncertainty analysis using a two-stage Monte Carlo simulation. Details pertinent to the two-stage MCS are provided in Maslia and Aral (2004, p. 185-186), Maslia et al. (2007, 2009b). Typically, 500, 1,000, or 10,000 MCS runs are conducted to get a sense of the variation and uncertainty of model parameters and output. These results are shown graphically in Figure 7.16. Based on probabilistic analyses, the most likely dates that finished water first exceeded the current MCL ranged from October 1957 to August 1958 (95 percent probability), with an average (most likely) first exceedance date of November 1957. Exposure to PCE and PCE degradation by-products from contaminated drinking water ceased after February 1987; the TTWTP was closed March 1987 (Table 7.1).

7.5.2 Hadnot Point (HP)

The Hadnot Point area represented a far more complex analysis than for Tarawa Terrace. HP had multiple locations and multiple contaminant sources compared to the single source at TT (ABC One-Hour Cleaners). Contaminants for HP were PCE (PCE degradation products), TCE, and benzene (BTEX). These contaminants were found in multiple locations such as the Hadnot Point landfill (HPLF; PCE and TCE), the Hadnot Point Industrial Area (HPIA; PCE, TCE, and benzene), and the Hadnot Pont fuel farm (HPFF; benzene), which is located within the HPIA. Tables A4 and A5 in Maslia et al. (2013, p. A21–A22) lists contaminant data with detections of PCE, TCE, 1,1-DCE, 1,2-tDCE, 1,2-cDcE, VC, and benzene in water-supply wells for the HP-HB study area. An extensive effort was put into the identification and documentation of source areas, timelines, primary contaminants, and location of major dissolved sources for the HP area, and these data are listed in Table 7.13. There are substantially more sources in the HP area than at TT (one source), making data analysis and historical reconstruction substantially more complex. The areal distribution of contaminant sources and impacted water-supply wells in the HP area are shown in Figure 7.17.

Calibration of models for the HP-HB area used a similar hierarchical, 4-level approach, previously described for the TT models, namely: (1) predevelopment (steady or nonpumping) groundwater-flow conditions, (2) transient (time varying or pumping) groundwater-flow conditions, (3) the fate and transport (migration) of VOCs (PCE, TCE, and benzene) from their sources at the HPIA, HPLF , and HPFF areas to HP water-supply wells, and (4) comparing measured concentrations of VOCs in finished water at the HPWTP with the flow-weighted mixing model concentrations. Because of multiple sources, additional analysis methods and modeling approaches were used for the HP area. The following ATSDR reports contain specific details pertinent to the different modeling approaches and calibration results:

- Three-dimensional groundwater flow (predevelopment and transient)—described in Suárez-Soto et al. (2013),
- Three-dimensional contaminant fate and transport of PCE, TCE, and benzene in the vicinities of the HPIA and HPLF area—described in Jones et al. (2013),
- Linear control theory methodology to reconstruct contaminant concentrations of PCE, TCE, 1,2-tDCE, and VC in water-supply well HP-651—described in Guan et al. (2013),
- Dissolution of benzene from an LNAPL source area and subsequent three-dimensional fate and transport of dissolved-phase benzene in the HP Industrial Area—described in Jang et al. (2013), and
- Distribution of finished water from the HPWTP to the HB water-distribution system—described in Sautner et al. (2013b).

Table 7.13. Identification of documented source areas, primary contaminants, and location of major dissolved-phase sources, Hadnot Point area (Figure references are to the Chapter A report [Maslia et al. 2013]).

[HPFF, Hadnot Point fuel farm; UST, underground storage tank; AS/SVE; air sparging/soil vapor extraction; MW, monitor well; µg/L, microgram per liter; gal, gallon; LUST, leaking underground storage tank; CERCLA, Comprehensive Environmental Response, Compensation, and Liability Act of 1980; TCE, trichloroethylene; PCE, tetrachloroethylene]

[1] Source-area timeline [reference documents]	Primary contaminant; number of major sources	Location of major dissolved-phase sources
Hadnot Point Industrial Area (see Figure A13)		
Hadnot Point fuel farm events **1941**, HPFF USTs installed [UST #669, UST #670] **1942**, Building 1115 USTs installed [UST #670] **1993 January**, HPFF and Building 1115 USTs removed [UST #1186, UST #670] **2000 December**, Piping removal (extensive) at HPFF/Building 1115 [UST #417] **Building 1613 events** **1950s**, USTs installed [UST #548, UST #546] **1995 January**, USTs and contaminated soil removed [UST #535, UST #548] **1998–2004**, AS/SVE remediation system operated **Building 1601 events** **1940s**, Building 1601 built [UST #172, UST #195] UST removal date unknown	Benzene; three sources	HPFF/Building 1115/Building 1101 free product footprint Building 1613 free product footprint Building 1601 locations of maximum measured benzene in groundwater (78-GW75-1 and 78-GW74) and former location of USTs and dispenser island at southeast corner of building; MW 78-GW75-1 (5,500 µg/L in 2003; 3,200 µg/L in 2004); MW 78-GW74 (3,200 µg/L in 2004) (See Figure A9 for building and monitor well [MW] locations)
Building 1601 events **1940s**, Building 1601 built [UST #172, UST #195] **1942**, 1,500-gal UST install date listed in LUST study completed in 1990 by Geraghty and Miller [UST #504, UST #507] **1993 June 29**, UST excavated/removed [UST #624] **Building 901/902/903 events** **1948**, Buildings 900, 901, 902, 903 constructed [CERCLA #258, p. 149] TCE UST installation date unknown; removal/abandonment date unknown, but probably occurred prior to onset of remediation efforts around January 1995 [Sovereign Consulting, Inc. 2007]	TCE; two sources	Building 1601 locations of maximum measured TCE in groundwater (MW 78-GW09-1 (old) and (new)) and former location of 1,500-gal waste UST on north side of building; MW 78-GW09-1 (old) (5,000–14,000 µg/L during 1987–1991); MW 78-GW09-1 (new) (at/above 1,000 µg/L during 1993–1996) Building 901/902/903 locations of max measured TCE in groundwater (MW 78-GW23; 13,000 µg/L in 1987), maximum measured vinyl chloride in groundwater (MW 78-GW44; 1,600–6,700 µg/L during 2000–2004), and former locations of USTs containing TCE/solvent waste at Building 901 and between Buildings 902/903. (See Figure A9 for building and monitor well [MW] locations)
Hadnot Point landfill area (see Figure A14)		
Landfill **1940s**, reportedly used as a waste disposal area (Site 6 and Site 82; Figure A8) beginning in the 1940s	PCE and TCE; one source	Location of maximum measured concentration of TCE and PCE in groundwater (MW 06-GW01D) TCE ranged from 6,400 to 180,000 µg/L during 1992–2004; PCE ranged from 210 to 6,500 µg/L during 1992–2004 (See Figure A10 for monitor well [MW] locations)

[1] UST # refers to UST Web Management Portal file number (see References section of this report for complete details); CERCLA # refers to CERCLA Administrative Record file number (provided on digital video disc [DVD] in Maslia et al. 2007)

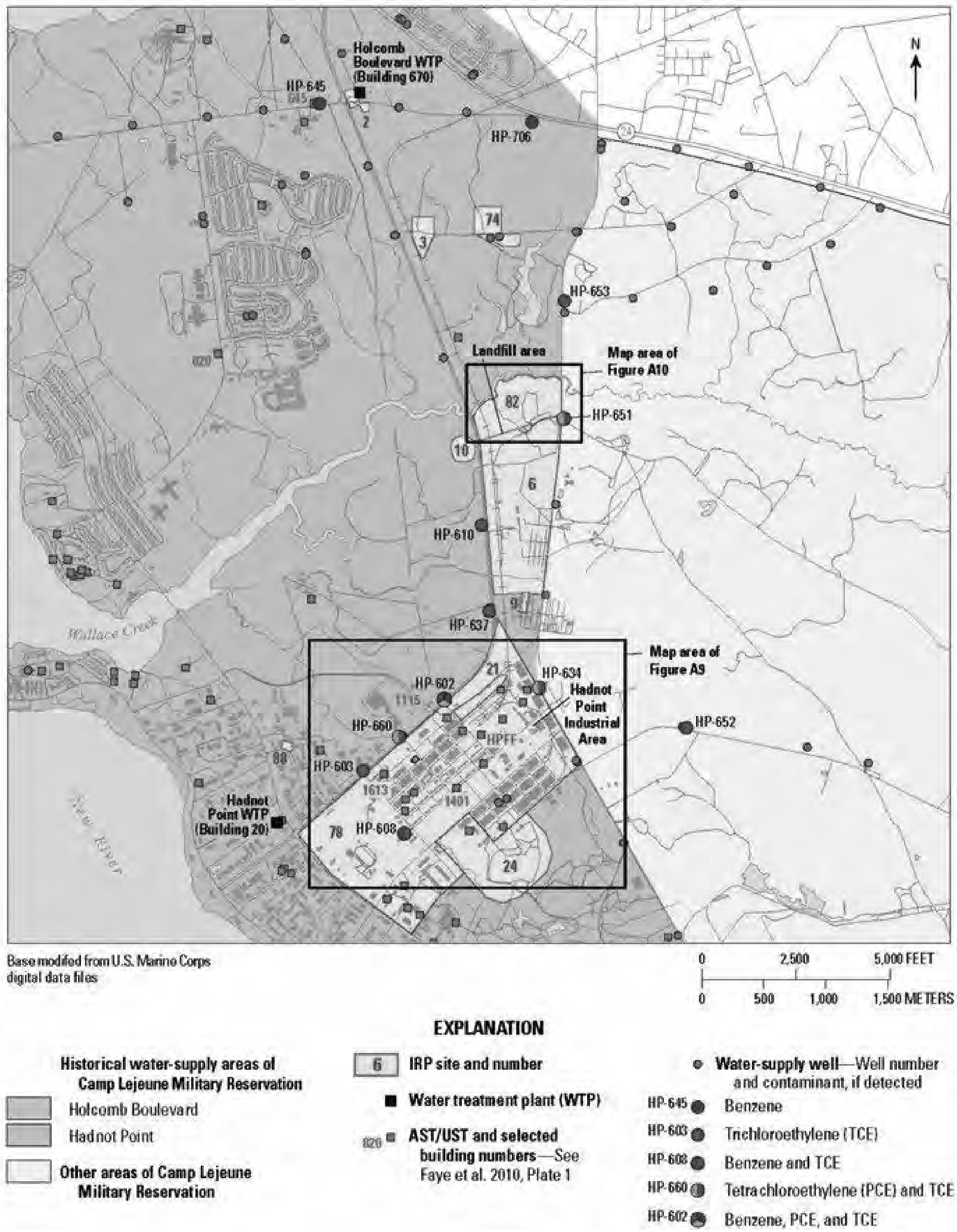


Figure 7.17. Locations of historically contaminated water-supply wells, Installation Restoration Program (IRP) sites, and above-ground and underground storage tank (AST/UST) sites, Hadnot Point–Holcomb Boulevard study areas (map area figures refer to the Chapter A report [Maslia et al. 2013]).

Level 1 Calibration (Predevelopment Conditions)

In Level 1 calibration, more than 700 water-level measurements were used to calibrate the steady-state model by using an automated parameter-estimation approach. A highly parameterized model—with more than 3,800 parameters—was calibrated using regularization and singular value decomposition. PEST 12 (Doherty 2010) was used to conduct simulations and optimization. The parameters included 970 pilot points for each of four parameter groups—horizontal hydraulic conductivity for layers 1, 3, and 5 and recharge. A graph of simulated versus observed potentiometric levels (heads or water-level measurements, Figure 7.18, top graph) shows a generally good agreement about the line of equality (diagonal line on Figure 7.18). A residual analysis (lower graph on Figure 7.18) was used to evaluate the goodness of the fit of the solution. Residual analysis includes a plot of observed potentiometric levels versus residuals and a spatial analysis of the residuals.

Level 2 Calibration (Transient Conditions)

Level 2 calibration included a trial-and-error approach in which hydrographs for multiple wells were compared against simulated water levels. In this Level 2 calibration, vertical anisotropy and temporal variation in recharge were adjusted to improve the match between observed and simulated water levels. Level 1 and 2 calibrations for the HP-HB study area are shown in Figures 7.18 and 7.19, respectively. Figure 7.18 demonstrates close agreement between simulated and measured values for the predevelopment (non-pumping) condition (Level 1) and Figure 7.19 shows good agreement between simulated and measured values for pumping conditions (Level 2). Thus, Levels 1 and 2 calibrations were successful for the HP-HB study area.

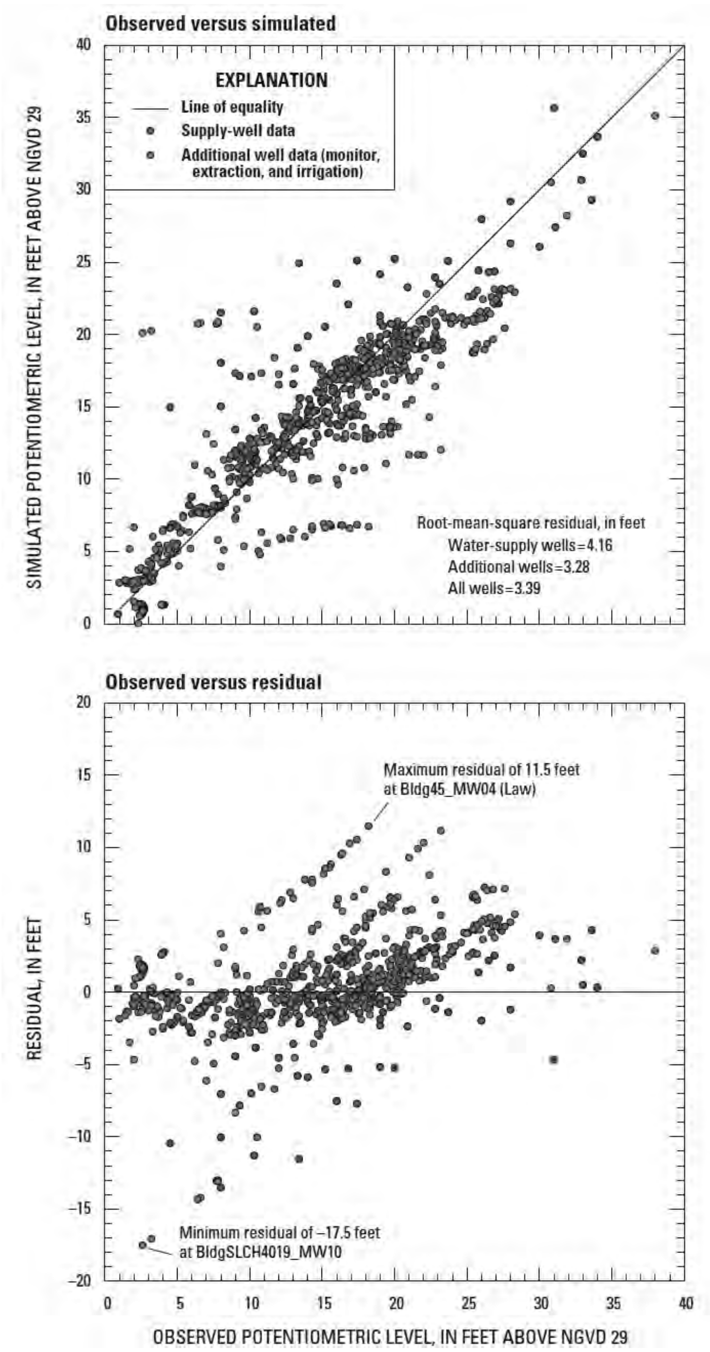


Figure 7.18. Steady-state groundwater-flow model results shown as observed and simulated potentiometric levels, and observed potentiometric levels and corresponding residuals, steady-state groundwater-flow model calibration, Hadnot Point–Holcomb Boulevard study area (from Suárez-Soto et al. 2013).

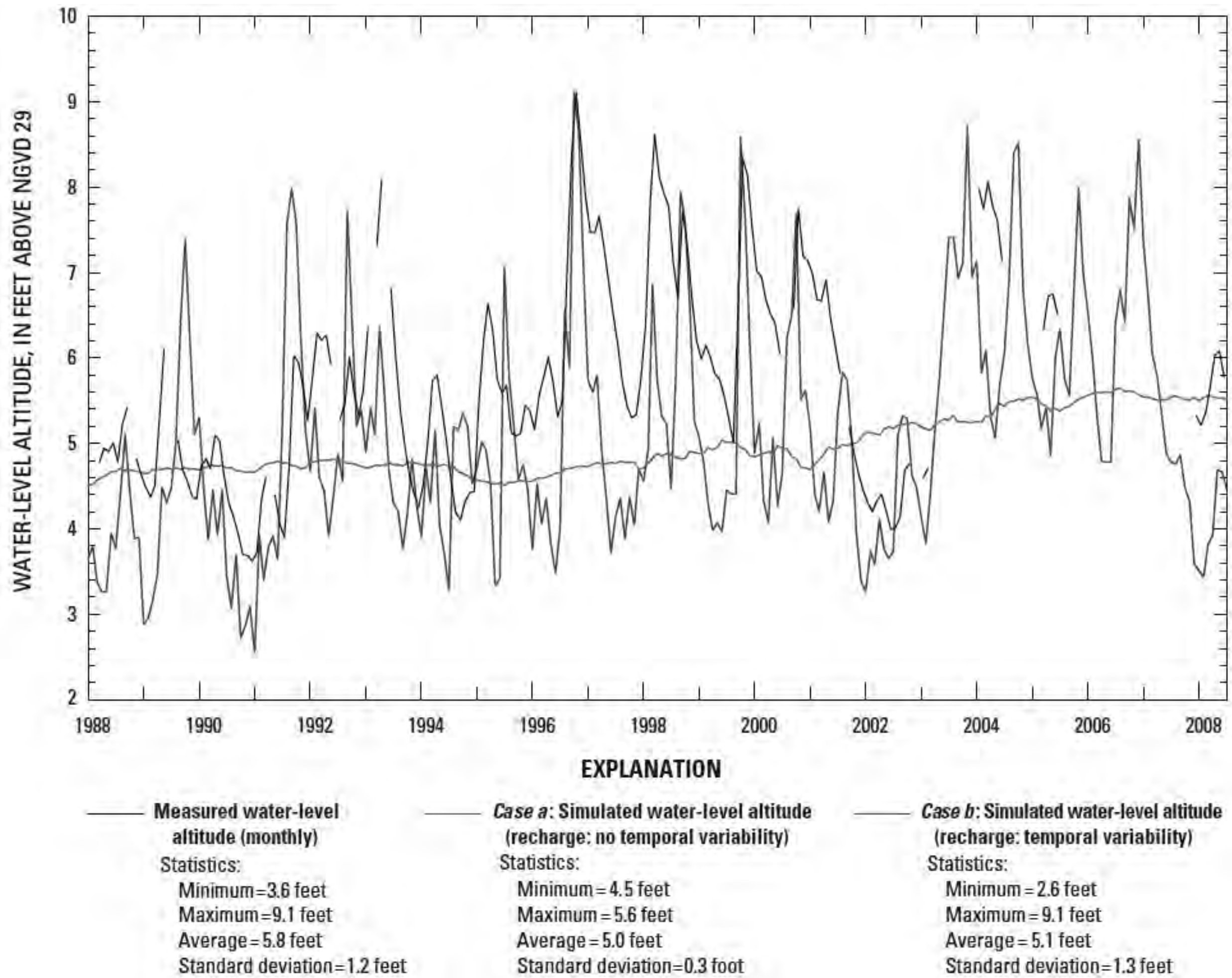


Figure 7.19. Comparison of observed water-level altitude and simulated water-level altitude for well X24S6 for two cases of the transient groundwater-flow model: *case a* with temporal variability of recharge, and *case b* without temporal variability of recharge, Hadnot Point–Holcomb Boulevard study area (from Suárez-Soto et al. 2013). [Note: Date range for measured and simulated water-level altitude for *cases a* and *b* is March 1988 to June 2008].

Level 3 Calibration (Contaminant Fate and Transport)

PCE and TCE

Level 3 calibration for the HP-HB study area involved fitting contaminant migration (fate and transport) parameters to maximize agreement between simulated and measured values at water supply wells. Figure 7.20 shows good agreement between simulated and measured values at four water supply wells. Table 7.14 summarizes calibrated fate and transport parameters.

Figure 7.20 shows the reconstructed (simulated) TCE concentrations for water-supply wells HP-601/660, HP-602, HP-608, and HP-634 within the HPIA. Note, water-supply well HP-660 replaced HP-601 and likely operated from July 1984 to December 1984. Monthly reconstructed TCE concentration results occur on the last day of the month (e.g., 31 January); they are interpreted as being representative of simulated values on any given day of that month. The results are monthly mean concentrations of TCE. The reconstructed concentrations at water-supply wells are flow-weighted concentration values for supply wells that are open to multiple water-bearing units. As can be seen in the graphs of Figure 7.20, observation data in water-supply wells are limited and, in some instances, provide as few as one data point by which to compare reconstructed TCE concentrations (e.g., HP-634). Given the above limitations, the reconstructed (simulated) TCE concentrations provide reasonable agreement with both observed data and "real-world" conditions.

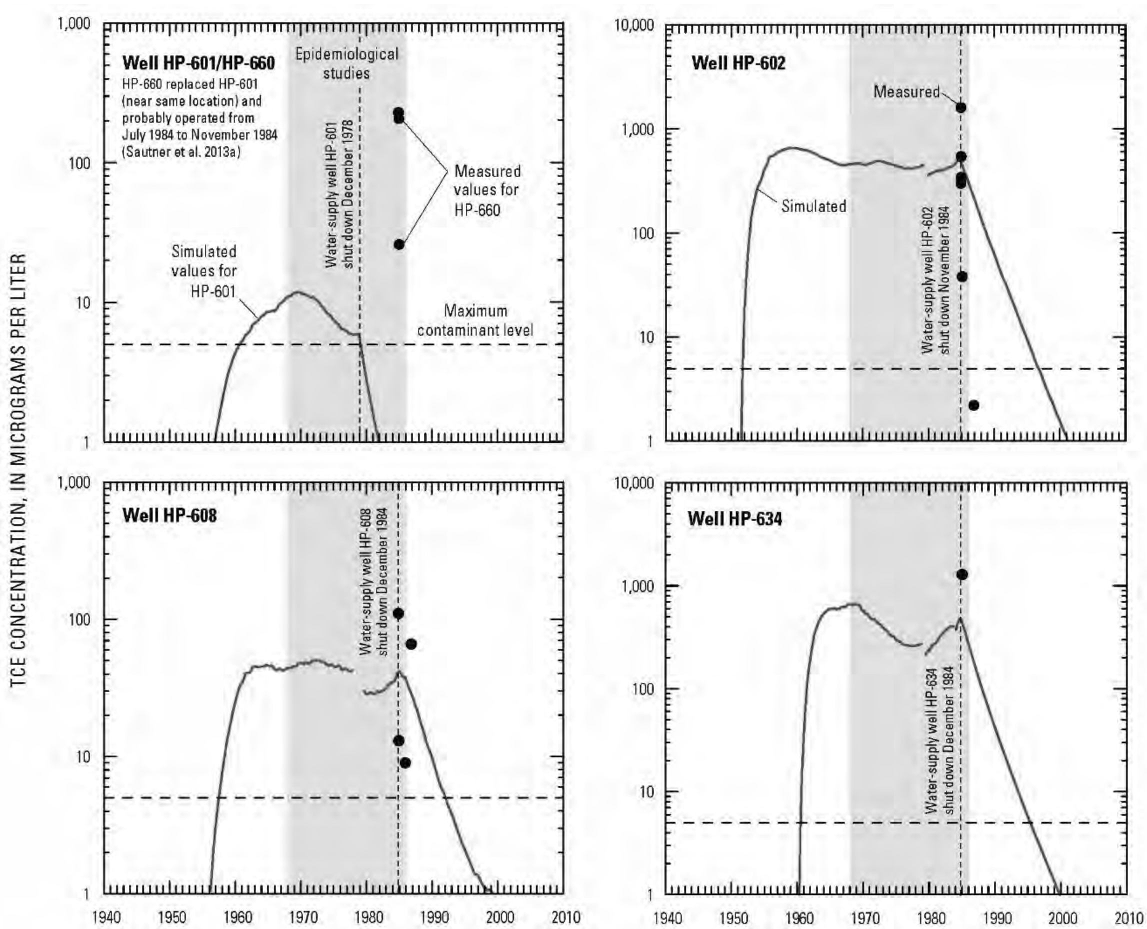


Figure 7.20. Reconstructed (simulated) and measured concentrations of trichloroethylene (TCE) at selected water- supply wells within the Hadnot Point Industrial Area, Hadnot Point-Holcomb Boulevard study area. Groundwater-flow simulation using MODFLOW (Harbaugh 2005) and contaminant fate and transport simulation using MT3DMS (Zheng and Wang 1999), see Figure 7.17 for well location (Jones et al. 2013).

Table 7.14. Calibrated model parameter values used to simulate groundwater flow and contaminant fate and transport, Hadnot Point Industrial Area, Hadnot Point-Holcomb Boulevard study area (Maslia 2013)[1]

[—, not applicable; in/yr, inch per year; ft, foot; ft³, cubic foot; d, day; g, gram; mg, milligram; L/kg, liter per kilogram; PCE, tetrachloroethylene; TCE, trichloroethylene; HPIA, Hadnot Point Industrial Area; HPLF, Hadnot Point landfill]

[2]Model parameter	[3]Model layer number						
	1	2	3	4	5	6	7
[4]Pre-development (steady-state) groundwater-flow model, conditions prior to 1942—Uniform grid (300-ft × 300-ft cells)							
Horizontal hydraulic conductivity, K_{xx} (ft/d)	0.5–46.8	1.0–20.0	1.0–50.0	1.0–35.0	2.3–50.0	1.0–20.0	20.0
Ratio of vertical to horizontal hydraulic conductivity, K_{zz}/K_{xx}	1:10	1:15	1:10	1:15	1:10	1:15	1:10
Infiltration (recharge), $I_{i,j}$ (in/yr)	2.5–22.0	—	—	—	—	—	—
[4]Transient groundwater-flow model, January 1942–June 2008—Variably spaced grid (300-ft × 300-ft – 50-ft × 50-ft cells)							
Specific yield, S_y	0.05	—	—	—	—	—	—
[5]Specific storage, S_s (1/ft) range of values	—	1.3×10^{-5} to 1.9×10^{-4}	4.3×10^{-6} to 3.6×10^{-5}	1.0×10^{-5} to 3.8×10^{-5}	4.0×10^{-6} to 8.3×10^{-6}	1.4×10^{-5} to 3.6×10^{-5}	3.4×10^{-6} to 7.7×10^{-6}
Infiltration (recharge), $I_{i,j}$ (in/yr)	Varies[6]	—	—	—	—	—	—
[7]Pumpage, Q (ft³/d)	Varies	Varies	Varies	Varies	Varies	Varies	Varies
[4]Contaminant fate and transport models, January 1942–June 2008—Subdomain area (50-ft × 50-ft cells)							
[8]Distribution coefficient, K_d (ft³/mg):							
PCE	1.1×10^{-8}	1.1×10^{-8}	1.1×10^{-8}	1.1×10^{-8}	1.1×10^{-8}	1.1×10^{-8}	1.1×10^{-8}
TCE	5.3×10^{-9}	5.3×10^{-9}	5.3×10^{-9}	5.3×10^{-9}	5.3×10^{-9}	5.3×10^{-9}	5.3×10^{-9}
Benzene	4.0×10^{-9}	4.0×10^{-9}	4.0×10^{-9}	4.0×10^{-9}	4.0×10^{-9}	4.0×10^{-9}	4.0×10^{-9}
Bulk density, ρ_b (g/ft³)	46,700	46,700	46,700	46,700	46,700	46,700	46,700
Effective porosity, n_E	0.2	0.2	0.2	0.2	0.2	0.2	0.2
Biodegradation, λ (d⁻¹):							
HPIA (TCE)	2.0×10^{-3}	2.0×10^{-3}	2.0×10^{-3}	2.0×10^{-3}	2.0×10^{-3}	2.0×10^{-3}	2.0×10^{-3}
HPIA (benzene)	1.0×10^{-4}	1.0×10^{-4}	1.0×10^{-4}	1.0×10^{-4}	1.0×10^{-4}	1.0×10^{-4}	1.0×10^{-4}
HPLF (PCE and TCE)	1.4×10^{-4}	1.4×10^{-4}	1.4×10^{-4}	1.4×10^{-4}	1.4×10^{-4}	1.4×10^{-4}	1.4×10^{-4}
Effective molecular diffusion coefficient, D^*(ft²/d)	1.0×10^{-3}	1.0×10^{-3}	1.0×10^{-3}	1.0×10^{-3}	1.0×10^{-3}	1.0×10^{-3}	1.0×10^{-3}
Dispersivity (ft):							
Longitudinal, α_L	25	25	25	25	25	25	25
Transverse, α_T	2.5	2.5	2.5	2.5	2.5	2.5	2.5
Vertical, α_V	0.25	0.25	0.25	0.25	0.25	0.25	0.25
Source concentration, C (mg/L):							
HPIA (TCE)	640	640	640	0	0	0	0
HPIA (benzene—dissolved)	1.7	—	—	—	—	—	—
HPIA (benzene—LNAPL)	17	—	—	—	—	—	—
HPLF (PCE)	42–105	33–83	27–66	18–46	6–16	0	0
HPLF (TCE)	256–384	256–384	256–384	256–384	256–384	256–384	256–384

[1]Refer to Suárez-Soto et al. (2013), Jones et al. (2013), and Jang et al. (2013) for details

[2]Symbolic notation used to describe model parameters obtained from Harbaugh (2005), Zheng and Wang (1999), and Zheng (2010)

[3]See Table A11 for correlation between geologic and hydrogeologic units and model layers for the HPHB study area; refer to Faye (2012) and Suárez-Soto et al (2013) for details; aquifers are designated as model layers 1, 3, 5, and 7; confining units are designated as model layers 2, 4, and 6

[4]See Figures A12–A14 for groundwater-flow model domain and contaminant fate and transport model subdomains

[5]Specific storage (S_s) was specified as input for MODFLOW-2005 (Harbaugh 2005); based on cell-by-cell thicknesses, storage coefficient (or storativity) of 4×10^{-4} determined using the equation $S = S_s \times b$, where S is the storage coefficient (dimensionless), S_s is specific storage (1/ft), and b is the cell thickness (ft)

[6]Transient infiltration was varied on a monthly basis using the ratio of monthly precipitation divided by average, long-term precipitation; see Suárez-Soto (2013 for details

[7]Pumpage varies by month and model cell; refer to Sautner et al. (2013a) and Telci et al. (2013) for details on the derivation of historical monthly water-supply well operations; refer to Suárez-Soto et al. (2013) for details pertaining to assigning monthly water-supply well pumpage to cells and model layers using the multi-node well-flow package for MODFLOW-2005

[8]Refer to Jones et al. (2013) for derivation of K_D values based on a survey reported in the scientific literature; to convert from model K_D units of ft³/mg to units c L/kg reported in Jones et al. (2013), multiply model K_D values by 28,381,652.21.

Figure 7.21 (top-left graph) shows the reconstructed (simulated) TCE and PCE concentrations at water-supply well HP-651, located to the east of the TCE contaminant sources and the HPLF (Figure 7.17). Monthly reconstructed results for water-supply well HP-651 also are listed in Maslia et al. (2013, Appendix A3). Observation data at water-supply wells are limited, and in the case of HP-651, three of the five TCE water-quality samples were obtained between January 16 and February 4, 1985, and range from 3,200 µg/L to 18,900 µg/L. Given the data measurement limitations, substantial variation in concentration range within a 1-month period, and interpretive constraints, the reconstructed (simulated) TCE and PCE concentrations shown in Figure 7.21 for water-supply well HP-651 are in reasonable agreement with observed data and “real world” conditions.

As further evidence of successful Level 3 model calibration for the HP-HB area, Figure 7.21 shows good agreement between measured and simulated values for four extraction wells. The additional panels in Figure 7.21 represent four remediation extraction wells (DRW01 to DRW04) that were installed over a decade after HP-651 was decommissioned to clean up the groundwater contamination during the USEPA Installation Restoration Program (IRP). While the historical reconstruction simulation efforts were not focused on (optimized for) remediation activities, comparing simulated values for these groundwater extraction wells with measured values during remediation is instructive. It is encouraging to see that the simulated values generally agree with the observed concentrations, capturing the overall concentration trends versus time. This is even more encouraging given that the remediation values are over a decade after the contaminated well HP-651 was abandoned, providing a longer-term basis for model calibration and increased confidence in the model's ability to reconstruct historical concentrations accurately. It is also instructive to note that concentrations in the remediation wells are similar to or higher than those in HP-651, providing additional data to support the limited measurements available when the contaminated water supply well HP-651 was decommissioned. The higher extraction well values for certain remediation wells in Figure 7.22 reflect the placement of these wells closer to the contamination to maximize contaminant withdrawal. Further, the rise and fall of simulated HP-651 concentrations (Figure 7.22) correspond to that water supply well being activated and decommissioned, while increasing and decreasing simulated values in the remediation wells reflect remediation pumps being turned on and off.

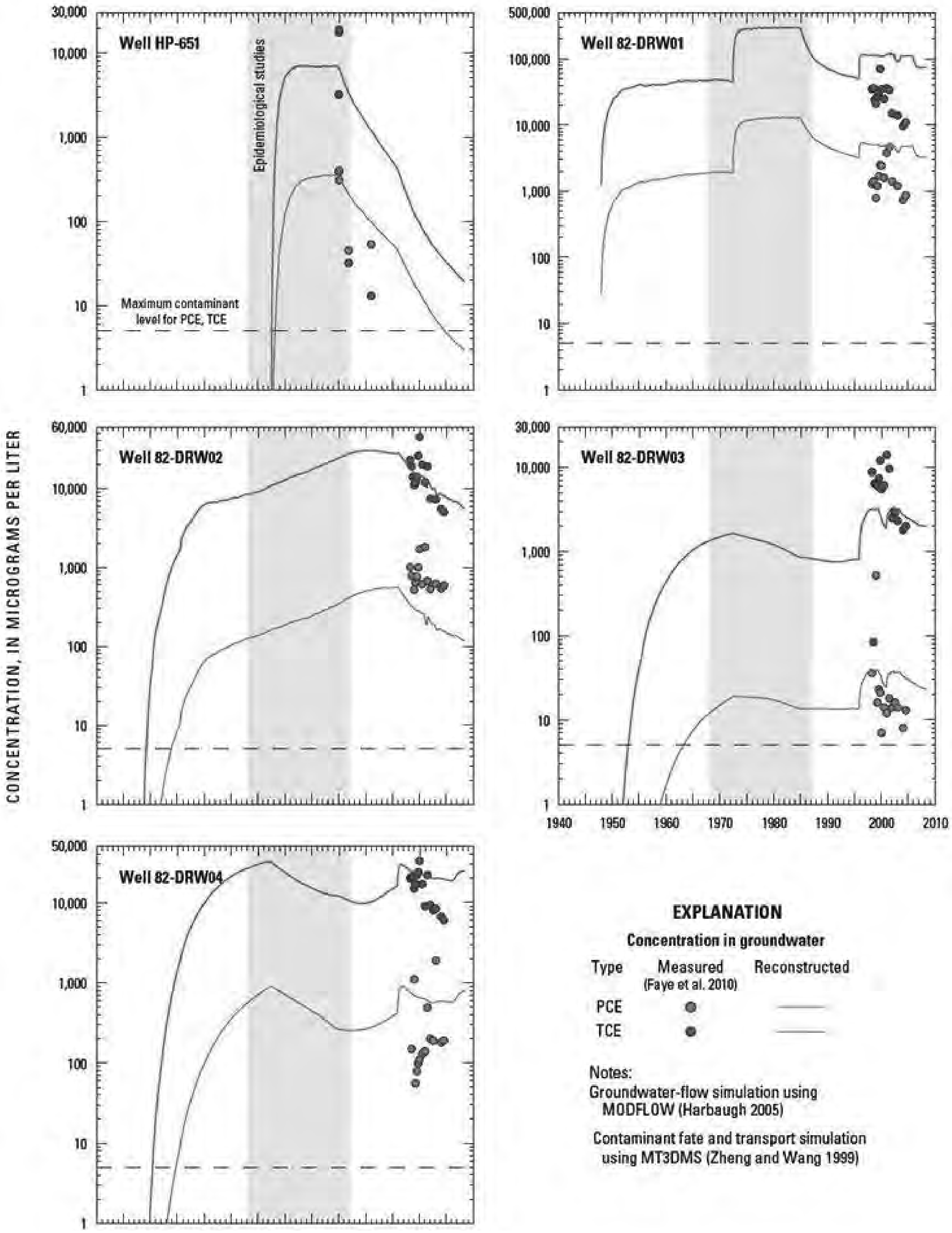


Figure 7.21. Reconstructed (simulated) and measured observed concentrations of trichloroethylene (TCE) and tetrachloroethylene (PCE) at water supply well HP-651 and extraction wells 82-DRW01, 82-DRW02, 82- DRW03, and 82-DRW04, model layer 5, Hadnot Point landfill area, Hadnot Point–Holcomb Boulevard study area (Jones et al. 2013).

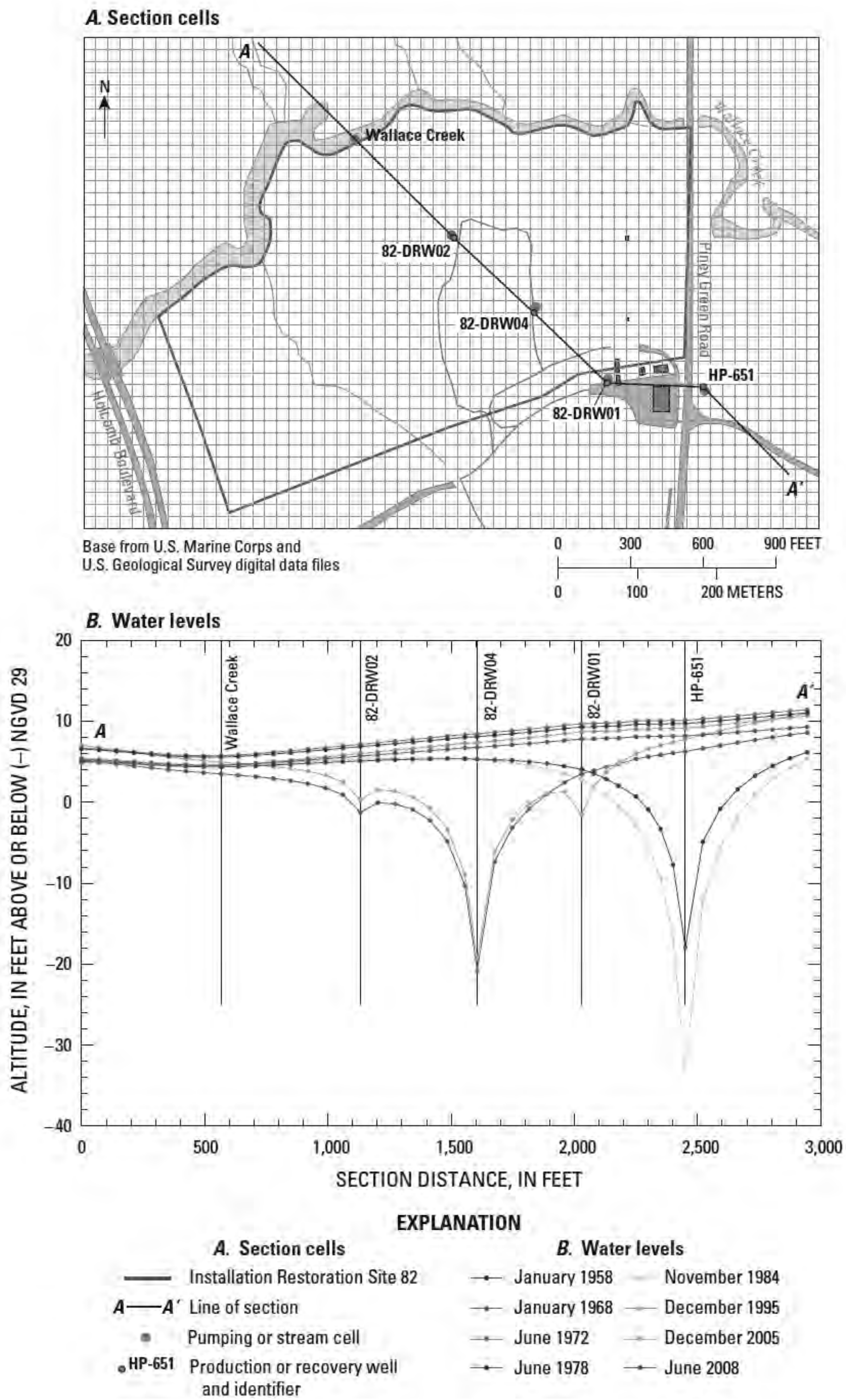


Figure 7.22. *(A)* Line of section *A–A′* and *(B)* simulated water levels within the Hadnot Point landfill area fate and transport model subdomain, model layer 5, Hadnot Point–Holcomb Boulevard study area (Jones et al. 2013).

Benzene

Benzene contamination of groundwater within the HPIA occurred primarily as a result of operations in and around the HPFF and Building 1115 areas (Figure 7.17). Benzene occurs as free product (or "floating light nonaqueous phase liquid (LNAPL)") in vicinity of the HPFF, Building 1115, and IRP site 94/Building 1613 areas and as dissolved-phase benzene contamination in the vicinity of Building 1601 (Faye et al. 2010, 2012). Because benzene occurs as both free product and dissolved phase within the HPIA, *three modeling approaches* were necessary to reconstruct benzene concentrations in groundwater: (1) estimation of the volume of fuel loss and mass of LNAPL in the subsurface using site data and the model TechNAPLVol (Jang et al. 2013), (2) simulation of the dissolution of benzene from LNAPL and the subsequent fate and transport of dissolved benzene using the model TechFlowMP (Jang and Aral 2008) at the HPFF, and in Building 1115 and Building 1613 areas, and (3) simulation of the fate and transport of dissolved-phase benzene in groundwater in the Building 1601 area using the model MT3DMS (Jones et al 2013). Details on the specific simulation approaches are described in these topical ATSDR reports and in Maslia et al. (2013).

The LNAPL source area characterized using the TechNAPLVol model served as input to the three-dimensional finite-element model, TechFlowMP (Jang and Aral 2005, 2007), which was used to reconstruct benzene concentrations in groundwater and at historically operated water-supply wells within the HPIA. Additionally, the three-dimensional finite-difference model, MT3DMS (Zheng and Wang 1999; Zheng 2010), was used to reconstruct benzene concentrations within the HPIA where the benzene source was characterized as dissolved-phase benzene in the vicinity of Building 1601.

Figure 7.23 shows reconstructed (simulated) benzene concentrations in water-supply wells HP-602, HP-603, and HP-608. Reconstructed (simulated) monthly mean benzene concentrations in these water-supply wells and selected others in the HP-HB are listed **Appendix I** (from Maslia et al (2013, Appendix A3) for the entire historical reconstruction period (January 1942–June 2008). During November 1984, 32 water-supply wells provided water to the HPWTP. The reconstructed combined flow rate for all wells was 417,012 cubic feet per day (ft^3/d), whereas the corresponding flow rate for well HP-602 was 10,012 ft^3/d. Comparison of the combined flow rate for all water-supply wells to the flow rate for well HP-602 for November 1984 indicates that the benzene contribution from water-supply well HP-602 to the finished water benzene concentration at the HPWTP is substantially reduced by dilution, both under actual and simulated operating conditions. Simulated (reconstructed) benzene concentrations in water-supply wells HP-602 and HP-603 (**Appendix I**) indicate approximately the same range of concentrations during the core period of interest (1968–1985) to the epidemiological studies. Reconstructed benzene concentrations for well HP-602 are in reasonable agreement with field data. However, reconstructed benzene concentrations for water-supply well HP-603 are inconsistent with field data. One or all of several lines of reasoning possibly explain the disparity between reconstructed and sampled benzene concentrations in well HP-603: (1) the release date of hydrocarbon fuels in the vicinity of Building 1613 is unknown and its representation in the numerical model is uncertain, (2) the source concentration and size of the source area during much of the period of simulation are unknown and their representation in a numerical model is consequently highly uncertain, and (3) local hydraulic, fate, and transport characteristics in the vicinity of Building 1613 and water-supply well HP-603 may be different from the average hydraulic, fate, and transport properties defined within the model subdomain (Figure 7.17 Table 7.14). Issues pertaining to source release and concentration were addressed by conducting sensitivity analyses varying model source area location, concentration, release date, and the contribution of benzene-contaminated and TCE-contaminated groundwater to finished-water concentrations at the HPWTP. For benzene, results indicated somewhat improved reconstructed concentrations in well HP-603 (Maslia et al. 2013, Figure A35 and Table A25) compared to field data; however, the corresponding changes in reconstructed benzene concentrations at the HPWTP are minimal (Maslia et al. 2013, Figure A36, p. A83).

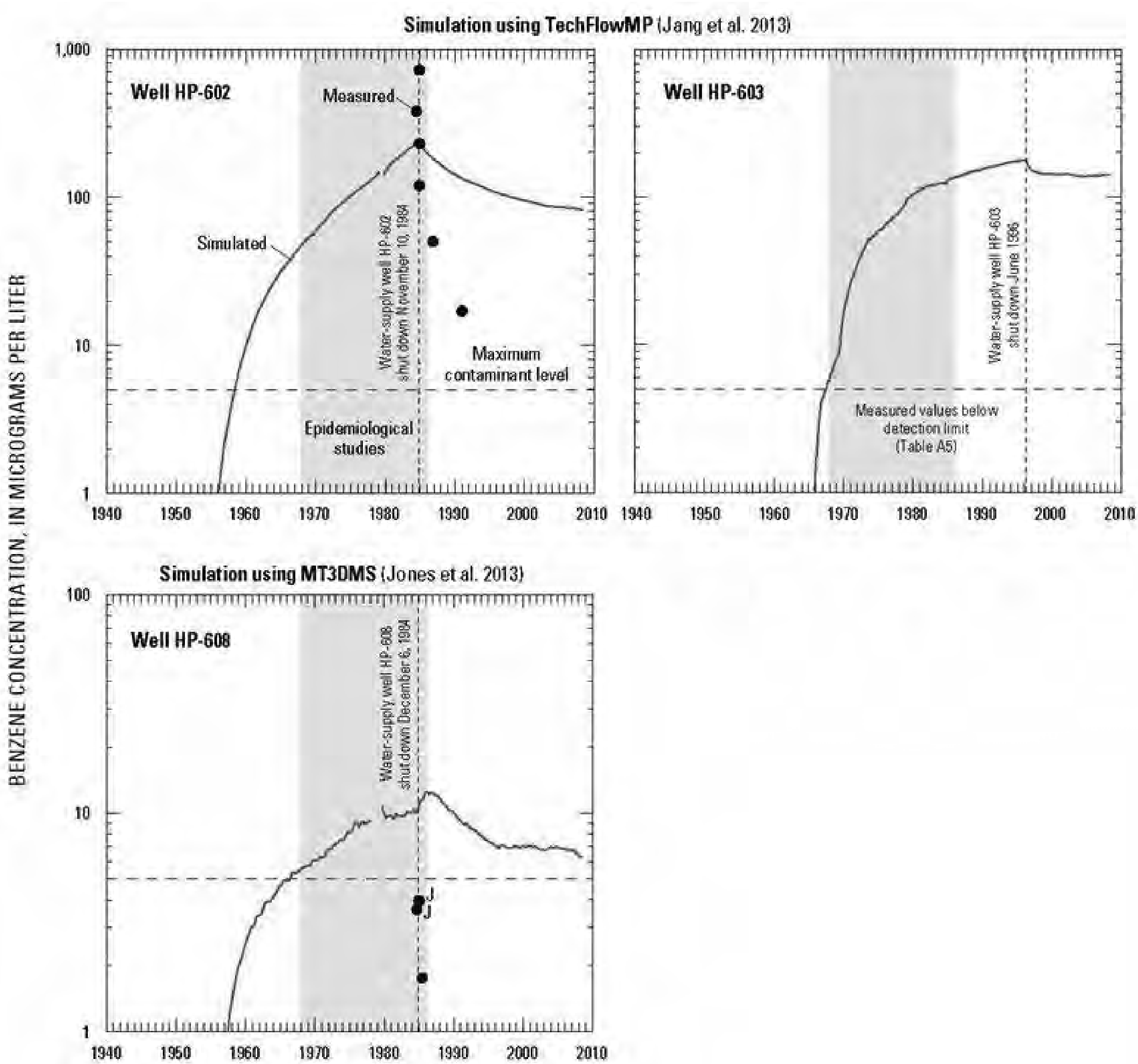


Figure 7.23. Reconstructed (simulated) and measured concentrations of benzene at selected water-supply wells within the Hadnot Point Industrial Area, Hadnot Point study area (Maslia et al. 2013).

Liner Control Model (LCM) Methodology

An alternative and simpler computational method, the Linear Control Model (LCM) methodology, which is a linear state-space representation of a contaminated groundwater aquifer system, was developed to reconstruct contaminant concentrations in water-supply wells and compare results with the MODFLOW and MT3DMS numerical modeling approach. The LCM methodology was investigated because (1) perhaps a simpler computational method requiring fewer resources could yield reliable historical reconstruction results and (2) results from an alternative computational method, if reliable, could be used to assess confidence in results derived from the MODFLOW and MT3DMS simulations. The LCM methodology, which is based on linear control theory, relies on two matrices to describe (1) the subsurface movement of a contaminant under predevelopment or natural conditions and (2) the effects of pumping operations on contaminant concentrations. This method, therefore, *characterizes the aquifer, contaminant sources, and the dynamics of contaminant migration as a "black box."* [10]

Deactivation of water-supply well HP-651, located adjacent to the HPLF (Figure 7.17), presented an opportunity to test and apply the LCM because there were sufficient, although limited, observation data once the well was secured and taken out of service on February 4, 1985 (CLW #4913; Sautner et al. 2013a). Measured data for PCE, TCE, 1,2-tDCE, and VC are shown graphically in Figure 7.24. Reconstructed historical monthly concentrations at water-supply well HP-651, derived using the LCM methodology, are shown in Figure 7.24 for PCE, TCE, 1,2-tDCE, and VC. For PCE and TCE, corresponding reconstructed (simulated) concentrations using the numerical contaminant fate and transport model MT3DMS (Zheng and Wang 1999; Zheng 2010) also are shown for comparison. **The results shown in Figure 7.24 demonstrate very good agreement between the LCM results, the numerical contaminant fate and transport model (MT3DMS) results, and observation data for water-supply well HP-651.** Thus, the application of the LCM to a contaminated water-supply well such as HP-651 demonstrates that historical contaminant concentrations can be reconstructed using a simpler modeling approach; results are reliable when compared with field data and historical reconstruction results from a numerical contaminant fate and transport model (MT3DMS). Details of the development of the LCM methodology and application to water-supply well HP-651 are presented in Guan et al. (2013).

[10] In science and engineering, the term "black box" refers to a device or system that can be analyzed in terms of inputs, transfer properties, and outputs, without specific knowledge of its internal dynamic workings.

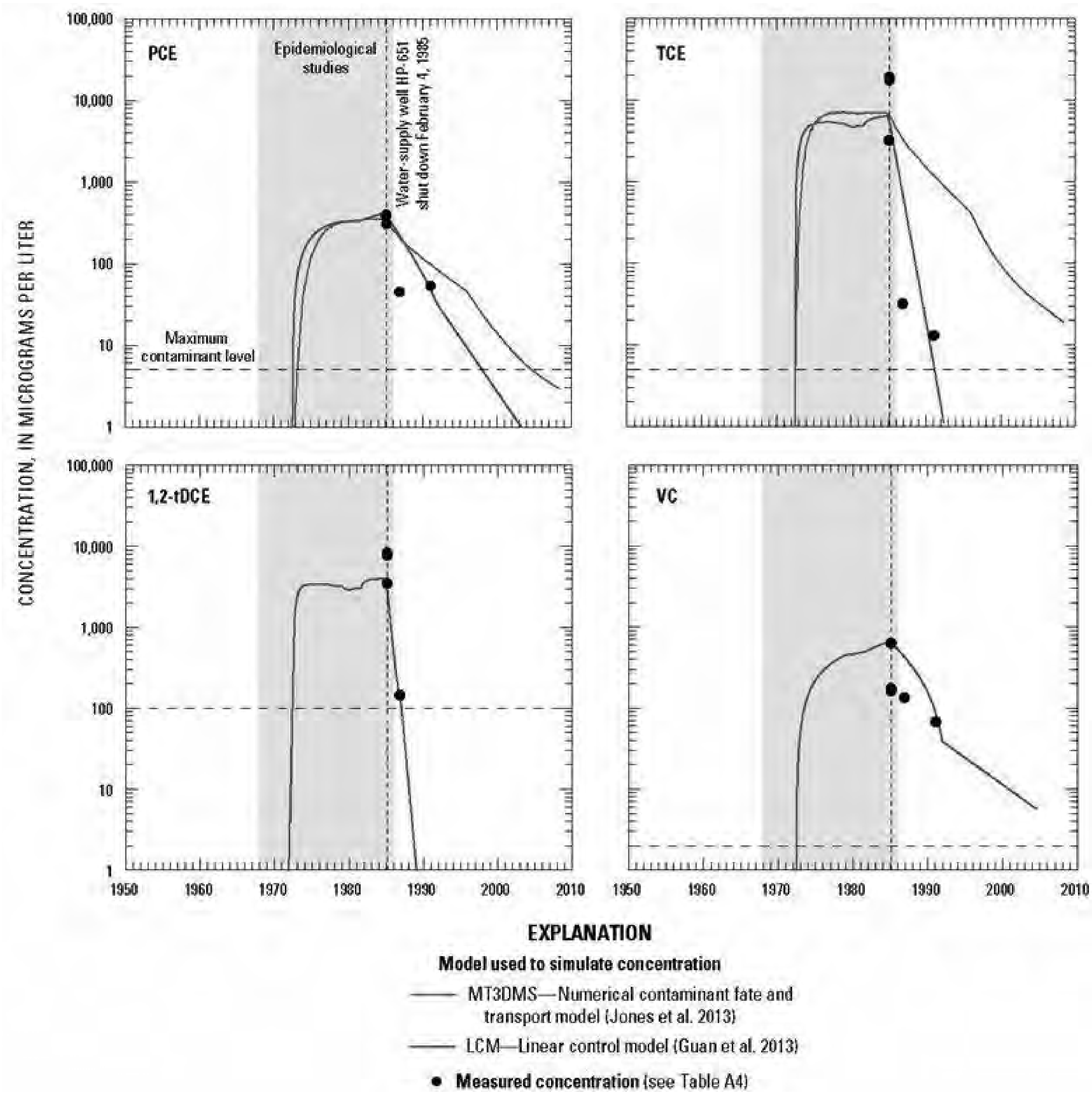


Figure 7.24. Reconstructed (simulated) and measured concentrations of tetrachloroethylene (PCE) and trichloroethylene (TCE), trans-1,2-dichloroethylene (1,2-tDCE), and vinyl chloride (VC) at water-supply well HP-651 using numerical (MT3DMS) and linear control methodology (LCM; TechControl) models, Hadnot Point study area (from Guan and Aral 2013, Maslia et al. 2013).

Level 4 Calibration (Mixing Model)

As discussed in the report section on Level 4 calibration for TT, the final level of model calibration employed a simple mixing (flow-weighted average) model to compute contaminant concentrations delivered to the HPWTP from all active water-supply wells and subsequently to the Hadnot Point water-distribution system. The model is based on the principles of continuity and conservation of mass (Masters 1998) and is used to compute the flow-weighted average concentration of contaminants in the HPIA, HPLF, and HPFF (PCE, TCE, 1,2-tDCE, VC, and benzene). Reconstructed (simulated) monthly mean concentrations of PCE, TCE, 1,2-tDCE, VC, and benzene in finished water delivered by the HPWTP and measured concentrations of VOCs in finished water are shown in Figure 7.25. Monthly reconstructed concentrations at the HPWTP for the entire historical period (1942–2008) are listed in **Appendix J**. Because the range in values for reconstructed and measured concentrations span several orders of magnitude, Figure 7.25 is plotted using a logarithmic ordinate (y-axis). Of note in Figure 7.25 is the effect of the contribution of contaminated groundwater when pumping began at water-supply well HP-651 (July 1972). TCE concentrations in finished water at the HPWTP ranged from about 10 to 30 µg/L for the period 1955–1972, prior to the onset of pumping from water-supply well HP-651 (Figure 7.25, and Appendix **I**). Subsequent to the onset of pumping of water-supply well HP-651 during July 1972, finished-water concentrations increased to a maximum computed value of 783 µg/L during November 1983 (Figure 7.25, Table 7.5, and **Appendix J**).

The reconstructed concentrations versus the observed data in Table 7.15 and Figure 7.25 demonstrate successful Level 4 calibration as the observed data from the HPWTP represents a separate, unique data set that has been used assess the "goodness of fit" of the calibrated HP-HB models. Table 7.15 Figure 7.25 demonstrate close agreement between simulated and measured contaminant concentrations (PCE, TCE, 1,2-tDCE, VC, and benzene) at the HPWTP. This close agreement between simulated and measured values (within a factor of ten – Maslia et al., 2016) is acceptable for the complexity of this site and supports the collective ability of the four-level modeling and calibration process to capture the HP-HB system behavior with acceptable accuracy.

Summary statistics of reconstructed (simulated) concentrations of selected water-supply wells located at the HPIA and the HPLF are listed in Table 7.16. Summary statistics for finished water at the HPWTP are also listed in Table 7.16. Results are provided for reconstructed concentrations of PCE, TCE, 1,2-tDCE, VC, and benzene. Included in the statistics of Table 7.16 is the duration in months that these contaminants exceeded their respective MCLs. The reconstructed (simulated) concentrations in finished water at the HPWTP are shown in Figure 7.25 for PCE, TCE, 1,2-tDCE, VC, and benzene. These estimates were computed using a materials mass balance model (simple mixing) to compute the flow-weighted mean concentrations of VOCs as described earlier in this report (using Equations 7.1 and 7.2). Measured concentrations of PCE, TCE, 1,2-tDCE, VC, and benzene and historical reconstruction (simulated) results for the HPWTP are listed in Table 7.15. Given the limited number of measured finished-water concentration data and their substantial variations, **there is reasonable agreement between measured finished-water concentrations and historical reconstruction results for the HPWTP**.

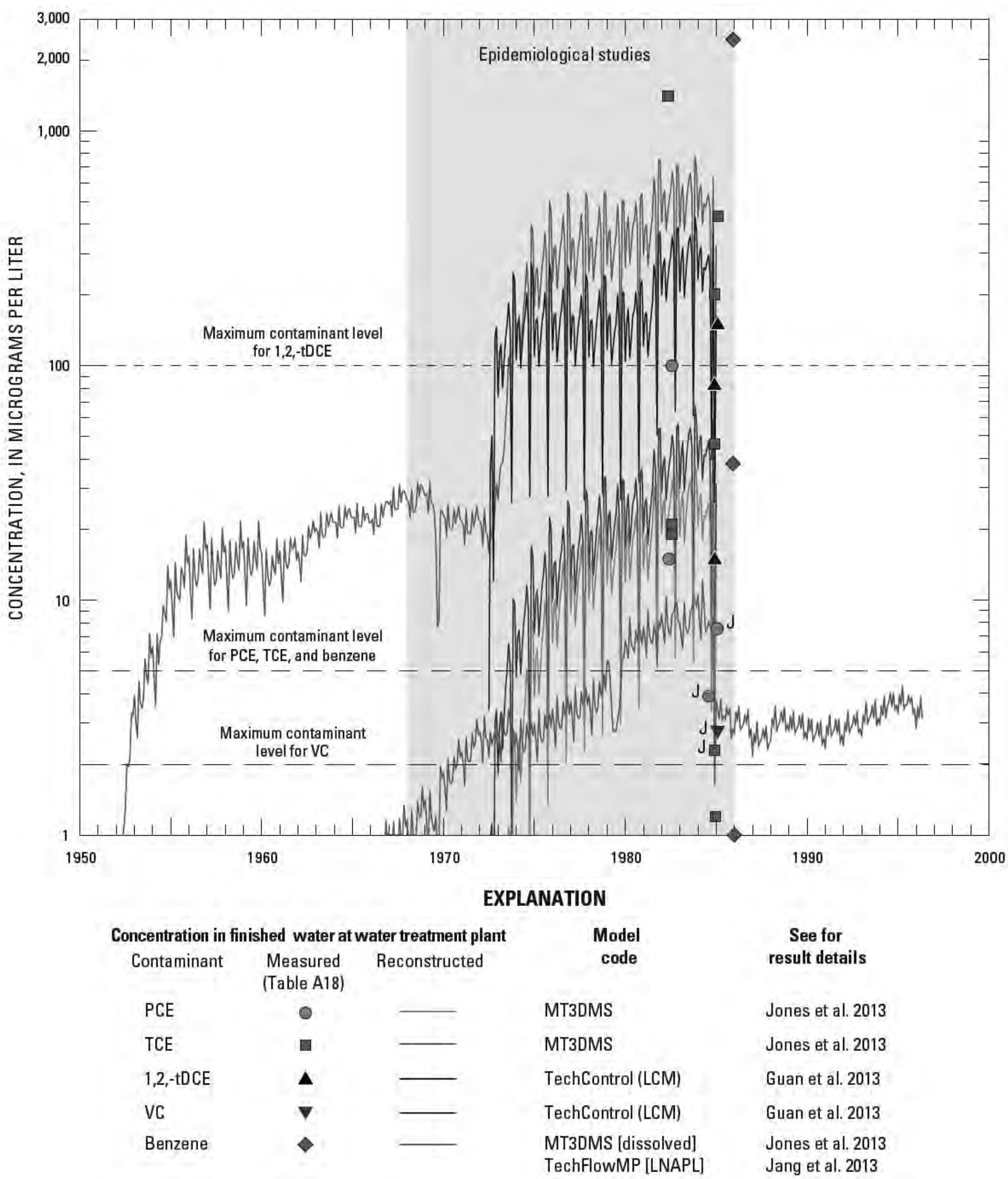


Figure 7.25. Reconstructed (simulated) finished-water concentrations of tetrachloroethylene (PCE), trichloroethylene (TCE), *trans*-1,2-dichloroethylene (1,2-tDCE), vinyl chloride (VC), and benzene, and measured concentrations (Faye et al. 2010), Hadnot Point water treatment plant, Hadnot Point–Holcomb Boulevard study area. (Note: See Appendix J for monthly mean finished-water concentration). (From Maslia et al. 2013) [J, estimated; LCM, linear control model; LNAPL, light nonaqueous phase liquid].

Table 7.15. Selected measured and reconstructed (simulated) concentrations of tetrachloroethylene (PCE), trichloroethylene (TCE), *trans*-1,2-dichloroethylene (1,2-tDCE), vinyl chloride (VC), and benzene at the Hadnot Point water treatment plant, Hadnot Point study area (Maslia et al. 2013).

Contaminant	[1]Measured data		[2]Reconstructed (simulated)		[2]Reconstructed (maximum value)	
	Sample date	Concentration, in µg/L	Simulation date	Concentration, in µg/L	Simulation date	Concentration, in µg/L
PCE	5/27/1982[3]	15	May 1982	21	Nov. 1983	39
	7/27/1982[4]	100	July 1982	27		
	12/4/1984[6]	3.9J	Nov. 1984	31		
	2/5/1985[7]	7.5J	Jan. 1985	16		
TCE	5/27/1982[3]	1,400	May 1982	438	Nov. 1983	783
	7/27/1982[5]	19	Aug. 1982	670		
	7/27/1982[6]	21	Aug. 1982	670		
	12/4/1984[5]	46	Nov. 1984	639		
	12/4/1984[6]	200	Nov. 1984	639		
	12/12/1984[6]	2.3J	Dec. 1984	43		
	12/19/1984	1.2	Dec. 1984	43		
	2/5/1985[7]	429	Jan. 1985	324		
1,2-tDCE	12/4/1984[6]	83	Nov. 1984	358	Nov. 1983	435
	12/4/1984[5]	15	Dec. 1984	26		
	12/12/1984[6]	2.3J	Dec. 1984	26		
	2/5/1985[7]	150	Jan. 1985	163		
VC	2/5/1985[7]	2.9J	Jan. 1985	31	Nov. 1983	67
Benzene	11/19/1985[7,8,9]	2,500	Nov. 1985	3	Apr. 1984	12
	12/10/1985[7]	38	Dec. 1985	3		
	12/18/1985[7]	1.0	Dec. 1985	3		

[1] Data from Faye et al. (2010, Tables C11 and C12)
[2] Simulation results represent the last day of each month (e.g., May 31); results reported for simulation month nearest the sample date; refer to Appendix A7 for complete listing of reconstructed finished-water concentrations
[3] Water sample collected at Building NH-1; data reported as unreliable
[4] Water sample collected at Building FC-530
[5] Untreated water
[6] Treated water
[7] Treatment status unknown
[8] Laboratory analysis noted with: “Sample appears to have been contaminated with benzene, toluene, and methyl chloride” (JTC Environmental Consultants 1985)
[9] Data noted with: “Not Representative” (U.S. Marine Corp Base Camp Lejeune Water Document CLW #1356)

Table 7.16. Summary statistics for reconstructed contaminant concentrations at selected water-supply wells and the Hadnot Point water treatment plant, Hadnot Point-Holcomb Boulevard study area (Maslia et al. 2013).[1,2]

Water-supply identification (contaminant)	Reconstructed (simulated) concentration, in micrograms per liter				[2]Duration in months exceeding MCL (month and year first exceeding MCL)	Date well stopped pumping in model
	[3]July 1942–June 1996			Range during health study period of interest (January 1968–February 1985)		
	Maximum (date of maximum)	Mean	Standard deviation			
[4]Hadnot Point Industrial Area (HPIA)						
HP-602 (TCE)	658 (Jan. 1959)	359	222	357–499	390 (Oct. 1951)	Dec. 1984
HP-608 (TCE)	50 (Sept. 1972)	25	20	28–50	307 (Aug. 1957)	Dec. 1984
HP-634 (TCE)	659 (Oct. 1968)	391	170	212–659	283 (Aug. 1960)	Dec. 1984
HP-602 (benzene)	236 (Nov. 1984)	53	65	48–236	309 (July 1958)	Dec. 1984
HP-603 (benzene)	179 (May 1996)	29	43	6–129	345 (Aug. 1967)	June 1996
HP-608 (benzene)	11 (Sept. 1979)	4	4	6–11	201 (June 1966)	Dec. 1984
[4]Hadnot Point landfill (HPLF)						
HP-651 (PCE)	353 (Dec. 1982)	249	122	[5]0–353	142 (Apr. 1973)	Feb. 1985
HP-651 (TCE)	7,135 (Dec. 1978)	5,831	2,071	[5]1–7,135	150 (Aug. 1972)	Feb. 1985
HP-651 (1,2-tDCE)	4,037 (Dec. 1984)	3,284	572	[5]69–4,037	150 (Aug. 1972)	Feb. 1985
HP-651 (VC)	660 (Nov. 1984)	391	173	[5]8–660	151 (July 1972)	Feb. 1985
[6]Hadnot Point water treatment plant (HPWTP)						
HPWTP (PCE)	39 (Nov. 1983)	4	8	0–39	114 (Aug. 1974)	N/A
HPWTP (TCE)	783 (Nov. 1983)	107	180	0–783	374 (Aug. 1953)	N/A
HPWTP (1,2-tDCE)	435 (Nov. 1983)	53	95	0–435	128 (Nov. 1972)	N/A
HPWTP (VC)	67 (Nov. 1983)	6	13	0–67	144 (Nov. 1972)	N/A
HPWTP (benzene)	12 (Apr. 1984)	2	3	0–12	63 (Jan. 1979)	N/A

[1]For periods of time when concentrations are equal to or exceed the current MCLs for TCE, PCE, and benzene; non-rounded concentration values used to calculate statistics
[2] Current MCLs are as follows: vinyl chloride, 2 µg/L; PCE, TCE, and benzene, 5 µg/L; 1,2-tDCE, 100 µg/L (see Maslia et al.
[3] Statistics are computed solely for periods of operation
[4] See Maslia et al. (2013, Appendix A3) for complete listing
[5] Water-supply well HP-651 did not start pumping until July 1972; values shown represent dates of July 1972–February 1985
[6] Finished-water concentrations; see Maslia et al. (2013, Appendix A7) for complete listing

Uncertainty

Best modeling practice requires that evaluations be conducted to ascertain confidence in models and model results by assessing parameter sensitivity, variability, and uncertainty associated with the modeling process and with the outcomes attributed to models (ASTM 1994; Saltelli et al. 2000). There are numerous methods for characterizing a model's sensitivity and uncertainty based on variations of calibrated parameter values (ASTM 1994; Cullen and Frey 1999; Salltelli et al. 2000; Tung and Yen 2005; Hill and Tiedeman 2007). These methods are generally classified into two groups: (1) sensitivity analysis, wherein calibrated model parameter values are varied either manually or through some automated method, and (2) probabilistic uncertainty analysis, wherein probabilistic methods are used to characterize and quantify the input and output parameter variation and uncertainty.

Sensitivity Analysis

A sensitivity analysis enables the modeler to evaluate how model output (simulated concentrations) responds to changes in model input parameters. By identifying parameter sensitivity, the modeler can better determine which input parameters have the greatest and least impact on model output. For the HP models, a number of sensitivity analyses were conducted. These included: varying hydraulic, fate and transport model parameters, benzene source-area and source-release, TCE source-release-date, and numerical model grid size and time-step variations. These sensitivity analyses are discussed in much detail in Maslia et al. (2013, p. A79–A91).

Figure 7.26 shows reconstructed (simulated) values of the HPWTP finished water for three different sensitivity analysis scenarios. Scenario 1, adjusting four variables, Scenario 2, adjusting five variables , and Scenario 3, adjusting seven variables. These sensitivity analyses were conducted to see how increasing levels of uncertainty in the input parameters impact the reconstructed values (see Figure 7.26 explanation for information on which parameters were varied). The darker interior (center) lines on Figure 7.26 represent the average (mean) reconstructed contaminant concentration levels. In contrast, the shaded region represents the variability in reconstructed contaminant concentration levels ranging from minimum (lower end of the shaded region) to maximum (higher end of the shaded region) reconstructed values for varying parameter input.

Based on these results, it is scientifically defensible to conclude that during the period of the 1950s to the mid-1980s, contaminant concentration levels would have occurred within this range of values (the shaded region) at HPWTP, with the average (most likely) values being the solid line in the interior. Although reconstructed concentrations were found to vary for these scenarios (the reconstructed levels were found to be sensitive to input parameter values), **exceedance of the MCL was shown to have occurred in all cases**.

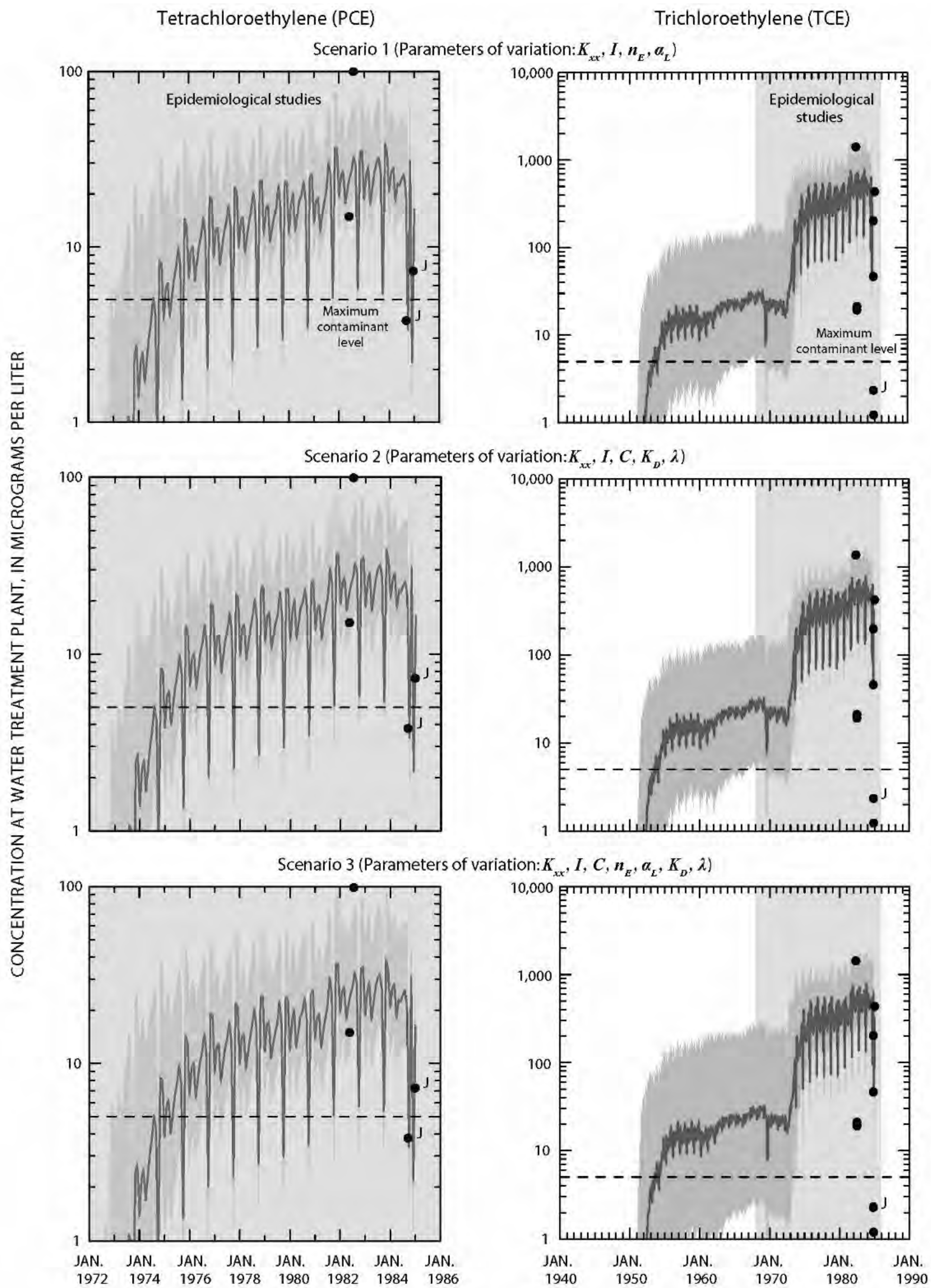


Figure 7.26. Concentrations of tetrachloroethylene (PCE) and trichloroethylene (TCE) in finished water at the Hadnot Point water treatment plant derived from model calibration and hydraulic, fate, and transport model parameter sensitivity analysis, Hadnot Point–Holcomb Boulevard study area, U.S. Marine Corps Base Camp Lejeune, North Carolina. [K_{xx}, horizontal hydraulic conductivity; I, infiltration; C, source concentration; n_E, porosity; α_L, longitudinal dispersivity; K_D, distribution coefficient; λ, biodegradation rate; J, estimated]

EXPLANATION

Maximum—Derived using parameters of variation

Calibrated parameters

Minimum—Derived using parameters of variation

Measured concentration (Table A18)

In all cases, the average of reconstructed values (the values represented by the dark solid line in the center of the shaded region) indicate that contaminant concentration levels were above the drinking water standard (MCL), as do the vast majority of reconstructed values in the sensitivity analyses (the vast majority of the shaded regions are above the drinking water MCL shown by the horizontal dashed line in Figure 7.26). The sensitivity analysis thus demonstrates that even in the worst-case scenario (if all seven input parameters deviated substantially from actual calibrated values and field data), **the historically reconstructed values still indicate PCE and TCE concentration levels above the drinking water MCL**.

Probabilistic Analysis

As discussed in the TT study area of this report, a probabilistic analysis is used to generate uncertainties in model inputs (for example, hydraulic conductivity or contaminant source mass loading rate) so that estimates of uncertainties in model outputs (for example water level or TCE concentration at the HPWTP) can be made. Of particular interest was the uncertainty and variability of water-supply well monthly operational schedules and the impact that the uncertainty and variability would have on the TCE concentrations at the HPWTP. To demonstrate the effect of uncertainty in the pumping schedules of water-supply wells, the Latin Hypercube Sampling (LHS) methodology was used. LHS is a useful tool for generating a limited number of random samples that are evenly distributed over a multidimensional random field. In this respect, LHS is an ideal approach to overcome the computational expense posed by the MCS by reducing the number of simulations required.

Details of applying the LHS method are described in Maslia et al. (2013, p. A93-A94) and Telci et al. (2013). The revised pumping schedules due to uncertainty and variability relative to the calibrated schedules reported in Telci et al. (2013) are used as an input to the contaminant fate and transport models of the HPIA and HPLF area to reconstruct TCE concentrations delivered to the HPWTP by each well. Reconstructed TCE concentrations at the HPWTP derived from applying the LHS methodology to water-supply well monthly operational schedules are shown in Figure 7.27. In this figure, the red line indicates the TCE concentration obtained from the calibrated models (Figure 7.25). The gray lines indicate the TCE concentration variation over time for 10 random scenarios obtained by LHS methodology. Results shown in Figure 7.27 indicate that observed data exhibit substantially greater variation than reconstructed concentrations generated using the LHS-Monte Carlo uncertainty analysis. It also shows that even under uncertainty, there is substantially high concentrations of TCE in finished water at the HPWTP after the onset of pumping at well HP-651.

In summary, effects of parameter uncertainty and variability were analyzed using two approaches—sensitivity analysis and probabilistic analysis. Individually and combined, these analyses demonstrate the high reliability of and confidence in results determined using the calibrated MODFLOW and MT3DMS models.

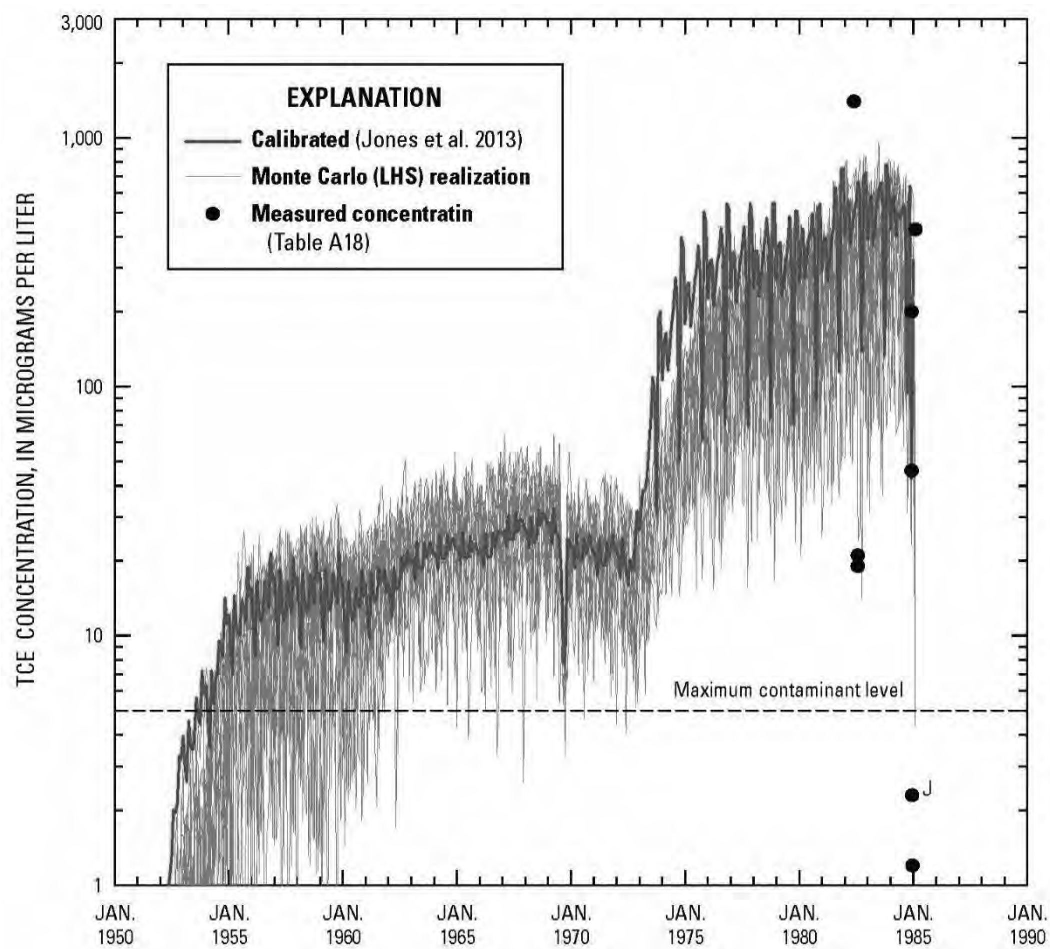


Figure 7.27. Variations in reconstructed (simulated) finished-water concentrations of trichloroethylene (TCE) derived using Latin hypercube sampling (LHS) methodology on water-supply well monthly operational schedules, Hadnot Point water treatment plant, Hadnot Point–Holcomb Boulevard study area (Maslia et al. 2013). [J, estimated].

Conclusions Regarding Hadnot Point

Based on information sources, field data, modeling analyses and results, and the historical reconstruction process, the following conclusions are made with respect to groundwater and finished-water contamination for Hadnot Point:

- **For the Hadnot Point water treatment plant (HPWTP) service area:**
  - The reconstructed contamination of finished water exceeding the current maximum contaminant level (MCL) for TCE was 374 months (August 1953–January 1985) (Table 7.14). With the onset of pumping at well HP-651 during July 1972, the concentration of TCE in well HP-651 affected the resulting finished-water concentrations of TCE at the HPWTP, which exceeded 750 µg/L during November 1983 (Table 7.16). Measured TCE concentrations in finished water at the HPWTP during the period May 1982 through February 1985 ranged from 1.2 µg/L to 1,400 µg/L (Table 7.15).

- The reconstructed contamination of finished water exceeding the current MCL for PCE was 114 months (August 1974–January 1985) (Table 7.16), also a consequence of the onset of pumping of well HP-651. The maximum reconstructed finished-water concentration of PCE was about 40 µg/L during November 1983 (Table 7.14). Measured PCE concentrations at the HPWTP ranged from below detection limits (1–10 µg/L) to 100 µg/L during the period May 1982–February 1985 (Table 7.16).
- The reconstructed duration of contamination of finished water exceeding the current MCL for benzene was 63 months (January 1979–November 1984) (Table 7.16); the maximum reconstructed finished water concentration of benzene was about 12 µg/L during April 1984 (Table 7.16). Measured benzene concentrations at the HPWTP ranged from below detection limits (10 µg/L) to 38 µg/L during the period December 1984–December 1985. An unexplained value of 2,500 µg/L of benzene was measured on November 11, 1985 (Table 7.16).
- Monthly mean reconstructed contaminant-specific concentrations at selected water-supply wells and at the HPWTP for the entire historical period are included with this report as **Appendix I** and **Appendix J**, respectively. They represent, within reasonable scientific and engineering certainty, the contaminant levels in supply wells and in finished water (HPWTP) from 1953 to 1987.

- **For the Hadnot Point Industrial Area (HPIA):**
    - The maximum reconstructed (simulated) monthly mean TCE concentrations at water-supply wells HP-602, HP-608, and HP-634 were 658 micrograms per liter (µg/L) during January 1959, 50 µg/L during September 1972, and 659 µg/L during October 1968, respectively (**Appendix I**). Measured TCE concentrations at well HP-602 ranged from an estimated 0.7 µg/L to 1,600 µg/L during the period of record, July 1984 to January 1991 (Table A4(H)). Corresponding concentrations at well HP-608 ranged from 9 µg/L to110 µg/L during the period of record, December 1984 to November 1986. In well HP-634 between December 1984 and January 1991, TCE concentrations ranged from less than detection limits to 1,300 µg/L.
    - At water-supply wells with measured benzene concentrations exceeding detection limits (HP-602 and HP-608), the maximum reconstructed (simulated) monthly benzene concentration was 236 µg/L at well HP-602 during November 1984 and 11 µg/L at well HP-608 during September 1979 (Table 7.16 and **Appendix I**). Measured benzene concentrations at well HP-602 during the period of record, July 1984 to January 1991, ranged from less than 1.0 µg/L to 720 µg/L. Measured benzene concentrations at well HP-608 during the period of record, December 1984 to November 1986, ranged from 1.6 µg/L to an estimated 4.0 µg/L. All measured benzene concentrations in well HP-603 were below detection limits (Maslia et al. 2013, Table A5, p. A32).

- **For the Hadnot Point landfill (HPLF) area:**
  - The maximum reconstructed (simulated) monthly mean TCE concentration at water-supply well HP-651 was 7,135 µg/L during December 1978 (Table 7.16). Measured TCE concentrations during the period of record, January 1985 to January 1991, ranged from 13 µg/L to 18,900 µg/L (Maslia et al. 2013, Table A4, p.A31).
  - The maximum reconstructed (simulated) monthly PCE concentration at water-supply well HP-651 was 353 µg/L during December 1982 (Table 7.16). Measured PCE concentrations during the period of record, January 1985 through January 1991, ranged from 45 µg/L to 400 µg/L (Maslia et al. 2013, Table A4, p.A31).
  - The maximum reconstructed (simulated) monthly mean 1,2-tDCE concentration at water-supply well HP-651 was 4,037 µg/L during December 1984 (Table 7.16). Measured 1,2-tDCE concentrations during the period of record, January 1985 to November 1986, ranged from 140 µg/L to 8,070 µg/L (Maslia et al. 2013, Table A4, p.A31).
  - The maximum reconstructed (simulated) monthly mean VC concentration at water-supply well HP-651 was 660 µg/L during November 1984 (Table 7.16). Measured VC concentrations during the period or record, January 1985 to January 1991, ranged from 70 µg/L to 655 µg/L (Maslia et al. 2013, Table A4, p.A31).

7.5.3 Holcomb Boulevard (HB)

During the period June 1972–December 1985, the HP and HB water-distribution systems were intermittently interconnected during dry spring and summer months. During these periods, contaminated HP finished water (Figure 7.25) was transferred to and distributed within the uncontaminated HB water-distribution system. The interconnection of the two water-distribution systems was primarily accomplished by operating booster pump 742, although on rare occasions, the valve at Marston Pavilion (near Wallace Creek) also was opened (Figure 7.1). Operational records indicating booster pump 742 operations and Marston Pavilion valve openings are only partially documented. Interconnection information and data that are available were obtained from the Camp Lejeune water utility log books (CLW #7023–CLW #8735).

Because of the interconnection of the HP and HB water-distribution systems, a more complex analysis was necessary (compared to the simple mixing-model approach described by Equations 7.1 and 7.2 and used to reconstruct finished-water concentrations for the TTWTP and HPWTP) to determine the concentration of finished water in the HB water-distribution system (Figure 7.28) during periods of interconnection. This required the application of the EPANET 2 water-distribution system model (Rossman 2000) and extended period simulation (EPS). The EPANET 2 water-distribution system model was calibrated for the HB water-distribution system using field data collected by the ATSDR water-modeling team; field data represented operational conditions during 2004 (Sautner et al. 2013). EPSs were used to reconstruct water-distribution system flow and mass transport patterns during discrete interconnection events when booster pump 742 was intermittently operated, resulting in the transfer of contaminated finished water from the HP water-distribution system to the “uncontaminated” HB water-distribution system. Pipelines represented in the water-distribution system network models coincide with locations of streets within the HP and HB study areas (Maslia et al. 2009b, Figure I3).

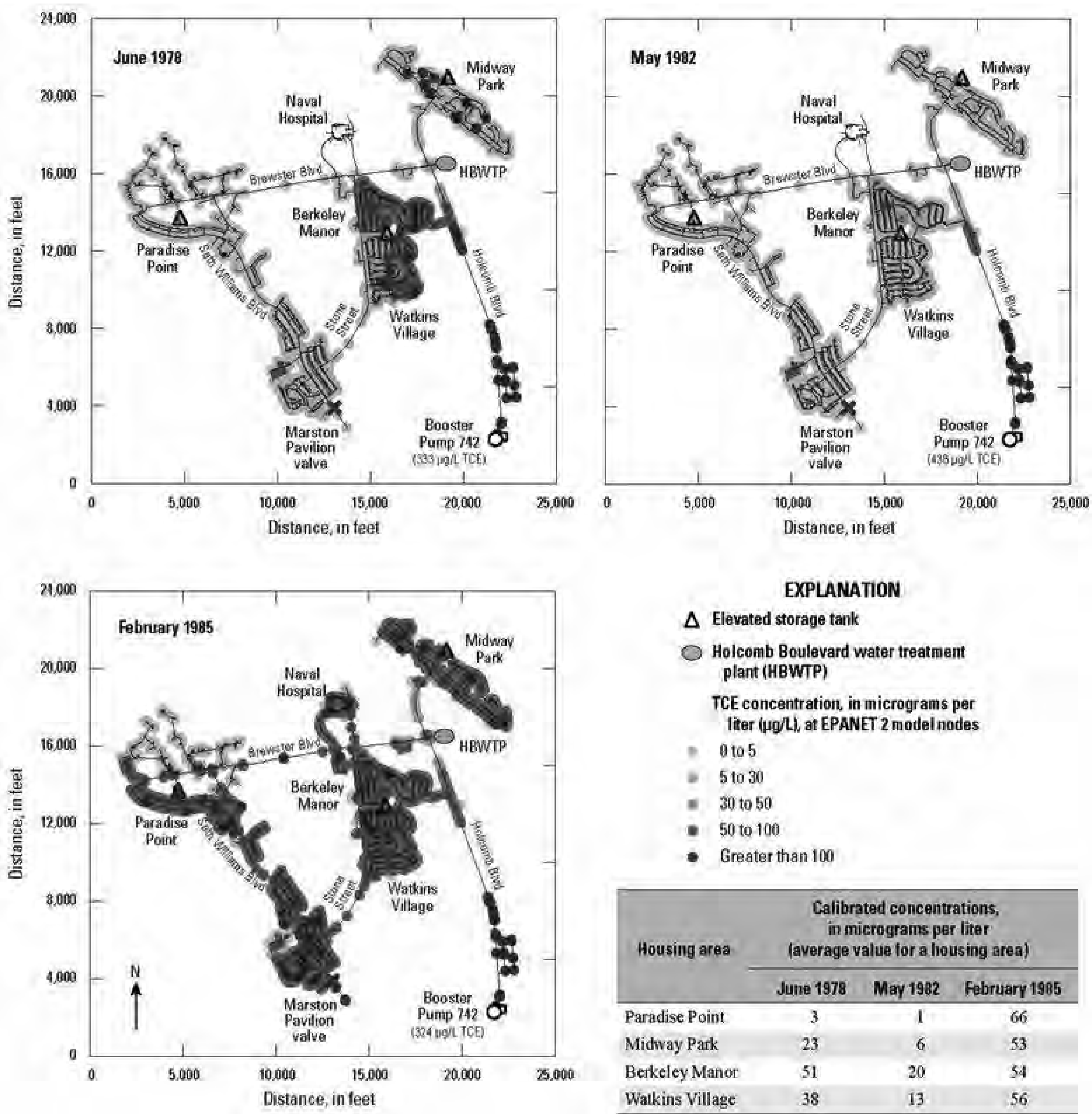
A complete listing of reconstructed contaminant concentrations (PCE, TCE, 1,2-tDCE, VC, and benzene) for the HB water-distribution system for 1972–1985 is provided in **Appendix K**. Spatial distributions of TCE levels within HB housing areas for three time periods—June 1978, May 1982, and February 1985—are shown in Figure 7.28 and listed in Table 7.17. These historical reconstruction results were obtained using the EPANET 2 water-distribution system model for interconnection events. The HB reconstructed drinking-water mean TCE concentrations for the Berkeley Manor and Watkins Village housing areas during June 1978 are 51 µg/L and 38 µg/L, respectively (Figure 7.28, Table 7.17, and **Appendix K**). For May 1982, the Berkeley Manor and Watkins Village housing areas show reconstructed mean TCE concentrations of 20 µg/L and 13 µg/L, respectively. During the 8-day period of 28 January–4 February 1985 (represented by the February 1985 map in Figure 7.28), when the HBWTP was shut down, the reconstructed mean TCE concentrations in all housing areas exceeded 50 µg/L with the exception of the northernmost extent of Paradise Point and a small area to the north of the Marston Pavilion valve (the current MCL for TCE in drinking water is 5 µg/L). Overall, during intermittent transfers of contaminated HP drinking water, the Paradise Point family housing area shows the lowest reconstructed mean TCE concentrations, whereas Berkeley Manor followed by Watkins Village show the greatest reconstructed mean TCE concentrations (except for the pipeline that directly connects booster pump 742 to the HB water-distribution system along Holcomb Boulevard). Spatial distribution maps for the other contaminants of concern (similar to Figure 7.28) are provided in Sautner et al. (2013b). Reconstructed concentrations for the other contaminants of concern (PCE, 1,2-tDCE, VC, and benzene) rarely equaled or exceeded their current MCLs during interconnection periods of interest to the ATSDR health studies (Table 7.17 and **Appendix K**).

Conclusions Regarding Holcomb Boulevard

Based on information sources, field data, modeling analyses and results, and the historical reconstruction process, the following conclusions are made with respect to the contaminated finished water delivered to Holcomb Boulevard:

- When this housing area was serviced by the HPWTP (prior to June 1972), the maximum reconstructed (simulated) monthly mean TCE concentration in finished water of interest to the ATSDR health studies (January 1968–December 1985) was 32 µg/L during August 1968 and August 1969 (**Appendix J**). The minimum reconstructed (simulated) monthly mean TCE concentration in finished water of interest to the health studies (January 1968–December 1985) was 8 µg/L (September and October 1969). TCE concentrations in finished water first exceeded the MCL during August 1953 (**Appendix J**).

- After June 1972 when the HBWTP came online to service this housing area, an interconnection analysis indicates that the maximum reconstructed (simulated) TCE concentration in finished water was 66 µg/L during February 1985 for the Paradise Point area (Figure 7.28, Table 7.17, and **Appendix K**).



Housing area	Calibrated concentrations, in micrograms per liter (average value for a housing area)		
	June 1978	May 1982	February 1985
Paradise Point	3	1	66
Midway Park	23	6	53
Berkeley Manor	51	20	54
Watkins Village	38	13	56

Figure 7.28. Reconstructed (simulated) distribution of trichloroethylene (TCE) contamination within the Holcomb Boulevard water treatment plant service area resulting from supply of contaminated Hadnot Point finished water, June 1978, May 1982, and February 1985 (see Maslia et al. 2013, Figure A1 for location map of Holcomb Boulevard water-distribution system).

Table 7.17. Reconstructed (simulated) mean concentrations of tetrachloroethylene, trichloroethylene, *trans*-1,2-dichloroethylene, vinyl chloride, and benzene in finished water distributed to Holcomb Boulevard family housing areas for selected months, Hadnot Point– Holcomb Boulevard study area (Maslia et al. 2013, Sautner et al. 2013b)[1,2]

[µg/L, microgram per liter; PP, Paradise Point; MP, Midway Park; BM, Berkeley Manor; WV, Watkins Village; —, not applicable]

Month Year	Concentration, in µg/L				Month Year	Concentration, in µg/L				Month Year	Concentration, in µg/L			
	PP	MP	BM	[3]WV		PP	MP	BM	[3]WV		PP	MP	BM	[3]WV
Tetrachloroethylene (PCE)[4]														
June 1978	0	1	2	2	May 1982	0	0	1	1	Jan. 1985[5]	2	2	2	2
June 1980	0	0	1	1	June 1982	0	0	1	0	Feb. 1985[5]	3	3	3	3
Apr. 1981	0	0	2	1	July 1982	0	0	1	0					
May 1981	0	0	1	0	May 1983	0	0	1	0					
Trichloroethylene (TCE)[4]														
Jan. 1972	22	22	22	—	May 1978	0	2	6	4	Apr. 1982	0	3	9	7
Feb. 1972	21	21	21	—	June 1978	3	23	51	38	May 1982	1	6	20	13
Mar. 1972	17	17	17	—	July 1978	0	0	1	1	June 1982	0	4	10	7
Apr. 1972	24	24	24	—	Apr. 1979	0	1	2	1	July 1982	0	4	12	8
May 1972	19	19	19	—	May 1979	0	1	3	2	Aug. 1982	1	3	6	4
June 1972	19	19	19	—	June 1979	0	2	6	4	May 1983	1	5	14	10
July 1972	1	0	0	—	July 1979	0	1	4	2	June 1983	0	0	2	2
June 1973	0	0	1	—	Aug. 1979	0	2	5	3	July 1983	0	0	3	2
June 1976	1	2	3	—	June 1980	2	8	17	13	Aug. 1983	0	2	5	3
Apr. 1977	0	1	2	—	Apr. 1981	0	4	39	28	Apr. 1984	0	2	5	3
May 1977	1	1	3	—	May 1981	0	4	13	10	Jan. 1985[5]	34	31	32	34
June 1977	1	2	3	—	June 1981	0	4	10	7	Feb. 1985[5]	66	53	54	56
July 1977	1	2	3	—	July 1981	0	2	4	3					
Aug. 1977	1	2	4	—	Aug. 1981	0	2	6	4					
***Trans*-1,2-dichloroethylene (1,2-tDCE)[4]**														
June 1973	0	1	1	—	June 1979	0	1	3	2	June 1982	0	2	6	4
June 1976	0	1	2	—	July 1979	0	0	1	1	July 1982	0	2	6	4
Apr. 1977	0	1	1	—	Aug. 1979	0	1	2	1	Aug. 1982	0	2	3	2
May 1977	0	1	1	—	June 1980	1	3	7	5	May 1983	0	3	8	5
June 1977	0	1	1	—	Apr. 1981	0	2	16	12	June 1983	0	0	1	1
July 1977	0	1	2	—	May 1981	0	2	6	4	July 1983	0	0	2	1
Aug. 1977	0	1	2	—	June 1981	0	2	4	3	Aug. 1983	0	1	3	2
May 1978	0	1	3	2	July 1981	0	1	2	1	Apr. 1984	0	1	2	2
June 1978	2	10	22	17	Aug. 1981	0	1	3	2	Jan. 1985[5]	17	16	16	17
Apr. 1979	0	1	1	1	Apr. 1982	0	2	4	3	Feb. 1985[5]	33	27	27	27
May 1979	0	0	1	1	May 1982	0	3	10	7					
Vinyl chloride (VC)[4]														
June 1978	0	1	3	2	June 1981	0	0	1	0	July 1982	0	0	1	1
June 1980	0	1	1	1	Apr. 1982	0	0	1	0	May 1983	0	0	1	1
Apr. 1981	0	0	3	2	May 1982	0	0	1	1	Jan. 1985[5]	3	3	3	3
May 1981	0	0	1	1	June 1982	0	0	1	1	Feb. 1985[5]	6	5	5	5
Benzene[4]														
Jan. 1972	3	3	3	—	Apr. 1972	3	3	3	—	June 1978	0	0	1	0
Feb. 1972	3	3	3	—	May 1972	3	3	3	—	Apr. 1981	0	0	1	1
Mar. 1972	2	2	2	—	June 1972	3	3	3	—	Feb. 1985[5]	1	1	1	1

[1] See Appendix A8 (Tables A8.1–A8.5) for complete monthly listing, January 1972–December 1985

[2] Values for January–June 1972 represent Hadnot Point finished water without any mixing (dilution) with Holcomb Boulevard water treatment plant (WTP) finished water because the Holcomb Boulevard WTP came online after June 1972 (Scott A. Brewer, U.S. Marine Corps Base Camp Lejeune, written communication, September 29, 2005)

[3] Watkins Village housing was not built and occupied until about 1978 (Faye et al. 2010), and the first documented interconnection occurs during May 1978 (U.S. Marine Corps Base Camp Lejeune Water Documents CLW #7023, #7031, and #7033)

[4] Current maximum contaminant level (MCL) for PCE, TCE, and benzene is 5 µg/L; current MCL for 1,2-tDCE is 100 µg/L; current MCL for VC is 2 µg/L; see Table A3

[5] For the 8-day period January 28–February 4, 1985, the Holcomb Boulevard water treatment plant was shut down, and contaminated Hadnot Point finished water was continuously provided to Holcomb Boulevard family housing areas

- After June 1972 when the HBWTP came online to service this housing area, the maximum reconstructed (simulated) monthly concentrations for PCE, 1,2-tDCE, and VC in finished water for the HB housing area occurred during February 1985 and were 3 μg/L, 33 μg/L, and 6 μg/L, respectively (**Appendix K**). The maximum reconstructed (simulated) monthly concentration for benzene was 3 μg/L, occurring during January, February, April, May, and June 1972 (Table 7.15).

- Monthly mean reconstructed contaminant-specific concentrations delivered to HB for the entire historical period included with this report as **Appendix K** represent, within reasonable scientific and engineering certainty, the contaminant levels in finished water from 1953 to 1987.

7.5.4 Discussion and Conclusions

The application and use of water modeling techniques to assist epidemiological studies has been proven to be a reliable and accepted method for obtaining environmental exposure concentrations. Three high-profile, public sites—Woburn, Massachusetts, Dover Township (Toms River), New Jersey, and USMCB Camp Lejeune, North Carolina—have all obtained **definitive results** by using water-modeling techniques (Costas 2002, NJDHSS 2003, Bove et al. 2014a, 2014b, Ruckart et al. 2013, 2014, 2015). The historical reconstruction process, which includes information and data mining activities and water-modeling methods can be used to reliably quantify estimates of mean monthly contaminant-specific concentrations. Based on data, analyses, interpretations, model calibrations, sensitivity analysis, and probabilistic uncertainty analyses, the historical reconstruction process provides reliable and defensible evidence within a reasonable degree of scientific and engineering certainty that drinking-water at Camp Lejeune during the periods of interest was contaminated with VOCs that exceeded drinking-water standards (MCLs) for PCE, TCE, 1,2-tDCE, VC, and benzene. This is demonstrated by the finished water concentrations at the TTWTP and HPWTP for PCE and TCE, respectively, shown in Figure 7.29. The historical reconstruction process was used to reliably quantify estimates of monthly mean contaminant-specific concentrations such as those shown in Figure 7.25 and 7.29, and the results were used in ATSDR's epidemiological studies to estimate the level and duration of exposures. Thus, water-modeling methods described and discussed in this report provide **reliable analysis tools and definitive results** for simulating historical contaminant concentration levels in finished water.

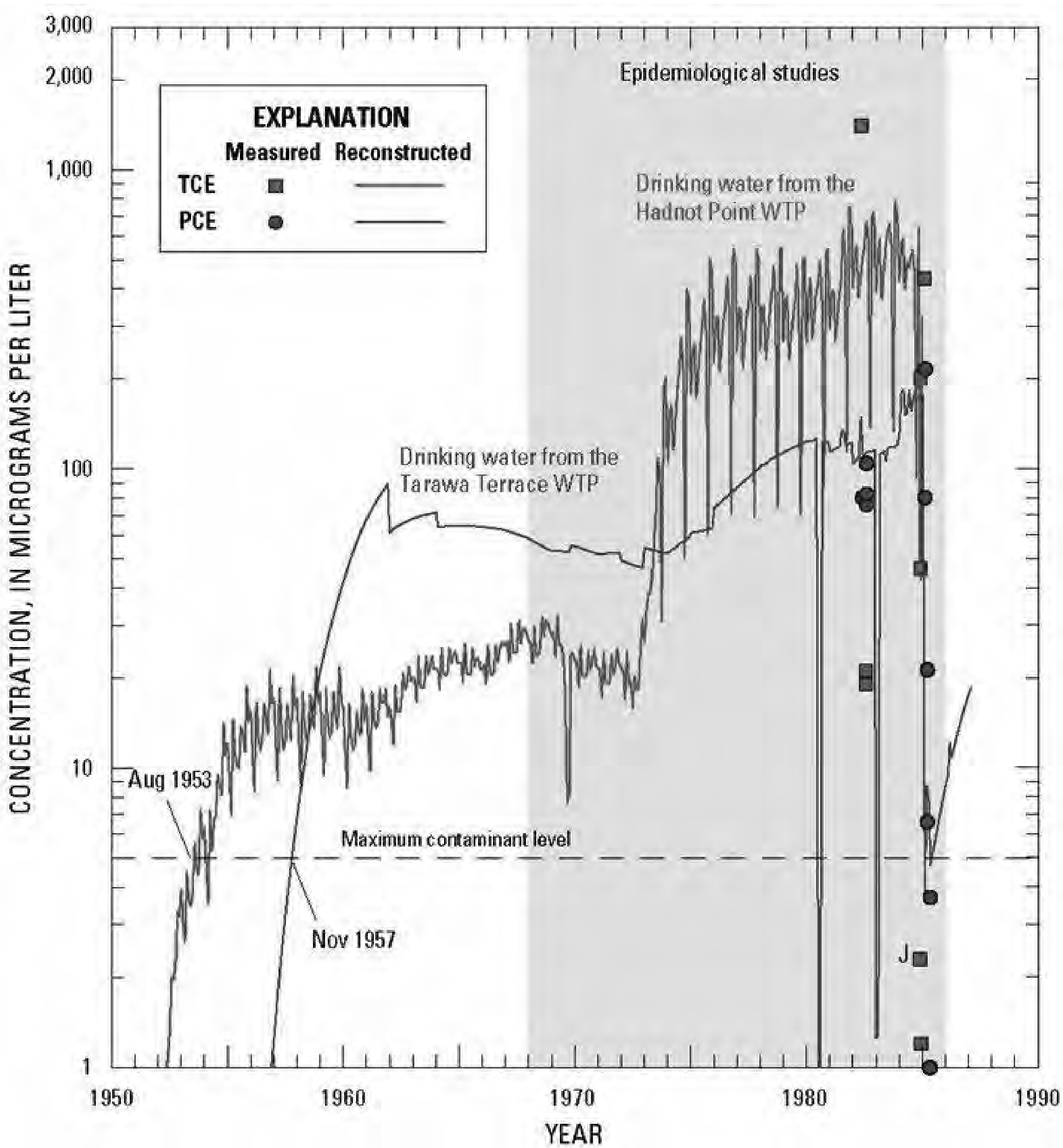


Figure 7.29. Reconstructed (simulated) and measured finished-water concentrations of tetrachloroethylene (PCE) and trichloroethylene (TCE) at the Tarawa Terrace and Hadnot Point water treatment plants (Maslia et al. 2016).

7.6 Peer Review of ATSDR Analyses, Results, and Reports

Throughout the historical reconstruction analysis for USMCB Camp Lejeune, I through the ATSDR sought independent external expert scientific input and review of project methods, approaches, and interpretations to assure scientific credibility of the analyses described in the TT and HP-HB reports. The review process included convening two expert review panels and submitting individual chapter reports to outside experts for peer review. On March 28–29, 2005, ATSDR convened an external expert panel to review the approaches used in conducting the historical reconstruction analysis for Tarawa Terrace and to provide input and recommendations on preliminary analyses and modeling results (available on the ATSDR website and in Maslia 2005). On April 29–30, 2009, ATSDR convened a second external expert panel to review the approaches used in conducting the historical reconstruction analysis for HP and HB and to provide input and recommendations on preliminary analyses and modeling results (available on the ATSDR website and in Maslia 2009). The panels were composed of nationally and internationally recognized experts with professional backgrounds from government, academia, and the private sector. Technical representatives for the Department of the Navy (DON) and the Camp Lejeune Community Assistance Panel (CAP) also served on the panels. Areas of expertise included numerical model development and simulation, groundwater-flow and contaminant fate and transport analyses and model calibration, hydraulic and water-quality analysis of water-distribution systems, epidemiology, and public health. After reviewing data and initial approaches and analyses provided by ATSDR, panel members made recommendations that ATSDR addressed. These panel recommendations and ATSDR responses are found in Maslia (2005, 2009).

In addition to the expert panels and implementing their recommendations, ATSDR sought out independent, external peer review for every chapter report for the TT and HP-HB reports. These peer reviewers were subject matter experts in all topics covered by the ATSDR historical reconstruction analysis reports. Review comments provided by external peer reviewers were used to address technical issues and to improve the scientific credibility of all final reports.

The series of ATSDR reports on historical reconstruction of drinking-water contamination also resulted in two peer reviewed journal articles (Maslia et al. 2009, 2016). Submission of the manuscripts to the scientific journals resulted in another level of external (and independent) peer review for the methods, analyses, and results applied by ATSDR for reconstructing historical drinking-water concentrations at TT, HP, and HB.

An additional endorsement of the quality and scientific validity of the ATSDR Camp Lejeune water-modeling studies came from the American Academy of Environmental Engineers and Scientists, which awarded our team the 2015 Grand Prize for Excellence in Environmental Engineering and Science. This distinguished award was given to the ATSDR team for "Using Environmental Engineering, Scientific Analyses, and Epidemiological Studies to Quantify Human Exposure to Contaminated Drinking Water and to Benefit Public Health."

7.7 Scientific Discourse

When characterizing, analyzing, and investigating sites with historical contamination, limited data, and potential for human exposure, there can naturally arise differences in opinions within the scientific community. The fact that there are differences is not the issue. Rather, if questions and differences are pointed out to investigators in scientific discourse, the issue becomes, have investigators— ATSDR Exposure-Dose Reconstruction Program scientists and engineers—addressed these questions and responded in an objective, transparent, and professional scientific manner to defend their analyses and results? ATSDR did so in all cases. Discussed below are review comments and ATSDR responses pertinent to DON's comments on ATSDR's Tarawa Terrace Model (ATSDR 2009), the National Research Council report on contaminated drinking-water supplies at Camp Lejeune (NRC 2009), and ATSDR's response to the editor (Maslia et al. 2012) to a published journal article in *Ground Water* that used the Camp Lejeune historical reconstruction analyses as a case study (Clement 2010).

7.7.1 Department of the Navy (DON) Comments on the Tarawa Terrace Models and ATSDR Response

On June 19, 2008, the DON (B.P. Harrison) wrote a letter to ATSDR's Deputy Director, Dr. Thomas Sinks. The letter in part stated, "*As with all modeling efforts, there is a great deal of uncertainty in trying to recreate the past. ATSDR has gone to great efforts to test and validate the model, and the resulting estimated results, using limited available data.*" The DON letter contained an attachment with specific concerns and recommendations. ATSDR Exposure-Dose Reconstruction staff, cooperators, and contractors reviewed the DON's concerns and recommendations and responded to them, point by point. The ATSDR response to the DON letter is provided in this report as **Appendix L** and is also available on the ATSDR website and in ATSDR (2009). An example of one of DON's concerns with the Tarawa Terrace model and ATSDR's response is provided below.

DON Comment

"Furthermore, all of the measured concentrations were used during model calibration, leaving no data available for model validation. As a result, the Tarawa Terrace model was not validated."

ATSDR Response

"A number of terms have been used throughout the published literature that reference the adequacy of model simulation to reliably reproduce real-world conditions based on the fidelity of the model and its intended use. Many groundwater modelers and hydrologists have abandoned the use of terms such as model verification and validation for the terms of history matching and post audits (Bredehoeft and Konikow 1993, Oreskes et al. 1994). However, ATSDR understands that the DON comment was intended to express the DON's concern that the calibrated Tarawa Terrace models were not compared to multiple independent sets of measured data (water levels and concentrations) as part of ATSDR's model calibration process and strategy. To address this concern, definitions of terms such as "verification" and "validation" should be agreed upon, and the consequences of undertaking a useful "validation" program for Tarawa Terrace should be completely understood by ATSDR and the DON. Model verification requires that multiple sets of field data be available for model calibration. These sets of field data should be sufficiently large in quantity and distribution and of sufficient quality to provide at least two equally useful calibration data sets. Each data set also should be sufficiently separated in time so as to represent significantly different water-level and contaminant conditions within the model domain. The field data set at Tarawa Terrace used for model calibration was not of sufficient quantity and was too compressed in time to implement a verification procedure. To appropriately calibrate the Tarawa Terrace models, all available field data were required for a single calibration data set and effort. This is consistent with and follows ASTM D5981-96 (1996), Standard Guide for Calibrating a Ground-Water Flow Model Application, that states (Note 4): *"When only one data set is available, it is inadvisable to artificially split it into separate 'calibration' and 'verification' data sets. It is usually more important to calibrate to data spanning as much of the modeled domain as possible."*

"Note, once an acceptable calibration was achieved (using a four-stage calibration strategy described in Maslia et al. (2007), Faye and Valenzuela (2007), and Faye (2008), the calibrated models were used to reconstruct historical monthly PCE and PCE degradation by-product concentrations in groundwater and drinking water (Jang and Aral 2008). This is standard practice in the modeling community–using a calibrated model to "predict" (in ATSDR's situation, "reconstruct") results for a period of time when data are not available or cannot be obtained."

7.7.2 National Research Council Report on Camp Lejeune and ATSDR Response

The NRC report (NRC 2009) on contaminated drinking water supplies at Camp Lejeune reviewed, in part, ATSDR's Tarawa Terrace analysis. In the NRC report's Section 2 (Exposure to Contaminants in Water Supplies at Camp Lejeune), the report made a number of comments that were generally at odds with and at times completely contradictory of data and information published in ATSDR's peer-reviewed Tarawa Terrace report series and provided to the NRC by ATSDR. On July 1, 2009, the Exposure-Dose Reconstruction Program staff at ATSDR submitted a response to ATSDR Management and Leadership pertinent to the NRC report Section 2 review of ATSDR's Tarawa Terrace Analyses. The complete Exposure-Dose Reconstruction Program staff response is provided in **Appendix M** of this report. A summary of the response to the NRC report is provided below.

> "The Agency for Toxic Substances and Disease Registry's (ATSDR) Exposure-Dose Reconstruction Program staff has reviewed the National Research Council (NRC) report titled, "*Contaminated Water Supplies at Camp Lejeune—Assessing Potential Health Effects*." Specifically, our review focused on Section 2 of the report (p. 28–66), "Exposure to Contaminants in Water Supplies at Camp Lejeune." Based on our review of Section 2, we conclude the following:
>
> "The National Research Committee report (NRC 2009) contains numerous misrepresentations and distortions of ATSDR water-modeling analyses, field data and related interpretations and conclusions that are clearly contradicted by findings in ATSDR technical reports. Those ATSDR reports that describe groundwater contamination and the results of model studies related to contamination of drinking water at the Tarawa Terrace base housing area, Camp Lejeune, North Carolina, along with additional supporting information from the Department of Navy, the U.S. Marine Corps, and other sources were provided to the NRC committee during the course of their deliberations. Because the NRC report contains many errors and misrepresentations with respect to the findings of the ATSDR water-modeling analyses and because conclusions and recommendations contained in the NRC report are at such odds with recommendations rendered by several review panels consisting of national and international experts in water modeling and epidemiology, the NRC report cannot be considered an authoritative interpretation or guidance document related to the historical exposure assessment of contaminated drinking water at Camp Lejeune.

> "We base the aforementioned statements on four overarching issues discussed below. In addition, we present specific examples wherein the NRC committee arrived at erroneous conclusions by using incorrect data and otherwise misrepresenting data and information contained in reports that summarize ATSDR investigations at Tarawa Terrace and vicinity. Additional supporting documentation and in-depth technical reviews related to specific NRC report comments are provided in Appendix I and II of this document."

The four overarching issues pertinent to ATSDR's Exposure-Dose Reconstruction Group's response to the NRC report are listed below:

- **Issue 1: Use of Historical Reconstruction for Exposure Assessment**
- **Issue 2: Characterization of PCE as a Dense Non-Aqueous Phase Liquid (DNAPL)**
- **Issue 3: Evaluation of Uncertainty**
- **Issue 4: Reliability of Reconstructed Historical Concentrations**

Refer to **Appendix M** for the complete, point-by-point ATSDR Exposure-Dose Reconstruction Program staff's response to the NRC (2009) report.

7.7.3 ATSDR Response to Ground Water Journal Article on Camp Lejeune

In issue number 5 (September-October) of the 2010 *Ground Water* Journal, author T.P. Clement published the article, "*Complexities in Hindcasting Models-When Should We Say Enough is Enough?*" (Clement, 2010).[11] The goal of the article appeared to be to use the USMCB Camp Lejeune water-modeling studies (specifically Tarawa Terrace analyses) to highlight issues that the author saw as relating to complexities in fate and reactive transport modeling of contaminants in groundwater systems. While the author correctly pointed out limitations with models in general and specifically reactive fate and transport models and shares some thought-provoking points of view, ATSDR believed that there was a lack of detail on several key issues with respect to modeling approaches and methods, the physics of contaminant transport in the subsurface, and agency policies for the review and dissemination of data and reports. Therefore, ATSDR submitted an editorial response to Clement's article (Clement, 2010) and this response was published in issue number 1 (January-February) of the 2012 *Ground Water* journal. A copy of the ATSDR editorial response (Maslia et al. 2012) is provided in **Appendix N** of this report.

The ATSDR editorial response discusses several issues and topics mentioned in the Clement article (2010). These include: (1) "Hindcasting" vs. Historical Reconstruction, (2) Application of "Complex" Models vs. "Simple" Models to simulate subsurface reactive transport, (3) Correction and clarifications of specific contaminant data analyses and modeling issues, (4) Research models vs. public domain codes, (5) Uncertainty and variability of simulation results, and (6) review and dissemination of water-modeling results. In their editorial response, Maslia et al. (2012) conclude:

[11] Dr. T. P. Clement was a member of the NRC Committee reviewing ATSDR's water-modeling analyses at Camp Lejeune (NRC 2009). It appears that he was the only recognized groundwater expert on the NRC committee.

(1) In the situation of the case-control health study at Camp Lejeune, models are powerful tools used to assist epidemiologists in facilitating the estimation of historical exposures during each month of the mother's pregnancy,

(2) Although the case-control health study at Camp Lejeune is a complex endeavor, ATSDR continues to maintain the scientific credibility and thoroughness of its analyses—from both the water-modeling and epidemiological perspectives—by using expert panels and external peer review, and

(3) It is our aim that by addressing the complex issues associated with the process of historical reconstruction in this discussion, our colleagues who have developed and applied models solely in the groundwater modeling and remediation fields, will broaden their horizons and come to appreciate the need and usefulness of extending and incorporating modeling into the multidisciplinary field of exposure assessment science.

8.0 References

Anderson B.A., Maslia M.L., Caparoso J.L., and Ausdemore D., **2007**. Probabilistic Analysis of Pesticide Transport in Shallow Groundwater at the Oatland Island Education Center, Oatland Island, Georgia. Atlanta, GA: Agency for Toxic Substances and Disease; September 2007.

Aral, M.M., Maslia, M.L., Ulirsch, and Reyes, J.J., **1996**. Estimating exposure to VOCs from municipal water supply systems: Use of a better computational model: *Archives of Environmental Health*, 1996, v. 51, no. 4, pp. 300-309.

Aral, M.M., **1998**. Analytical contaminant transport analysis system (ACTS). Multimedia Environmental Simulations Laboratory Report No. MESL-02-98, School of Civil and Environmental Engineering, Georgia Institute of Technology, 1998, Atlanta.

ASTM, **1996**. Standard Guide for Calibrating a Ground-Water Flow Model Application. D5981–96 (Reapproved 2002). West Conshohocken, PA: ASTM International; 1996.

ASTM International, **1994**. Standard Guide for Conducting a Sensitivity Analysis for a Ground-Water Flow Model Application; ASTM Guide D5611-94 (Reapproved 2002); ASTM International: West Conshohocken, PA, USA, October 1994.

ATSDR (Agency for Toxic Substances and Disease Registry), **2009**. Analyses of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water at Tarawa Terrace and Vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina: Historical Reconstruction and Present-Day Conditions—**Response to the Department of the Navy's Letter on: Assessment of ATSDR Water Modeling for Tarawa Terrace**, March 2009.

Bove, F.J.; Ruckart, P.Z.; Maslia, M.; Larson, T.C., **2014a**. Evaluation of mortality among marines and navy personnel exposed to contaminated drinking water at USMC base Camp Lejeune: A retrospective cohort study. *Environmental Health* 2014, *14*, 1–14.

Bove, F.J.; Ruckart, P.Z.; Maslia, M.; Larson, T.C., **2014b**. Mortality study of civilian employees exposed to contaminated drinking water at USMC Base Camp Lejeune: A retrospective cohort study. Environmental Health 2014, 13, 1–13.

Bredehoeft J.D., and Konikow L.F., **1993**. Ground-Water Models: Validate or Invalidate. Ground Water. 1993; 31(2):178‐179.

CDC/NECH/ATSDR, **2016**. Possible health implications from exposure to formaldehyde emitted from laminate flooring samples tested by the Consumer Product Safety Commission, 2016, Atlanta.

Camp Lejeune Water (CLW), **2007**. Camp Lejeune Water Documents, 0001–8761 (not consecutively available), provided on CD-ROM format. In Analyses of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water at Tarawa Terrace and Vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina: Historical Reconstruction and Present-Day Conditions—**Chapter A:** Summary of Findings; Maslia, M.L., Suárez-Soto, R.J., Sautner, J.B., Anderson, B.A., Jones, L.E., Faye, R.E., Aral, M.M., Guan, J., Jang, W., Telci, I.T., et al. Eds.; Agency for Toxic Substances and Disease Registry: Atlanta, GA, USA, July 2007.

Clement, T.P., **2010**. Complexities in hindcasting models—When should we say enough is enough. *Ground Water* 49, no. 5: 620–629.

Costas, K.; Knorr, R.S.; Condon, S.K., **2002**. A Case-Control Study of Childhood Leukemia in Woburn, Massachusetts: The Relationship between Leukemia Incidence and Exposure to Public Drinking Water. Science of the Total Environment. 2002, 300, 23–35.

Cullen, A.C., and Frey, H.C., **1999**. Probabilistic Techniques in Exposure Assessment: A Handbook for Dealing with Variability and Uncertainty in Models and Inputs; Plenum Press: New York, USA, 1999.

Davis, J.H., **2003**. Fate and Transport Modeling of Selected Chlorinated Organic Compounds at Hangar 1000, U.S. Naval Air Station, Jacksonville, Florida. Tallahassee, FL: U.S. Geological Survey Water-Resources Investigations Report 03-4089; 2003.

Davis, J.H., **2007**. Fate and Transport Modeling of Selected Chlorinated Organic Compounds at Operable Unit 1, U.S. Naval Air Station, Jacksonville, Florida. Tallahassee, FL: U.S. Geological Survey Scientific Investigations Report 2007-5043; 2007.

Deutsch, C.V., and Journel, A.G., **1998**. GSLIB Geostatical Software Library and User's Guide. 2nd ed. New York, NY: Oxford University Press; 1998.

Doherty, J., **2003**. Ground water model calibration using pilot points and regularization. *Ground Water*. 2003; 41(2):107–177.

Doherty, J., **2005**. Groundwater Data Utilities/Part B: Program Descriptions. Available from *http://www.sspa.com/pest/utilities.shtml*

Doherty, J., **2010**. PEST: Model Independent Parameter Estimation: User Manual; 2010. Available from*http://www.pesthomepage.org/Downloads.php*.

Doherty, J., **2011**. MODFLOW-ASP: Using MODFLOW-2000 with PEST-ASP; 2011. Available from *http://www.pesthomepage.org/getfiles.php?file=mf2pest.pdf*.

Doherty, J.E., Fienen, M.N., and Hunt, R.J., **2010**. Approaches to Highly Parameterized Inversion: Pilot-Point Theory, Guidelines, and Research Directions: U.S. Geological Survey Scientific Investigations Report 2010–5168; 2010, 36 p.

Faye, R.E., **2007**. Analyses of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water at Tarawa Terrace and Vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina: Historical Reconstruction and Present-Day Conditions—**Chapter B:** Geohydrologic Framework of the Castle Hayne Aquifer System. Atlanta, Georgia: Agency for Toxic Substances and Disease Registry; 2007.

Faye, R.E., **2008**. Analyses of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water at Tarawa Terrace and Vicinity, U.S. Marine Corps Base Camp Lejeune, North

Carolina: Historical Reconstruction and Present-Day Conditions—**Chapter F:** Simulation of the Fate and Transport of Tetrachloroethylene (PCE). Atlanta, GA: Agency for Toxic Substances and Disease Registry; 2008.

Faye, R.E., **2012**. Analyses and Historical Reconstruction of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water Within the Service Areas of the Hadnot Point and Holcomb Boulevard Water Treatment Plants and Vicinities, U.S. Marine Corps Base Camp Lejeune, North Carolina—**Chapter B:** Geohydrologic Framework of the Brewster Boulevard and Castle Hayne Aquifer Systems and the Tarawa Terrace Aquifer. Atlanta, GA: Agency for Toxic Substances and Disease Registry; 2012.

Faye, R.E., and Green, J.W., Jr., **2007**. Analyses of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water at Tarawa Terrace and Vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina: Historical Reconstruction and Present-Day Conditions—**Chapter E:** Occurrence of Contaminants in Groundwater. Atlanta, GA: Agency for Toxic Substances and Disease Registry; In press 2007.

Faye, R.E., and Valenzuela, C., **2007**. Analyses of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water at Tarawa Terrace and Vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina: Historical Reconstruction and Present-Day Conditions—**Chapter C:** Simulation of Groundwater Flow. Atlanta, GA: Agency for Toxic Substances and Disease Registry; 2007.

Faye, R.E.; Anderson, B.A.; Suárez-Soto, R.J.; Sautner, J.B., **2010**. Analyses and Historical Reconstruction of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water within the Service Areas of the Hadnot Point and Holcomb Boulevard Water Treatment Plants and Vicinities, U.S. Marine Corps Base Camp Lejeune, North Carolina—**Chapter C:** Occurrence of Selected Contaminants in Groundwater at Installation Restoration Program Sites; Agency for Toxic Substances and Disease Registry: Atlanta, GA, USA, October 2010.

Faye, R.E., Jones, L.E., and Suárez-Soto, R.J., **2013**. Descriptions and Characterizations of Data Pertinent to Water-Level Data and Groundwater Flow for the Brewster Boulevard and Castle Hayne Aquifer Systems and the Tarawa Terrace Aquifer—**Supplement 3.** In: Maslia ML, Suárez-Soto RJ, Sautner JB, Anderson BA, Jones LE, Faye RE, Aral MM, Guan J, Jang W, Telci IT, Grayman WM, Bove FJ, Ruckart PZ, and Moore SM. Analyses and Historical Reconstruction of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water Within the Service Areas of the Hadnot Point and Holcomb Boulevard Water Treatment Plants and Vicinities, U.S. Marine Corps Base Camp Lejeune, North Carolina—Chapter A: Summary and Findings. Atlanta, GA: Agency for Toxic Substances and Disease Registry; 2013.

Faye, R.E.; Suárez-Soto, R.J.; Maslia, M.L., **2012**. Analyses and Historical Reconstruction of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water within the Service Areas of the Hadnot Point and Holcomb Boulevard Water Treatment Plants and Vicinities, U.S. Marine Corps Base Camp Lejeune, North Carolina—**Chapter D:** Occurrence of Selected

Contaminants in Groundwater at Above-Ground and Underground Storage Tank Sites; Agency for Toxic Substances and Disease Registry: Atlanta, GA, USA, December 2012.

Grayman, W.M., Clark, R.M., Harding, B.L., Maslia, M., Aramini, J., **2004**. Chapter 10: Reconstructing Historical Contamination Events. In: Mays, L.W., editor. Water Supply Systems Security, McGraw-Hill, New York, 2004, pp. 10.1-10.55.

Grayman, W.M.; Maslia, M.L.; Sautner, J.B., **2006**. Calibrating Distribution Systems Models with Fire-Flow Tests. *Optflow* 2006, *32*, 10–12.

Guan, J.; Anderson, B.A.; Aral, M.M.; Maslia, M.L., **2013**. Theory, Development, and Application of Linear Control Model Methodology to Reconstruct Historical Contaminant Concentrations at Selected Water-Supply Wells—**Supplement 5**. In *Analyses and Historical Reconstruction of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water within the Service Areas of the Hadnot Point and Holcomb Boulevard Water Treatment Plants and Vicinities, U.S. Marine Corps Base Camp Lejeune, North Carolina—Chapter A: Summary and Findings*; Maslia, M.L., Suárez-Soto, R.J., Sautner, J.B., Anderson, B.A., Jones, L.E., Faye, R.E., Aral, M.M., Guan, J., Jang, W., Telci, I.T., et al. Eds.; Agency for Toxic Substances and Disease Registry: Atlanta, GA, USA, March 2013.

Harbaugh, A.W., **2005**. The U. S. Geological Survey modular ground-water model—the ground-water flow processes. Reston, VA: U. S. Geological Survey Techniques and Methods 6-A 16; 2005.

Harbaugh, A.W., Banta, E.R., Hill, M.C., and McDonald, M.G, **2000**. MODFLOW-2000, The U.S. Geological Survey Modular Ground-Water Model: User Guide to Modularization Concepts and the Ground-Water Flow Process. Reston, VA: U.S. Geological Survey Open-File Report 00-92; 2000.

Harbaugh, A.W., and McDonald, M.G., **1996**. User's Documentation of MODFLOW-96, an Update to the U.S. Geological Survey Modular Finite-Difference Ground-Water Flow Model. Reston, VA: U.S. Geological Survey Open-File Report 96-458; 1996.

Hayes, L.R., Maslia, M.L., and Meeks, W.C., **1983**. Hydrology and model evaluation of the principal artesian aquifer, Dougherty Plain, southwest Georgia. Atlanta, GA: Georgia Geologic Survey Bulletin 97; 1997.

Hill, M.C., and Tiedeman, C.R., **2007**. Effective Groundwater Model Calibration; John Wiley & Sons, Inc.: Hoboken, NJ, USA, 2007.

IHmod (Version 0,209), downloaded May **2015**. Available from https://www.aiha.org/get-involved/VolunteerGropus/Pages/Exposure-Assessment-Strategies-Committee.aspx

Jang, W., and Aral, M.M., **2005**. Three-Dimensional Multiphase Flow and Multi-Species Transport Model, TechFlowMP. Report No. MESL-02-05. Multimedia Environmental Simulations Laboratory, School of civil and Environmental Engineering, Georgia Institute of Technology; 2005.

Jang, W., and Aral, M.M. **2007**.Desity-Driven Transport of Volatile Organic Compounds and Its Impact on Contaminated Groundwater Plume Evolution and Natural Attenuation. Transport in Porous Media. 2007; 67(3):353–374.

Jang, W., and Aral, M.M., **2008**. Analyses of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water at Tarawa Terrace and Vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina: Historical Reconstruction and Present-Day Conditions–**Chapter G:** Simulation of Three-Dimensional Multispecies, Multiphase Mass Transport of Tetrachloroethylene (PCE) and Associated Degradation By-Products. Atlanta, GA: Agency for Toxic Substances and Disease Registry; 2008.

Jang, W.; Anderson, B.A.; Suárez-Soto, R.J.; Aral, M.M.; Maslia, M.L., **2013**. Source Characterization and Simulation of the Migration of Light Nonaqueous Phase Liquids (LNAPLs) in the Vicinity of the Hadnot Point Industrial Area—**Supplement 7**. In *Analyses and Historical Reconstruction of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water within the Service Areas of the Hadnot Point and Holcomb Boulevard Water Treatment Plants and Vicinities, U.S. Marine Corps Base Camp Lejeune, North Carolina—Chapter A: Summary and Findings*; Maslia, M.L., Suárez-Soto, R.J., Sautner, J.B., Anderson, B.A., Jones, L.E., Faye, R.E., Aral, M.M., Guan, J., Jang, W., Telci, I.T., et al. Eds.; Agency for Toxic Substances and Disease Registry: Atlanta, GA, USA, March 2013.

Jones, L.E., and Maslia, M.L., **1994**. Selected ground-water data, and results of aquifer tests for the Upper Floridan aquifer, Brunswick, Glynn County, Georgia, area: U.S. Geological Survey Open-File Report 94-520, 1994, 107 pp.

Jones, L.E., Prowell, D.C., and Maslia, M.L., **2002**. Hydrogeology and water quality (1978) of the Floridan aquifer system at U.S. Geological Survey TW-26, on Colonels Island, near Brunswick, Georgia: U.S. Geological Survey Water-Resources Investigation Report 02-4020, 2002, 44 p.

Jones, L.E., Suárez-Soto R.J., Anderson B.A., and Maslia M.L., **2013**. Characterization and Simulation of Fate and Transport of Selected Volatile Organic Compounds in the Vicinities of the Hadnot Point Industrial Area and Landfill—**Supplement 6**. In: Maslia ML, Suárez-Soto RJ, Sautner JB, Anderson BA, Jones LE, Faye RE, Aral MM, Guan J, Jang W, Telci IT, Grayman WM, Bove FJ, Ruckart PZ, and Moore SM. Analyses and Historical Reconstruction of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water Within the Service Areas of the Hadnot Point and Holcomb Boulevard Water Treatment Plants and Vicinities, U.S. Marine Corps Base Camp Lejeune, North Carolina—Chapter A: Summary and Findings. Atlanta, GA: Agency for Toxic Substances and Disease Registry; 2013.

Jones, N.L. and Davis, R.J., 2024. Tarawa Terrace Flow and Transport Model Post-Audit, Integral Consulting, Inc., October 24, 2024.

JTC Environmental Consultants, Inc., **1985**. Laboratory Analyses on Naval Samples, JTC Report #85-513; 1985. Contract No.: N62470-84-B-6932.

Lawrence, S.J., **2007**. Analyses of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water at Tarawa Terrace and Vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina: Historical Reconstruction and Present-Day Conditions—**Chapter D:** Properties and Degradation Pathways of Common Organic Compounds in Groundwater. Atlanta, GA: Agency for Toxic Substances and Disease Registry; 2007.

Kopecky, K.J.; Davis, S.; Hamilton, T.E.; Saporito, M.S.; Onstad, L.E., **2004**. Estimation of Thyroid Radiation Doses for the Hanford Thyroid Disease Study: Results and Implications for Statistical Power of the Epidemiological Analyses. Health Phys. 2004, 87, 15–32.

McLaren/Hart-ChemRisk, **2000**. Oak Ridge Dose Reconstruction Project Summary Report; McLaren/Hart-ChemRisk: Alameda, CA, USA, March 2000.

Maslia, M.L., **1980**. Numerical modeling of saturated-unsaturated fluid flow through porous media. MSCE thesis. Atlanta, GA: School of Civil Engineering, Georgia Institute of Technology; March 1980.

Maslia, M.L., and Johnston, R.H., **1982**. Simulation of ground-water flow in the vicinity of Hyde Park landfill, Niagara Falls, New York: U.S. Geological Survey Open-File Report 82-159, 1982, 19 p.

Maslia, M.L., and Johnston, R.H., **1984**. Use of a digital model to evaluate hydrogeologic controls on ground-water flow in a fractured rock aquifer at Niagara Falls, New York: *Journal of Hydrology*, 1984, v. 75, no. 1/4, p. 167-194.

Maslia, M.L., and Randolph, R.H., **1986**. Methods and computer program documentation for determining anisotropic transmissivity tensor components of two-dimensional ground-water flow: U.S. Geological Survey Open-File Report 86-227,1986, 64 p.

Maslia, M.L., and Randolph, R.H., **1987**. Methods and computer program documentation for determining anisotropic transmissivity tensor components of two-dimensional ground-water flow: U.S. Geological Survey Water-Supply Paper 2308, 1987, 46 p.

Maslia, M.L., and Hayes, L.R., **1988**. Hydrogeology and simulated effects of ground-water development of the Floridan aquifer system, southwest Georgia, northwest Florida, and southernmost Alabama: U.S. Geological Survey Professional Paper 1403-H, 1988, 71 p.

Maslia, M.L., and Prowell, C.D., **1990**. Effect of faults on fluid flow and chloride contamination in a carbonate aquifer system: *Journal of Hydrology*, 1990, v. 115, p. 1-49.

Maslia, M.L., Aral, M.M., Houlihan, M.F., **1992**. Evaluation of ground-water flow regime at a landfill with liner system: *Journal of Environmental Science and Health, Part A: Environmental Science and Engineering*, 1992, v. A27, no. 7, p. 1793-1816.

Maslia, M.L., **1994**. Note on "Modifications to the computer program TENSOR2D": *Ground Water*, 1994, v. 32, no. 3, pp. 501-502.

Maslia, M.L., Aral, M.M., Williams, R.C., Williams-Fleetwood, S., Hayes, L.C., and Wilder, L.C., **1996**. Use of computational models to reconstruct and predict trichloroethylene exposure, *Toxicology and Industrial Health*, 1996, v. 12, no. 2, pp. 139-152.

Maslia, M.L., Aral, M.M., and Williams, R.C., **1997**. Exposure assessment using analytical and numerical models: Case study: *ASCE Practice Periodical of Hazardous, Toxic, and Radioactive Waste Management*, 1997, v. 1, no. 2, pp. 50-60.

Maslia, M.L, Sautner, J.B., Aral, M.M., **2000a**. Analysis of the 1998 Water-Distribution System Serving the Dover Township Area, New Jersey: Field-data Collection Activities and Water-distribution System Modeling. Agency for Toxic Substances and Disease Registry, Atlanta, GA.

Maslia, M.L., Sautner, J.B., Aral, M.M., Reyes, J.J., Abraham, J.E., Williams, R.E., **2000b**. Using water-distribution system modeling to assist epidemiologic investigations. ASCE J. Water Resources Planning Manage. 126 (4), 180–198.

Maslia, M.L., Sautner, J.B., Aral, M.M., Gillig, R.E., Reyes, R.E., Williams, R.C., **2001**. Historical reconstruction of the water-distribution system serving the Dover Township area, New Jersey: January 1962–December 1996. Agency for Toxic Substances and Disease Registry, Atlanta, GA.

Maslia, M.L., and Aral, M.M., **2004**. ACTS—Analytical Contaminant Transport Analysis System (ACTS)—Multimedia Environmental Fate and Transport. *ASCE Practice Periodical of Hazardous, Toxic, and Radioactive Waste Management*, 2004, v. 8, no. 3, pp.181-198.

Maslia, M.L., editor, **2005**. Expert Peer Review Panel Evaluating ATSDR's Water-Modeling Activities in Support of the Current Study of Childhood Birth Defects and Cancer at U.S. Marine Corps Base Camp Lejeune, North Carolina: Atlanta, GA: Agency for Toxic Substances and Disease Registry; 2005.

Maslia, M.L., Reyes, J.J., Gillig, R.E., Sautner, J.B., Fagliano, J.A., and Aral, M.M., **2005**. Public Health Partnerships Addressing Childhood Cancer Investigations: Case Study of Toms River, Dover Township, New Jersey, USA. *International Journal of Hygiene and Environmental Health*, 2005, v. 208, no. 1–2, pp. 45–54.

Maslia, M.L., Sautner J.B., Faye R.E., Suárez-Soto R.J., Aral M.M., Grayman W.M., Jang W., Wang J., Bove F.J., Ruckart P.Z., Valenzuela C., Green J.W. Jr., and Krueger A.L., **2007**. Analyses of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water at Tarawa Terrace and Vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina: Historical Reconstruction and Present-Day Conditions—**Chapter A:** Summary of Findings. Atlanta, GA: Agency for Toxic Substances and Disease Registry; July 2007.

Maslia, M.L., editor, **2009**. Expert Panel Assessing Methods and Analyses for Historical Reconstruction of Groundwater Resources and Distribution of Drinking Water at Hadnot Point, Holcomb Boulevard, and Vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina, April 29–30, 2009; *Prepared by* Eastern Research Group, Inc., Atlanta, GA; *Prepared for* Agency for Toxic Substances and Disease Registry (ATSDR), Atlanta, GA, 149 p.

Maslia, M.L., Aral, M.M., Faye, R.E., Suárez-Soto, R.J., Sautner, J.B., Wang, J., Jang, W., Bove, F.J., and Ruckart, P.Z., **2009a**. Reconstructing Historical Exposures to Volatile Organic Compound-Contaminated Drinking Water at a U.S. Military Base. *Journal of Water Quality, Exposure and Health*, 2009, Vol. 1, No. 1, p. 49–68.

Maslia, M.L., Suárez-Soto, R.J., Wang J., Aral M.M., Faye, R.E., Sautner J.B., Valenzuela C., and Grayman, W.M., **2009b**. Analyses of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water at Tarawa Terrace and Vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina: Historical Reconstruction and Present-Day Conditions—**Chapter I:** Parameter Sensitivity, Uncertainty, and Variability Associated with Model Simulations of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water. Atlanta, GA: Agency for Toxic Substances and Disease Registry; February 2009.

Maslia, M.L., Aral, M.M., Faye, R.E., Grayman, W.M., Suárez-Soto, R.J., Anderson, B.A., Bove, F.J., Ruckart, P.Z., and Moore, S.M. **2012**. **Comment on:** "*Complexities in Hindcasting Models—When Should We Say Enough Is Enough,"* by T. Prabhakar Clement, v. 49, no. 5, 620–629: *Ground Water*, v. 50, no. 1, 10–16.

Maslia, M.L., Suárez-Soto R.J., Sautner J.B., Anderson, B.A., Jones, L.E., Faye, R.E., Aral, M.M, Guan, J., Telci, I.T., Grayman, W.M., Bove, F.J., Ruckart, P.Z., and Moore, S.M., **2013**. Analyses and Historical Reconstruction of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water Within the Service Areas of the Hadnot Point and Holcomb Boulevard Water Treatment Plants and Vicinities, U.S. Marine Corps Base Camp Lejeune, North Carolina—**Chapter A:** Summary and Findings. Atlanta, GA: Agency for Toxic Substances and Disease Registry; February 2013.

Maslia, M.L., Aral, M.M., Ruckart, P.Z., and Bove, F.B., **2016**. Reconstructing Historical VOC Concentrations in Drinking Water for Epidemiological Studies at a U.S. Military Base: Summary of Results. *Water*. 2016, 8 (10), 1–23. Available online: http://www.mdpi.com/2073-4441/8/10/449 (accessed on 13 October 2015).

Masters, G.M., **1998**. Introduction to Environmental Engineering and Science. 2nd ed: Prentice Hall; 1998.

New Jersey Department of Health and Senior Services (NJDHSS), **2003**. Case–Control Study of Childhood Cancers in Dover Township (Ocean County), New Jersey. New Jersey Department of Health and Senior Services, Division of Epidemiology, Environmental and Occupational.

NRC (National Research Council), **2009**. Contaminated water supplies at Camp Lejeune: Assessing potential health effects. In: *Board on Environmental Studies and Toxicology*, 328. Washington, DC: National Academies Press.

Oreskes N., Shrader-Frechette K., and Belitz K., **1994**. Verification, Validation, and Confirmation of Numerical Models in the Earth Sciences. Science. 1994; 263:641‐646.

Papadopulas, I.S., **1965**. Nonsteady flow to a well in an infinite anisotropic aquifer: Proceedings of the Dubrovnik Symposium on the Hydrology of Fractured Rocks, International Association of Scientific Hydrology, 1965, p. 21–31.

Randolph, R.B., Krause, R.E., and Maslia, M.L., **1985**. Comparison of aquifer characteristics derived from local and regional aquifer tests: *Ground Water*, 1985, v. 23, no. 3, p. 309-316.

Reif, J.S.; Burch, J.B.; Nuckols, J.R.; Metzger, L.; Ellington, D.; Anger, K.W., **2003**. Neurobehavioral Effects of Exposure to Trichloroethylene Through a Municipal Water Supply. *Environ. Res.* 2003, *93*, 248–258.

Rodenbeck, S.E., and Maslia, M.L., **1998**. Use of groundwater modeling and GIS to determine population exposure to trichloroethylene (TCE) at the Tucson International Airport area National Priorities List site, Tucson, Arizona, USA: *ASCE Practice Periodical of Hazardous, Toxic, and Radioactive Waste Management*, 1998, v.2, no. 2, pp. 53-61.

Ross, S.M, **1977**. Introduction to Probability Models. Academic Press; 1997.

Rossman, L.A., **1994**. EPANET Users Manual. U.S. Environmental Protection Agency, Risk Reduction Engineering Laboratory, 1994, Cincinnati.

Rossman LA., **2000**. EPANET 2 Users Manual. Cincinnati: U.S. Environmental Protection Agency, National Risk Management Research Laboratory; 2000 September. Report No.: EPA/600-R-00/057.

Roy F. Weston, Inc., **1992**. Remedial Investigation Report, ABC One-Hour Cleaners, Jacksonville, North Carolina: Roy F. Weston, Inc.; 1992.

Roy F. Weston, Inc.,**1994**. Remedial Investigation, ABC One-Hour Cleaners, Operable Unit 2, Jacksonville, North Carolina: Roy F. Weston, Inc.; 1994.

Ruckart, P.Z.; Bove, F.J.; Maslia, M, **2013**. Evaluation of exposure to contaminated drinking water and specific birth defects and childhood cancers at Marine Corps Base Camp Lejeune, North Carolina: A case–control study. *Environ. Health* 2013, *12*, 1–10.

Ruckart, P.Z.; Bove, F.J.; Maslia, M., **2014**. Evaluation of contaminated drinking water and preterm birth, small for gestational age, and birth weight at Marine Corps Base Camp Lejeune, North Carolina: A cross-sectional study. Environmental Health 2014, 13, 1–10.

Ruckart, P.Z.; Bove, F.J.; Shanley, E.; Maslia, M., **2015**. Evaluation of contaminated drinking water and male breast cancer at Marine Corps Base Camp Lejeune, North Carolina: A case control study. *Environmental Health* 2015, *14*, 1–16.

Saltelli, A.; Chan, K.; Scott, E.M. (Eds.), **2000**. Sensitivity Analysis; John Wiley & Sons, Ltd.: Chichester, UK.

Samhel, J.; Devlin, D.; Paustenbach, D.; Hollins, D.; Gaffney, S., **2010**. The Role of Exposure Reconstruction in Occupational Human Health Risk Assessment: Current Methods and a Recommended Framework. *Critical Reviews in Toxicology.* 2010, *40*, 799–843.

Sautner, J.B., Maslia, M.L., Valenzuela, C., and Grayman, W.M., Aral, M.MN., and Green Jr., J.W., **2005**. Filed testing of water-distribution systems at the U.S. Marine Corps Base, Camp Lejeune, North Carolina, in support of an epidemiologic study. Proceedings: World Environmental and Water Resources Congress, 2005 May 15–19; Anchorage, AK.

Sautner, J.B., Anderson, B.A., Suárez-Soto, R.J., and Maslia, M.L., **2013**. Descriptions and Characterizations of Data Pertinent to Water-Supply Well Capacities, Histories, and Operations—**Supplement 1.** In: Maslia ML, Suárez-Soto RJ, Sautner JB, Anderson BA, Jones LE, Faye RE, Aral MM, Guan J, Jang W, Telci IT, Grayman WM, Bove FJ, Ruckart PZ, and Moore SM. Analyses and Historical Reconstruction of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water Within the Service Areas of the Hadnot Point and Holcomb Boulevard Water Treatment Plants and Vicinities, U.S. Marine Corps Base Camp Lejeune, North Carolina—Chapter A: Summary and Findings. Atlanta, GA: Agency for Toxic Substances and Disease Registry; 2013.

Sautner, J.B., Grayman, W.M., Telci, I.T., Maslia, M.L., and Aral, M.M., **2013**. Field Tests, Data Analyses, and Simulation of the Distribution of Drinking Water with Emphasis on Intermittent Transfers of Drinking Water Between the Hadnot Point and Holcomb Boulevard Water-Distribution Systems—**Supplement 8**. In: Maslia ML, Suárez-Soto RJ, Sautner JB, Anderson BA, Jones LE, Faye RE, Aral MM, Guan J, Jang W, Telci IT, Grayman WM, Bove FJ, Ruckart PZ, and Moore SM. Analyses and Historical Reconstruction of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water Within the Service Areas of the Hadnot Point and Holcomb Boulevard Water Treatment Plants and Vicinities, U.S. Marine Corps Base Camp Lejeune, North Carolina—Chapter A: Summary and Findings. Atlanta, GA: Agency for Toxic Substances and Disease Registry; 2013b.

Suárez-Soto R.J., Jones L.E., and Maslia M.L., **2013**. Simulation of Three-Dimensional Groundwater Flow—**Supplement 4**. In: Maslia ML, Suárez-Soto RJ, Sautner JB, Anderson BA, Jones LE, Faye RE, Aral MM, Guan J, Jang W, Telci IT, Grayman WM, Bove FJ, Ruckart PZ, and Moore SM. Analyses and Historical Reconstruction of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water Within the Service Areas of the Hadnot Point and Holcomb Boulevard Water Treatment Plants and Vicinities, U.S. Marine Corps Base Camp Lejeune, North Carolina—Chapter A: Summary and Findings. Atlanta, GA: Agency for Toxic Substances and Disease Registry; 2013.

Telci, I.T.; Sautner, J.B.; Suárez-Soto, R.J.; Anderson, B.A.; Maslia, M.L.; Aral, M.M., **2013**. Development and Application of a Methodology to Characterize Present-Day and Historical Water-Supply Well Operations—**Supplement 2**. In *Analyses and Historical Reconstruction of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water within the Service Areas of the Hadnot Point and Holcomb Boulevard Water Treatment Plants and Vicinities, U.S. Marine Corps Base Camp Lejeune, North Carolina—Chapter A: Summary and Findings*; Maslia, M.L., Suárez-Soto, R.J., Sautner, J.B., Anderson, B.A., Jones, L.E., Faye, R.E., Aral, M.M., Guan, J., Jang, W., Telci, I.T., et al. Eds.; Agency for Toxic Substances and Disease Registry: Atlanta, GA, USA, March 2013.

Tung, Y.-K., and Yen, B.-C, **2005**. Hydrosystems Engineering Uncertainty Analysis; McGraw-Hill: New York, NY, USA, 2005.

USEPA (U.S. Environmental Protection Agency), **1997**. Guiding Principles for Monte Carlo Analysis. Washington, DC: United States Environmental Protection Agency; 1997 March. Report No.: EPA 630-R-97-001.

USEPA (U.S. Environmental protection Agency), **2009**. Guidance on the Development, Evaluation, and Application of Environmental Models. Washington, DC: U.S. Environmental Protection Agency, Office of the Science Advisor, Council for Regulatory Environmental Modeling; 2009 March. Report No.: EPA/100/K-09/003. Available from *http://www.epa.gov/crem/cremlib.html*

Wang, J., and Aral, M.M., **2008**. Analyses of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water at Tarawa Terrace and Vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina: Historical Reconstruction and Present-Day Conditions—Chapter H: Effect of Groundwater Pumping Schedule Variation on Arrival of Tetrachloroethylene (PCE) at Water-Supply Wells and the Water Treatment Plant. Atlanta, GA: Agency for Toxic Substances and Disease Registry; 2008.

Zheng C., **2010**. MT3DMS v5.3 Supplemental User's Guide. Technical Report to the U.S. Army Engineer Research and Development Center. Tuscaloosa, AL: Department of Geological Sciences, University of Alabama; 2010.

Zheng C., and Wang P.P., **1999**. MT3DMS: A Modular Three-Dimensional Multi-Species Model for Simulation of Advection, Dispersion, and Chemical Reactions of Contaminants in Groundwater Systems: Documentation and User's Guide. Vicksburg, MS: U.S. Army Engineer Research and Development Center; 1999. Report No.: SERDP-99.

9.0 Glossary and Abbreviations

Definitions of terms and abbreviations used throughout this report are listed below.

A

AAEE American Association of Environmental Engineers

AAEES American Association of Environmental Engineers and Scientists

ACTS Analytical contaminant transport analysis system, a computational p[platform to assist with assessing and quantifying environmental multimedia fate and transport within air, soil, surface water and groundwater; can be run in deterministic or probabilistic mode (Aral 1998, Maslia and Aral 2004)

ATSDR Agency for Toxic Substances and Disease Registry; https://www.atsdr.cdc.gov

ASCE American Society of Civil Engineers

AST Above-ground storage tank

B

BAH Booz-Allen-Hamilton

BHC Benzene hexachloride, HCH, or hexachlorocyclohexane

BTEX Benzene, toluene, ethylbenzene, and xylenes

C

CAP Community assistance panel

CDC U.S. Centers for disease Control and Prevention: https://www.cdc.gov

CERCLA The Comprehensive Environmental Response, Compensation, and Liability Act of 1980, also known as Superfund

CLW Camp Lejeune Water document

CPSC Consumer Product Safety Commission

CV Curriculum vitae

D

DCE 1,1-dichloroethylene or 1,1-dichloroethene

1,2-DCE *cis*-1,2-dichloroethylene or *trans*-1,2-dichloroethylene

1,2-cDCE *cis*-1,2-dichloroethylene or *cis*-1,2-dichloroethene

1,2-tDCE *trans*-1,2-dichloroethylene or *trans*-1,2-dichloroethene

DON Department of the Navy

DNAPL Dense nonaqueous phase liquid

E

EDB Ethylene dibromide

EDRP Exposure-Dose Reconstruction Program developed by ATSDR in 1993

EPA U.S. Environmental Protection Agency, https://www.epa.gov, also see USEPA

EPANET A water-distribution system (network) model developed by the USEPA (Rossman 1994)

EPANET 2 Version 2 of the EPANET model (Rossman 2000)

EPM Equivalent porous medium

EPS Extended period simulation

F

F-D Finite-difference solver; a transport equation solution method used by MT3DMS

ft Foot or feet

ft^3/d Cubic foot per day

G

Ga. Tech Georgia Institute of Technology, Atlanta, Georgia

GIS Geographic information system

g Grams

H

HB Holcomb Boulevard

HBWTP Holcomb Boulevard water treatment plant

HCOH Formaldehyde

HP Hadnot Point

HPFF Hadnot Point fuel farm

HPIA Hadnot Point Industrial Area

HPLF Hadnot Point landfill

HPWTP Hadnot Point water treatment plant

I

IHMod A suite of mathematical models used to estimate air concentrations of chemicals; can be run in deterministic or probabilistic modes; available from the American Industrial Hygiene Association (AIHA)

IRP Installation Restoration Program

L

LCL Lower confidence limit

LCM Linear control model; a model based on linear control theory methodology developed to reconstruct historical contaminant concentrations in water-supply wells (Guan et al. 2013)

LHS Latin hypercube sampling

LNAPL Light nonaqueous phase liquids

M

Markov process A process that analyzes the tendency of one event to be followed by another event based on the sequence of events. Using this analysis, one can generate a new sequence of random but related events, which will look similar to the original; a stream of events is called a Markov Chain

MCS Monte Carlo simulation; see Monte Carlo analysis

MOC Method of characteristics solver; a transport equation solution method used by MT3DMS

Monte Carlo analysis Also referred to as Monte Carlo simulation; a computer-based method of analysis that uses statistical sampling techniques to obtain a probabilistic approximation to the solution of a mathematical equation or model

MODFLOW A family of three-dimensional groundwater-flow models, developed by the U.S. Geological Survey, https://www.usgs.gov/mission-areas/water-resources/science/modflow-and-related-programs

MT3DMS Three-dimensional mass transport, multispecies model developed on behalf of the U.S. Army Engineer Research and Development Center. MT3DMS-5.3 (Zheng and Wang 1999) is the specific version of MT3DMS code used for the Hadnot Point–Holcomb Boulevard study area analyses

MCL Maximum contaminant level

MESL Multimedia Environmental Simulations Laboratory, School of Civil and Environmental Engineering, Georgia Institute of Technology

mg/L micrograms per liter; 1 part per billion

Model calibration The process of adjusting model input parameter values until reasonable agreement is achieved between model-predicted outputs or behavior and field observations

N

NAVFAC Naval Facilities Engineering Command, Norfolk, Virginia

NCEH National Center for Environmental Health; a center within the U.S. Centers for Disease Control and Prevention (CDC)

ND nondetect

NJDHSS New Jersey Department of Health and Senior Services

NPL National Priorities List

NRC National Research Council

P

PCE Tetrachloroethene, tetrachloroethylene, 1,1,2,2-tetrachloroethylene, or perchloroethylene; also known as PERC® or PERK®

PDF Probability density function

PRNG Pseudo-random number generator

R

RASA Regional Aquifer System Analysis program of the U.S. Geological Survey

S

SCADA Supervisory control and data acquisition

SGS Sequential Gaussian simulation

T

TCE 1,1,2-trichloroethene, or 1,1,2-trichloroethylene, or trichloroethylene

TechFlowMP A three-dimensional multispecies, multiphase mass transport model developed by the Multimedia Environmental Simulations Laboratory at the Georgia Institute of Technology, Atlanta, Georgia

TechNAPLVoL LNAPL estimate model developed by the Multimedia Environmental Simulations Laboratory at the Georgia Institute of Technology, Atlanta, Georgia

TENSOR2D A computer program to automate computing components of the two-dimensional anisotropic transmissivity tensor (Maslia and Randolph 1986, 1987)

TT Tarawa Terrace

TTWTP Tarawa Terrace water treatment plant

TVD Total variation diminishing solver; a transport equation solution method used by MT3DMS

U

UCL Upper confidence limit

USEPA U.S. Environmental Protection Agency, https://www.epa.gov, also see EPA

USGS U. S. Geological Survey

USMC U.S. Marine Corps

USMCB U.S. Marine Corp Base

UST Underground storage tank

V

VC Vinyl chloride

VOC Volatile organic compound

W

WTP Water treatment plant

Appendix A — Curriculum Vitae for Morris L. Maslia, P.E.

Curriculum Vitae

MORRIS L. MASLIA, P.E., D.WRE, DEE, Fellow EWRI
Water Resources — Environmental Analyses — Public Health
3360 Norfolk Chase Drive, Peachtree Corners, GA 30092
Mobile: +1 404-431-0035 — Email: H2OBoy54@gmail.com

EDUCATION

Georgia Institute of Technology, Atlanta, Georgia

- Coursework towards Ph.D. (Water Resources and Environmental Analysis)
- Master of Science, Civil Engineering (Water Resources), 1980
- Bachelor of Civil Engineering, 1976

PROFESSIONAL HISTORY

M. L. Maslia Consulting Engineer, Peachtree Corners, Georgia
Owner, 2018–Present

Agency for Toxic Substances and Disease Registry, Atlanta, Georgia
Environmental Engineer and Project Officer, 1992–2017

Rollins School of Public Health, Emory University, Atlanta, Georgia
Adjunct Faculty, Department of Environmental Health, 2000–2018

Geosyntec Consulting Engineers, Norcross, Georgia
Water Resources Group Manager and Hydrologist, 1989–1992

U.S. Geological Survey, Water Resources Division, Doraville, Georgia
Research Hydrologist, 1980–1989

Federal Energy Regulatory Commission, Washington, DC/Atlanta, Georgia
Civil Engineer, 1976–1980

PROFESSIONAL LICENSE AND CERTIFICATION

Registered Professional Engineer (GA), #PE012689 (active)
Certified Ground Water Professional, National Ground Water Association #115205
Diplomate, American Academy of Water Resources Engineers, D.WRE #00066
Diplomate, American Academy of Environmental Engineers & Scientists, DEE #00-20013
OSHA HAZWOPR 40-hour certification with annual 8-hour refresher; CPR/AED certified

REPRESENTATIVE EXPERIENCE

Morris L. Maslia, PE, has conducted consulting engineering, research, and scientific studies in the areas of environmental fate and transport, water resources (including water-distribution systems), hazardous waste remediation, environmental health, exposure assessment, and public health. He has worked with international organizations, non-profit organizations, U.S. federal agencies, state government agencies, engineering consulting firms, and private industry. He has developed and presented workshops, lectures, and training courses for international, government, and academic institutions (*e.g.*, Emory University and Georgia Tech). His areas of experience, expertise, and continued interests include environmental and public health, water resources and sanitation, global impacts of contamination of water resources, environmental analyses, epidemiological studies, exposure assessment, water-distribution system analysis, engineering and research report review, and volunteering and working with non-profit organizations.

KNOWLEDGE, SKILLS, AND ABILITIES

- Consultant to Bell Legal Group (Georgetown, SC) on historical reconstruction of groundwater contamination, fate and transport modeling of contaminants in groundwater, and water-distribution system analyses; July 2022–Present.
- Professional engineering review of "Semiannual Groundwater Monitoring and Corrective Action Reports, Plant McManus Inactive Ash Pond 1," for Resolute Environmental & Water Resources Consulting, LLC; 2022–2024.
- Consultant to Resolute Environmental & Water Resources Consulting, LLC, on groundwater monitoring, groundwater modeling, and fate and transport modeling at a site in Athens, GA; August 2021–March 2022.
- Member of Review Panel evaluating a National Science Foundation EPSCoR Track-2 IGM Project, The University of Alabama, Tuscaloosa, AL; June 2023 and June 2024.
- Developed and lead agency wide (ATSDR) program for estimating human exposures to environmental contaminants and documenting resulting public health impacts. Direct involvement with three of the most high-profile U.S. environmental contamination and public health cases to date: (1) Love Canal/Hyde Park, NY; (2) Toms River (Dover Township), NJ; and (3) Marine Corps Base Camp Lejeune, NC.
- Deployment to San Juan, Puerto Rico for Hurricane Maria response (October—November 2017) Deployment to CDC Emergency Operations Center for ZIKA response (May 2016)
- International teaching and travel experience; volunteer work with international environmental, water resources, and non-profit organizations.
- Outstanding project proposal/request for proposal development and writing skills.

- Outstanding written and oral communication skills. Presentations given to academic audiences, to top military officers at the Pentagon, to an Assistant Secretary of the Navy, and to Congressional staff. Ability to communicate highly scientific and technical analyses for a lay person's and media understanding at community and public meetings.
- Extensive experience, abilities, and skills to interface with the public in meetings and diverse settings.
- Ability to work effectively with minimal supervision in a multidisciplinary and diverse team environment.
- Outstanding skills with WIN OS, MAC OS, MS Office Suite, ADOBE, geographic information systems (GIS), multimedia presentations, and scientific visualization.
- OSHA 40-hour HAZWOPER certified with annual 8-hour refresher, CPR/AED certified, annual ethics, scientific integrity, and diversity training certifications.
- National Incident Management System (NIMS, IS-00700.a) training and certification.
- Knowledge and experience with CERCLA and RCRA sites and regulations.
- Extensive experience with water resources, water-distribution systems analysis, environmental and public health analyses (including epidemiological studies).
- Non-profit organization volunteer experiences ranging from being a Board of Directors member to President where I was responsible for engaging clergy, hiring and directing administrative and educational staff, and balancing an annual budget.

INTERNATIONAL ASSISTANCE, TEACHING AND TRAINING

Provided international government representatives with technical advice, training, and consultation. Coordinated workshops and presented seminars at training centers and universities in the areas of water resources, exposure assessment, public health implications of exposure to contaminated environmental media, and the use and application of geographic information systems (GIS) and spatial analysis techniques. Mr. Maslia is an Adjunct Faculty Member in the Department of Environmental Health, Rollins School of Public Health, Emory University, Atlanta, Georgia, USA.

- Requested by the Pan American Health Organization's Center for Human Ecology and Health, to develop, coordinate, and present a two-week workshop on Geographic Information Systems and Human Exposure to Chemical Substances. The course was presented at the Autonomous University of San Luis Potosi', Mexico; February 1996.
- Requested by the Autonomous University of San Luis Potosi', Mexico, to develop a three-day course on Quantitative Exposure Assessment. Course conducted as part of the universities Health Risk Assessment graduate course, San Luis Potosi, Mexico; May 24–30, 2003.

- Invited to present a seminar at the Munro Center for Civil and Environmental Engineering at the University of New South Wales, Australia; October 1995.
- Provided technical advice on modeling variably saturated flow and contaminant transport to a representative from the People's Republic of China visiting the USGS's Georgia office; 1988.
- Requested by USGS (on behalf of USAID) to provide advice to Jordanian Government on flow and transport modeling of contamination of a carbonate aquifer system underlying Amman, Jordan; 1986.
- Provided training, technical advice, and consultation to the Head of the Water Authority of Jordan on use of USGS documented groundwater-flow and transport computer models; 1985.
- Requested by the Director, Department of Environmental and Occupational Health, Rollins School of Public Health of Emory University, to develop and teach a course in Environmental and Occupational Hazards (EOH541) for students enrolled in the Master's of Public Health Degree; September 1999.
- Adjunct Faculty, Rollins School of Public Health of Emory University, Department of Environmental and Occupational Health, 2000–2015; taught EOH541, Environmental and Occupation Health, Hazards II course, January – May 2000–2004; Faculty advisor/student mentor; guest seminar presenter.
- Co-developed Water Distribution System Analysis (WDSA) Workshop on "Distribution System Tracer Studies: Design, Implementation and Case Studies." Presented at 8th WDSA Symposium 2006, Cincinnati, OH; August 27, 2006.
- Developed a five-day workshop for ATSDR and Cooperative State Health Assessors on the use and application of the Analytical Contaminant Transport Analysis System (ACTS) computational software; June 1999.

ADMINISTRATIVE ACCOMPLISHMENTS

- Authored and project officer of U.S. Government agency (ATSDR) strategy for Exposure-Dose Reconstruction.
- Organized administrative logistics and technical aspects for expert panels to review water-modeling analyses conducted at U.S. Marine Corps Base Camp Lejeune, North Carolina (April 2009 and March 2005) and Dover Township (Toms River), New Jersey (August 2001 and December 1998).
- Detailed to the National Center for Injury Prevention and Control (NCIPC), Office of the Associate Director for Science, 2003. Served as the acting Executive Secretary for NCIPS's study

section and as a Designated Federal Official (DFO) during the NCIPC peer review of extramural grant proposals.

- Developed and wrote sole-source contracts for external technical assistance on behalf of ATSDR.
- Developed and wrote cooperative agreement for ATSDR's Research Program on Exposure-Dose Reconstruction, 1993, 1998, 2003, and 2008.
- Developed and wrote interagency agreements (IAA) with the U.S. Geological Survey (Connecticut, North Carolina, Georgia, and National Research Program) to provide technical assistance, hydrogeologic site characterization, training in geochemical modeling, and report preparation, 1995, 1996, and 2004–2013.
- Developed technical and computational specifications and reviewed interim and final analyses for conducting a multi-pathway environmental exposure assessment at the Otis Air Force Base site, Massachusetts, on behalf of ATSDR's Division of Health Studies and the Massachusetts Department of Health.
- Developed ATSDR's analytical, computational, and scientific visualization capabilities so that the agency now has a state-of-the-art computational laboratory that is the envy of many state environmental and public health agencies. The analysis capabilities of the laboratory are respected throughout the environmental and public health community.

TECHNICAL AND SCIENTIFIC ACCOMPLISHMENTS

- Briefed Deputy Assistant Secretary of the Navy for Environment and U.S. Marine Corps General Staff on water-modeling analyses at U.S. Marine Corps Base Camp Lejeune, North Carolina, April 29, 2011, The Pentagon, Washington, DC
- Presented scientific findings before the National Academies, National Research Council Committee on Contaminated Drinking Water at Camp Lejeune, September 24, 2007, Washington, DC.
- Responded to Congressional Inquiry on Contamination of Drinking Water at U.S. Marine Corps Base Camp Lejeune, North Carolina. U.S. House of Representatives Committee on Energy and Commerce, Subcommittee on Oversight and Investigations, June 13, 2007, Washington, DC.
- Provided technical assistance to ATSDR's Division of Health Studies in assessing potential associations between drinking-water contamination at U.S. Marine Corps Base Camp Lejeune, North Carolina and birth defects and childhood cancer.
- Assisted U.S. Environmental Protection Agency in providing Federal Circuit Judge in Buffalo, New York with groundwater flow analyses of the Hyde Park landfill area near Niagara Falls; this

formed the basis for one of the first consent decrees under CERCLA (Superfund) legislation for a hazardous waste site analysis and clean up.

- Assisted the New Jersey Department of Health with determining the possible locations and extent of historical exposures from environmental contaminants that have led to an increased number of cases of childhood brain cancers in the Toms River section of Dover Township, NJ. Developed strategy and protocol for using water-distribution system model to assist with estimating proportionate amount of public water used by residents of Dover Township in a case-control epidemiologic investigation.
- Developed and successfully implemented a protocol for continuous and simultaneous monitoring and recording of pipeline pressures and hydraulic characteristics for a large water-distribution system. Pressures were recorded at 25 locations throughout the system that was operating under winter-time and summer-time demand conditions.
- Assisted the U.S. Environmental Protection Agency's (USEPA), National Risk Management Laboratory (Cincinnati, OH), with refining and upgrading the EPANET water-distribution system model for use with large-scale distribution systems (>10,000 pipe) in simulating hydraulics and contaminant transport.
- Provided technical assistance and expertise to CDC's National Center for Environmental Health (NCEH) in the area of integrating the use of GIS, numerical modeling, and demographic analysis.
- In conjunction with the Multimedia Environmental Simulations Laboratory in the Georgia Tech School of Civil and Environmental Engineering, developed and tested ATSDR's analytical contaminant transport and health risk analysis system software (ACTS/RISK). This is a WINDOWS-based software platform that is used to compute fate and transport of contaminants and exposure to contaminants by the groundwater, surface-water, air, and biota pathways. The ACTS/RISK software can be run in deterministic (single parameter value) or Monte Carlo (uncertainty) modes.
- Requested by the National Cancer Institute to serve on a panel of national experts to assess the use of geographic information system (GIS) technology as it relates to exposure assessment.
- Provided assistance to health assessors working on Tucson International Airport NPL site. Used innovative analysis and application of flow and transport modeling to assess TCE contamination of Tucson, AZ area in order to reconstruct historical exposures.
- Requested by the attorney general's office for the State of Connecticut and citizens of Somers, CT to conduct groundwater flow and contaminant transport modeling to characterize the extent and duration of citizens' exposure to PCE.
- Requested by the Connecticut Department of Health to conduct analysis of municipal water distribution system to assess exposure to VOC contamination. Hydrodynamic and water-quality modeling were integrated with geographic information systems (GIS) and demographic characteristics for the Town of Southington, CT.

- Assisted health assessors in determining historical exposures by conducting groundwater flow and contaminant transport modeling of the Gratuity Road site, Groton, MA.

VOLUNTEER AND OUTSIDE ACTIVITIES

- Coordinated and raised more than $58,000 in scholarship funds for the Arava Institute for Environmental Studies (www.arava.org) that brings together Palestinians, Jordanians, and Israel Jews and Arabs to work on local and regional Middle-East issues at the grass-roots level using environmental study as a framework. Cycled more than 280 miles during a five-day period during November 2014 and November 2016 from Jerusalem to Eilat as part of the scholarship fundraising program; Team Captain and coordinator for the 16-person Atlanta cycling team that raised the scholarship funds.
- Participated in a cycling event to honor the 50th anniversary of the Selma to Montgomery Voting Rights March during February 2015. More than 300 cyclists participated in the ride sponsored by the Montgomery Bicycle Club on February 21, 2015. The ride began at the historic Edmund Pettus Bridge in Selma, Alabama and ended 54 miles away at the steps of the Alabama state capital in Montgomery.
- Presented with the Jewish National Fund's Community Service Award, May 2014.
- Associate Editor, American Society of Civil Engineers (ASCE) Journal of Water Resources Planning and Management.
- Associate Editor, International Journal of Water Quality, Exposure, and Health (Springer).
- Adjunct Faculty, Department of Environmental Health, Rollins School of Public Health, Emory University.

AWARDS AND HONORS

Presentation of Opening Keynote Address: *Hurricane Maria Deployment Experiences, October 23-November 20, 2017*. EWRI World Environmental & Water Resources Congress, 2017 Extreme Weather Events Panel, Minneapolis, MN, June 3-7, 2018. **Invited Presentation**

American Academy of Environmental Engineers and Scientists (AAEES), 2015 Excellence in Environmental Engineering Award, Grand Prize, Research Category, April 2015.

Environmental and Water Resources Institute, American Society of Civil Engineers (ASCE), Elected to Fellow-Grade Member, May 2013.

American Society of Civil Engineers (ASCE), 2011 James R. Croes Medal, for the paper, "*Optimal Design of Sensor Placement in Water Distribution Networks*," Journal of Water Resources Planning and Management, January-February 2010.

U.S. Public Health Service Engineering Literary Award (Peer-Reviewed Publication Category) for the publication: *Reconstructing Historical Exposures to Volatile Organic Compound-Contaminated Drinking Water at a U.S. Military Base*, April 2010.

U.S. Public Health Service Engineering Literary Award (Publications Category) for the publication: *Analytical Contaminant Transport Analysis System (ACTS)—Multimedia Environmental Fate and Transport*, June 2005.

American Academy of Environmental Engineers (AAEE), 2003 Excellence in Environmental Engineering Award, Grand Prize, Research Category, April 2003.

Assistant Administrator's Award for Special Service to ATSDR, June 2002.

U.S. Public Health Service, ATSDR, Quality Increase Award, February 2002.

Cumming Award, American Society of Military Engineers, 2000 to the Dover Township Water-Distribution System Modeling Team.

Environmental and Water Resources Research Institute (EWRI), American Society of Civil Engineers (ASCE), Best Practice-Oriented Paper of 2000 for the paper, *"Using Water-Distribution System Modeling to Assist Epidemiologic Investigations,"* ASCE Journal of Water Resources Planning and Management, Vol. 126, July/August 2000.

Agency for Toxic Substances and Disease Registry, Engineer of the Year Award, 1998. Agency for Toxic Substances and Disease Registry, Science Award, 1998.

U.S. Public Health Service Engineering Literary Award (Publications Category) for the publication:

Exposure Assessment Using Analytical and Numerical Models: Case Study, May 1998.

U.S. Public Health Service Engineering Literary Award (Publications Category) for the publication: *Estimating Exposure to VOCs from Municipal Water System Pipelines: Use and Application of a Computational Model*, May 1996.

AFFILIATIONS

American Academy of Environmental Engineers and Scientists (Diplomate)

American Academy of Water Resources Engineers (Diplomate)

American Society of Civil Engineers–ASCE (Member)

Environmental & Water Resources Institute (EWRI) of ASCE (Fellow-Grade Member)

- Vice-Chair, Hydraulic Fracturing Committee, EWRI/ASCE
- Chair, Hydraulic Fracturing Task Committee, EWRI/ASCE

- Fellow, Environmental and Water Resources Institute (EWRI)
- Vice-Chair, Water Distribution Systems Analysis Committee (October 2014–2016)
- Chair, Groundwater Hydrology Committee (2009–2011)
- Chair, Emerging and Innovative Technologies Technical Committee (2008–2009)
- Co-Chair, 17th Water Distribution Systems Analysis Symposium, EWRI Congress, May 2015
- Co-Chair, 15th Water Distribution Systems Analysis Symposium, EWRI Congress, May 2013
- Member, Organizing Committee, 12th International Symposium on Water-Distribution System Analysis, Tucson, AZ, 2011
- Member, Organizing Committee, 8th International Symposium on Water Distribution System Analysis, Cincinnati, OH, 2007

American Water Resources Association

American Water Works Association

Georgia Ground Water Association

International Society for Exposure Science

- Co-Chairman, 2002 Joint Symposium on Computation Techniques/Multimedia Multipathway Models

Associate Editor, ASCE Journal of Water Resources, Planning, and Management, https://ascelibrary.org/page/jwrmd5/editorialboard; July 2006—2016.

Member, Peer Review Committee for Massachusetts Department of Health on, "*An Epidemiologic Study of Childhood Cancer and Exposure to Drinking Water Contaminated with N-nitrosodimethylamine (NDMA), Wilmington, Massachusetts*," 2014–2018.

Member, External Advisory Board to University of Kentucky, for National Institute of Hometown Security funded project, "*Studying Distribution System Hydraulics and Flow Dynamics to Improve Utility Operational Decisions*," 2011–2014.

Member, External Advisory Board to University Consortium, for National Institute of Hometown Security funded project, "*Protocols for Response and Recovery Operations in Contaminated Water Systems*," 2010–2013.

PUBLICATIONS: Books, Journal Articles, Reports, and Proceedings

Books and Book Chapters

Aral, M.M., Brebbia, C.A., Maslia, M.L., and Sinks, T., editors. Environmental Exposure and Health, WIT Press, Southampton, UK, 2005.

Grayman, W.M., Clark, R.M., Harding, B.L., Maslia, M., Aramini, J. Chapter 10: Reconstructing Historical Contamination Events. In: Mays, L.W., editor. Water Supply Systems Security, McGraw-Hill, New York, 2004, pp. 10.1-10.55.

Maslia, M.L., and Hayes, L.R. Hydrogeology and simulated effects of ground-water development of the Floridan aquifer system, southwest Georgia, northwest Florida, and southernmost Alabama: U.S. Geological Survey Professional Paper 1403-H, 1988, 71 p.

Maslia, M.L., and Randolph, R.H. Methods and computer program documentation for determining anisotropic transmissivity tensor components of two-dimensional ground-water flow: U.S. Geological Survey Water-Supply Paper 2308, 1987, 46 p.

Peer-Reviewed Journal Articles

Maslia, M.L., Aral, M.M., Ruckart, P.Z., and Bove, F.B. Reconstructing Historical VOC Concentrations in Drinking Water for Epidemiological Studies at a U.S. Military Base: Summary of Results. *Water*. **2016**, 8 (10), 1–23. Available on line: http://www.mdpi.com/2073-4441/8/10/449 (accessed on 13 October 2015).

Ruckart, Perri Zeits, Bove, Frank J., Shanley III, Edwin, and Maslia, Morris. Evaluation of contaminated drinking water and male breast cancer at Marine Corps Base Camp Lejeune, North Carolina: a case control study. *Journal of Environmental Health*, 2015, v. 14, no. 74. Available at: https://doi.org/10.1186/s12940-015-0061-4

Bove, F. J., Ruckart, P. Z., Maslia, M. L., and Larson, T. C. Evaluation of mortality among marines and navy personnel exposed to contaminated drinking water at USMC Base Camp Lejeune: A retrospective cohort study. *Journal of Environmental Health*, v. 13, no. 10, 1-14. Available at: http://www.ehjournal.net/content/13/1/10.

Ruckart, P.Z., Bove, F.J., and Maslia, M.L. Evaluation of contaminated drinking water and preterm birth, small for gestational age, and birth weight at Marine Corps Base Camp Lejeune, North Carolina: A Cross-sectional Study. *Journal of Environmental Health*, 2014, v. 13, no. 99. Available at: http://www.ehjournal.net/content/13/1/99.

Ruckart, P.Z., Bove, F.J., Maslia, M.L., and Larson, T.C. Evaluation of Mortality Among Marines and Navy Personnel Exposed to Contaminated Drinking Water at USMC Base Camp Lejeune: A Retrospective Cohort Study. *Journal of Environmental Health*, 2014, v. 13, no. 10. Available at: http://www.ehjournal.net/content/13/1/10.

Ruckart, P.Z., Bove, F.J., and Maslia, M.L. Evaluation of Exposure to Contaminated Drinking water and Specific Birth Defects and Childhood Cancers at Marine Corps Base Camp Lejeune, North Carolina: A Case-Control Study. *Journal of Environmental Health*, 2013, v. 12, no. 104. Available at: http://www.ehjournal.net/content/12/104.

Maslia, M.L., Aral, M.M., Faye, R.E., et al. Comment on the Discussion Paper, "*Complexities in Hindcasting Models—When Should We Say Enough Is Enough*," by T. Prabhakar Clement. *Ground Water*, 2012, v. 50, no. 1, p. 10–16.

Anderson, B.A., Maslia, M.L., Caparoso, J.L., Ausdemore, D., and Aral, M.M. Stochastic Analysis of Pesticide Transport in the Shallow Groundwater of Oatland Island, Georgia, USA. *Journal of Water Quality, Exposure and Health*, 2010, Vol. 2, No. 1, p. 47-64 [Published online: 08 April 2010].

Aral, M.M., Guan, J., and Maslia, M.L. Optimal Design of Sensor Placement in Water distribution Networks. *ASCE Journal of Water Resources Planning and Management*, 2010, Vol. 131, No. 1, pp. 5–18.

Maslia, M.L., Aral, M.M., Faye, R.E., Suárez-Soto, R.J., Sautner, J.B., Wang, J., Jang, W., Bove, F.J., and Ruckart, P.Z. Reconstructing Historical Exposures to Volatile Organic Compound-Contaminated Drinking Water at a U.S. Military Base. *Journal of Water Quality, Exposure and Health*, 2009, Vol. 1, No. 1, p. 49–68.

Perelman, L., Maslia, M.L., Ostfeld, A., and Sautner, J.B. Using Aggregation/Skeletonization Network Models for Water Quality Simulations in Epidemiologic Studies. *Journal, American Water Works Association*, 2008, v.100, no. 6, pp. 122–133.

Guan J., Aral, M.M., Maslia, M.L., and Grayman, W.M. Identification of Contaminant Sources in Water Distribution Systems Using Simulation–Optimization Method: Case Study. *ASCE Journal of Water Resources Planning and Management*, 2006, Vol. 132, No. 4, pp. 252–262.

Grayman, W.M., Maslia, M.L., and Sautner, J.B. Calibrating Distribution System Models with Fire-Flow Tests. *Opflow, American Water Works Association*, 2006, v.32, no. 4, pp. 10–12.

Maslia, M.L., Reyes, J.J., Gillig, R.E., Sautner, J.B., Fagliano, J.A., and Aral, M.M. Public Health Partnerships Addressing Childhood Cancer Investigations: Case Study of Toms River, Dover Township, New Jersey, USA. *International Journal of Hygiene and Environmental Health*, 2005, v. 208, no. 1–2, pp. 45–54.

Evans, M. and Maslia, M.L. Hydrogeology and Human Exposure Assessment. *Hydrogeology Journal: Special Issue*, 2005, v. 13, pp. 325–327.

Aral, M.M., Guan, J., Maslia, M.L., Sautner, J.B., Gillig, R.E., Reyes, J.J., and Williams, R.C. Optimal Reconstruction of Historical Water Supply to a Distribution System: A. Methodology. *Journal of Water and Health*, 2004, v. 2, no. 3, pp. 123–136.

Aral, M.M., Guan, J., Maslia, M.L., Sautner, J.B., Gillig, R.E., Reyes, J.J., and Williams, R.C. Optimal Reconstruction of Historical Water Supply to a Distribution System: B. Applications. *Journal of Water and Health,* 2004*,* v. 2, no. 3, pp. 137-156.

Maslia, M.L., and Aral, M.M. ACTS—Analytical Contaminant Transport Analysis System (ACTS)—Multimedia Environmental Fate and Transport. *ASCE Practice Periodical of Hazardous, Toxic, and Radioactive Waste Management*, 2004, v. 8, no. 3, pp.181-198.

Aral, M.M., Guan, J., and Maslia, M.L. Identification of contaminant source location and release history in aquifers, Closure: *ASCE Journal of Hydrologic Engineering*, v. 7, no. 5, pp. 399–401.

Aral, M.M., Guan, J., and Maslia, M.L. Identification of contaminant source location and release history in aquifers: *ASCE Journal of Hydrologic Engineering*, 2001, v. 6, no. 3, pp. 225-234.

Maslia, M.L., Sautner, J.B., Aral, M.M. Abraham, J.E., Williams, R.C., and Reyes, J.J Using water-distribution system modeling to assist epidemiologic investigations: *ASCE Journal of Water Resources Planning and Management*, 2000, v. 126, no. 4, July/August, pp. 180-197.

Maslia, M.L. Models refine exposure-dose reconstruction, in: *Hazardous Substances and Public Health*, G. Moore, editor, 1998, v. 7, no. 4, Winter 1998, pp. 1-3.

Rodenbeck, S.E., and Maslia, M.L. Use of groundwater modeling and GIS to determine population exposure to trichloroethylene (TCE) at the Tucson International Airport area National Priorities List site, Tucson, Arizona, USA: *ASCE Practice Periodical of Hazardous, Toxic, and Radioactive Waste Management*, 1998, v.2, no. 2, pp. 53-61.

Maslia, M.L., Aral, M.M., and Williams, R.C. Exposure assessment using analytical and numerical models: Case study: *ASCE Practice Periodical of Hazardous, Toxic, and Radioactive Waste Management*, 1997, v. 1, no. 2, pp. 50-60.

Williams, R.C., and Maslia, M.L. Making a map of public health hazards: *Civil Engineering*, 1997, v. 67, no. 9, September, pp. 64-65.

Aral, M.M., Maslia, M.L., Ulirsch, and Reyes, J.J. Estimating exposure to VOCs from municipal water supply systems: Use of a better computational model: *Archives of Environmental Health*, 1996, v. 51, no. 4, pp. 300-309.

Maslia, M.L., Aral, M.M., Williams, R.C., Williams-Fleetwood, S., Hayes, L.C., and Wilder, L.C. Use of computational models to reconstruct and predict trichloroethylene exposure, *Toxicology and Industrial Health*, 1996, v. 12, no. 2, pp. 139-152.

Maslia, M.L. Note on "Modifications to the computer program TENSOR2D": *Ground Water*, 1994, v. 32, no. 3, pp. 501-502.

Aral, M.M., Maslia, M.L., and Williams, R.C. Discussion of "Ground-water remediation using smart pump and treat", by Fredric Hoffman, January-February 1993 issue, 1993, v. 31, no. 1, pp. 98-106: *Ground Water*, v. 31, no. 4, pp. 680-681.

Maslia, M.L., Aral, M.M., Houlihan, M.F. Evaluation of ground-water flow regime at a landfill with liner system: *Journal of Environmental Science and Health, Part A: Environmental Science and Engineering*, 1992, v. A27, no. 7, p. 1793-1816.

Maslia, M.L., and Prowell, C.D. Effect of faults on fluid flow and chloride contamination in a carbonate aquifer system: *Journal of Hydrology*, 1990, v. 115, p. 1-49.

Maslia, M.L., Aral. M.M., Williams, R.C., Susten, A.S., and Heitgerd, J.L. Exposure assessment of populations using environmental modeling, demographic analysis, and GIS: *Water Resources Bulletin*, 1994, v. 30, no. 6, pp. 1025-1041.

Randolph, R.B., Krause, R.E., and Maslia, M.L. Comparison of aquifer characteristics derived from local and regional aquifer tests: *Ground Water*, 1985, v. 23, no. 3, p. 309-316.

Maslia, M.L., and Johnston, R.H. Use of a digital model to evaluate hydrogeologic controls on ground-water flow in a fractured rock aquifer at Niagara Falls, New York: *Journal of Hydrology*, 1984, v. 75, no. 1/4, p. 167-194.

Aral, M.M., and Maslia, M.L. Unsteady seepage analysis of Wallace Dam: *ASCE Journal of Hydraulic Engineering*, 1983, v. 109, no. 6, p. 809-826.

Maslia, M.L., and Aral, M.M., 1982, Evaluation of a chimney drain design in an earthfill dam: *Ground Water*, v. 20, no. 1, p. 22-31.

Reports

Maslia M.L., Suárez-Soto R.J., Sautner J.B., Anderson, B.A., Jones, L.E., Faye, R.E., Aral, M.M, Guan, J., Telci, I.T., Grayman, W.M., Bove, F.J., Ruckart, P.Z., and Moore, S.M. Analyses and Historical Reconstruction of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water Within the Service Areas of the Hadnot Point and Holcomb Boulevard Water Treatment Plants and Vicinities, U.S. Marine Corps Base Camp Lejeune, North Carolina—Chapter A: Summary and Findings. Atlanta, GA: Agency for Toxic Substances and Disease Registry; February 2013.

Maslia M.L., Suárez-Soto R.J., Wang J., Aral M.M., Faye, R.E., Sautner J.B., Valenzuela C., and Grayman, W.M. Analyses of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water at Tarawa Terrace and Vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina: Historical Reconstruction and Present-Day Conditions—Chapter I: Parameter Sensitivity, Uncertainty, and Variability Associated with Model Simulations of Groundwater Flow, Contaminant Fate and

Transport, and Distribution of Drinking Water. Atlanta, GA: Agency for Toxic Substances and Disease Registry; February 2009.

Anderson B.A., Maslia M.L., Caparoso J.L., and Ausdemore D. Probabilistic Analysis of Pesticide Transport in Shallow Groundwater at the Oatland Island Education Center, Oatland Island, Georgia. Atlanta, GA: Agency for Toxic Substances and Disease; September 2007.

Maslia M.L., Sautner J.B., Faye R.E., Suárez-Soto R.J., Aral M.M., Grayman W.M., Jang W., Wang J., Bove F.J., Ruckart P.Z., Valenzuela C., Green J.W. Jr., and Krueger A.L. Analyses of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water at Tarawa Terrace and Vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina: Historical Reconstruction and Present-Day Conditions—Chapter A: Summary of Findings. Atlanta, GA: Agency for Toxic Substances and Disease Registry; July 2007.

Maslia M.L., Sautner J.B., Faye R.E., Suárez-Soto R.J., Aral M.M., Grayman W.M., Jang W., Wang J., Bove F.J., Ruckart P.Z., Valenzuela C., Green J.W. Jr., and Krueger A.L. Analyses of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water at Tarawa Terrace and Vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina: Historical Reconstruction and Present-Day Conditions—Executive Summary. Atlanta, GA: Agency for Toxic Substances and Disease Registry; June 2007.

Maslia, M.L., editor. Expert peer review panel evaluating ATSDR's water-modeling activities in support of the current study of childhood birth defects and cancer at U.S. Marine Corps base Camp Lejeune, North Carolina—Analyses of groundwater resources and present-day (2004) water-distribution systems, March 28–29, 2005: Prepared by Eastern Research Group, Inc., Atlanta, Georgia; Prepared for Agency for Toxic Substances and Disease Registry (ATSDR), 2005, Atlanta, 31 pp., 4 app.

Jones, L.E., Prowell, D.C., and Maslia, M.L. Hydrogeology and water quality (1978) of the Floridan aquifer system at U.S. Geological Survey TW-26, on Colonels Island, near Brunswick, Georgia: U.S. Geological Survey Water-Resources Investigation Report 02-4020, 2002, 44 p.

Maslia, M.L., Sautner, J.B., Aral, M.M., Gillig, R.E., Reyes, J.J., and Williams, R.C. Historical reconstruction of the water-distribution system serving the Dover Township area, New Jersey: January 1962-December 1996. Atlanta, GA: Agency for Toxic Substances and Disease Registry; October 2001.

Aral, M.M., Guan, J., Maslia, M.L., and Sautner, J.B. Reconstruction of hydraulic management of a water distribution system using optimization: Multimedia Environmental Simulation Laboratory report MESL-01-01. Atlanta, GA: School of Civil and Environmental Engineering, Georgia Institute of Technology; 2001.

Maslia, M.L., Sautner, J.B., Aral, M.M., Gillig, R.E., Reyes, J.J., and Williams, R.C. Summary of findings: historical reconstruction of the water-distribution system serving the Dover Township area, New Jersey: January 1962-December 1996. Atlanta, GA: Agency for Toxic Substances and Disease Registry; September 2001.

Maslia, M.L., Sautner, J.B., and Aral, M.M. Analysis of the 1998 water-distribution system serving the Dover Township Area, New Jersey. Atlanta, GA: Agency for Toxic Substances and Disease Registry; June 2000.

Aral, M.M., and Maslia, M.L. Multi-pathway environmental exposure assessment using ACTS and SAINTS software: Multimedia Environmental Simulation Laboratory report MESL-05-98. Atlanta, GA: School of Civil and Environmental Engineering, Georgia Institute of Technology; October 1998

Aral, M.M., Babar Sani, A.F., and Maslia, M.L. Geographic information systems integrated groundwater flow and contaminant fate and transport modeling: Multimedia Environmental Simulation Laboratory report MESL-03-98. Atlanta, GA; School of Civil and Environmental Engineering, Georgia Institute of Technology, October 1998.

Maslia, M.L., and Sautner, J.B. Water-distribution system, pressure measurement work plan, Dover Township area, Ocean County, New Jersey. Atlanta, GA: Agency for Toxic Substances and Disease Registry; February 1998.

Sautner, J.B., and Maslia, M.L. Water-distribution system pressure test, March 23-26, 1998, Dover Township, Ocean County, New Jersey. Atlanta, GA: Agency for Toxic Substances and Disease Registry; June 1998.

Maslia, M.L., Aral, M.M., Abraham, J.E., and Reyes, J.J. Childhood cancer investigation: A work plan for environmental exposure assessment, Dover Township (Toms River), Ocean County, New Jersey. Atlanta, GA: Agency for Toxic Substances and Disease Registry; February 1997.

Maslia, M.L., Henriques, W.D., and McRae, T. Hydraulic device location, Dover Township water-distribution system, Dover Township (Toms River), Ocean County, New Jersey. Atlanta, GA: Agency for Toxic Substances and Disease Registry; June 1997.

Maslia, M. ATSDR engineers use new tools to simplify and enhance exposure assessment analyses: U.S. Public Health Service, *Office of the Chief Engineer Newsletter*, 1996, v. 1, no. 3, pp. 4-5.

Jones, L.E., and Maslia, M.L. Selected ground-water data, and results of aquifer tests for the Upper Floridan aquifer, Brunswick, Glynn County, Georgia, area: U.S. Geological Survey Open-File Report 94-520, 1994, 107 pp.

Aral, M.M., and Maslia, M.L. A public health analysis of exposure to contaminated municipal water supplies at Southington, Hartford County, Connecticut. Atlanta, GA: Agency for Toxic Substances and Disease Registry; December 1994.

Susten, A.S., and Maslia, M.L. Exposure-dose reconstruction program, overview of strategy. Atlanta, GA: Agency for Toxic Substances and Disease Registry; March 1993.

Maslia, M.L., and Randolph, R.H. Methods and computer program documentation for determining anisotropic transmissivity tensor components of two-dimensional ground-water flow: U.S. Geological Survey Open-File Report 86-227,1986, 64 p.

Hayes, L.R., Maslia, M.L., and Meeks, W.C. Hydrology and model evaluation of the principal artesian aquifer, Dougherty Plain, southwest Georgia. Atlanta, GA: Georgia Geologic Survey Bulletin 97; 1983.

Maslia, M.L., and Johnston, R.H. Simulation of ground-water flow in the vicinity of Hyde Park landfill, Niagara Falls, New York: U.S. Geological Survey Open-File Report 82-159, 1982, 19 p.

Aral, M.M., Mayer, P.G., and Maslia, M.L. Mathematical modeling of aquatic dispersion of effluents. Prepared for Oak Ridge National Laboratories. Atlanta, GA: School of Civil Engineering, Georgia Institute of Technology; 1980.

Maslia, M.L. Numerical modeling of saturated-unsaturated fluid flow through porous media. MSCE thesis. Atlanta, GA: School of Civil Engineering, Georgia Institute of Technology; March 1980.

Conference, Symposium, and Workshop Proceedings

Maslia, M.L. Reconstructing VOC-Contaminated Drinking Water Concentrations for Epidemiological Studies at U.S. Marine Corps Base Camp Lejeune, North Carolina. *American College of Toxicology, 40th Annual Meeting*, Phoenix, AZ, November 17–20, 2019. **Invited Presentation**.

Maslia, ML. Hurricane Maria Deployment Experiences: Assessing Health Care Facilities in Puerto Rico.

13th CECIA-IAUPR Biennial Symposium on Potable Water Issues in Puerto Rico, February 13–15, 2019, San Juan, Puerto Rico. **Invited Presentation**.

Maslia, ML. Reconstructing Historical Drinking Water Contamination Events. EWRI, 10th International Perspectives on Water and the Environment (IPWE), December 4–7, 2018, Cartagena, Colombia. **Invited Course Lecturer.**

Maslia, ML. Hurricane Maria Deployment Experiences, October 23-November 20, 2017. EWRI World Environmental & Water Resources Congress, 2017 Extreme Weather Events Panel, Minneapolis, MN, June 3-7, 2018. **Invited Presentation**

Maslia, ML. Application of Water-Modeling Tools to Reconstruct Historical Drinking Water Contaminant Concentrations for Epidemiological Studies. Proceedings of the World Environmental and Water Resources Congress, Austin, TX: American Society of Civil Engineers, Environmental and Water Resources Institute Congress 2015 Floods, Droughts, and Ecosystems: Managing Our Resources Despite Growing Demand and Diminishing Funds, May 17-21, 2015.

Maslia, ML. Using Environmental Engineering Tools, Scientific Analyses, and Epidemiological Studies to Quantify Human Exposure to Contaminated Drinking Water and to Benefit Public Health. 2015 Excellence in Environmental Engineering & Science Awards Luncheon & Conference, Washington, DC: American Academy of Environmental Engineers & Scientists, National Press Club, April 23, 2015. **Invited Presentation**

Maslia, M.L. Water Mapping—From Exposure to Disease. *TEDMed@CDC/Ignite*, U.S. Centers for Disease Control and Prevention, U.S. Department of Health and Human Services, Atlanta, Georgia, April 30, 2014. **Invited Presentation**

Maslia, ML and Aral, MM. Application of Water-Modeling Tools to Reconstruct Historical Drinking Water Contaminant Concentrations in Epidemiological Studies. Proceedings of the 24th Annual Meeting of the International Society of Exposure Science, Cincinnati, OH: International Society of Exposure Science, Exposure Science Integration to Protect Ecological Systems, Human Well-Being, and Occupational Health, October 12-16, 2014.

Maslia, ML. Reconstructing Historical VO-Contaminated Drinking Water Concentrations for Exposure Classification at U.S. Marine Corps Base Camp Lejeune, North Carolina. The Augusta Founding Fathers Conference, Augusta, GA: American Society of Civil Engineers, A Joint ASCE Georgia/South Carolina Event, March 14-15, 2014.

Sautner JB, Grayman W, and Maslia ML. Modeling Discrete Interconnection Events of Two Water-Distribution Systems to Reconstruct Historical Human Exposure. In: Beighley II RE and Kilgore MW, ed. Proceedings of the World Environmental & Water Resources Congress, Palm Springs, CA: American Society of Civil Engineers, Environmental and Water Resources Congress 2011 Bearing Knowledge for Sustainability, May 22-26, 2011 [on CD-ROM].

Maslia, ML. Reconstructing Historical VOC-Contaminated Drinking Water Concentrations for Exposure Classification at U.S. Marine Corps Base Camp Lejeune, North Carolina. The Augusta Founding Fathers Conference A Joint Georgia/South Carolina ASCE Event, Augusta, GA, March 13-15, 2014.

Guan J., Jang W., Maslia ML, and Aral MM. Historical Reconstruction of Groundwater Contamination at Contaminated Sites and Uncertainty Analysis. In: Palmer RN, ed. Proceedings of the World Environmental & Water Resources Congress, Providence, RI: American Society of Civil Engineers, Environmental and Water Resources Congress 2010 Challenges of Change, May 16-20, 2010 [on CD-ROM].

Jang W, Maslia ML, and Aral MM. The Effect of Atmospheric Chemical Release on the Reduction in Groundwater Pollution by CVOCs. In: Palmer RN, ed. Proceedings of the World Environmental & Water Resources Congress, Providence, RI: American Society of Civil Engineers, Environmental and Water Resources Congress 200 Challenges of Change, May 16-20, 2010 [on CD-ROM].

Guan J., Maslia, MM, and Aral MM. A Methodology to Reconstruct Groundwater Contamination History with Limited Field Data. In: Starrett S, ed. Proceedings of the World Environmental & Water Resources Congress, Kansas City, MO: American Society of Civil Engineers, Environmental and Water Resources Congress 2009 Great Rivers, May 17-21, 2009 [on CD-ROM].

Aral MM, Guan J, and Maslia ML. A Multi-Objective Optimization Algorithm for Sensor Placement in Water distribution Systems. In: Babcock RW Jr and Walton R, eds. Proceedings of the World Environmental & Water Resources Congress, Honolulu, HI: American Society of Civil Engineers, Environmental and Water Resources Congress 2008 Ahupua'a, May 12-16, 2008 [on CD-ROM].

Suárez-Soto RJ, Wang J, Faye RE, Maslia ML, Aral MM, and Bove FJ. Historical Reconstruction of PCE-Contaminated Drinking Water Using Probabilistic Analysis at U.S. Marine Corps Base Camp Lejeune, North Carolina. In: Babcock RW Jr and Walton R, eds. Proceedings of the World Environmental & Water Resources Congress, Honolulu, HI: American Society of Civil Engineers, Environmental and Water Resources Congress 2008 Ahupua'a, May 12-16, 2008 [on CD-ROM].

Suárez-Soto RJ, Anderson BA, Maslia ML, and Aral MM. A Comparison Between BIOCHLOR and the Analytical Contaminant Transport Analysis System (ACTS) for a Case Study in Coastal Georgia. In: Babcock RW Jr and Walton R, eds. Proceedings of the World Environmental & Water Resources Congress, Honolulu, HI: American Society of Civil Engineers, Environmental and Water Resources Congress 2008 Ahupua'a, May 12-16, 2008 [on CD-ROM].

Anderson BA, Maslia ML, Caparoso JL, and Ausdemore D. Probabilistic Analysis of Pesticide Transport in Shallow Groundwater at the Oatland Island, Georgia. In: Krabbes KC, ed. Proceedings of the World Environmental & Water Resources Congress. Tampa, FL: American Society of Civil Engineers, Environmental and Water Resources Institute, May 15-19, 2007 [on CD-ROM].

Rogers SW, Gaun J, Maslia ML, and Aral MM. Nodal Importance Concept for Computational Efficiency in Optimal Sensor Placement in Water Distribution Systems. In: Krabbes KC, ed. Proceedings of the World Environmental & Water Resources Congress. Tampa, FL: American Society of Civil Engineers, Environmental and Water Resources Institute, May 15-19, 2007 [on CD-ROM].

Sautner JB, Maslia ML, and Grayman WM. Storage Tank Mixing Models: Comparison of Tracer Data with Model Simulation. In: Krabbes KC, ed. Proceedings of the World Environmental & Water Resources Congress. Tampa, FL: American Society of Civil Engineers, Environmental and Water Resources Institute, May 15-19, 2007 [on CD-ROM].

Suárez-Soto RJ, Maslia ML, Faye RE, Wang J, and Aral MM. Using Uncertainty Analysis to Reconstruct Historical Tetrachloroethylene (PCE) Exposure for an Epidemiological Study. In: Krabbes KC, ed.

Proceedings of the World Environmental & Water Resources Congress. Tampa, FL: American Society of Civil Engineers, Environmental and Water Resources Institute, May 15-19, 2007 [on CD-ROM].

Wang J, Aral MM, Maslia ML, and Faye RE. Tetrachloroethylene (PCE) Exposure Reconstruction for an Epidemiological Study: The Effect of Historical Supply-Well Schedule Variation on Arrival Time. In: Krabbes KC, ed. Proceedings of the World Environmental & Water Resources Congress. Tampa, FL: American Society of Civil Engineers, Environmental and Water Resources Institute, May 15-19, 2007 [on CD-ROM].

Grayman, W.M., Maslia, M., and Boccelli, D. Distribution System Tracer Studies: Design, Implementation and Case Studies. Water Distribution System Analysis Symposium Workshop: Cincinnati, OH: WDSA Symposium 2006, August 27, 2006.

Guan, J., Aral, M.M., and Maslia, M.L. Identification of contaminant sources in a water-distribution system using an optimization-simulation method. In: Aral, M.M., Brebbia, C.A., Maslia, M.L., and Sinks, T, editors. Environmental Exposure and Health, WIT Press, Southampton, 2005, pp. 175–184.

Maslia, M.L., and Aral, M.M. Reconstructing historical contamination events: Use of computational tools to assist environmental engineers and health scientists. In: Aral, M.M., Brebbia, C.A., Maslia, M.L., and Sinks, T, editors. Environmental Exposure and Health, WIT Press, Southampton, 2005, pp. 175– 184.

Boccelli, D.L., Shang, F., Uber, J.G., Orcevic, A., Moll, D., Hooper, S., Maslia, M., Sautner, J., Blount, B., and Cardinali, F. Tracer Tests for Network Model Calibration. In: Sehlke, G., Hayes, D.F., and Stevens, D.K., editors. Proceedings of the 2004 World Water and Environmental Resources Congress, American Society of Civil Engineers, [CD ROM document]. Salt Lake City, UT: 2004 June 27–July1.

Aral, M.M., and Maslia, M.L. Application of Monte Carlo Simulation to Analytical Contaminant Transport Modeling: In: S. Mishra, editor. Proceedings of the Symposium, Groundwater Quality Modeling and Management Under Uncertainty, Environmental and Water Resources Institute of the American Society of Civil Engineers, Philadelphia, PA, June 23–25, 2003, American Society of Civil Engineers, pp. 305–312.

Maslia, M.L., Aral, M.M., and Sautner. Reconstructing Historical Operations of Water-Distribution Systems. In: Bizier, P., and DeBarry, P., editors. Proceedings of the American Society of Civil Engineers, World Water & Environmental Resources Congress 2003 [CD ROM document]. Philadelphia, PA: 2003 June 23–26.

Aral, M.M., Guan, J., Maslia, M.L., Sautner, J.B., Reyes, R.R., and Williams, R.C. Optimal Reconstruction of Hydraulic Management of a Water Distribution System. Final Programs and Abstracts, 12th Conference of the International Society of Exposure Analysis (ISEA) and the 14th Conference of the International Society for Environmental Epidemiology. Vancouver, BC, Canada: 2002 August 11-15, p. 251.

Fagliano, J., Berry, M., Goun, B., Hlatimeier, P., Savrin, J., Blando, J., Imtiaz, R., Maslia, M., Kaye, W., Georgopolous, P., Klotz, J., Bresnitz, E., Reyes, J., Gillig, R., and Lioy, P. Case-Control Study of Childhood Cancers and Environmental factors in Dover Township, New Jersey. Final Programs and Abstracts, 12th Conference of the International Society of Exposure Analysis (ISEA) and the 14th Conference of the International Society for Environmental Epidemiology. Vancouver, BC, Canada: 2002 August 11-15, p. 250.

Maslia, M.L., Sautner, J.B., Aral, M.M., Gillig, R.E., Reyes, J.J., and Williams, R.C. Using Water-Distribution System Modeling to Assist Epidemiologic Investigations. Final Programs and Abstracts, 12th Conference of the International Society of Exposure Analysis (ISEA) and the 14th Conference of the International Society for Environmental Epidemiology. Vancouver, BC, Canada: 2002 August 11- 15, p. 252.

Reyes, J.J., Gillig, R.E., Fagliano, J.A., and Maslia, M.L. Partnerships Addressing Childhood Caner: Case Study of Toms River, Dover Township, NJ. Final Programs and Abstracts, 12th Conference of the International Society of Exposure Analysis (ISEA) and the 14th Conference of the International Society for Environmental Epidemiology. Vancouver, BC, Canada: 2002 August 11-15, p. 250.

Aral, M.M., Maslia, M.M., and Guan, J, 2002 ACTS, A multi-media contaminant transport modeling platform: *in* Development and Application of Computer Techniques to Environmental Studies, Ninth International Conference on the Modelling, Monitoring, and Management of Environmental Problems, ENVIROSOFT 2002, Bergen, Norway, May 6–8, 2002, Brebbia, C.A. and Zannetti, P., eds., WIT Press, Southampton, pp. 403–412.

Sautner, J.B., Maslia, M.L., and Aral, M.M., 1999, Water-distribution system modeling as a tool to enhance epidemiologic case-control investigations. A case study: The Dover Township childhood cancer investigation: *in* Proceedings of the 26th Annual Water Resources Planning and Management Conference, American Society of Civil Engineers: Preparing for the 21st Century, Tempe, Arizona, June 6-9, 1999, E.M. Wilson, ed.

Aral, M.M., and Maslia, M.M., 1996, Evaluation of human exposure to contaminated water supplies using GIS and modeling: *in* Proceedings, HydroGIS96: Application of Geographic Information Systems in Hydrology and Water Resources Management, Vienna, Austria, April 1996, Kovar, K. and Nachtnebel, H.P, eds. IAHS Publication No. 235, pp. 243-252.

Maslia, M.L., 1996, Exposure assessment: Integrating GIS and modeling: *in* Technical Papers of Fourteenth Annual Environmental Management and Technology Conference International, Atlantic City, New Jersey, June 18-20, 1996, pp. 21-24.

Maslia, M.L., Aral, M.M., and Radtke, T.M., 1995, Conducting exposure assessment of populations by integrating environmental transport models, demographic analysis, and geographic information systems: *in* Proceedings, Assessing and Managing Health Risks from Drinking Water Contamination: Approaches and Applications, Rome, Italy, September 13-17, 1994, Reichard, E.G. and Zapponi, G.A., eds. IAHS Publication No. 233, pp. 221-233.

Aral, M.M., Maslia, M.L., Williams, R.C., and Abraham, J.E., 1995, ATSDR's exposure-dose reconstruction program: Case studies in public health analysis of exposure to environmental

contamination: *in* Abstracts and Papers, 1995 Pacific Rim Conference on Occupational and Environmental Health, October 4-6, 1995, Sydney, Australia.

Holm, D.M., Maslia, M.L., Reyes, J.J., Williams, R.C., and Aral, M.M., 1995, Geographic Information Systems: A critical resource in exposure assessment: *in* Proceedings, SUPERFUND XVI Conference and Exhibition, Washington, D.C., November 6-8, 1995, pp. 857-866.

Maslia, M.L., Aral, M.M., Williams, R.C., Williams-Fleetwood, S., Hayes, L., and Wilder, L.C., 1994, Use of computational models to reconstruct and predict trichloroethylene exposure, *in* Hazardous Waste and Public Health: International Congress on the Health Effects of Hazardous Waste, Andrews, J.S, and others, eds. May 3-6, 1993, Atlanta, Georgia, pp. 271-283.

Maslia, M. L., and Prowell, D. C., 1988, Relation between concealed faults and ground-water quality in a carbonate aquifer system, Brunswick, Georgia, U.S.A., *in* Hitchon, Brian, and Bachu, Stephan, eds. Proceedings, Fourth Canadian/American Conference on Hydrogeology, Fluid flow, Heat Transfer, and Mass Transport in Fractured Rocks: Dublin, Ohio, National Water Well Association, p. 231-244.

Maslia, M.L. Regional and local tensor components of a fractured carbonate aquifer, in Farmer, I.W., and others, *eds.* Rock Mechanics: Proceedings of the 28th U.S. Symposium, University of Arizona, Tucson, June 29-July 1, 1987, p. 441-452.

UNIVERSITY LECTURES

Reconstructing Historical VOC-Contaminated Drinking Water Concentrations at U.S. Marine Corps Base Camp Lejeune, North Carolina: Advanced Risk Assessment Class (EH 760), Department of Environmental Health, Rollins School of Public Health of Emory University, April 17, 2014, Atlanta, Georgia. **Invited Lecture**.

Quantifying Exposure to Contaminated Drinking Water—Case Study: Camp Lejeune, NC: Risk Assessment II Class (EOH 525), Department of Environmental and Occupational Health, Rollins School of Public Health of Emory University, March 16, 2010, Atlanta, Georgia. **Invited Lecture**.

Quantifying Exposure to Contaminated Drinking Water—Concepts and Case Studies: Risk Assessment I Class (EOH 522), Department of Environmental and Occupational Health, Rollins School of Public Health of Emory University, November 19, 2008, Atlanta, Georgia. **Invited Lecture**.

Using Water-Distribution System Analyses to Benefit Public Health: Environmental Hydraulics Class (CE633), Department of Civil and Environmental Engineering, University of Cincinnati, February 9, 2006, Cincinnati, Ohio. **Invited Lecture**.

Engineering Graduate Seminar, School of Civil and Environmental Engineering, Georgia Institute of Technology, January 21, 2004, Atlanta, Georgia. **Invited Lecture**.

Quantitative Exposure Assessment: Health Risk Assessment Course, Autonomous University of San Luis Potosi, May 27–29, 2003, San Luis Potosi, Mexico. **Invited Lecture**.

Computational Tools for Conducting Exposure Assessments and Assisting Epidemiologic Investigations: CEE 8094, Graduate Environmental Engineering Seminar, School of Civil and Environmental Engineering, Georgia Institute of Technology, October 3, 2001, Atlanta, Georgia. **Invited Lecture**.

Environmental and Occupational Hazards II: EOH 541 graduate class, Rollins School of Public Health of Emory University, Atlanta, Georgia, January – May 2001–2004. **Adjunct Professor**.

MISCELLANEOUS LECTURES

Using Environmental Engineering Tools, Scientific Analyses, and Epidemiological Studies to Quantify Human Exposure to Contaminated Drinking Water and to Benefit Public Health. American Academy of Environmental Engineers & Scientists Awards Luncheon and Conference, National Press Club, Washington, DC, April 23, 2015. **Invited Presentation**.

Water Mapping—From Exposure to Disease: TEDMed@CDC/Ignite, Centers for Disease Control and Prevention, U.S. Department of Health and Human Services, April 30, 2014, Atlanta, Georgia. **Invited Presentation**.

Update on ATSDR's Camp Lejeune Water-Modeling Activities: Presentation to U.S. Marine Corps Headquarters Staff, February 4, 2013, The PENTATGON, Washington, DC.

Status and Update—Data and Modeling Analyses of Historical Drinking-Water Contamination at Camp Lejeune. Camp Lejeune Community Assistance Panel Meeting and Public Forum, July 20, 2011, Wilmington, NC.

Data and Modeling Analyses of Historical Drinking Water Contamination at Camp Lejeune, North Carolina: Pentagon Briefing for Deputy Assistant Secretary of the Navy and USMC General Staff, April 29, 2011, Pentagon, Washington, DC.

Using Computational Tools to Models to Reconstruct Historical Drinking-Water Contamination at U.S. Marine Corps Base Camp Lejeune, North Carolina: The National Academies, National Research Council Committee on Contaminated Drinking Water at Camp Lejeune, September 24, 2007, Washington, DC.

Summary of Findings: Water Modeling Analyses at U.S. Marine Corps Base Camp Lejeune, North Carolina, Tarawa Terrace and Vicinity—Final Results. U.S. Environmental Protection Agency, Region IV, July 11, 2007, Atlanta, Georgia.

Probabilistic Analysis of Pesticide Transport in Shallow Groundwater at Oatland Island, Georgia. Site Rounds Seminar, ATSDR Division of Health Assessment and Consultation, February 13, 2007, Atlanta, Georgia.

Marine Corps Base Camp Lejeune, North Carolina. Site Rounds Seminar, ATSDR Division of Health Assessment and Consultation, March 21, 2006, Atlanta, Georgia.

Reconstructing Historical Operations of Water-Distribution Systems: Integrating Modeling, GIS, and Epidemiology. National Center for Environmental Health, Environmental Public Health Tracking Workshop, July 22, 2003, Chicago, Illinois.

Introduction to Environmental Fate and Transport Models. National Center for Environmental Health, Environmental Public Health Tracking Workshop, July 22, 2003, Chicago, Illinois.

Computational tools assisting epidemiologic investigations: Concepts and case studies. National Center for Environmental Health, May 1, 2003, Atlanta, Georgia.

Computational techniques for exposure assessment to assist with epidemiologic investigations: Methods and case studies from the DHAC arsenal of tools. ATSDR Division of Health Studies Seminar, February 20, 2002, Atlanta, Georgia.

Using Water-Distribution System Modeling to Assist Epidemiologic Investigations. New Jersey Department of Health and Senior Services Expert Panel Meeting, May 22, 2001, Environmental and Occupational Health Sciences Institute, Piscataway, New Jersey.

Concepts of models and the modeling process: use and application of screening-level models. 2001 ATSDR Partners in Public Health Meeting, April 1-4, 2001, Atlanta, Georgia.

Hands-On Use of the Analytical Contaminant Transport Analysis System (ACTS) Software. ATSDR Environmental Public Health Training Module, June 14-18, 1999, Atlanta, Georgia.

Uncertainty and Variability of Measurements. ATSDR Exposure Investigations Workshop, March 11, 1999, Atlanta, Georgia.

Appendix B — The ATSDR Water Modeling Team for Historical Reconstruction at U.S. Marine Corps Base Camp Lejeune, North Carolina

Name	Occupation	Position	Company	TT-A	TT-B	TT-C	TT-D	TT-E	TT-F	TT-G	TT-H	TT-I	HP-A	HP-S1	HP-S2	HP-S3	HP-S4	HP-S5	HP-S6	HP-S7	HP-S8	HP-B	HP-C	HP-D	Total
				Tarawa Terrace									Hadnot Point												
Morris L. Maslia, MSCE, PE, D.WRE, DEE	Research Environmental Engineer and Project Officer	Exposure-Dose Reconstruction Project	Agency for Toxic Substances and Disease Registry, Atlanta GA	X	O	O	O	O	O	O	O	X	X	X	X	O	X	X	X	X	X	O	O	X	11
René J. Suárez-Soto, MS EnvE, EIT	Environmental Health Scientist	Division of Health Assessment and Consultation	Agency for Toxic Substances and Disease Registry, Atlanta GA	X								X	X	X	X	X	X		X	X			X	X	11
Robert E. Faye, MSCE, PE	Civil Engineer/Hydrologist	Robert E. Faye and Associates, Inc	Consultant to Eastern Research Group, Inc. Lexington, Massachusetts	X	X	X		X	X			X	X			X						X	X	X	11
Mustafa M. Aral, PhD, PE	Director and Professor	Multimedia Environmental Simulations Laboratory	School of Civil and Environmental Engineering Georgia Institute of Technology Atlanta, Georgia	X						X	X	X	X		X			X		X	X				9
Jason B. Sautner, MSCE, EIT	Environmental Health Scientist	Division of Community Health Investigations	Agency for Toxic Substances and Disease Registry, Atlanta, Georgia	X								X	X	X	X						X		X		7
Barbara A. Anderson, MSEnvE, PE	Environmental Health Scientist	Division of Community Health Investigations	Agency for Toxic Substances and Disease Registry, Atlanta, Georgia										X	X	X			X	X	X			X		7
L. Elliott Jones, MS, PE	Hydrologist	Georgia Water Science Center	U.S. Geological Survey, Atlanta, Georgia										X			X	X		X						4
Wonyong Jang, PhD	Post Doctoral Fellow	Multimedia Environmental Simulations Laboratory	School of Civil and Environmental Engineering Georgia Institute of Technology Atlanta, Georgia	X						X			X							X					4
Walter M. Grayman, PhD, PE	Consulting Engineer		W.M. Grayman Consulting Engineer, Cincinnati OH	X								X	X								X				4
Jinjun Wang, MSCE	Ph.D. Candidate	Multimedia Environmental Simulations Laboratory	School of Civil and Environmental Engineering Georgia Institute of Technology Atlanta, Georgia	X							X	X													3
Claudia Valenzuela, MSCE	Post Graduate Research Fellow	Oak Ridge Institute for Science and Education	Agency for Toxic Substances and Disease Registry, Atlanta, Georgia	X		X						X													3
Jiabao Guan, PhD	Research Engineer	Multimedia Environmental Simulations Laboratory	School of Civil and Environmental Engineering Georgia Institute of Technology Atlanta, Georgia										X					X							2
Frank J. Bove, ScD	Senior Epidemiologist	Division of Toxicology and Human Health Services	Agency for Toxic Substances and Disease Registry, Atlanta, Georgia	X									X												2
Perri Z. Ruckart, MPH	Epidemiologist and Principal Investigator	Division of Toxicology and Human Health Services	Agency for Toxic Substances and Disease Registry, Atlanta, Georgia	X									X												2
Ilker T. Telci, PhD	Post-Graduate Research Fellow	Oak Ridge Institute for Science and Education	Agency for Toxic Substances and Disease Registry, Atlanta, Georgia												X						X				2
Joseph W. Green, Jr., MA	Post Graduate Research Fellow	Oak Ridge Institute for Science and Education	Agency for Toxic Substances and Disease Registry, Atlanta, Georgia	X				X																	2
Ilker T. Telci, PhD	Post-Graduate Research Fellow	Oak Ridge Institute for Science and Education	Agency for Toxic Substances and Disease Registry, Atlanta, Georgia										X												1
Susan M. Moore, MS	Environmental Health Scientist and Branch Chief	Division of Community Health Investigations	Agency for Toxic Substances and Disease Registry, Atlanta, Georgia										X												1
Amy L. Krueger, MPH	Post Graduate Research Fellow	Oak Ridge Institute for Science and Education	Agency for Toxic Substances and Disease Registry, Atlanta, Georgia	X																					1
Stephen J. Lawrence	Water-Quality Specialist	Georgia Water Science Center	U.S. Geological Survey, Atlanta, Georgia				X																		1
				13	1	2	1	2	1	2	2	8	14	4	6	3	3	4	4	5	5	1	4	3	

Senior Author	X
Contributing Author	X
Project Management & Coordination	O

Appendix C — Exposure-Dose Reconstruction Program: Overview of Strategy, Agency for Toxic Substances and Disease Registry, March 1993

March 26, 1993

From: Assistant Administrator, ATSDR, (E28)

Subject: ATSDR's Exposure-Dose Reconstruction Program
Overview of Strategy

To: Division Directors
Office Directors
Dose Reconstruction Committee Members

A critical activity in achieving ATSDR's mission is characterizing past and current human exposures to, and doses received from hazardous substances. On December 23, 1992 I requested that a coordinated, comprehensive plan be developed that would serve as the agency's strategy for exposure dose reconstruction activities. Since that time, members of the Dose Reconstruction Committee have developed a plan that will enable ATSDR to address issues ranging from total human exposure to early biological effects.

Attached to this memorandum is the document developed by the Dose Reconstruction Committee. The document sets forth the agency's program objectives and priorities for conducting exposure-dose reconstruction activities. As agency and division needs and requirements are identified, specific projects under the auspices of the Exposure-Dose Reconstruction Program will be proposed, developed, and funded.

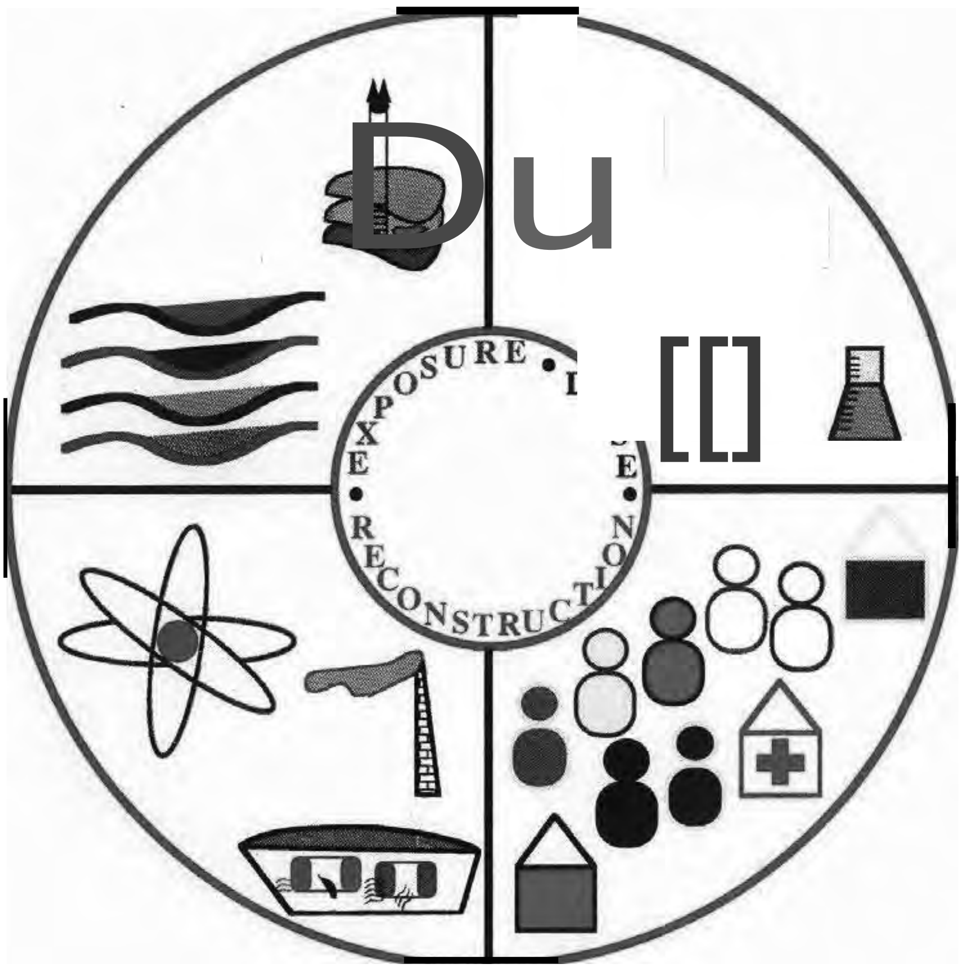
If additional copies of the report are needed, they may be obtained from Dr. Allan S. Susten, Assistant Director for Science, DHAC (E32).

Barry L. Johson, Ph.D.

AGENCY FOR TOXIC SUBSTANCES AND DISEASE **REGISTRY**

EXPOSURE-DOSE RECONSTRUCTION **PROGRAM**

OVERVIEW OF STRATEGY



MARCH 1993

Agency for Toxic Substances and Disease Registry

EXPOSURE-DOSE RECONSTRUCTION PROGRAM

OVERVIEW OF STRATEGY

MARCH 1993

PREFACE

A critical activity in achieving ATSDR's mission is characterizing past and current human exposures to, and doses received from, hazardous substances. Because direct measures of exposure and dose are often unavailable to agency health assessors and health scientists, sensitive, integrated, science-based methods for exposure-dose characterization need to be developed. On December 23, 1992, Dr. Barry L. Johnson, Assistant Administrator, ATSDR, requested that a coordinated, comprehensive plan be developed that would serve as the agency's strategy for exposure-dose reconstruction activities. Since that time, members of the Dose Reconstruction Committee have developed a plan that will enable ATSDR to address issues ranging from total human exposure to early biological effects.

The overall goal of the Exposure-Dose Reconstruction Program is to enhance the agency's capacity to characterize exposure and dose to better support health assessments and consultations, health studies, and exposure registries. As agency and division needs and requirements are identified, specific projects under the auspices of the Exposure-Dose Reconstruction Program will be proposed and developed. This document, therefore, sets forth ATSDR's program objectives and priorities for conducting exposure-dose reconstruction activities.

AUTHORS AND CONTRIBUTORS

PRINCIPAL AUTHORS

Allan S. Susten, Ph.D., DABT

Assistant Director for Science
Division of Health Assessment and Consultation

Morris L. Maslia, MSCE, P.E.

Environmental Engineer
Division of Health Assessment and Consultation

CONTRIBUTORS

Paul A. Charp, Ph.D.

Chief, Energy Facilities Assessment Section Division of Health Assessment and Consultation

Mark W. Evans, Ph.D.

Environmental Geologist
Division of Health Assessment and Consultation

Joseph L. Hugart, MPH

Deputy Director
Office of Federal Programs

Dennis E. Jones, Ph.D.

Senior Toxicologist
Office of the Associate Administrator for Science

M. Moiz Mumtaz, Ph.D.
Senior Toxicologist Division of Toxicology

Ralph C. O'Connor, Jr., Ph.D.
Assistant Director for Science
Division of Health Education

Timothy M. Radtke, MSEH
Environmental Health Scientist
Division of Health Studies

Robert F. Spengler, Sc.D. Assistant Director for Science Division of Health Studies

Agency for Toxic Substances and Disease Registry

EXPOSURE-DOSE RECONSTRUCTION PROGRAM

OVERVIEW OF STRATEGY

INTRODUCTION

The Agency for Toxic Substances and Disease Registry (ATSDR) was created by the Comprehensive Environmental Response, Compensation, and Liability Act of 1980 (CERCLA), otherwise known as Superfund. ATSDR's mission is to mitigate the adverse human health effects and diminished quality of life resulting from hazardous substances in the environment (ATSDR, 1992). A critical activity necessary to achieve this mission is characterizing past and current human exposures to, and doses received from, hazardous substances.

Because direct measures of exposure and dose, especially historical exposures, are often unavailable to ATSDR's health assessors and health scientists, the agency is embarking on a coordinated, comprehensive effort to develop sensitive, integrated, science-based methods for exposure-dose characterization. The agency's Exposure-Dose Reconstruction Program will coordinate relevant intramural and extramural projects covering environmental, geochemical, and biomedical disciplines.

For its purposes, ATSDR defines exposure-dose reconstruction as *an approach that uses computational models and other approximation techniques to estimate cumulative amounts of hazardous substances internalized by persons at presumed or actual risk from contact with substances associated with hazardous waste sites*. The emphasis of the program is to estimate past exposures. ATSDR is also beginning an exposure-dose determination initiative that uses direct personal space and biologic sampling to determine current exposure levels. This initiative will complement the Exposure-Dose Reconstruction Program.

In complying with CERCLA, ATSDR conducts activities at hazardous waste sites contaminated with radioactive or non-radioactive substances. Complexity of the sites varies with respect to the number, type and concentrations of contaminants, the number and characteristics of waste disposal areas for a site, site use, weather patterns, and the hydrogeologic and geochemical features of the site and surrounding areas. Whether sites are simple or complex, agency scientists require improved tools and methods for assessing exposures and doses that have the potential to produce adverse health effects if they are to arrive at credible conclusions regarding the health impact of hazardous waste sites. Moreover, ATSDR's policy is to determine the dose of an exposure whenever that is practicable (Johnson, 1992). The continuum that relates sources of contamination to clinical disease is illustrated in Figure 1.

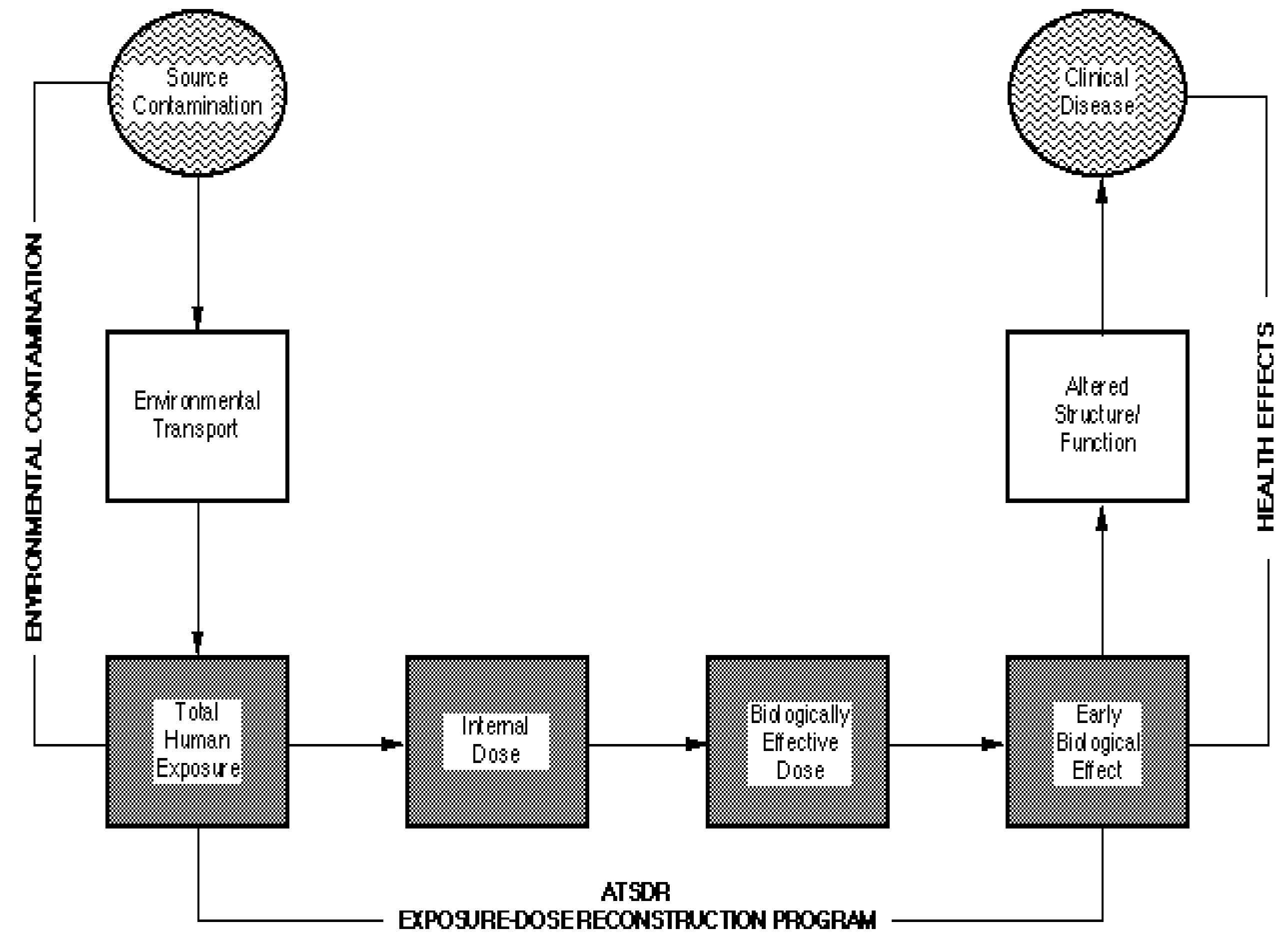


Figure 1. Continuum for relating environmental contamination with clinical disease. (From Lioy, 1990; Johnson and Jones, 1992)

PROGRAM GOAL

The goal of the Exposure-Dose Reconstruction Program is to enhance ATSDR's capacity to assess exposure and dose (with special emphasis on characterizing past exposures) to better support health assessments and consultations, health studies, and exposure registries.

PROGRAM OBJECTIVES

To set program priorities and focus activities, two objectives to meet the broad goal have been set. It is expected that the objectives will evolve over time as the agency begins to better understand the complexities of exposure-dose reconstruction. The objectives are these.

Over the next four years, significantly enhance the agency's ability to understand and use existing science-based methods and tools to assess past and current exposure and dose.

This objective will provide a stimulus to agency staff to focus on and identify specific areas of needs and activities, including training on existing tools and equipment, modifying existing techniques, and acquiring equipment and information.

Over the next four years, encourage developing new and improved technologies and methods that can be used by agency and non-agency scientists.

This objective can be met by developing a focused program that promotes using and developing mathematical models and computational tools for assessing total human exposure and by identifying and quantifying specific and sensitive biological indicators of exposure, disease, and susceptibility for assessing internal and biologically effective doses (Johnson and Jones, 1992)

STRATEGY

The strategy includes the following action elements:

- obtain and develop new and improved computational and mathematical tools for estimating past exposures and dose;
- obtain and develop tools for personal space monitoring and biologic testing for correlation with environmental sampling; and
- support research to fill specific information needs for use in environmental and biological models used for exposure-dose reconstruction.

The results of a number of completed agency projects (National Academy of Science (NAS) Studies) provide an important platform for planning future activities related to exposure-dose reconstruction. In addition, the results of several ongoing programs at ATSDR as well as programs at other agencies should provide additional relevant information.

A review of the approaches being used by other agencies revealed that a number of large-scale, exposure-dose reconstruction efforts are underway at several federal facility sites, including Hanford (Washington State), Idaho National Engineering Laboratory (Idaho), Rocky Flats Arsenal (Colorado), Fernald (Ohio), Oak Ridge (Tennessee), and Savannah River (South Carolina). At many of these sites, the primary concern is for radiological hazards; although, chemical hazards may also be present.

At several U.S. Department of Energy sites, the Centers for Disease Control and Prevention (CDC) have the lead in estimating public health impact of past and current radiation levels. Because many of ATSDR's efforts are directed toward hazardous substances and because techniques developed for quantifying radiological dose and risks are probably not applicable for estimating exposure to and dose received from chemicals, ATSDR, given resource constraints, believes it should focus its attention on the problems concerned with reconstructing exposures and doses to single and multiple chemicals. Completed, ongoing, and future activities relevant to the major action elements are presented below.

Obtain and develop improved computational and mathematical tools for estimating past exposures and dose:

Current Activities

An intramural project begun in FY93 will use existing computational and mathematical programs for assessing exposures to contaminated groundwater. This four-year project is the responsibility of the Division of Health Assessment and Consultation. Within the first two years, the existing programs will be applied to 12 sites, including four Exposure Registry sites. Advanced computer equipment and support hardware have been identified and purchased.

A four-year extramural project was begun in FY93 with first-year funding of $165,000 (recipient to be selected during 3rd Quarter FY93). The purpose of the project is to develop computational tools and a decision support system (software and a user's manual) for estimating exposures resulting from using contaminated groundwater at selected NPL sites. Deliverables scheduled in the 3rd and 4th years of the project are expected to provide agency staff with user-friendly methods that can be used to assess and reconstruct total exposures and estimates of dose from groundwater pathways.

The agency is continuing to develop a Geographic Information System (GIS) network. To date, six workstations have been purchased. The purpose of this activity is to use GIS technology to obtain information from geographic databases, and in conjunction with the agency's HAZDAT database, assess population demographics to assist in estimating past exposures in communities surrounding hazardous waste sites.

Future Activities

Additional equipment will be needed if the agency's capacity is to be expanded beyond the limited number of staff members currently able to apply and use the existing programs and equipment. Because the goal is total exposure/dose assessment, enhanced agency capacity to do exposure assessments in other media (air, soil, surface water) in addition to groundwater is also needed. Plans to expand present activities to include other media should be initiated during FY93 and FY94.

Plans should be developed to apply and evaluate the existing groundwater methods at additional sites. A formal ranking scheme or screening tool should be developed to identify other sites for analysis during FY94, FY95, and beyond, if appropriate.

Studies to validate the predictive capabilities of the exposure models should be conducted.

Protocols for conducting such studies, if feasible, could be a topic of a scientific meeting.

Support research to fill specific information needs for use in environmental and biological models used for exposure-dose reconstruction:

Of particular interest are the following:

- improved tools and methods for estimating past, **total human exposure or potential dose** (exposure multiplied by contact rate [NAS, 1991, p. 29]) to one or more hazardous substances as a result of contact with one or more media;
- improved approaches for estimating past internal doses (amount absorbed or deposited in the body of exposed individuals or interactions with membrane surfaces [NAS, 1991, p. 29]); and
- improved tools and methods for modeling and measuring **biologically effective doses** (amount of deposited or absorbed contaminant that reaches the cells or target site where an adverse effect occurs [NAS, 1991, p. 29]).

Current Activities

An extramural project was begun in FY93 to develop assessment methods that will bridge the gap between internalized dose and subtle alterations in structure/function (disease). The three-year project is being funded under a cooperative agreement with the Environmental & Occupational Health

Sciences Institute (EOHSI), Piscataway, New Jersey. First-year funding was $200,000. A workshop is planned in FY93 to prioritize future activities.

ATSDR is funding CDC's National Center for Health Statistics to develop reference ranges for 38 substances measured in biologic media. This is being accomplished through the latest population-based survey, the National Health and Nutrition Examination Survey (NHANES III). Such "baseline" data are useful when evaluating persons at health risk from exposure to any of the 38 substances.

Through a cooperative agreement with the National Research Council (NRC), ATSDR has sponsored biological marker studies that have resulted in four monographs that address biological markers for specific clinical or toxicologic endpoints (Johnson and Jones, 1992). The monographs address reproductive toxicology, pulmonary toxicology, neurotoxicology, and immunotoxicology. Ongoing projects include reports on Urinary Tract Biomarkers and Measuring Lead in Critical Populations.

ATSDR's Division of Toxicology is evaluating a model that estimates total body burdens of lead based on published slope factors for people exposed to known concentrations of lead in environmental media. Testing and validation of the model is planned for the latter part of FY93. This activity is also being monitored under the agency's lead program.

Future Activities

ATSDR's Division of Toxicology has formed a workgroup to focus on the development and use of integrated uptake/biokinetic (IU/BK) models for assessing the distribution and body burdens of environmental contaminants. The Exposure-Dose Reconstruction Committee should work closely with this group to promote development and validation of IU/BK models that will increase ATSDR's capacity to evaluate health impacts of specific site contaminants. Through an analysis of completed health assessments and consultations, a list of selected substances can be identified for which the development of IU/BK models should be considered.

The Division of Toxicology's substance-specific research program should be used to fill in data that will be needed for the environmental and biological models. These needs can be identified through the activities of the Dose-Reconstruction Program in addition to the to those identified by the Toxicological Profiles.

ATSDR's Division of Health Assessment and Consultation will develop an initiative to focus on exposure-dose determination. Exposure-dose measurements, taken as part of the public health assessment process when ongoing exposures appear likely, will help to prevent or mitigate adverse health effects. Levels of toxic substances in biologic samples and personal space will be correlated with environmental samples. This activity is critical because direct measurements of many substances such as volatile organic compounds (VOCs) cannot be obtained once exposure has ended. Site-specific exposure-dose information will complement exposure-dose reconstruction activities.

COORDINATION

In pursuing agency objectives, the Dose Reconstruction Committee will coordinate intramural and extramural activities with CDC, EPA, NTP, and other organizations that are actively involved with exposure-dose assessment and reconstruction. The committee will monitor and provide status reports on a regular basis to the Assistant Administrator, ATSDR.

REFERENCES

Agency for Toxic Substances and Disease Registry (ATSDR). Goals, objectives, and milestones: 1992. US Department of Health and Human Services, Public Health Service, Atlanta, GA. 1992.

Johnson, BL. A précis on exposure assessment. Journal of Environmental Health 1992;55(1):6- 9.

Johnson, BL, Jones, DE. ATSDR's activities and views on exposure assessment. Journal of Exposure and Environmental Epidemiology 1992; Suppl. 1:1-17.

Lioy, PJ. Assessing total human exposure to contaminants, a multidisciplinary approach. Environment, Science, and Technology 1990;24(7):938-945.

National Academy of Sciences (NAS). Human exposure assessment for airborne pollutants--advances and opportunities: National Academy Press: Washington, D.C. 1991.

Appendix D — Dover Township, Toms River, New Jersey Childhood Cancer Cluster Investigation

Background

Toms River, located in Dover Township, Ocean County, New Jersey, USA, experienced an increased incidence in childhood leukemia, brain, and central nervous system cancers from the mid-1980s through the early 1990s. (See Figure D.1 for location and Figure D.2 for cancer incidence, located at end of this section). These findings initiated a series of community-based activities that lead to the establishment of a successful partnership between the community, public health, and environmental agencies. The common goal of this partnership was to investigate linkages between environmental exposures and childhood cancers. The case–control study focused on two age groups in which elevated rates of cancer were previously found in Dover Township — children diagnosed before 20 years of age and children diagnosed before age five. The study was designed to focus on specific hypotheses about certain environmental exposure pathways. These hypotheses included: (1) exposure to two public drinking water supply sources with documented historical contamination (Parkway and Holly well fields), (2) exposure to contaminated private wells in Dover Township, and (3) exposure to major air pollution sources.

Exposure Indexes

To develop exposure indexes that would test the study hypotheses for drinking-water exposure, the study area's municipal drinking water distribution system was assessed using advanced numerical modeling techniques to reconstruct historical conditions (EPANET; Rossman 1994). For example, to derive exposure indexes for the municipal water supply and water-distribution system, modeling focused on reconstructing and estimating the percentage of water that a study subject might have received from each well and well field that historically supplied the water-distribution system. This modeling approach led to a novel development of the "proportionate contribution" concept wherein at any given point in the distribution system, water may be derived from one or more sources in differing proportions.

Using Water-Distribution System Modeling to Assist Exposure Assessment

Because the Dover Township area was primarily served by public water supply that relies solely on groundwater, ATSDR developed a protocol for using a water-distribution model as a tool to assist the exposure assessment component of the epidemiologic investigation (the EPANET model). Components of the water-distribution modeling approach included: (1) gathering data during field tests conducted in March and August 1998, (2) the development, calibration, and testing of the water-distribution system model for 1998 conditions, (3) a water-quality simulation of a naturally occurring conservative element in the groundwater, barium, to further test the reliability of the model calibration, (4) simulation of the proportionate contribution of water from points of entry (i.e., well fields) to various locations throughout the distribution system for 1998 conditions, and (5) reconstructing the water-distribution system networks on an monthly basis from 1962 through 1996 to determine the historical monthly "proportionate contribution" of water from all municipal well fields to any point served by the water-distribution system.

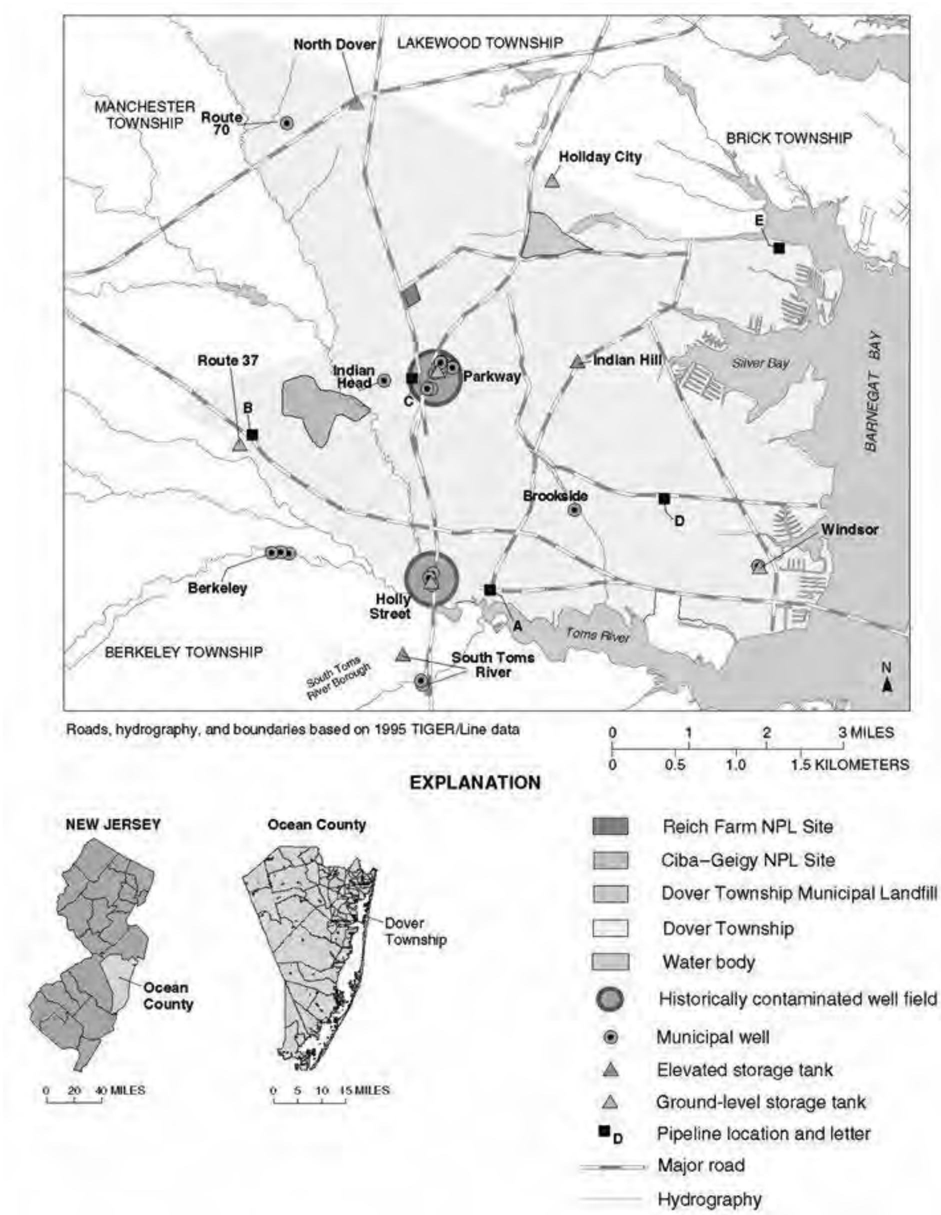


Figure D.1. Investigation area, Dover Township, Ocean County, New Jersey (modified from Maslia et al. 2001).

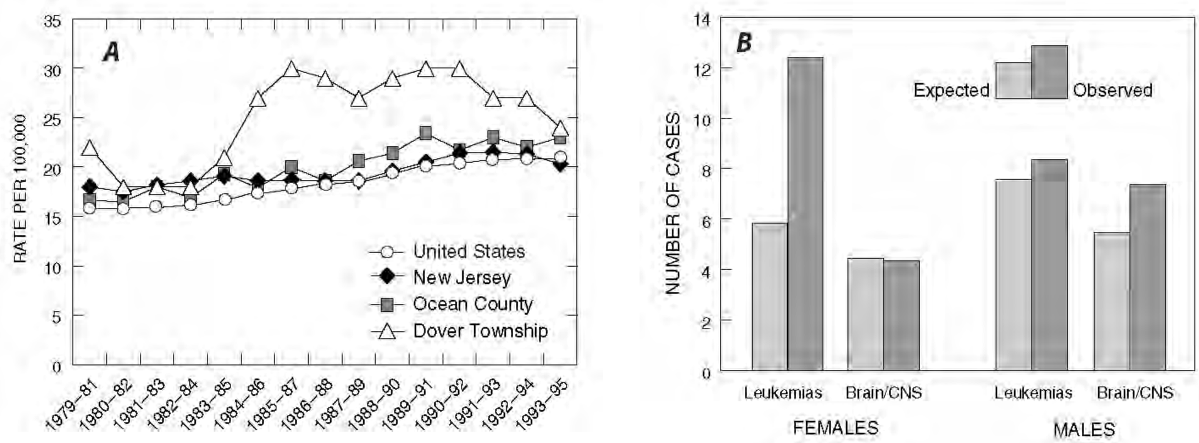


Figure D.2. Childhood cancer incidence analysis: (A) time trend in childhood cancer rates (1979–1995). (B) childhood cancer incidence, ages 0–19 years, Dover Township, New Jersey (1979–1995). (From Maslia et al. 2005).

Historical Reconstruction

Because of the lack of appropriate historical data, the EPANET model was calibrated to the present-day (1998) water-distribution system characteristics using data collected during March and August 1998. The reliability of the calibrated model was demonstrated by successfully conducting a water-quality simulation of the transport of a naturally occurring (in groundwater) conservative element—barium—and comparing results with data collected at 21 schools and 6 points of entry to the water-distribution system during March and April 1996. Results of the field-data collection activities, model calibration, and reliability testing are described in Maslia et al. (2000a, b). Following calibration, the model was used to reconstruct historical characteristics of the water-distribution system serving the Dover Township area on a monthly basis from 1962 through 1996.

Examples of historical results for the proportionate contribution of water are shown in Figure 5.3 (located at end of this section) for May 1962 and June 1996. In these examples, five geographically distinct locations (A–E) are selected from the historical distribution-system networks (see Figure 5.1 for locations A–E). In May 1962 (Fig. 5.3A), only two well fields (Holly and Brookside) provided water to any one location (e.g., locations A and C); whereas, in June 1996 (Fig. 5.3B), as many as seven well fields provided water to the distribution system (e.g., location E). Additionally, in May 1962, the Holly well field provided approximately 70% of the drinking water to location C (Fig. 5.3A), whereas, in June 1996 the Parkway well field provided approximately 70% of the drinking water to location C (Fig. 5.3B). Health scientists conducting the case–control epidemiologic study used the results described above (Fig. 5.3) to derive exposure indexes for each study subject.

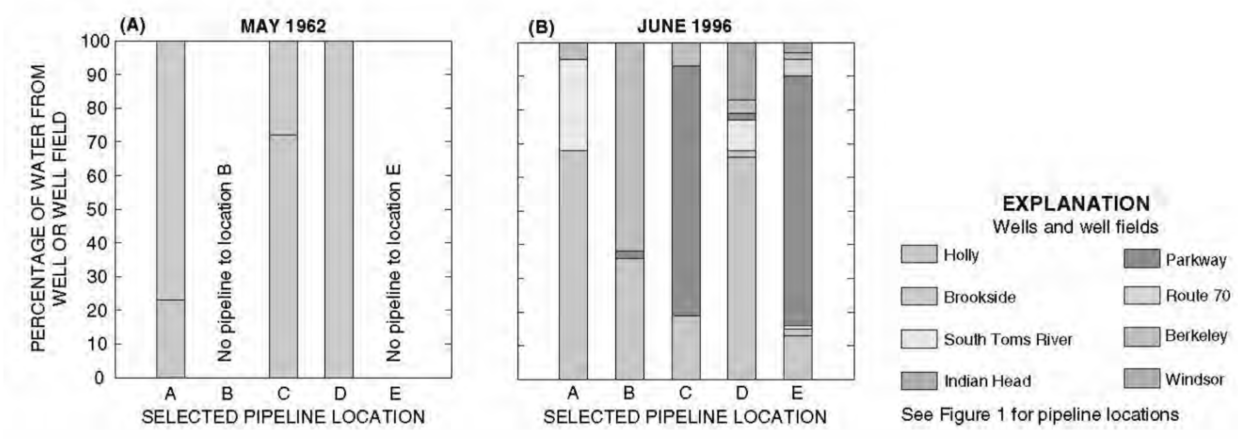


Figure D.3. Reconstructed (simulated) proportionate contribution of water from wells and well fields to selected locations in Dover Township area, New Jersey: (A) May 1962, and (B) June 1996 (see Figure 5.1 for locations A–E). (From Maslia et al. 2001, 2005).

Results from the case–control study showed (NJDHSS, 2003):

- A statistically significant association and consistency in multiple measures of association between prenatal exposure to time-specific Parkway well field water (1982–1996) and leukemia in female children of all ages, and
- a consistent elevation in the odds ratios and an apparent dose response effect was seen in interview and birth records studies between prenatal exposure to Ciba-Geigy ambient air and leukemia in female children diagnosed prior to age five.

Innovative methods were developed and used in the Toms River childhood cancer cluster investigation. With respect to characterizing the Dover Township water-distribution system, pressure data were gathered *simultaneously at 25 hydrants* throughout the distribution system using *continuous recording pressure data loggers* during 48-hour tests in March and August 1998. Data for storage tank water levels, system demand, and pump and well status (on/off) were obtained from the supervisory control and data acquisition (SCADA) system at the same time. Results of this aspect of the study were presented in the peer-reviewed American Society of Civil Engineers (ASCE) *Journal of Water Resources, Planning and Management* (Maslia et al. 2000). This paper was subsequently awarded (by ASCE in 2001), Best Practice-Oriented Paper of 2000 for the paper, *"Using Water-Distribution System Modeling to Assist Epidemiologic Investigations,"* ASCE Journal of Water Resources Planning and Management, Vol. 126, July/August 2000.

Results of the Dover Township, Toms River, New Jersey, childhood cancer cluster investigation are presented in ATSDR and NJDHSS reports (all independently peer reviewed) and published in peer-reviewed scientific journals (Maslia 2000a, b, 2001, 2005, NJDHSS 2003).

The American Academy of Environmental Engineers (AAEE) also recognized the Dover Township, Toms River, New Jersey, historical reconstruction effort. This environmental engineering professional organization awarded the

ATSDR and NJDHSS effort the 2003 Excellence in Environmental Engineering Award, Grand Prize, Research Category (April 2003) for the project, "*Enhancing Environmental Engineering Science to Benefit Public Health, Dover Township, Ocean County, New Jersey.*"

The Dover Township, Toms River, New Jersey childhood cancer investigation results are significant because out of hundreds of cancer cluster investigations, only two — Woburn, Massachusetts and Dover Township, New Jersey — have shown an association between environmental exposures and childhood cancer.

Appendix E — Information Sources Used to Extract Model-Related Data for Historical Reconstruction

Appendix A2. Information sources used to extract model-specific data for historical reconstruction analyses, U.S. Marine Corps Base Camp Lejeune, North Carolina.

[Refer to end of Appendix A2 for a list of abbreviations and acronyms]

Information source	Original media	Supplier or location of information source	Approximate quantity or size	Description	Date obtained (date of information)
ATSDR information requests and selected authored reports					
ATSDR information request, July 11, 2003	CD–ROM	Camp Lejeune	CD–ROMs with numerous files	Final Basewide Remediation Assessment Groundwater Study (Baker 1998a); GIS data for Camp Lejeune; historical water-supply well data from wellhead management program study (Geophex Ltd. 1991); wellhead protection plan update (AH Environmental Consultants 2002); historical water treatment plant booster pump information (Henry Von Oesen and Associates, Inc. 1979)	Aug. 2003 (varies)
ATSDR information request, 2004	CD–ROM, DVD	Camp Lejeune	About 25 gigabytes	Natural color digital orthophotography; data layers maintained in the integrated geographic information repository (IGIR) master database, Feb. 2004; TIFF files	Nov. 2004 (Feb. 2004)
ATSDR information request, 2005	Paper	Camp Lejeune	12 pages	Documentation for startup of Holcomb Boulevard water treatment plant; acquisition data form, April 1973; plant account record card, July 1990; Newspaper (Globe) article, August 1972; Command chronology, July–Dec 1972	Sept. 2005 (June–Dec 1972)
ATSDR information request, Dec. 1, 2005	CD–ROM	Camp Lejeune	3 CD–ROMs	VOC impacted drinking water document database (CLW database); TCE/PCE sample result summary spreadsheet; JTC historical laboratory analytical results (subset of CLW database, about 34 files)	Dec. 2005 (1980–1986)
ATSDR information request, 2006	CD–ROM, DVD	Camp Lejeune	1 CD–ROM, 1 DVD	Natural color digital orthophotography of entire base, Feb. 2004, MrSID image format; color infrared color digital orthophotography of entire base, Mar. 1996, MrSID image format	Sept. 2006 (Nov. 2004; Mar. 1996)
ATSDR information request, May 2009	CD–ROM, DVD, paper	Camp Lejeune	CD–ROM, DVD, paper	186 documents (PDFs) from the Camp Lejeune Historic Drinking Water Consolidated Document Repository (f/k/a BAH files); 31 sets of contract drawings from Public Works vault; Raw Water Master Plan (AH Environmental Consultants 2005); Draft (2009) USGS groundwater- level report, (published as McSwain 2010); Permit to Construct Municipal Solid Waste Landfill (Dewberry and Davis 1995); Evaluation of Cogdell's Creek (CH2M HILL, Inc. 1998); Corrosion Control Study, Hadnot Point and Marine Corps Air Station (MCAS) New River (Malcolm Pirnie 1999)	July 2009 (varies)
ATSDR information request, Nov. 2009	CD–ROM	Camp Lejeune	1 CD–ROM (about 160 megabytes)	Site Management Plans for 2007, 2008, 2009, and 2010 (CH2M HILL 2007a,b, 2008, 2009)	Dec. 2009 (Apr. 2007–Aug. 2009)
ATSDR information request, Apr. 2011	CD–ROM	USEPA, Region IV	57 files, 19 megabytes	JTC Laboratory analyses on Naval samples	Sept. 2011 (Feb. 1985–Apr. 1986)

Appendix A2. Information sources used to extract model-specific data for historical reconstruction analyses, U.S. Marine Corps Base Camp Lejeune, North Carolina.—Continued

[Refer to end of Appendix A2 for a list of abbreviations and acronyms]

Information source	Original media	Supplier or location of information source	Approximate quantity or size	Description	Date obtained (date of information)
		ATSDR information requests and selected authored reports—Continued			
Hadnot Point–Holcomb Boulevard reports	Paper; electronic (PDF)	ATSDR *http://www.atsdr.cdc.gov/sites/lejeune/watermodeling.html*	Three reports (Chapters B, C, and D), about 40 megabytes	Analyses and interpretations of data to develop geohydrologic framework of the Brewster Boulevard and Castle Hayne aqufier systems and the Tarawa Terrace aquifer; analyses of selected contaminants within the HPWTP and HBWTP service areas and vicinities at Camp Lejeune; among contaminants of interest in this report series, PCE, TCE, 1,2-tDCE, benzene, and vinyl chloride	Oct. 2010, Jan. 2012, Dec. 2012 (1940s–2008)
Public Health Assessment for ABC One-Hour Cleaners	Paper	ATSDR records room and LAN	1 folder in records room	Administrative records for 1990 public health assessment; 1996 site review and update also available	Aug. 1990; Sept. 1996 (Aug. 1990; Sept. 1996)
Public Health Assessment for Camp Lejeune	Paper	ATSDR records room and LAN	52 folders in records room and numerous electronic files	Administrative records for 1997 public health assessment	Aug. 1997 (Aug. 1997)
Tarawa Terrace reports	Paper; electronic (PDF)	ATSDR *http://www.atsdr.cdc.gov/sites/lejeune/watermodeling.html*	Executive summary report and 9 report volumes (Chapters A–I); about 100 megabytes	Analyses of the Tarawa Terrace drinking-water system at Camp Lejeune that was contaminated with PCE and its degradation by-products from the nearby, off-base, ABC One-Hour Cleaners	2007–2009 (1950s–1994)
		Databases and information portals			
ABC One-Hour Cleaners site reports	Paper; electronic (PDF)	USEPA Web site: *http://www.epa.gov/*	About 25 electronic files (PDF), 125 megabytes	Reports primarily related to CERCLA activities at ABC One-Hour Cleaners site; files vary in size from a few pages to several hundred pages	2003–2007 (1986–2007)
Camp Lejeune Historic Drinking Water Consolidated Document Repository (CLHDW CDR)	Electronic (PDF)	Camp Lejeune	514 pages (index only); about 8,000–10,000 documents	The index (f/k/a BAH index) is a list of documents compiled from a base-wide search of buildings and documents; a single index entry may reference several boxes to tens of boxes of documents and information records	Apr. 2009 (varies)
Camp Lejeune Historic Drinking Water Consolidated Document Repository (CLHDW CDR)	Electronic (PDF)	Camp Lejeune	7,403 files, 158 gigabytes	Documents, handwritten notes, reports, lab analyses, water-supply data, compiled from a base-wide search of buildings and documents; a single file may reference several one-page documents or several hundred pages of information and records	Mar. 2011 (varies)
Camp Lejeune water document (CLW files)	CD–ROM	Camp Lejeune	About 574 megabytes; about 1,100 files	Documents, handwritten notes, reports, lab analyses primarily related to water supply, distribution, and water-quality issues; files vary in size from a few pages to several hundred pages	Dec. 2005 (varies)
CERCLA administrative record for ABC One-Hour Cleaners	Paper and electronic (PDF)	USEPA Web site: *http://www.epa.gov/*	About 100 files listed on CERCLA administrative record index	Documents, handwritten notes, and reports primarily related to CERCLA activities at ABC One-Hour Cleaners site; files vary in size from a few pages to several hundred pages	2003–2007 (1986–1994)

Appendix A2. Information sources used to extract model-specific data for historical reconstruction analyses, U.S. Marine Corps Base Camp Lejeune, North Carolina.—Continued

[Refer to end of Appendix A2 for a list of abbreviations and acronyms]

Information source	Original media	Supplier or location of information source	Approximate quantity or size	Description	Date obtained (date of information)
			Databases and information portals—Continued		
CERCLA administrative record for Camp Lejeune	Hard drive (provided by Camp Lejeune)	Baker Engineers, Inc., Web portal; *http://www.bakerenv.com/camplejeune_irp*	About 15 gigabytes; about 3,700 files	Documents, handwritten notes, and reports primarily related to installation restoration program sites at Camp Lejeune; files vary in size from a few pages to several hundred pages	Jan. 2006 (varies)
Environmental Management Division (EMD) document index	Electronic (MS Excel; PDF)	Camp Lejeune	Hundreds to thousands of reports and documents	Reports and documents related to base IRP, wastewater, drinking water, surface water, groundwater, indoor air quality, vapor intrusion, solid waste, landfill activities, environmental conservation, compliance, wellhead management, etc.	2003–2010 (varies)
Terrabase—IRP sites	CD–ROM (MS Access)	Catlin/Camp Lejeune	About 1.3 million records of analytical data	Analytical data associated with base IRP provided to Catlin by Camp Lejeune; IRP data derived from other source documents	Apr. 2010 (1984–2010)
Terrabase—UST sites	CD–ROM (MS Access)	Catlin/Camp Lejeune	About 700,000 records of analytical data	Time frame of data is 1984 to 2005. Database developed from database provided to Catlin by Camp Lejeune during November 2005; contains analytical data for UST sites	Mar. 2010 (1984–2005)
UST files	Electronic (Web portal)	Camp Lejeune; Catlin Engineers and Scientists *http://lejeune.Webmainframe.com* (proprietary)	1,535 files	Information, site data, meeting minutes, monitoring data, etc., related to all UST sites and activities at Camp Lejeune; files vary in size from a few pages to exceeding 1,000 pages	Mar. 2010 (1986–2009)
			Drinking-water system information and data		
AH Environmental reports on drinking-water systems	Paper	Camp Lejeune	6 reports, about 250 pages	Cataloging and information gathering of drinking-water systems at Camp Lejeune; all reports by AH Environmental Consultants: (1) Long Term Water System Master Plan (Dec. 2001), (2) Wellhead Protection Plan—2002 Update (Aug. 2002), (3) Water Distribution System Modeling Support (Aug. 2004), (4) ATSDR Support—Estimation of VOC Removal (Dec. 2004), (5) Meter Installation Work Plan (Dec. 2004), and Raw Water Master Plan (March 2005)	Aug. 2003–Dec. 2005 (2001–2005)
Golf course watering information	Paper	Camp Lejeune	5 electronic files	Scanned images (PDFs and TIFFs) of golf course sprinkler locations and information	Sept. 2010 (Mar. 1969; Aug. 1991; June 1993)
Pump rating curves	Paper	Camp Lejeune	4 pages	Pump rating curves for finished water pumps at Hadnot Point and Holcomb Boulevard water treatment plants	Mar. 2004 (~1985?)

Appendix A2. Information sources used to extract model-specific data for historical reconstruction analyses, U.S. Marine Corps Base Camp Lejeune, North Carolina.—Continued

[Refer to end of Appendix A2 for a list of abbreviations and acronyms]

Information source	Original media	Supplier or location of information source	Approximate quantity or size	Description	Date obtained (date of information)
			Drinking-water system information and data—Continued		
Survey of selected water-distribution system locations	Electronic (MS Excel)	U.S. Geological Survey, North Carolina Water Science Center	27 fire hydrants and 7 water-storage tanks	Horizontal and vertical survey data for selected hydrants and water-storage tanks	May–July 2004 (May–July 2004)
Survey of selected water-distribution system locations	Electronic (MS Excel)	Parker and Associates (subcontractor to Eastern Research Group, Inc.)	56 fire hydrants, 21 monuments, and 6 water-storage tanks	Horizontal and vertical survey data for selected hydrants and water-storage tanks	Oct. 2004 (Oct. 2004)
Water treatment plant flow data	CD–ROM	Camp Lejeune	About 100 megabytes	2-minute SCADA data for various times during 2004–2005	2004–2007 (Mar. 2004–Sept. 2005)
Water treatment plant flow data	Electronic (MS Excel); paper	Camp Lejeune	About 15 megabytes	Daily and monthly flows from water treatment plants; 1995–1999 in paper format; 2000–2005 in electronic format	2004–2009 (1999–2005)
Water utility maps	CD–ROM; paper	Camp Lejeune	About 100–150 files, 500 megabytes	Historical (1956–1987) water utility maps, scanned in as TIFFs, showing water-distribution systems aboard Camp Lejeune	July 2006 (1956–1987)
Water utility and housing maps	CD–ROM	Camp Lejeune	About 500 files, 525 megabytes	Historical (1940s and 1950s) water utility and housing maps, scanned in as TIFFs, 50-ft and 500-ft scales	Oct. 2003 (1940s–1950s)
Water plant log books	Paper	Camp Lejeune	About 2,100 pages	CLW files 6610.pdf–8761.pdf; handwritten entries in water utility log books containing information on mechanical repairs, water-supply operations, water-quality issues, and customer contacts and complaints	Dec. 2005 (varies)
Water-supply wells capacity data	Paper	Camp Lejeune	About 110 wells	Historical and present-day notes, information and data on operations and capacity histories of Tarawa Terrace, Holcomb Boulevard, and Hadnot Point water-supply wells	Aug. 2003–Aug. 2010 (1940s–2010)
Water-supply well operational data	CD–ROM	Camp Lejeune	10,000 scanned pages	Ten years of daily records, 1999–2008, indicating water-supply well on-off cycling operations—handwritten entries	2009 (1999–2008)
			Housing records and information		
Housing maps	Paper	Camp Lejeune	About 10 maps (sheets)	Paper maps that show housing units, addition of housing units, and estimated number of housing units	Date unknown (1940s–1990s)
Housing records	Paper	Camp Lejeune	About 90,000 records	Camp Lejeune housing records used for identifying enlisted and officer personal housing locations; obtained for small for gestational age study (ATSDR 1998)	About 1994 (1950s–1995)

Appendix A2. Information sources used to extract model-specific data for historical reconstruction analyses, U.S. Marine Corps Base Camp Lejeune, North Carolina.—Continued

[Refer to end of Appendix A2 for a list of abbreviations and acronyms]

Information source	Original media	Supplier or location of information source	Approximate quantity or size	Description	Date obtained (date of information)
			Drinking-water system information and data—Continued		
Survey of selected water-distribution system locations	Electronic (MS Excel)	U.S. Geological Survey, North Carolina Water Science Center	27 fire hydrants and 7 water-storage tanks	Horizontal and vertical survey data for selected hydrants and water-storage tanks	May–July 2004 (May–July 2004)
Survey of selected water-distribution system locations	Electronic (MS Excel)	Parker and Associates (subcontractor to Eastern Research Group, Inc.)	56 fire hydrants, 21 monuments, and 6 water-storage tanks	Horizontal and vertical survey data for selected hydrants and water-storage tanks	Oct. 2004 (Oct. 2004)
Water treatment plant flow data	CD–ROM	Camp Lejeune	About 100 megabytes	2-minute SCADA data for various times during 2004–2005	2004–2007 (Mar. 2004–Sept. 2005)
Water treatment plant flow data	Electronic (MS Excel); paper	Camp Lejeune	About 15 megabytes	Daily and monthly flows from water treatment plants; 1995–1999 in paper format; 2000–2005 in electronic format	2004–2009 (1999–2005)
Water utility maps	CD–ROM; paper	Camp Lejeune	About 100–150 files, 500 megabytes	Historical (1956–1987) water utility maps, scanned in as TIFFs, showing water-distribution systems aboard Camp Lejeune	July 2006 (1956–1987)
Water utility and housing maps	CD–ROM	Camp Lejeune	About 500 files, 525 megabytes	Historical (1940s and 1950s) water utility and housing maps, scanned in as TIFFs, 50-ft and 500-ft scales	Oct. 2003 (1940s–1950s)
Water plant log books	Paper	Camp Lejeune	About 2,100 pages	CLW files 6610.pdf–8761.pdf; handwritten entries in water utility log books containing information on mechanical repairs, water-supply operations, water-quality issues, and customer contacts and complaints	Dec. 2005 (varies)
Water-supply wells capacity data	Paper	Camp Lejeune	About 110 wells	Historical and present-day notes, information and data on operations and capacity histories of Tarawa Terrace, Holcomb Boulevard, and Hadnot Point water-supply wells	Aug. 2003–Aug. 2010 (1940s–2010)
Water-supply well operational data	CD–ROM	Camp Lejeune	10,000 scanned pages	Ten years of daily records, 1999–2008, indicating water-supply well on-off cycling operations—handwritten entries	2009 (1999–2008)
			Housing records and information		
Housing maps	Paper	Camp Lejeune	About 10 maps (sheets)	Paper maps that show housing units, addition of housing units, and estimated number of housing units	Date unknown (1940s–1990s)
Housing records	Paper	Camp Lejeune	About 90,000 records	Camp Lejeune housing records used for identifying enlisted and officer personal housing locations; obtained for small for gestational age study (ATSDR 1998)	About 1994 (1950s–1995)

Appendix A2. Information sources used to extract model-specific data for historical reconstruction analyses, U.S. Marine Corps Base Camp Lejeune, North Carolina.—Continued

[Refer to end of Appendix A2 for a list of abbreviations and acronyms]

Information source	Original media	Supplier or location of information source	Approximate quantity or size	Description	Date obtained (date of information)
			Map information and data		
Airborne laser digital imagery; spatial data, Onslow County, NC	DVD	Spectrum Mapping Corporation, North Carolina	44 DVDs (about 170 gigabytes)	Digital orthophotographs of Onslow County, North Carolina	Nov. 2004 (Feb. 2003?)
AutoCAD files	CD–ROM	Camp Lejeune	About 100 megabytes; 70 files	Quadrangle maps of Camp Lejeune containing features such as topography, utility lines, wastewater and water-distribution systems, housing locations, etc.	Oct. 2003 (1996)
Camp Lejeune survey control data	Paper	Camp Lejeune	1 report (85 pages)	Report on geodetic survey to upgrade and update horizontal control aboard U.S. Marine Corps Base Camp Lejeune	2005 (Sept. 1984)
Digital elevation model (DEM) data	DVD	U.S. Geological Survey, North Carolina Water Science Center	1.9 gigabytes	LIDAR-derived DEM data for Camp Lejeune area, 20-ft and 5-ft grids; obtained from the NC Flood Mapping Program	Jan. 2004; Aug. 2010 (May 31, 2002)
Digital topographic contour data	CD–ROM	U.S. Geological Survey, North Carolina Water Science Center	650 megabytes	2-ft contours created from the 20-ft LIDAR-derived DEM, available from the NC Flood Mapping Program; projection is NC State Plane, NAD 83, units feet	Feb. 2004 (May 31, 2002)
Geographic information system files	CD–ROM; DVD	Camp Lejeune	Several dozen CD–ROMs and DVDs	Installation geospatial information and historical satellite imagery files	Aug. 2003–July 2009 (1938–June 2009)
Soil Survey Geographic (SSURGO) database for Onslow County, North Carolina	Electronic	Natural Resources Conservation Service, United States Department of Agriculture *http://soildatamart.nrcs.usda.gov*	1.6 megabytes	Georeferenced digital map data and tabular data of soils and attribute data for Onslow County, NC, provided in ESRI Arcview shapefile format	Nov. 2010 (Sept. 2003–June 2009)
			North Carolina documents and reports		
Central Coastal Plain Capacity Use Investigation Report	Electronic (PDF)	NCDENR, Division of Water Resources	1 report (24 pages)	Report describing the central coastal plain capacity use area under the 1967 Water Use Act (NCDENR 1998)	Nov. 2003 (Nov. 1998)
Detailed soil maps for Onslow County, NC	CD–ROM	North Carolina Center for Geographic Information and Analysis	52 megabytes	Detailed digital soils maps for Onslow County, North Carolina	Apr. 2005 (2003–2004)
North Carolina water-supply plan	Electronic (PDF)	North Carolina Department of Environment and Natural Resources (NCDENR)	1 report and 20 appendixes (about 150 pages)	Compilation of more than 500 water-supply plans developed by local government water systems to assess water-supply needs over the next 20 years; report dated January 2001 and based on local water-supply plans developed during 1998 and 1999	Nov. 2003 (1998–1999)

Appendix A2. Information sources used to extract model-specific data for historical reconstruction analyses, U.S. Marine Corps Base Camp Lejeune, North Carolina.—Continued

[Refer to end of Appendix A2 for a list of abbreviations and acronyms]

Information source	Original media	Supplier or location of information source	Approximate quantity or size	Description	Date obtained (date of information)
North Carolina documents and reports—Continued					
State of North Carolina Records	CD–ROM, DVD, paper	NCDENR and historical archives in Raleigh and Wilmington[1]	5 CD–ROMs, 1 DVD, (historical files unknown)	Historical and present-day water-supply information; water-supply well construction information; site information for Hadnot Point fuel farm (IR site 22) and Hadnot Point Industrial Area (IR site 78)	Mar. 2004; June 2010; Aug. 2010 (1980–2007)
State of North Carolina vital statistics data files	Paper	NCDENR	1 report (116 pages)	Documentation of North Carolina vital statistic data files available for public use	Unknown (Oct. 1993)
Miscellaneous information, data, and reports					
Community group Web sites	Electronic	*http://www.watersurvivors.com* *http://www.tftptf.com/*	N/A	Former marine's and citizen's Web sites containing miscellaneous information and numerous Camp Lejeune documents (current and historical). Historical obtained from the U.S. Marine Corps through FOIA requests	N/A (N/A)
National Climatic Data Center (NCDC)	Electronic	NCDC, Asheville, NC *http://www.ncdc.noaa.gov/oa/ncdc.html*	6 files, about 6 megabytes	Precipitation and evaporation data for the Hoffman/Maysville station, NC	Dec. 2008 (Dec. 1945–Dec. 2008)
National Geophysical Data Center (NGDC)	Electronic	NGDC, Boulder, CO *http://www.ngdc.noaa.gov*	4 files, about 600 kilobytes	Bathymetry survey data for New River area of Camp Lejeune, NC; 5 surveys: H04697 (1927), H05277 (1933), H05301 (1933), H05302 (1933), and H09882 (1980)	Dec. 2008 (1927, 1933, 1980)
Onslow County, NC Soil Survey	Paper	U.S. Department of Agriculture, Soil Conservation Service	1 report (152 pages)	Information that can be used for land-planning programs in Onslow County; report contains predictions of soil behavior for selected land uses	May 2003 (1982)
Specific DON and USMC reports	CD–ROM; electronic (PDF); paper	Camp Lejeune	10–15 volumes	Base Master Plans for 1972 (CERCLA Administrative Record File #0368) and 1988 (NAVFAC 1988?); Water Conservation Study (ECG Inc. 1999); Site Management Plans 2005–2011 (CH2M HILL and Baker Environmental, Inc. 2005; CH2M HILL 2006, 2007a, 2007b, 2008, 2009, 2010); Range Environmental Vulnerability Assessment report (Malcolm Pirnie 2009); Vapor Intrusion report (AGVIQ–CH2M HILL 2009)	2005–2010 (1984–2009)
Technical Memoranda	Electronic (PDF)	Camp Lejeune	Several electronic files	SWMU 350, IR site 88, Area of Potential Concern reports 9, 10, and 11	May 2010 (Mar.–May 2010)
U.S. Geological Survey open files and reports	Paper	USGS, North Carolina Water Science Center, Raleigh	Several hundred to thousand pages; published reports	Files on well construction, well locations, and water use at Camp Lejeune; published reports on Camp Lejeune	Mar. 2004 (1940s–1987)
Vapor intrusion activities	Electronic (PDF); paper	USEPA; NAVFAC (Camp Lejeune)	Several reports including one 6-volume report	Reports describing vapor intrusion activities at ABC One-Hour Cleaners, Tarawa Terrace Elementary School, and Camp Lejeune (Mainside)	2007–2009 (2007–2009)

[1] In searching the historical archives in Raleigh, North Carolina, information contained in files folders dated 1969–1989 were missing.

Appendix A2. Information sources used to extract model-specific data for historical reconstruction analyses, U.S. Marine Corps Base Camp Lejeune, North Carolina.—Continued

[Refer to end of Appendix A4 for a list of abbreviations and acronyms]

List of abbreviations and acronyms:
- 1,2-tDCE, *trans*-1,2-dichloroethylene
- ATSDR, Agency for Toxic Substances and Disease Registry
- BAH, Booze Allen Hamilton
- Catlin, Richard Catlin and Associates, Inc. or Catlin Engineers and Scientists (see Rerference Section)
- CD–ROM, computer disc, read-only memory
- CERCLA, Comprehensive Environmental Response, Compensation, and Liability Act of 1980
- CLW, Camp Lejeune water document
- DEM, digital elevation model
- DON, Department of the Navy
- DVD, digital video disc
- ESRI, Environmental Systems Research Institute
- f/k/a, formerly known as
- FOIA, Freedom of Information Act
- ft, foot
- GIS, geographic information system
- HBWTP, Holcomb Boulevard water treatment plant
- HPWTP, Hadnot Point water treatment plant
- IGIR, integrated geographic information repository
- IRP, Installation Restoration Program
- JTC, JTC Environmental Consultants, Inc. (see Reference Section)
- LAN, local area network
- LIDAR, line detection and ranging
- MS, Microsoft, Excel, and Access are either registered trademarks or trademarks of Microsoft Corporation in the United States and/or other countries
- N/A, not available
- NAD 83, North American Datum of 1983
- NAVFAC, Naval Facilities Engineering Command
- NC, North Carolina
- NCDC, National Climatic Data Center
- NCDENR, North Carolina Department of Environment and Natural Resources
- NGDC, National Geophysical Data Center
- PCE, tetrachloroethylene
- PDF, portable document file format
- PHA, public health assessment
- SCADA, supervisory control and data acquisition
- SWMU, solid waste management unit
- TCE, trichloroethylene
- TIFF, tagged image file format
- USEPA, U.S. Environmental Protection Agency
- USGS, U.S. Geological Survey
- USMC, U.S. Marine Corps
- UST, underground storage tank
- VOC, volatile organic compound

Appendix F — Summaries of ATSDR's Tarawa Terrace Chapter Reports

Summaries of **Tarawa Terrace** chapter reports are described below. Electronic versions of each chapter report and their supporting information and data will be made available on the ATSDR Camp Lejeune Web site at *http://www.atsdr.cdc.gov/sites/lejeune/index.html.*

Chapter A: Summary of Findings (Maslia et al. 2007) provides a summary of detailed technical findings (described in Chapters B–K) focusing on the historical reconstruction analysis and present-day conditions of groundwater flow, contaminant fate and transport, and distribution of drinking water at Tarawa Terrace and vicinity. Among the topics that this report summarizes are: (1) methods of analyses, (2) data sources and requirements, (3) the four-stage hierarchical approach used for model calibration and estimating PCE concentrations in drinking water, (4) presentation, discussion, and implications of selected simulation results for PCE and its degradation by-products, and (5) quantifying confidence in simulation results by varying water- supply well historical pumping schedules and by using sensitivity and probabilistic analyses to address issues of uncertainty and variability in model parameters. In addition, this report provides a searchable electronic database—using digital video disc (DVD) format—of information and data sources used to conduct the historical reconstruction analysis. Data were obtained from a variety of sources, including ATSDR, USEPA, Environmental Management Division of U.S. Marine Corps Base Camp Lejeune, U.S. Geological Survey, private consulting organizations, published scientific literature, and community groups representing former marines and their families.

Chapter B: Geohydrologic Framework of the Castle Hayne Aquifer System (Faye 2007) provides detailed analyses of well and geohydrologic data used to develop the geohydrologic framework of the Castle Hayne aquifer system at Tarawa Terrace and vicinity. Potentiometric levels, horizontal hydraulic conductivity, and the geohydrologic framework of the Castle Hayne aquifer system east of the New River are described and quantified. The geohydrologic framework is com- posed of 11 units, 7 of which correspond to the Upper, Middle, and Lower Castle Hayne aquifers and related confining units. Overlying the Upper Castle Hayne aquifer are the Brewster Boulevard and Tarawa Terrace aquifers and confining units. Much of the Castle Hayne aquifer system is composed of fine, fossiliferous sand, limestone, and shell limestone. The sands are frequently silty and contain beds and lenses of clay. Limestone units are probably discontinuous and occasionally cavernous. Confining units are characterized by clays and silty clays of significant thickness and are persistent across much of the study area. Maximum thickness of the Castle Hayne aquifer system within the study area is about 300 ft. In general, geohydrologic units thicken from northwest to the south and southeast. The limestones and sands of the Castle Hayne aquifer system readily yield water to wells. Aquifer-test analyses indicate that horizontal hydraulic conductivities of water-bearing units at supply wells commonly range from 10 to 30 feet per day. Estimated predevelopment potentiometric levels of the Upper and Middle Castle Hayne aquifers indicate that groundwater- flow directions are from highland areas north and east of the study area toward the major drainages of New River and Northeast Creek.

Chapter C: Simulation of Groundwater Flow (Faye and Valenzuela 2007) provides detailed analyses of groundwater flow at Tarawa Terrace and vicinity, including the development of a predevelopment (steady-state) and transient groundwater-flow model using the model code MODFLOW-96 (Harbaugh and McDonald 1996). Calibration and testing of the model are thoroughly described. The groundwater-flow model was designed with seven layers largely representing the Castle Hayne aquifer system. Com- parison of 59 observed water levels representing esti- mated predevelopment conditions and corresponding simulated potentiometric levels indicated a high degree of similarity throughout most of the study area. The average absolute difference between simulated and observed predevelopment water levels was 1.9 ft, and the root-mean-square (RMS) of differences was 2.1 ft. Transient simulations represented pumping at Tarawa Terrace supply wells for 528 stress periods representing 528 months—January 1951–December 1994. Assigned pumpage at supply wells was estimated using reported well-capacity rates and annual rates of raw water treated at the Tarawa Terrace water treatment plant (WTP) during 1975 –1986. Calibrated model results of 263 paired water levels representing observed and simulated water levels at monitor wells indicated an average absolute difference between simulated and observed water levels of 1.4 ft, a standard deviation of water-level difference of 0.9 ft, and a RMS of water-level difference of 1.7 ft. Calibrated model results of 526 paired water levels representing observed and simulated water levels at water-supply wells indicated an average absolute difference between simulated and observed water levels of 7.1 ft, a standard deviation of water-level difference of 4.6 ft, and a RMS of water-level difference of 8.5 ft.

Chapter D: Properties of Degradation Pathways of Common Organic Compounds in Groundwater (Lawrence 2007) describes and summarizes the properties, degradation pathways, and degradation by-products of VOCs (non-trihalomethane) commonly detected in groundwater contamination sites in the United States. This chapter also is published as U.S. Geological Survey Open-File Report 2006-1338 (Lawrence 2006) and provides abridged information describing the most salient properties and biodegradation of 27 VOCs. This report cross-references common names and synonyms associated with VOCs with the naming conventions supported by the IUPAC. In addition, the report describes basic physical characteristics of those compounds such as Henry's Law constant, water solubility, density, octanol-water partition (log *Kow*), and organic carbon partition (log *Koc*) coefficients. Descriptions and illustrations are provided for natural and laboratory biodegradation rates, chemical by-products, and degradation pathways.

Chapter E: Occurrence of Contaminants in Groundwater (Faye and Green, Jr. 2007) describes the occurrence and distribution of PCE and related contaminants within the Tarawa Terrace aquifer and the Upper Castle Hayne aquifer system at and in the vicinity of the Tarawa Terrace housing area. The occurrence and distribution of benzene, toluene, ethylbenzene, and xylene (BTEX) and related compounds also are briefly described. This report describes details of historical investigations of VOC contamination of groundwater at Tarawa Terrace with emphasis on water-supply wells TT-23, TT-25, and TT-26 (Figure A1). Detailed analyses of concentrations of PCE at monitor wells, at hydrocone sample locations, and at Tarawa Terrace water-supply wells during the period 1991–1993 were sufficient to estimate the mass of PCE remaining in the Tarawa Ter- race and Upper Castle Hayne aquifers. Similar methods were applied to compute the mass of PCE in the unsaturated zone (zone above the water table) at and in the vicinity of ABC One-Hour Cleaners using concentration- depth data determined from soil borings. The total mass of PCE computed in groundwater and within the unsaturated zone equals about 6,000 pounds and equates to a volume of about 430 gallons. This volume represents an average minimum loss rate of PCE to the subsurface at ABC One-Hour Cleaners of about 13 gallons per year for the period 1953–1985.

Chapter F: Simulation of the Fate and Transport of Tetrachloroethylene (PCE) in Groundwater (Faye 2008) describes: (1) the fate and transport of PCE in groundwater from the vicinity of ABC One-Hour Cleaners to the intrusion of PCE into individual water- supply wells (for example, TT-23 and TT-26, Figure A1), and (2) the concentration of PCE in finished water at the Tarawa Terrace WTP computed using a materials mass balance model (simple mixing). The materials mass balance model was used to compute a flow-weighted average PCE concentration, which was assigned as the finished water concentration at the Tarawa Terrace WTP for a specified month. The contaminant fate and trans- port simulation was conducted using the code MT3DMS (Zheng and Wang 1999) integrated with the calibrated groundwater-flow model (Faye and Valenzuela In press 2007) based on the code

MODFLOW-96. Simulated mass loading occurred at a constant rate of 1,200 grams per day using monthly stress periods representing the period January 1953–December 1984. The complete simulation time was represented by the period January 1951–December 1994. Until 1984, the vast majority of simulated PCE-contaminated groundwater was supplied to the Tarawa Terrace WTP by well TT-26. Simulated breakthrough of PCE at well TT-26 at the current MCL of 5 µg/L occurred during January 1957. Corresponding breakthrough at the location of well TT-23 occurred during December 1974; however, well TT-23 was not operational until about August 1984.

Simulated maximum and average PCE concentrations at well TT-26 following breakthrough were 851 µg/L and 414 µg/L, respectively. Corresponding maximum and average concentrations at well TT-23 subsequent to the onset of operations were 274 µg/L and 252 µg/L, respectively. Simulated breakthrough of PCE in finished water at the Tarawa Terrace WTP occurred at the current MCL concentration of 5 µg/L during November 1957 and remained at or above a concentration of 40 µg/L from May 1960 until the termination of pumping at water-supply well TT-26 during February 1985. Computed maximum and average PCE concentrations at the WTP were 183 µg/L and 70 µg/L, respectively, during the period November 1957–February 1985, when well TT-26 was removed from service.

Chapter G: Simulation of Three-Dimensional Multispecies, Multiphase Mass Transport of Tetra- chloroethylene (PCE) and Associated Degradation By-Products (Jang and Aral 2008) provides detailed descriptions and analyses of the development and application of a three-dimensional model (TechFlowMP) capable of simulating multispecies and multiphase (water and vapor) transport of PCE and associated degradation by-products—TCE, 1,2-tDCE, and VC. The development of the TechFLowMP model is described in Jang and Aral (2005) and its application to Tarawa Terrace and vicinity also is published as report MESL-02-07 by the Multimedia Environmental Simulations Laboratory in the School of Civil and Environmental Engineering, Georgia Institute of Technology (Jang and Aral 2007). Simulation results show that the maxi- mum concentrations of PCE degradation by-products, TCE, 1,2-tDCE, and VC, generally ranged between10 µg/L and 100 µg/L in Tarawa Terrace water-supply well TT-26 and between 2 µg/L and 15 µg/L in finished water delivered from the Tarawa Terrace WTP. As part of the degradation by-product simulation using the TechFlowMP model, results were obtained for PCE and PCE degradation by-products dissolved in groundwater and in the vapor phase (above the water table in the unsaturated zone). Analyses of the distribution of vapor- phase PCE and PCE degradation by-products indicate there is potential for vapors to enter buildings at Tarawa Terrace, thereby providing a potential exposure pathway from inhalation of PCE and PCE degradation by-product vapors. At Tarawa Terrace these buildings would include family housing and the elementary school.

Chapter H: Effect of Groundwater Pumping Schedule Variation on Arrival of Tetrachloroethylene (PCE) at Water-Supply Wells and the Water Treatment Plant (Wang and Aral 2008) describes a detailed analysis of the effect of groundwater pumping schedule variation on the arrival of PCE at water-supply wells and at the Tarawa Terrace WTP. Analyses contained in this chapter used the calibrated model parameters described in Chapter C (Faye and Valenzuela In press 2007) and Chapter F (Faye In press 2007b) reports in combination with the groundwater pumping schedule optimization system simulation tool (PSOpS) to assess the influence of unknown and uncertain historical well operations at Tarawa Terrace water-supply wells on PCE concentrations at water-supply wells and at the Tarawa Terrace WTP. This chapter also is published as report MESL-01-07 by the Multimedia Environmental Simulations Laboratory in the School of Civil and Environ- mental Engineering, Georgia Institute of Technology (Wang and Aral 2007). Variation in the optimal pumping schedules indicates that the arrival time of PCE exceeding the current MCL of 5 µg/L at water-supply well TT-26 varied between May 1956 and August 1959. The corresponding arrival time of PCE exceeding the current MCL of 5 µg/L at the Tarawa Terrace WTP varied between December 1956 and June 1960.

Chapter I: Parameter Sensitivity, Uncertainty, and Variability Associated with Model Simulations of Groundwater Flow, Contaminant Fate and Trans- port, and Distribution of Drinking Water (Maslia et al. 2009b) describes the development and application of a probabilistic analysis using Monte Carlo and sequential Gaussian simulation analysis to quantify uncertainty and variability of groundwater hydraulic and transport parameters. These analyses demonstrate quantitatively the high reliability and confidence in results determined using the calibrated parameters from the MODFLOW-96 and MT3DMS models. For example, 95% of Monte Carlo simulations indicated that the current MCL for PCE of 5 µg/L was exceeded in finished water at the Tarawa Terrace WTP between October 1957 and August 1958; the corresponding breakthrough simulated by the calibrated fate and transport model (Chapter F report, Faye 2008) occurred during November 1957.

Appendix G — Summaries of ATSDR's Hadnot Point–Holcomb Boulevard Chapter Reports and Supplemental Information

Summaries of Hadnot Point–Holcomb Boulevard (HP-HB) chapter reports (A, B, C, and D) and supplemental information sections of Chapter A (Supplements 1–8) are described below. Electronic versions of each chapter report and each Chapter A supplement are on the computer disc, read-only memory (CD-ROM) media provided in the back pocket of the Chapter A report. The chapter reports and supplements will be made available on the ATSDR Camp Lejeune Web site at *http://www.atsdr.cdc.gov/sites/lejeune/index.html*.

Chapter A: Summary and Findings (Maslia et al. 2013—this report) provides both a summary of technical findings and detailed analyses of historical reconstruction of groundwater flow, contaminant fate and transport, and distribution of finished water within the Hadnot Point and Holcomb Boulevard water treatment plant (HPWTP and HBWTP, respectively) service areas. Contaminants of concern to the ATSDR health studies described in this report are tetrachloroethylene (PCE), trichloroethylene (TCE), *trans*-1,2-dichloroethylene (1,2-tDCE), vinyl chloride (VC), and benzene. Among the topics covered in this chapter are (1) the purpose of the HPHB study area historical reconstruction analysis, (2) review of contaminants of concern (volatile organic compounds [VOCs])for ATSDR health studies, (3) base-housing information and water-supply data (4) methods for reconstructing historical concentrations in finished water, which include data mining and contaminant-source identification and characterization, (5) application of numerical models and computational tools, (6) historical reconstruction analyses and results for the Hadnot Point Industrial Area (HPIA) and Hadnot Point landfill (HPLF) area, (7) reconstructed concentrations in finished water at the HPWTP, (8) analyses of intermittent transfers of contaminated finished water from the HPWTP to the Holcomb Boulevard family housing areas during years 1972–1985, and (9) selected bounding estimates of historical reconstruction results using sensitivity and uncertainty analyses. Historical reconstruction results summarized in Chapter A provide considerable evidence that concentrations of several contaminants of interest in finished water delivered by the HPWTP substantially exceeded current maximum contaminant levels (MCLs) during all or much of the epidemiological study period of 1968–1985. Included in this chapter report is a comprehensive table listing disparate information sources used to extract pertinent information and data that were needed to develop model input databases used to conduct historical reconstruction analyses. In this report, a CD-ROM is included that contains all chapter reports (A–D), Chapter A supplements (1–8), selected calibrated model input files, and reconstructed (simulated) concentrations at selected water-supply wells and in finished-water at the HPWTP and within the Holcomb Boulevard water-distribution system.

Chapter A–Supplement 1: Descriptions and Characterizations of Data Pertinent to Water-Supply Well Capacities, Histories, and Operations (Sautner et al. 2013a) provides specific documentation for 96 water-supply wells in terms of capacities, histories, and operations that operated during the period 1942–June 2008 and provided groundwater to the HPWTP and HBWTP. Hundreds of documents and reports were reviewed, and numerous discussions with former and current water treatment plant (WTP) operators took place. Notable information was recorded and analyzed for each specific water-supply well to determine the chronological record of a well's operation (well history) starting from the time the well was placed into service and ending with the time the well was abandoned. A listing of the documented historical well operations has been created for each water-supply well and is used to better understand how the Hadnot Point and Holcomb Boulevard water-distribution systems were historically operated. This information and data are used to assist with the reconstruction of historical monthly operations for each water-supply well when little or no information is available. Tabulated well histories from the 96 water-supply wells described in this Supplement 1 report were used to reconstruct historical monthly operations for water-supply wells.

Information contained in Chapter A–Supplement 1 was necessary to conduct groundwater-flow and contaminant fate and transport modeling as part of the historical reconstruction process.

Chapter A–Supplement 2: Development and Application of a Methodology to Characterize Present-Day and Historical Water-Supply Well Operations (Telci et al. 2013) describes a methodology that is developed to estimate the historical monthly volume of groundwater pumped from water-supply wells in the HPHB study area. The available data on operational patterns of water-supply wells consist of the capacities of the wells, the operational state of the wells on a daily basis, and the volume of water delivered to the WTPs on a daily and monthly bases. The overall operational timeframe of the Hadnot Point and Holcomb Boulevard water-distribution systems is divided into two periods: "present-day" (1998–2008) and "Reconstruction" (1942–1997). In Supplement 2, the present-day period is defined as the time during which daily water-supply well operational data are available. The reconstruction period is defined as the time when water-supply well operational data are limited or unavailable. The methodology is an efficient and effective way of integrating available data for present-day conditions (1998–2008) with the prediction process for the historical years (1942–1998). Results demonstrate that historical estimates of water-supply well operations using this methodology are reasonable, and therefore, can be readily applied to groundwater-flow and contaminant fate and transport model simulations for the HPHB study area.

Chapter A–Supplement 3: Descriptions and Characterizations of Water-Level Data and Groundwater Flow for the Brewster Boulevard and Castle Hayne Aquifer Systems and the Tarawa Terrace Aquifer (Faye et al. 2013) provides summaries of the results of analyses of groundwater-level data and describes corresponding elements of groundwater flow such as vertical hydraulic gradients useful for groundwater-flow model calibration. Field data and theoretical concepts indicate that potentiometric surfaces within the study area are shown to resemble to a large degree a subdued replica of surface topography. Consequently, precipitation that infiltrates to the water table flows laterally from highland to lowland areas and eventually discharges to streams such as Northeast and Wallace Creeks and New River. Vertically downward hydraulic gradients occur in highland areas, resulting in the transfer of groundwater from shallow relatively unconfined aquifers to underlying confined or semi-confined aquifers. Conversely, in the vicinity of large streams such as Wallace and Frenchs Creeks, diffuse upward leakage occurs from underlying confined or semi-confined aquifers. Point water-level data indicating water-table altitudes, water-table altitudes estimated using a regression equation, and estimates of stream levels determined from a digital elevation model (DEM) and topographic maps were used to estimate a predevelopment water-table surface in the study area. Approximate flow lines along hydraulic gradients are shown on a predevelopment potentiometric surface map and extend from highland areas where potentiometric levels are greatest toward streams such as Northeast and Wallace Creeks. The distribution of potentiometric levels and corresponding groundwater-flow directions conform closely to related descriptions of the conceptual model.

Chapter A–Supplement 4: Simulation of Three-Dimensional Groundwater Flow (Suárez-Soto et al. 2013**)** provides detailed analyses of groundwater flow based on data and model simulations for the HPHB study area. Predevelopment (steady state) and transient three-dimensional groundwater-flow models were developed using MODFLOW-2005 (Harbaugh 2005). Multiple groundwater-flow models were necessary to describe both predevelopment and transient conditions, which focused on the HPIA and HPLF subdomain areas. The predevelopment model is characterized by a uniform finite-difference grid consisting of 300-ft × 300-ft cells. Transient models—one for the HPIA and one for the HPLF subdomain areas—were characterized by variably spaced finite-difference grids consisting of cells ranging in size from 300 ft × 300 ft to 50 ft × 50 ft—the 50-ft × 50-ft cells being necessary to meet fate and transport numerical modeling requirements. The variably spaced grid models were used to simulate local transient conditions and contaminant fate and transport in the HPIA and HPLF subdomain areas (Jones et al. 2013). All models consist of seven layers representing the Brewster Boulevard and Castle Hayne aquifer systems and Tarawa Terrace aquifer described by Faye (2012). The predevelopment calibration represents long-term average conditions, and transient simulations represent conditions occurring as a consequence of water-supply well operations. The 798 monthly stress periods were used to represent transient conditions during the period January 1942–June 2008. Model cells coincident with water-supply wells were assigned reconstructed pumpage values based on the methodology described in Telci et al. (2013).

Chapter A–Supplement 5: Theory, Development, and Application of Linear Control Model Methodology to Reconstruct Historical Contaminant Concentrations at Selected Water-Supply Wells (Guan et al. 2013) describes the development of an alternate modeling approach using a linear state-space representation of a contaminated aquifer system, designated in this Supplement 5 report as a linear control model (LCM). The LCM is used to reconstruct historical concentrations at water-supply wells. The LCM approach is substantially less resource-intensive and requires less effort in terms of model parameter identification and calibration than traditional (numerical) groundwater-flow and contaminant fate and transport modeling approaches. The mathematical development for the LCM approach is described in detail and then verified by using synthesized data from the numerical groundwater model developed for the Tarawa Terrace study area (Faye and Green 2007; Faye and Valenzuela 2007). The LCM (TechControl) is then applied to the HPLF to reconstruct the history of chlorinated solvent contamination at water-supply well HP-651; the well was shut down in early 1985 when chlorinated solvents were detected in the well. The LCM approach utilizes the historical operating schedule of water-supply well HP-651 in conjunction with post-shutdown (1985–2004) measured contaminant concentrations in groundwater to reconstruct the history of contaminants in the water-supply well prior to 1985.

Chapter A–Supplement 6: Source Characterization and Simulation of Fate and Transport of Selected Volatile Organic Compounds in the Vicinities of the Hadnot Point Industrial Area and Landfill (Jones et al. 2013) describes reconstruction (simulation) of historical concentrations of tetrachloroethylene (PCE), trichloroethylene (TCE), and benzene in finished water in the vicinities of the HPIA and the HPLF area. A contaminant fate and transport model was used to simulate contaminant migration from source locations through the groundwater system and to estimate monthly mean contaminant concentrations in water withdrawn from production wells in the vicinity of the HPIA and the HPLF area. The monthly mean contaminant concentrations were subsequently input to a mixing model to quantify monthly mean concentrations of the contaminants in finished water that supplied the housing areas and other facilities served by the HPWTP. Review of available records indicates that the earliest production wells began operation in the early 1940s, and contaminants leaked into the subsurface as early as the late 1940s. Concentrations of the contaminants were simulated using monthly intervals for the entire period of production-well operation from January 1942 through June 2008, the date of the most recently available data. The applied and calibrated fate and transport models, described in Supplement 6, were based on the groundwater-flow models that are described in Suárez-Soto et al. (2013).

Chapter A–Supplement 7: Source Characterization and Simulation of the Migration of Light Nonaqueous Phase Liquids (LNAPLs) in the Vicinity of the Hadnot Point Industrial Area (Jang et al. 2013) describes (1) the migration potential and distribution of LNAPLs for several hypothetical scenarios, (2) the estimation of LNAPL volume based on field measurements of LNAPL thicknesses in the HPIA, and (3) the transport of dissolved contaminants within the HPIA. The analysis was carried out by using complex modeling of multiphase flow through pore spaces. The analysis of LNAPL flow delineated the migration and expansion of free-phase LNAPL plumes and the spatial variation in LNAPL saturation in the modeling domain with time. Based on available field data of LNAPL thickness from observation wells, the mass distribution and volume of LNAPLs in the subsurface at the HPIA were estimated using the TechNAPLVol model code. The computed LNAPL volume ranged from approximately 0.9 to 1.6 million gallons. The mass distribution (or saturation profile) of LNAPLs in the subsurface was used as the contaminant-source input for a fate and transport analysis of dissolved LNAPL components in groundwater at the HPIA. The TechFlowMP multiphase flow and multispecies contaminant transport model was used to simulate the dissolution and subsequent fate and transport of dissolved-phase benzene and xylenes in the HPIA.

Chapter A–Supplement 8: Field Tests, Data Analyses, and Simulation of the Distribution of Drinking Water with Emphasis on Intermittent Transfers of Drinking Water Between the Hadnot Point and Holcomb Boulevard Water-Distribution Systems (Sautner et al. 2013b) provides detailed information on the design of field tests conducted during 2004 to ascertain water-distribution system properties for Hadnot Point and Holcomb Boulevard. By using information and data gathered during the field tests, along with data provided by Camp Lejeune water utility staff, an extended period simulation model for water-distribution system hydraulics and water-quality dynamics was developed and calibrated using EPANET 2 (Rossman 2000). The calibrated EPANET 2 model of the Holcomb Boulevard water-distribution system was used in conjunction with Markov Chain analysis to estimate the concentrations of VOCs during the period 1972–1985. During this time, contaminated Hadnot Point finished water was intermittently provided to the Holcomb Boulevard housing areas. Within the Holcomb Boulevard housing area, except for the 8-day period of January 28–February 4, 1985, when the HBWTP was out of service, only TCE routinely exceeded its MCL during intermittent periods of connection with the Hadnot Point water-distribution system.

Chapter B: Geohydrologic Framework of the Brewster Boulevard and Castle Hayne Aquifer Systems and the Tarawa Terrace Aquifer (Faye 2012) provides detailed analyses and interpretations of well, borehole, and geophysical data used to develop the geohydrologic framework of the Brewster Boulevard and Castle Hayne aquifer systems and the Tarawa Terrace aquifer. The geometry and lithology of seven aquifers and related confining units are described in a series of sections, maps, and tables. Hydraulic characteristics, including hydraulic conductivity, transmissivity, storativity, and leakance parameters, are tabulated for several geohydrologic units. Where data density is sufficient, maps showing spatial distributions of hydraulic conductivity are included.

Chapter C: Occurrence of Selected Contaminants in Groundwater at Installation Restoration Program Sites (Faye et al. 2010) provides detailed accounting of the known occurrences of contaminants of concern (e.g., PCE and TCE) and their related degradation products in groundwater at selected Installation Restoration Program (IRP) sites within the HPWTP and HBWTB service areas at U.S. Marine Corp Base (USMCB) Camp Lejeune. These sites were identified by the Department of the Navy under the auspices of the Comprehensive Environmental Response, Compensation, and Liability Act (CERCLA). Concentrations of these constituents in water-supply wells and in finished water of the HPWTP and HBWTP also are described. Collectively, these data provide most of the base of information necessary to construct the fate and transport models used to reconstruct (simulate) historical concentrations of contaminants within the water-distribution systems serviced by the HPWTP and HBWTP. Additionally, this report provides a detailed summary of historical information useful to ongoing and future exposure and health studies at USMCB Camp Lejeune, including a chronology of residential housing areas served by the HPWTP and HBWTP, annual operational capacities of the WTPs, locations and construction details of water-supply wells and water-quality monitor wells, and a summary and discussion of relevant environmental investigations at 18 IRP sites within the study area where contaminated groundwater occurred or was thought to have occurred.

Chapter D: Occurrence of Selected Contaminants in Groundwater at Above-Ground and Underground Storage Tank Sites (Faye et al. 2012) provides summaries of results of investigations at 64 designated Resource Conservation and Recovery Act (RCRA) study areas and emphasizes the occurrence and distribution of benzene, toluene, ethylbenzene, and xylenes (BTEX) components within groundwater of the areas served by the HPWTP and HBWTP. The volume of BTEX mass removed from the subsurface during remediation at selected locations within the service areas also is summarized. Results of analyses of samples collected in monitor wells at several CERCLA investigation study areas co-located with RCRA areas are also included herein. Concentrations of chlorinated alkenes such as PCE and TCE are also described where plumes of BTEX and chlorinated alkenes are mixed at several locations.

Appendix H1 — Tarawa Terrace Water Treatment Plant Reconstructed (Simulated) Mean Monthly Finished Water Concentrations for Single-Specie Tetrachloroethylene (PCE) Using MT3DMS Model and for Multispecies, Multiphase PCE (Trichloroethylene [TCE], *trans*-1,2-Dichlorothylene [1,2-*t*DCE], and Vinyl Chloride [VC]) Using TechFlowMP Model

Appendix A2. Simulated tetrachloroethylene and its degradation by-products in finished water, Tarawa Terrace water treatment plant, January 1951–March 1987.[1]

[PCE, tetrachloroethylene; µg/L, microgram per liter; 1,2-tDCE, *trans*-1,2-dichloroethylene; TCE, trichloroethylene; VC, vinyl chloride; WTP, water treatment plant]

Stress period	Month and year	Single specie using MT3DMS model[2]	Multispecies, multiphase using TechFlowMP model[3]			
		[4]PCE, in µg/L	[5]PCE, in µg/L	[5]1,2-tDCE, in µg/L	[5]TCE, in µg/L	[5]VC, in µg/L
1–12	Jan–Dec 1951	WTP not operating	WTP not operating	WTP not operating	WTP not operating	WTP not operating
13	Jan 1952	0.00	0.00	0.00	0.00	0.00
14	Feb 1952	0.00	0.00	0.00	0.00	0.00
15	Mar 1952	0.00	0.00	0.00	0.00	0.00
16	Apr 1952	0.00	0.00	0.00	0.00	0.00
17	May 1952	0.00	0.00	0.00	0.00	0.00
18	June 1952	0.00	0.00	0.00	0.00	0.00
19	July 1952	0.00	0.00	0.00	0.00	0.00
20	Aug 1952	0.00	0.00	0.00	0.00	0.00
21	Sept 1952	0.00	0.00	0.00	0.00	0.00
22	Oct 1952	0.00	0.00	0.00	0.00	0.00
23	Nov 1952	0.00	0.00	0.00	0.00	0.00
24	Dec 1952	0.00	0.00	0.00	0.00	0.00
25	Jan 1953	0.00	0.00	0.00	0.00	0.00
26	Feb 1953	0.00	0.00	0.00	0.00	0.00
27	Mar 1953	0.00	0.00	0.00	0.00	0.00
28	Apr 1953	0.00	0.00	0.00	0.00	0.00
29	May 1953	0.00	0.00	0.00	0.00	0.00
30	June 1953	0.00	0.00	0.00	0.00	0.00
31	July 1953	0.00	0.00	0.00	0.00	0.00
32	Aug 1953	0.00	0.00	0.00	0.00	0.00
33	Sept 1953	0.00	0.00	0.00	0.00	0.00
34	Oct 1953	0.00	0.00	0.00	0.00	0.00
35	Nov 1953	0.00	0.00	0.00	0.00	0.00
36	Dec 1953	0.00	0.00	0.00	0.00	0.00
37	Jan 1954	0.00	0.00	0.00	0.00	0.00
38	Feb 1954	0.00	0.00	0.00	0.00	0.00
39	Mar 1954	0.00	0.00	0.00	0.00	0.00
40	Apr 1954	0.00	0.00	0.00	0.00	0.00
41	May 1954	0.00	0.00	0.00	0.00	0.00
42	June 1954	0.00	0.00	0.00	0.00	0.00
43	July 1954	0.00	0.00	0.00	0.00	0.00
44	Aug 1954	0.00	0.00	0.00	0.00	0.00
45	Sept 1954	0.00	0.00	0.00	0.00	0.00
46	Oct 1954	0.00	0.00	0.00	0.00	0.00
47	Nov 1954	0.00	0.00	0.00	0.00	0.00
48	Dec 1954	0.00	0.00	0.00	0.00	0.00

Appendix A2. Simulated tetrachloroethylene and its degradation by-products in finished water, Tarawa Terrace water treatment plant, January 1951–March 1987[1].—Continued

[PCE, tetrachloroethylene; µg/L, microgram per liter; 1,2-tDCE, *trans*-1,2-dichloroethylene; TCE, trichloroethylene; VC, vinyl chloride; WTP, water treatment plant]

Stress-period	Month and year	Single specie using MT3DMS model[2]	Multispecies, multiphase using TechFlowMP model[3]			
		[4]PCE, in µg/L	[5]PCE, in µg/L	[5]1,2-tDCE, in µg/L	[5]TCE, in µg/L	[5]VC, in µg/L
49	Jan 1955	0.00	0.00	0.00	0.00	0.01
50	Feb 1955	0.00	0.00	0.01	0.00	0.01
51	Mar 1955	0.00	0.01	0.01	0.00	0.01
52	Apr 1955	0.00	0.01	0.01	0.00	0.02
53	May 1955	0.00	0.01	0.01	0.00	0.02
54	June 1955	0.01	0.01	0.02	0.00	0.03
55	July 1955	0.01	0.02	0.03	0.00	0.03
56	Aug 1955	0.01	0.03	0.03	0.00	0.04
57	Sept 1955	0.02	0.04	0.04	0.00	0.05
58	Oct 1955	0.03	0.05	0.05	0.00	0.07
59	Nov 1955	0.04	0.06	0.07	0.00	0.08
60	Dec 1955	0.06	0.08	0.08	0.01	0.10
61	Jan 1956	0.08	0.11	0.10	0.01	0.12
62	Feb 1956	0.10	0.14	0.12	0.01	0.14
63	Mar 1956	0.13	0.17	0.15	0.01	0.17
64	Apr 1956	0.17	0.22	0.18	0.01	0.20
65	May 1956	0.23	0.27	0.21	0.02	0.23
66	June 1956	0.29	0.33	0.25	0.02	0.26
67	July 1956	0.36	0.40	0.29	0.02	0.30
68	Aug 1956	0.46	0.49	0.33	0.03	0.34
69	Sept 1956	0.57	0.59	0.38	0.03	0.39
70	Oct 1956	0.70	0.70	0.44	0.04	0.44
71	Nov 1956	0.85	0.83	0.50	0.05	0.49
72	Dec 1956	1.04	0.97	0.57	0.06	0.55
73	Jan 1957	1.25	1.14	0.64	0.06	0.61
74	Feb 1957	1.47	1.33	0.72	0.07	0.68
75	Mar 1957	1.74	1.52	0.79	0.08	0.74
76	Apr 1957	2.04	1.75	0.88	0.10	0.81
77	May 1957	2.39	2.00	0.97	0.11	0.89
78	June 1957	2.77	2.28	1.08	0.12	0.97
79	July 1957	3.21	2.59	1.18	0.14	1.05
80	Aug 1957	3.69	2.93	1.29	0.16	1.13
81	Sept 1957	4.21	3.30	1.41	0.17	1.23
82	Oct 1957	4.79	3.69	1.53	0.19	1.32
83	Nov 1957	5.41	4.13	1.66	0.22	1.41
84	Dec 1957	6.10	4.59	1.80	0.24	1.51

Appendix A2. Simulated tetrachloroethylene and its degradation by-products in finished water, Tarawa Terrace water treatment plant, January 1951–March 1987[1].—Continued

[PCE, tetrachloroethylene; µg/L, microgram per liter; 1,2-tDCE, *trans*-1,2-dichloroethylene; TCE, trichloroethylene; VC, vinyl chloride; WTP, water treatment plant]

Stress period	Month and year	Single specie using MT3DMS model[2]	Multispecies, multiphase using TechFlowMP model[3]			
		[4]PCE, in µg/L	[5]PCE, in µg/L	[5]1,2 tDCE, in µg/L	[5]TCE, in µg/L	[5]VC, in µg/L
85	Jan 1958	6.86	5.11	1.94	0.26	1.62
86	Feb 1958	7.60	5.65	2.09	0.29	1.72
87	Mar 1958	8.47	6.17	2.22	0.31	1.81
88	Apr 1958	9.37	6.79	2.38	0.34	1.92
89	May 1958	10.37	7.41	2.53	0.37	2.02
90	June 1958	11.39	8.10	2.70	0.41	2.13
91	July 1958	12.91	9.09	2.96	0.45	2.32
92	Aug 1958	14.12	9.88	3.14	0.49	2.44
93	Sept 1958	15.35	10.73	3.33	0.53	2.56
94	Oct 1958	16.69	11.58	3.52	0.57	2.68
95	Nov 1958	18.03	12.52	3.72	0.61	2.81
96	Dec 1958	19.49	13.46	3.92	0.66	2.94
97	Jan 1959	20.97	14.48	4.13	0.71	3.07
98	Feb 1959	22.35	15.54	4.34	0.76	3.21
99	Mar 1959	23.92	16.54	4.54	0.80	3.33
100	Apr 1959	25.49	17.70	4.77	0.85	3.48
101	May 1959	27.15	18.84	4.99	0.91	3.61
102	June 1959	28.81	20.09	5.23	0.96	3.77
103	July 1959	30.56	21.34	5.46	1.02	3.91
104	Aug 1959	32.36	22.66	5.69	1.08	4.05
105	Sept 1959	34.14	24.01	5.93	1.14	4.19
106	Oct 1959	36.01	25.35	6.16	1.20	4.32
107	Nov 1959	37.85	26.77	6.40	1.27	4.46
108	Dec 1959	39.78	28.18	6.64	1.33	4.60
109	Jan 1960	41.86	29.67	6.88	1.40	4.74
110	Feb 1960	43.85	31.17	7.12	1.46	4.86
111	Mar 1960	46.03	32.58	7.33	1.52	4.97
112	Apr 1960	48.15	34.16	7.57	1.59	5.10
113	May 1960	50.37	35.67	7.79	1.66	5.21
114	June 1960	52.51	37.24	8.03	1.73	5.33
115	July 1960	54.74	38.79	8.26	1.80	5.45
116	Aug 1960	56.96	40.45	8.51	1.87	5.59
117	Sept 1960	59.09	42.13	8.76	1.94	5.73
118	Oct 1960	61.30	43.80	9.02	2.02	5.86
119	Nov 1960	63.42	45.57	9.28	2.09	6.01
120	Dec 1960	65.61	47.31	9.54	2.17	6.15

Appendix A2. Simulated tetrachloroethylene and its degradation by-products in finished water, Tarawa Terrace water treatment plant, January 1951–March 1987[1].—Continued

[PCE, tetrachloroethylene; µg/L, microgram per liter; 1,2-tDCE, *trans*-1,2-dichloroethylene; TCE, trichloroethylene; VC, vinyl chloride; WTP, water treatment plant]

Stress period	Month and year	Single specie using MT3DMS model[2]	Multispecies, multiphase using TechFlowMP model[3]			
		[4]PCE, in µg/L	[5]PCE, in µg/L	[5]1,2-tDCE, in µg/L	[5]TCE, in µg/L	[5]VC, in µg/L
121	Jan 1961	67.69	49.15	9.82	2.25	6.30
122	Feb 1961	69.54	51.03	10.10	2.33	6.46
123	Mar 1961	71.56	52.73	10.35	2.41	6.61
124	Apr 1961	73.49	54.69	10.64	2.49	6.77
125	May 1961	75.49	56.57	10.92	2.58	6.92
126	June 1961	77.39	58.53	11.20	2.66	7.07
127	July 1961	79.36	60.43	11.46	2.75	7.22
128	Aug 1961	81.32	62.42	11.74	2.83	7.36
129	Sept 1961	83.19	64.40	12.01	2.92	7.51
130	Oct 1961	85.11	66.32	12.27	3.00	7.64
131	Nov 1961	86.95	68.33	12.55	3.09	7.79
132	Dec 1961	88.84	70.28	12.80	3.17	7.92
133	Jan 1962	60.88	47.74	8.63	2.15	5.32
134	Feb 1962	62.10	49.86	9.00	2.25	5.56
135	Mar 1962	62.94	51.28	9.17	2.31	5.64
136	Apr 1962	63.59	52.37	9.25	2.36	5.67
137	May 1962	64.17	53.18	9.28	2.39	5.66
138	June 1962	64.70	53.88	9.28	2.41	5.63
139	July 1962	65.23	54.48	9.28	2.43	5.60
140	Aug 1962	65.74	55.06	9.26	2.45	5.56
141	Sept 1962	66.22	55.59	9.24	2.46	5.52
142	Oct 1962	66.71	56.07	9.22	2.48	5.47
143	Nov 1962	67.18	56.54	9.19	2.49	5.42
144	Dec 1962	67.65	56.97	9.16	2.50	5.38
145	Jan 1963	68.06	57.40	9.13	2.51	5.33
146	Feb 1963	68.39	57.78	9.09	2.52	5.28
147	Mar 1963	68.73	58.11	9.06	2.53	5.24
148	Apr 1963	69.03	58.49	9.02	2.54	5.20
149	May 1963	69.33	58.81	8.98	2.55	5.15
150	June 1963	69.62	59.14	8.94	2.56	5.11
151	July 1963	69.90	59.42	8.90	2.57	5.06
152	Aug 1963	70.17	59.70	8.86	2.57	5.02
153	Sept 1963	70.43	59.97	8.82	2.57	4.98
154	Oct 1963	70.69	60.21	8.78	2.58	4.94
155	Nov 1963	70.93	60.45	8.74	2.58	4.90
156	Dec 1963	71.17	60.67	8.70	2.59	4.86

Appendix A2. Simulated tetrachloroethylene and its degradation by-products in finished water, Tarawa Terrace water treatment plant, January 1951–March 1987[1].—Continued

[PCE, tetrachloroethylene; µg/L, microgram per liter; 1,2-tDCE, *trans*-1,2-dichloroethylene; TCE, trichloroethylene; VC, vinyl chloride; WTP, water treatment plant]

Stress period	Month and year	Single specie using MT3DMS model[2]	Multispecies, multiphase using TechFlowMP model[3]			
		[4]PCE, in µg/L	[5]PCE, in µg/L	[5]1,2 tDCE, in µg/L	[5]TCE, in µg/L	[5]VC, in µg/L
157	Jan 1964	71.40	60.89	8.67	2.59	4.83
158	Feb 1964	63.77	54.39	7.69	2.31	4.27
159	Mar 1964	63.95	54.42	7.58	2.30	4.17
160	Apr 1964	64.08	54.43	7.50	2.29	4.10
161	May 1964	64.19	54.36	7.42	2.29	4.04
162	June 1964	64.27	54.29	7.35	2.28	3.98
163	July 1964	64.34	54.21	7.28	2.27	3.93
164	Aug 1964	64.39	54.14	7.22	2.26	3.88
165	Sept 1964	64.43	54.06	7.16	2.26	3.84
166	Oct 1964	64.47	53.99	7.10	2.25	3.79
167	Nov 1964	64.49	53.92	7.05	2.24	3.75
168	Dec 1964	64.50	53.85	7.00	2.24	3.72
169	Jan 1965	64.50	53.78	6.95	2.23	3.68
170	Feb 1965	64.49	53.72	6.90	2.23	3.65
171	Mar 1965	64.47	53.64	6.86	2.22	3.61
172	Apr 1965	64.45	53.59	6.82	2.22	3.58
173	May 1965	64.42	53.52	6.78	2.21	3.55
174	June 1965	64.38	53.47	6.74	2.21	3.52
175	July 1965	64.33	53.40	6.70	2.20	3.50
176	Aug 1965	64.27	53.34	6.66	2.20	3.47
177	Sept 1965	64.20	53.27	6.63	2.19	3.44
178	Oct 1965	64.13	53.20	6.59	2.19	3.42
179	Nov 1965	64.05	53.14	6.56	2.18	3.40
180	Dec 1965	63.97	53.07	6.53	2.18	3.37
181	Jan 1966	63.88	53.00	6.50	2.17	3.35
182	Feb 1966	63.79	52.93	6.47	2.17	3.33
183	Mar 1966	63.68	52.84	6.44	2.16	3.31
184	Apr 1966	63.57	52.78	6.41	2.16	3.29
185	May 1966	63.46	52.70	6.38	2.15	3.27
186	June 1966	63.34	52.63	6.35	2.15	3.25
187	July 1966	63.21	52.54	6.33	2.14	3.23
188	Aug 1966	63.08	52.46	6.30	2.14	3.21
189	Sept 1966	62.94	52.38	6.27	2.13	3.20
190	Oct 1966	62.80	52.28	6.25	2.13	3.18
191	Nov 1966	62.65	52.20	6.22	2.12	3.16
192	Dec 1966	62.50	52.11	6.19	2.12	3.14

Appendix A2. Simulated tetrachloroethylene and its degradation by-products in finished water, Tarawa Terrace water treatment plant, January 1951–March 1987[1].—Continued

[PCE, tetrachloroethylene; µg/L, microgram per liter; 1,2-tDCE, *trans*-1,2-dichloroethylene; TCE, trichloroethylene; VC, vinyl chloride; WTP, water treatment plant]

Stress-period	Month and year	Single specie using MT3DMS model[2]	Multispecies, multiphase using TechFlowMP model[3]			
		[4]PCE, in µg/L	[5]PCE, in µg/L	[5]1,2-tDCE, in µg/L	[5]TCE, in µg/L	[5]VC, in µg/L
193	Jan 1967	62.25	52.02	6.17	2.11	3.13
194	Feb 1967	61.99	51.90	6.14	2.11	3.11
195	Mar 1967	61.67	51.76	6.11	2.10	3.09
196	Apr 1967	61.35	51.61	6.08	2.09	3.07
197	May 1967	61.02	51.43	6.04	2.08	3.05
198	June 1967	60.69	51.23	6.00	2.07	3.03
199	July 1967	60.37	51.02	5.96	2.06	3.00
200	Aug 1967	60.05	50.79	5.92	2.05	2.98
201	Sept 1967	59.74	50.57	5.87	2.04	2.95
202	Oct 1967	59.43	50.34	5.83	2.03	2.92
203	Nov 1967	59.13	50.11	5.79	2.02	2.90
204	Dec 1967	58.83	49.89	5.75	2.01	2.87
205	Jan 1968	58.41	49.66	5.70	2.00	2.85
206	Feb 1968	57.95	49.40	5.66	1.99	2.82
207	Mar 1968	57.43	49.10	5.60	1.97	2.79
208	Apr 1968	56.94	48.77	5.55	1.96	2.76
209	May 1968	56.45	48.43	5.49	1.94	2.73
210	June 1968	55.98	48.07	5.43	1.93	2.69
211	July 1968	55.49	47.67	5.36	1.91	2.65
212	Aug 1968	55.02	47.26	5.29	1.89	2.61
213	Sept 1968	54.58	46.84	5.23	1.87	2.57
214	Oct 1968	54.13	46.43	5.16	1.85	2.54
215	Nov 1968	53.71	46.03	5.10	1.84	2.50
216	Dec 1968	53.28	45.63	5.04	1.82	2.46
217	Jan 1969	53.07	45.24	4.98	1.80	2.43
218	Feb 1969	52.97	44.91	4.93	1.79	2.40
219	Mar 1969	52.94	44.64	4.88	1.78	2.37
220	Apr 1969	52.93	44.47	4.86	1.77	2.35
221	May 1969	52.93	44.32	4.83	1.76	2.34
222	June 1969	52.92	44.20	4.81	1.76	2.32
223	July 1969	52.90	44.09	4.79	1.75	2.31
224	Aug 1969	52.86	44.01	4.78	1.75	2.30
225	Sept 1969	52.81	43.92	4.77	1.75	2.29
226	Oct 1969	52.75	43.83	4.76	1.74	2.29
227	Nov 1969	55.19	45.75	4.97	1.82	2.38
228	Dec 1969	55.19	45.96	5.01	1.83	2.42

Appendix A2. Simulated tetrachloroethylene and its degradation by-products in finished water, Tarawa Terrace water treatment plant, January 1951–March 1987[1].—Continued

[PCE, tetrachloroethylene; µg/L, microgram per liter; 1,2-tDCE, *trans*-1,2-dichloroethylene; TCE, trichloroethylene; VC, vinyl chloride; WTP, water treatment plant]

Stress period	Month and year	Single specie using MT3DMS model[2]	Multispecies, multiphase using TechFlowMP model[3]			
		[4]PCE, in µg/L	[5]PCE, in µg/L	[5]1,2 tDCE, in µg/L	[5]TCE, in µg/L	[5]VC, in µg/L
229	Jan 1970	55.01	46.05	5.03	1.84	2.43
230	Feb 1970	54.79	46.03	5.03	1.84	2.43
231	Mar 1970	54.49	45.94	5.03	1.83	2.43
232	Apr 1970	54.20	45.84	5.03	1.83	2.44
233	May 1970	53.90	45.70	5.01	1.82	2.44
234	June 1970	53.61	45.54	5.00	1.82	2.43
235	July 1970	53.32	45.37	4.98	1.81	2.43
236	Aug 1970	53.04	45.20	4.96	1.80	2.42
237	Sept 1970	52.78	45.00	4.94	1.79	2.41
238	Oct 1970	52.53	44.79	4.91	1.78	2.40
239	Nov 1970	52.29	44.58	4.89	1.78	2.39
240	Dec 1970	52.05	44.37	4.87	1.77	2.38
241	Jan 1971	51.96	44.17	4.84	1.76	2.37
242	Feb 1971	51.93	43.99	4.82	1.75	2.35
243	Mar 1971	51.95	43.86	4.80	1.74	2.34
244	Apr 1971	51.99	43.76	4.79	1.74	2.34
245	May 1971	52.03	43.66	4.78	1.74	2.33
246	June 1971	52.08	43.60	4.78	1.73	2.33
247	July 1971	52.12	43.53	4.77	1.73	2.33
248	Aug 1971	52.16	43.47	4.77	1.73	2.33
249	Sept 1971	52.20	43.41	4.77	1.73	2.33
250	Oct 1971	52.23	43.35	4.77	1.72	2.33
251	Nov 1971	52.26	43.31	4.77	1.72	2.33
252	Dec 1971	52.29	43.26	4.77	1.72	2.34
253	Jan 1972	49.34	41.02	4.53	1.63	2.22
254	Feb 1972	49.01	40.49	4.44	1.61	2.17
255	Mar 1972	48.68	40.01	4.37	1.58	2.13
256	Apr 1972	48.40	39.51	4.30	1.56	2.09
257	May 1972	48.14	39.03	4.24	1.54	2.06
258	June 1972	47.90	38.55	4.17	1.52	2.02
259	July 1972	47.67	38.11	4.11	1.50	1.98
260	Aug 1972	47.45	37.68	4.05	1.48	1.95
261	Sept 1972	47.25	37.26	3.99	1.46	1.92
262	Oct 1972	47.05	36.88	3.94	1.45	1.89
263	Nov 1972	46.87	36.51	3.89	1.43	1.86
264	Dec 1972	46.69	36.15	3.85	1.42	1.84

Appendix A2. Simulated tetrachloroethylene and its degradation by-products in finished water, Tarawa Terrace water treatment plant, January 1951–March 1987[1].—Continued

[PCE, tetrachloroethylene; µg/L, microgram per liter; 1,2-tDCE, *trans*-1,2-dichloroethylene; TCE, trichloroethylene; VC, vinyl chloride; WTP, water treatment plant]

Stress-period	Month and year	Single specie using MT3DMS model[2]	Multispecies, multiphase using TechFlowMP model[3]			
		[4]PCE, in µg/L	[5]PCE, in µg/L	[5]1,2-tDCE, in µg/L	[5]TCE, in µg/L	[5]VC, in µg/L
265	Jan 1973	54.28	41.48	4.40	1.62	2.10
266	Feb 1973	54.19	42.32	4.57	1.67	2.21
267	Mar 1973	53.98	42.49	4.60	1.68	2.23
268	Apr 1973	53.76	42.42	4.60	1.68	2.24
269	May 1973	53.52	42.25	4.59	1.67	2.24
270	June 1973	53.30	42.05	4.58	1.66	2.25
271	July 1973	53.08	41.78	4.56	1.65	2.24
272	Aug 1973	52.87	41.53	4.53	1.64	2.23
273	Sept 1973	52.68	41.27	4.51	1.63	2.22
274	Oct 1973	52.51	41.01	4.48	1.62	2.21
275	Nov 1973	52.35	40.75	4.45	1.61	2.20
276	Dec 1973	52.20	40.48	4.42	1.60	2.19
277	Jan 1974	52.43	40.22	4.40	1.59	2.17
278	Feb 1974	52.82	40.13	4.39	1.59	2.17
279	Mar 1974	53.39	40.10	4.38	1.58	2.16
280	Apr 1974	53.99	40.20	4.40	1.59	2.17
281	May 1974	54.63	40.35	4.43	1.60	2.18
282	June 1974	55.25	40.59	4.48	1.61	2.21
283	July 1974	55.90	40.82	4.52	1.62	2.24
284	Aug 1974	56.53	41.08	4.57	1.63	2.27
285	Sept 1974	57.10	41.35	4.62	1.64	2.31
286	Oct 1974	57.70	41.61	4.68	1.65	2.34
287	Nov 1974	58.30	41.91	4.74	1.67	2.39
288	Dec 1974	58.92	42.19	4.81	1.68	2.43
289	Jan 1975	61.00	43.76	5.02	1.74	2.55
290	Feb 1975	61.24	43.90	5.06	1.75	2.59
291	Mar 1975	61.41	44.03	5.11	1.75	2.63
292	Apr 1975	61.57	44.18	5.16	1.76	2.68
293	May 1975	61.72	44.29	5.20	1.77	2.71
294	June 1975	61.88	44.38	5.24	1.77	2.75
295	July 1975	62.05	44.45	5.28	1.77	2.78
296	Aug 1975	62.25	44.52	5.31	1.78	2.81
297	Sept 1975	62.46	44.57	5.34	1.78	2.83
298	Oct 1975	62.69	44.62	5.36	1.78	2.85
299	Nov 1975	62.92	44.69	5.39	1.78	2.87
300	Dec 1975	63.18	44.74	5.41	1.78	2.89

Appendix A2. Simulated tetrachloroethylene and its degradation by-products in finished water, Tarawa Terrace water treatment plant, January 1951–March 1987[1].—Continued

[PCE, tetrachloroethylene; µg/L, microgram per liter; 1,2-tDCE, *trans*-1,2-dichloroethylene; TCE, trichloroethylene; VC, vinyl chloride; WTP, water treatment plant]

Stress period	Month and year	Single specie using MT3DMS model[2]	Multispecies, multiphase using TechFlowMP model[3]			
		[4]PCE, in µg/L	[5]PCE, in µg/L	[5]1,2 tDCE, in µg/L	[5]TCE, in µg/L	[5]VC, in µg/L
301	Jan 1976	73.96	51.53	6.24	2.06	3.34
302	Feb 1976	74.94	53.43	6.62	2.15	3.60
303	Mar 1976	75.97	54.44	6.80	2.20	3.72
304	Apr 1976	76.97	55.38	6.99	2.24	3.85
305	May 1976	78.00	56.21	7.16	2.28	3.98
306	June 1976	79.02	57.07	7.34	2.32	4.10
307	July 1976	80.07	57.86	7.51	2.35	4.22
308	Aug 1976	81.13	58.73	7.69	2.39	4.34
309	Sept 1976	82.17	59.58	7.86	2.43	4.46
310	Oct 1976	83.25	60.41	8.02	2.46	4.57
311	Nov 1976	84.31	61.28	8.19	2.50	4.68
312	Dec 1976	85.41	62.10	8.35	2.53	4.79
313	Jan 1977	86.61	62.97	8.52	2.57	4.89
314	Feb 1977	87.70	63.98	8.71	2.62	5.01
315	Mar 1977	88.91	64.81	8.86	2.65	5.11
316	Apr 1977	90.10	65.83	9.05	2.70	5.22
317	May 1977	91.32	66.76	9.21	2.74	5.32
318	June 1977	92.53	67.76	9.38	2.78	5.43
319	July 1977	93.75	68.70	9.55	2.82	5.53
320	Aug 1977	94.99	69.70	9.72	2.86	5.63
321	Sept 1977	96.20	70.70	9.88	2.90	5.72
322	Oct 1977	97.42	71.65	10.04	2.94	5.82
323	Nov 1977	98.62	72.71	10.21	2.99	5.92
324	Dec 1977	99.84	73.68	10.36	3.03	6.00
325	Jan 1978	101.18	74.73	10.53	3.07	6.10
326	Feb 1978	102.77	76.25	10.80	3.14	6.26
327	Mar 1978	103.04	78.73	11.26	3.26	6.56
328	Apr 1978	104.31	77.97	11.02	3.21	6.37
329	May 1978	105.18	79.28	11.27	3.27	6.53
330	June 1978	106.88	79.72	11.29	3.28	6.51
331	July 1978	107.95	82.31	11.78	3.41	6.83
332	Aug 1978	108.69	83.81	12.00	3.47	6.96
333	Sept 1978	109.61	84.16	12.00	3.48	6.93
334	Oct 1978	111.18	84.92	12.09	3.51	6.97
335	Nov 1978	111.08	87.48	12.55	3.63	7.25
336	Dec 1978	111.93	85.67	12.04	3.52	6.87

Appendix A2. Simulated tetrachloroethylene and its degradation by-products in finished water, Tarawa Terrace water treatment plant, January 1951–March 1987[1].—Continued

[PCE, tetrachloroethylene; µg/L, microgram per liter; 1,2-tDCE, *trans*-1,2-dichloroethylene; TCE, trichloroethylene; VC, vinyl chloride; WTP, water treatment plant]

Stress period	Month and year	Single specie using MT3DMS model[2]	Multispecies, multiphase using TechFlowMP model[3]			
		[4]PCE, in µg/L	[5]PCE, in µg/L	[5]1,2-tDCE, in µg/L	[5]TCE, in µg/L	[5]VC, in µg/L
337	Jan 1979	113.14	85.41	11.95	3.50	6.79
338	Feb 1979	114.05	86.75	12.16	3.56	6.91
339	Mar 1979	114.98	87.55	12.23	3.60	6.93
340	Apr 1979	115.82	88.43	12.32	3.63	6.97
341	May 1979	116.68	89.21	12.40	3.66	7.00
342	June 1979	117.47	90.09	12.49	3.70	7.05
343	July 1979	118.29	90.82	12.56	3.73	7.07
344	Aug 1979	119.08	91.67	12.65	3.76	7.11
345	Sept 1979	119.82	92.44	12.72	3.79	7.14
346	Oct 1979	120.59	93.22	12.81	3.82	7.18
347	Nov 1979	121.31	94.00	12.88	3.85	7.21
348	Dec 1979	122.04	94.78	12.96	3.89	7.24
349	Jan 1980	123.28	95.56	13.03	3.92	7.27
350	Feb 1980	122.98	98.20	13.49	4.04	7.56
351	Mar 1980	124.03	96.35	12.98	3.94	7.19
352	Apr 1980	123.90	97.86	13.28	4.01	7.39
353	May 1980	124.69	96.00	12.78	3.90	7.03
354	June 1980	125.83	96.23	12.80	3.91	7.03
355	July 1980	0.72	0.00	0.00	0.00	0.00
356	Aug 1980	0.75	0.00	0.00	0.00	0.00
357	Sept 1980	121.36	95.07	12.43	3.92	6.83
358	Oct 1980	121.72	91.40	11.24	3.63	5.84
359	Nov 1980	122.14	91.00	11.17	3.63	5.82
360	Dec 1980	122.95	90.64	11.14	3.62	5.81
361	Jan 1981	114.05	84.14	10.41	3.37	5.46
362	Feb 1981	114.39	84.80	10.53	3.41	5.55
363	Mar 1981	115.60	84.13	10.37	3.37	5.44
364	Apr 1981	116.55	85.90	10.74	3.46	5.69
365	May 1981	117.30	87.53	11.02	3.54	5.87
366	June 1981	118.36	88.90	11.26	3.60	6.03
367	July 1981	133.29	102.10	13.12	4.17	7.09
368	Aug 1981	134.31	105.46	13.75	4.33	7.50
369	Sept 1981	120.72	96.34	12.64	3.96	6.93
370	Oct 1981	121.04	96.29	12.60	3.95	6.90
371	Nov 1981	121.41	96.69	12.67	3.96	6.93
372	Dec 1981	121.81	97.27	12.74	3.98	6.97

Appendix A2. Simulated tetrachloroethylene and its degradation by-products in finished water, Tarawa Terrace water treatment plant, January 1951–March 1987[1].—Continued

[PCE, tetrachloroethylene; µg/L, microgram per liter; 1,2-tDCE, *trans*-1,2-dichloroethylene; TCE, trichloroethylene; VC, vinyl chloride; WTP, water treatment plant]

Stress-period	Month and year	Single specie using MT3DMS model[2]	Multispecies, multiphase using TechFlowMP model[3]			
		[4]PCE, in µg/L	[5]PCE, in µg/L	[5]1,2 tDCE, in µg/L	[5]TCE, in µg/L	[5]VC, in µg/L
373	Jan 1982	103.95	81.28	10.65	3.33	5.81
374	Feb 1982	105.86	83.47	11.06	3.43	6.09
375	Mar 1982	107.52	85.42	11.40	3.51	6.31
376	Apr 1982	108.83	87.32	11.75	3.60	6.55
377	May 1982	148.50	120.45	16.30	4.98	9.13
378	June 1982	110.78	92.65	12.81	3.86	7.26
379	July 1982	111.98	92.98	12.77	3.86	7.21
380	Aug 1982	113.07	94.09	12.97	3.91	7.34
381	Sept 1982	114.04	95.33	13.18	3.96	7.46
382	Oct 1982	114.60	96.51	13.37	4.01	7.57
383	Nov 1982	113.87	96.63	13.31	4.00	7.51
384	Dec 1982	115.16	93.14	12.43	3.80	6.88
385	Jan 1983	1.25	0.10	0.04	0.00	0.05
386	Feb 1983	1.29	0.12	0.05	0.01	0.07
387	Mar 1983	111.76	88.43	11.55	3.65	6.37
388	Apr 1983	112.66	86.39	10.85	3.43	5.77
389	May 1983	113.97	87.67	11.04	3.52	5.88
390	June 1983	106.10	82.26	10.54	3.33	5.70
391	July 1983	116.70	92.03	11.95	3.75	6.52
392	Aug 1983	117.72	94.46	12.45	3.87	6.87
393	Sept 1983	117.83	96.92	12.94	3.99	7.21
394	Oct 1983	117.97	96.60	12.82	3.96	7.12
395	Nov 1983	118.63	95.49	12.58	3.89	6.95
396	Dec 1983	120.78	95.52	12.60	3.89	6.96
397	Jan 1984	132.87	111.52	15.09	4.61	8.43
398	Feb 1984	180.39	145.48	19.20	5.94	10.56
399	Mar 1984	183.02	155.54	21.34	6.47	11.97
400	Apr 1984	151.46	132.07	18.23	5.52	10.26
401	May 1984	153.42	132.19	18.09	5.49	10.13
402	June 1984	182.13	158.14	21.85	6.60	12.28
403	July 1984	156.39	140.96	19.72	5.92	11.14
404	Aug 1984	170.47	118.88	16.05	4.81	8.94
405	Sept 1984	181.22	149.36	19.60	6.17	11.20
406	Oct 1984	173.73	136.04	17.33	5.56	9.39
407	Nov 1984	173.77	131.63	16.46	5.34	8.87
408	Dec 1984	173.18	128.47	15.83	5.18	8.46

Appendix A2. Simulated tetrachloroethylene and its degradation by-products in finished water, Tarawa Terrace water treatment plant, January 1951–March 1987[1].—Continued

[PCE, tetrachloroethylene; µg/L, microgram per liter; 1,2-tDCE, *trans*-1,2-dichloroethylene; TCE, trichloroethylene; VC, vinyl chloride; WTP, water treatment plant]

Stress period	Month and year	Single specie using MT3DMS model[2]	Multispecies, multiphase using TechFlowMP model[3]			
		[4]PCE, in µg/L	[5]PCE, in µg/L	[5]1,2-tDCE, in µg/L	[5]TCE, in µg/L	[5]VC, in µg/L
409	Jan 1985	176.12	127.80	15.48	5.13	8.20
410	Feb 1985	3.64	1.10	0.29	0.05	0.22
411	Mar 1985	8.71	3.88	0.68	0.17	0.47
412	Apr 1985	8.09	3.70	0.68	0.16	0.49
413	May 1985	4.76	1.65	0.44	0.07	0.35
414	June 1985	5.14	1.88	0.50	0.08	0.41
415	July 1985	5.54	2.10	0.56	0.09	0.47
416	Aug 1985	6.01	2.34	0.63	0.10	0.52
417	Sept 1985	6.50	2.62	0.71	0.12	0.59
418	Oct 1985	7.06	2.91	0.79	0.13	0.65
419	Nov 1985	7.64	3.24	0.87	0.15	0.71
420	Dec 1985	8.27	3.58	0.95	0.16	0.76
421	Jan 1986	8.85	3.95	1.04	0.18	0.82
422	Feb 1986	9.42	4.24	1.08	0.19	0.83
423	Mar 1986	12.14	5.40	1.34	0.24	1.01
424	Apr 1986	10.83	4.93	1.20	0.22	0.89
425	May 1986	11.56	5.25	1.25	0.23	0.91
426	June 1986	12.28	5.61	1.30	0.25	0.92
427	July 1986	13.06	5.97	1.35	0.26	0.94
428	Aug 1986	13.84	6.36	1.39	0.28	0.96
429	Sept 1986	14.61	6.75	1.44	0.30	0.97
430	Oct 1986	15.42	7.12	1.48	0.31	0.99
431	Nov 1986	16.21	7.52	1.52	0.33	1.00
432	Dec 1986	17.03	7.89	1.56	0.34	1.01
433	Jan 1987	17.85	8.28	1.59	0.36	1.01
434	Feb 1987	18.49	8.71	1.64	0.38	1.03
435	Mar 1987	**WTP closed**	**WTP closed**	**WTP closed**	**WTP closed**	**WTP closed**

[1]Current maximum contaminant levels (MCLs) are: tetrachloroethylene (PCE) and trichloroethylene (TCE), 5 µg/L; *trans*-1,2-dichloroethylene (1,2-tDCE), 100 µg/L; and vinyl chloride (VC), 2 µg/L (USEPA, 2003); effective dates for MCLs are as follows: TCE and VC, January 9, 1989; PCE and 1,2-tDCE, July 6, 1992 (40 CFR, Section 141.60, Effective Dates, July 1, 2002, ed.)

[2]MT3DMS: A three-dimensional mass transport, multispecies model developed by C. Zheng and P. Wang (1999) on behalf of the U.S. Army Engineer Research and Development Center in Vicksburg, Mississippi (*http://hydro.geo.ua.edu/mt3d/*)

[3]TechFlowMP: A three-dimensional multispecies, multiphase mass transport model developed by the Multimedia Environmental Simulations Laboratory (Jang and Aral 2007) at the Georgia Institute of Technology, Atlanta, Georgia (*http://mesl.ce.gatech.edu*)

[4]Results from Chapter F report (Faye In press 2007b)

[5]Results from Chapter G report (Jang and Aral In press 2007)

Appendix H2 — Tarawa Terrace Water Treatment Plant Reconstructed (Simulated) Mean Monthly Finished Water Concentration of Single-Specie Tetrachloroethylene (PCE) and Range of Concentrations Derived from Monte Carlo Simulation

Appendix I5. Simulated concentrations of tetrachloroethylene in finished water at the water treatment plant, Tarawa Terrace, U.S. Marine Corps Base Camp Lejeune, North Carolina.

[PCE, tetrachloroethylene; µg/L, microgram per liter; $P_{2.5}$, Monte Carlo simulation results for the 2.5 percentile; P_{50}, Monte Carlo simulation results for the 50 percentile; $P_{97.5}$, Monte Carlo simulation results for the 97.5 percentile; WTP, water treatment plant; Jan, January; Feb, February; Mar, March; Apr, April; Aug, August; Sept, September; Oct, October; Dec, December]

Stress period	Month and year	Calibrated PCE concentration, in µg/L[1]	Range of concentrations derived from Monte Carlo simulations[2]					
			Monte Carlo simulation (Scenario 1)[3]			Monte Carlo simulation (Scenario 2)[4]		
			$P_{2.5}$, in µg/L	P_{50}, in µg/L	$P_{97.5}$, in µg/L	$P_{2.5}$, in µg/L	P_{50}, in µg/L	$P_{97.5}$, in µg/L
1-12	Jan–Dec 1951	WTP not operating						
13	Jan 1952	0.00	0.00	0.00	0.00	0.00	0.00	0.00
14	Feb 1952	0.00	0.00	0.00	0.00	0.00	0.00	0.00
15	Mar 1952	0.00	0.00	0.00	0.00	0.00	0.00	0.00
16	Apr 1952	0.00	0.00	0.00	0.00	0.00	0.00	0.00
17	May 1952	0.00	0.00	0.00	0.00	0.00	0.00	0.00
18	June 1952	0.00	0.00	0.00	0.00	0.00	0.00	0.00
19	July 1952	0.00	0.00	0.00	0.00	0.00	0.00	0.00
20	Aug 1952	0.00	0.00	0.00	0.00	0.00	0.00	0.00
21	Sept 1952	0.00	0.00	0.00	0.00	0.00	0.00	0.00
22	Oct 1952	0.00	0.00	0.00	0.00	0.00	0.00	0.00
23	Nov 1952	0.00	0.00	0.00	0.00	0.00	0.00	0.00
24	Dec 1952	0.00	0.00	0.00	0.00	0.00	0.00	0.00
25	Jan 1953	0.00	0.00	0.00	0.00	0.00	0.00	0.00
26	Feb 1953	0.00	0.00	0.00	0.00	0.00	0.00	0.00
27	Mar 1953	0.00	0.00	0.00	0.00	0.00	0.00	0.00
28	Apr 1953	0.00	0.00	0.00	0.00	0.00	0.00	0.00
29	May 1953	0.00	0.00	0.00	0.00	0.00	0.00	0.00
30	June 1953	0.00	0.00	0.00	0.00	0.00	0.00	0.00
31	July 1953	0.00	0.00	0.00	0.00	0.00	0.00	0.00
32	Aug 1953	0.00	0.00	0.00	0.00	0.00	0.00	0.00
33	Sept 1953	0.00	0.00	0.00	0.00	0.00	0.00	0.00
34	Oct 1953	0.00	0.00	0.00	0.00	0.00	0.00	0.00
35	Nov 1953	0.00	0.00	0.00	0.00	0.00	0.00	0.00
36	Dec 1953	0.00	0.00	0.00	0.00	0.00	0.00	0.00
37	Jan 1954	0.00	0.00	0.00	0.00	0.00	0.00	0.00
38	Feb 1954	0.00	0.00	0.00	0.00	0.00	0.00	0.00
39	Mar 1954	0.00	0.00	0.00	0.00	0.00	0.00	0.00
40	Apr 1954	0.00	0.00	0.00	0.00	0.00	0.00	0.00
41	May 1954	0.00	0.00	0.00	0.00	0.00	0.00	0.00
42	June 1954	0.00	0.00	0.00	0.00	0.00	0.00	0.00
43	July 1954	0.00	0.00	0.00	0.00	0.00	0.00	0.00
44	Aug 1954	0.00	0.00	0.00	0.00	0.00	0.00	0.00
45	Sept 1954	0.00	0.00	0.00	0.00	0.00	0.00	0.00
46	Oct 1954	0.00	0.00	0.00	0.00	0.00	0.00	0.00
47	Nov 1954	0.00	0.00	0.00	0.00	0.00	0.00	0.00
48	Dec 1954	0.00	0.00	0.00	0.00	0.00	0.00	0.00
49	Jan 1955	0.00	0.00	0.00	0.00	0.00	0.00	0.00
50	Feb 1955	0.00	0.00	0.00	0.00	0.00	0.00	0.00
51	Mar 1955	0.00	0.00	0.00	0.00	0.00	0.00	0.00
52	Apr 1955	0.00	0.00	0.00	0.01	0.00	0.00	0.01
53	May 1955	0.00	0.00	0.00	0.01	0.00	0.00	0.01
54	June 1955	0.01	0.00	0.00	0.01	0.00	0.00	0.01
55	July 1955	0.01	0.00	0.01	0.02	0.00	0.01	0.02
56	Aug 1955	0.01	0.00	0.01	0.03	0.00	0.01	0.02
57	Sept 1955	0.02	0.00	0.01	0.04	0.00	0.01	0.03
58	Oct 1955	0.03	0.01	0.02	0.05	0.01	0.02	0.04
59	Nov 1955	0.04	0.01	0.03	0.07	0.01	0.03	0.07
60	Dec 1955	0.06	0.01	0.04	0.09	0.01	0.03	0.09

Appendix I5. Simulated concentrations of tetrachloroethylene in finished water at the water treatment plant, Tarawa Terrace, U.S. Marine Corps Base Camp Lejeune, North Carolina.—Continued

[PCE, tetrachloroethylene; µg/L, microgram per liter; $P_{2.5}$, Monte Carlo simulation results for the 2.5 percentile; P_{50}, Monte Carlo simulation results for the 50 percentile; $P_{97.5}$, Monte Carlo simulation results for the 97.5 percentile; WTP, water treatment plant; Jan, January; Feb, February; Mar, March; Apr, April; Aug, August; Sept, September; Oct, October; Dec, December]

Stress period	Month and year	Calibrated PCE concentration, in µg/L[1]	Range of concentrations derived from Monte Carlo simulations[2]					
			Monte Carlo simulation (Scenario 1)[3]			Monte Carlo simulation (Scenario 2)[4]		
			$P_{2.5}$, in µg/L	P_{50}, in µg/L	$P_{97.5}$, in µg/L	$P_{2.5}$, in µg/L	P_{50}, in µg/L	$P_{97.5}$, in µg/L
61	Jan 1956	0.08	0.02	0.05	0.12	0.02	0.04	0.12
62	Feb 1956	0.10	0.02	0.07	0.16	0.02	0.06	0.15
63	Mar 1956	0.13	0.03	0.09	0.21	0.03	0.08	0.18
64	Apr 1956	0.17	0.04	0.12	0.26	0.04	0.10	0.24
65	May 1956	0.23	0.05	0.15	0.33	0.05	0.12	0.29
66	June 1956	0.29	0.07	0.20	0.42	0.06	0.15	0.34
67	July 1956	0.36	0.09	0.25	0.52	0.08	0.18	0.41
68	Aug 1956	0.46	0.12	0.31	0.65	0.10	0.23	0.51
69	Sept 1956	0.57	0.15	0.38	0.79	0.13	0.29	0.65
70	Oct 1956	0.70	0.18	0.47	0.96	0.16	0.35	0.78
71	Nov 1956	0.85	0.23	0.57	1.16	0.22	0.47	1.03
72	Dec 1956	1.04	0.28	0.69	1.38	0.24	0.54	1.14
73	Jan 1957	1.25	0.35	0.83	1.63	0.31	0.63	1.38
74	Feb 1957	1.47	0.41	0.97	1.89	0.37	0.77	1.69
75	Mar 1957	1.74	0.49	1.16	2.21	0.43	0.88	1.84
76	Apr 1957	2.04	0.59	1.36	2.57	0.53	1.09	2.08
77	May 1957	2.39	0.70	1.59	2.97	0.60	1.20	2.40
78	June 1957	2.77	0.83	1.84	3.40	0.64	1.31	2.51
79	July 1957	3.21	0.98	2.12	3.87	0.74	1.50	3.08
80	Aug 1957	3.69	1.15	2.45	4.42	0.87	1.73	3.38
81	Sept 1957	4.21	1.33	2.80	4.99	1.07	2.11	3.83
82	Oct 1957	4.79	1.54	3.20	5.64	1.20	2.31	4.48
83	Nov 1957	5.41	1.77	3.61	6.32	1.46	2.95	5.33
84	Dec 1957	6.10	2.02	4.08	7.07	1.61	3.08	5.81
85	Jan 1958	6.86	2.29	4.60	7.87	1.81	3.43	6.42
86	Feb 1958	7.60	2.57	5.11	8.67	2.04	3.97	7.10
87	Mar 1958	8.47	2.88	5.71	9.58	2.36	4.36	7.74
88	Apr 1958	9.37	3.22	6.33	10.56	2.68	5.04	8.73
89	May 1958	10.37	3.61	7.02	11.61	2.99	5.37	9.15
90	June 1958	11.39	4.00	7.73	12.67	2.98	5.43	9.32
91	July 1958	12.91	4.59	8.78	14.26	4.03	6.88	11.46
92	Aug 1958	14.12	5.09	9.61	15.49	4.55	7.67	12.57
93	Sept 1958	15.35	5.62	10.47	16.74	4.62	8.07	13.12
94	Oct 1958	16.69	6.19	11.39	18.13	5.24	8.98	14.89
95	Nov 1958	18.03	6.79	12.32	19.54	5.71	9.88	16.33
96	Dec 1958	19.49	7.45	13.33	21.07	6.32	10.83	17.27
97	Jan 1959	20.97	8.11	14.36	22.62	6.84	11.56	18.53
98	Feb 1959	22.35	8.77	15.34	23.97	7.74	12.87	20.40
99	Mar 1959	23.92	9.53	16.47	25.59	7.80	13.07	20.81
100	Apr 1959	25.49	10.24	17.59	27.22	8.26	14.30	23.52
101	May 1959	27.15	11.08	18.81	29.01	8.82	15.02	23.60
102	June 1959	28.81	11.94	20.01	30.78	10.46	16.86	25.74
103	July 1959	30.56	12.79	21.37	32.69	11.14	17.71	27.35
104	Aug 1959	32.36	13.70	22.77	34.63	12.06	18.88	28.65
105	Sept 1959	34.14	14.62	24.11	36.56	12.39	19.29	28.82
106	Oct 1959	36.01	15.60	25.59	38.60	13.35	20.99	31.36
107	Nov 1959	37.85	16.60	27.04	40.57	13.30	22.66	35.03
108	Dec 1959	39.78	17.68	28.50	42.59	14.48	23.99	36.02

Appendix I5. Simulated concentrations of tetrachloroethylene in finished water at the water treatment plant, Tarawa Terrace, U.S. Marine Corps Base Camp Lejeune, North Carolina.—Continued

[PCE, tetrachloroethylene; µg/L, microgram per liter; $P_{2.5}$, Monte Carlo simulation results for the 2.5 percentile; P_{50}, Monte Carlo simulation results for the 50 percentile; $P_{97.5}$, Monte Carlo simulation results for the 97.5 percentile; WTP, water treatment plant; Jan, January; Feb, February; Mar, March; Apr, April; Aug, August; Sept, September; Oct, October; Dec, December]

Stress period	Month and year	Calibrated PCE concentration, in µg/L[1]	Range of concentrations derived from Monte Carlo simulations[2]					
			Monte Carlo simulation (Scenario 1)[3]			Monte Carlo simulation (Scenario 2)[4]		
			$P_{2.5}$, in µg/L	P_{50}, in µg/L	$P_{97.5}$, in µg/L	$P_{2.5}$, in µg/L	P_{50}, in µg/L	$P_{97.5}$, in µg/L
109	Jan 1960	41.86	18.82	30.15	44.74	15.99	24.99	38.89
110	Feb 1960	43.85	19.92	31.62	46.80	16.98	27.00	41.00
111	Mar 1960	46.03	21.13	33.16	49.07	17.85	26.94	41.01
112	Apr 1960	48.15	22.35	34.81	51.31	18.45	29.03	43.84
113	May 1960	50.37	23.59	36.60	53.65	19.84	30.13	44.48
114	June 1960	52.51	24.80	38.35	55.92	22.20	33.22	47.21
115	July 1960	54.74	26.08	40.12	58.27	23.30	34.55	50.18
116	Aug 1960	56.96	27.37	42.13	60.60	24.49	36.32	51.82
117	Sept 1960	59.09	28.64	43.80	62.82	24.27	35.66	51.64
118	Oct 1960	61.30	29.98	45.51	65.09	26.27	38.51	55.86
119	Nov 1960	63.42	31.31	47.25	67.22	26.43	40.46	59.79
120	Dec 1960	65.61	32.81	48.96	69.64	26.91	43.02	60.66
121	Jan 1961	67.69	34.22	50.74	71.88	28.21	43.30	63.65
122	Feb 1961	69.54	35.52	52.42	73.96	30.97	45.69	70.43
123	Mar 1961	71.56	36.93	54.16	76.28	31.47	45.72	66.14
124	Apr 1961	73.49	38.31	55.82	78.51	32.33	47.92	70.86
125	May 1961	75.49	39.76	57.54	80.74	32.37	49.12	70.32
126	June 1961	77.39	41.04	59.14	82.99	38.28	53.02	73.49
127	July 1961	79.36	42.45	60.87	84.92	36.88	54.13	75.55
128	Aug 1961	81.32	43.86	62.61	86.79	38.78	56.07	77.30
129	Sept 1961	83.19	45.25	64.23	88.82	38.62	54.74	76.56
130	Oct 1961	85.11	46.69	65.85	90.84	40.37	58.11	80.91
131	Nov 1961	86.95	48.10	67.44	92.75	39.55	59.92	87.09
132	Dec 1961	88.84	49.61	69.03	94.71	42.20	62.63	86.40
133	Jan 1962	60.88	34.23	47.47	64.96	27.60	42.46	62.20
134	Feb 1962	62.10	35.17	48.52	66.43	30.36	45.91	68.03
135	Mar 1962	62.94	35.84	49.35	67.26	31.00	45.13	66.06
136	Apr 1962	63.59	36.33	50.10	68.07	32.57	48.08	68.30
137	May 1962	64.17	36.80	50.73	68.98	31.10	46.57	66.06
138	June 1962	64.70	37.21	51.33	69.81	29.45	43.47	61.90
139	July 1962	65.23	37.65	51.82	70.45	28.63	44.36	62.01
140	Aug 1962	65.74	38.07	52.41	71.23	29.87	45.14	64.88
141	Sept 1962	66.22	38.47	52.91	71.97	32.00	47.51	67.91
142	Oct 1962	66.71	38.89	53.53	72.74	30.29	47.30	68.59
143	Nov 1962	67.18	39.30	54.16	73.38	35.13	53.53	77.51
144	Dec 1962	67.65	39.72	54.77	74.05	33.21	50.53	75.06
145	Jan 1963	68.06	40.19	55.24	74.67	32.41	49.74	74.10
146	Feb 1963	68.39	40.63	55.56	75.17	34.46	52.70	77.58
147	Mar 1963	68.73	41.15	56.03	75.76	35.61	52.41	73.73
148	Apr 1963	69.03	41.66	56.47	76.32	36.91	55.39	79.81
149	May 1963	69.33	42.03	56.98	77.17	34.47	53.02	77.36
150	June 1963	69.62	42.25	57.46	77.94	34.18	49.23	70.00
151	July 1963	69.90	42.45	57.98	78.48	32.75	49.62	71.03
152	Aug 1963	70.17	42.67	58.43	79.00	34.06	51.05	73.06
153	Sept 1963	70.43	42.87	58.82	79.47	36.62	52.90	76.53
154	Oct 1963	70.69	43.17	59.15	79.90	36.26	52.47	77.15
155	Nov 1963	70.93	43.60	59.49	80.31	38.46	59.09	84.58
156	Dec 1963	71.17	43.90	59.88	80.88	36.71	56.06	80.60

Appendix I5. Simulated concentrations of tetrachloroethylene in finished water at the water treatment plant, Tarawa Terrace, U.S. Marine Corps Base Camp Lejeune, North Carolina.—Continued

[PCE, tetrachloroethylene; µg/L, microgram per liter; $P_{2.5}$, Monte Carlo simulation results for the 2.5 percentile; P_{50}, Monte Carlo simulation results for the 50 percentile; $P_{97.5}$, Monte Carlo simulation results for the 97.5 percentile; WTP, water treatment plant; Jan, January; Feb, February; Mar, March; Apr, April; Aug, August; Sept, September; Oct, October; Dec, December]

Stress period	Month and year	Calibrated PCE concentration, in µg/L[1]	Range of concentrations derived from Monte Carlo simulations[2]					
			Monte Carlo simulation (Scenario 1)[3]			Monte Carlo simulation (Scenario 2)[4]		
			$P_{2.5}$, in µg/L	P_{50}, in µg/L	$P_{97.5}$, in µg/L	$P_{2.5}$, in µg/L	P_{50}, in µg/L	$P_{97.5}$, in µg/L
157	Jan 1964	71.40	44.18	60.32	81.34	35.81	55.22	80.71
158	Feb 1964	63.77	39.66	54.00	72.84	37.51	58.47	83.80
159	Mar 1964	63.95	39.92	54.36	73.38	37.37	57.84	81.58
160	Apr 1964	64.08	40.09	54.68	73.85	40.30	60.39	85.06
161	May 1964	64.19	40.31	54.98	74.28	39.56	57.23	84.15
162	June 1964	64.27	40.51	55.23	74.64	37.14	53.54	75.21
163	July 1964	64.34	40.61	55.45	74.98	35.59	54.24	76.87
164	Aug 1964	64.39	40.68	55.64	75.27	37.29	55.12	77.08
165	Sept 1964	64.43	40.75	55.82	75.62	39.55	57.96	80.84
166	Oct 1964	64.47	40.81	56.00	75.94	38.57	56.64	78.51
167	Nov 1964	64.49	40.88	56.18	76.19	42.49	63.10	91.13
168	Dec 1964	64.50	40.96	56.36	76.45	39.06	59.01	88.36
169	Jan 1965	64.50	41.10	56.58	76.70	37.87	59.05	88.52
170	Feb 1965	64.49	41.12	56.70	76.94	39.46	61.35	94.71
171	Mar 1965	64.47	41.14	56.78	77.17	41.20	60.99	89.98
172	Apr 1965	64.45	41.16	56.92	77.24	42.66	64.07	93.10
173	May 1965	64.42	41.20	57.06	77.13	41.03	61.17	87.07
174	June 1965	64.38	41.23	57.20	77.34	36.64	56.23	81.33
175	July 1965	64.33	41.26	57.22	77.80	38.15	57.32	81.83
176	Aug 1965	64.27	41.14	57.22	77.91	38.93	57.04	84.04
177	Sept 1965	64.20	41.03	57.22	77.92	41.40	60.36	84.29
178	Oct 1965	64.13	40.92	57.30	78.03	38.84	59.61	87.79
179	Nov 1965	64.05	40.85	57.34	78.10	44.47	66.00	95.45
180	Dec 1965	63.97	40.78	57.39	78.10	39.95	61.88	91.31
181	Jan 1966	63.88	40.81	57.48	78.26	39.34	61.61	91.59
182	Feb 1966	63.79	40.88	57.54	78.38	42.06	64.63	99.81
183	Mar 1966	63.68	41.01	57.62	78.45	41.44	63.87	94.47
184	Apr 1966	63.57	41.20	57.61	78.33	43.72	66.91	97.21
185	May 1966	63.46	41.28	57.64	78.43	42.05	64.21	91.37
186	June 1966	63.34	41.40	57.70	78.44	38.28	58.86	86.56
187	July 1966	63.21	41.54	57.70	78.65	39.70	58.20	87.29
188	Aug 1966	63.08	41.69	57.74	78.94	39.57	60.11	87.73
189	Sept 1966	62.94	41.79	57.79	78.91	41.82	62.94	91.60
190	Oct 1966	62.80	41.73	57.82	78.87	40.67	60.35	90.52
191	Nov 1966	62.65	41.67	57.78	78.78	44.43	68.76	99.82
192	Dec 1966	62.50	41.60	57.82	78.70	40.92	63.19	97.26
193	Jan 1967	62.25	41.42	57.70	78.67	40.95	62.45	96.88
194	Feb 1967	61.99	41.20	57.61	78.56	41.00	66.51	98.39
195	Mar 1967	61.67	40.98	57.36	78.37	43.47	64.42	95.01
196	Apr 1967	61.35	40.74	57.12	78.11	44.75	66.63	97.65
197	May 1967	61.02	40.52	56.84	77.78	42.71	64.23	95.11
198	June 1967	60.69	40.22	56.65	77.54	38.89	58.53	86.55
199	July 1967	60.37	40.03	56.43	77.45	38.46	59.64	87.57
200	Aug 1967	60.05	39.87	56.26	77.39	39.01	59.72	89.18
201	Sept 1967	59.74	39.69	56.04	77.26	40.93	61.91	90.19
202	Oct 1967	59.43	39.49	55.86	77.12	40.30	60.56	90.27
203	Nov 1967	59.13	39.31	55.71	76.98	44.01	68.01	99.90
204	Dec 1967	58.83	39.12	55.50	76.83	41.94	63.60	97.99

Appendix I5. Simulated concentrations of tetrachloroethylene in finished water at the water treatment plant, Tarawa Terrace, U.S. Marine Corps Base Camp Lejeune, North Carolina.—Continued

[PCE, tetrachloroethylene; µg/L, microgram per liter; $P_{2.5}$, Monte Carlo simulation results for the 2.5 percentile; P_{50}, Monte Carlo simulation results for the 50 percentile; $P_{97.5}$, Monte Carlo simulation results for the 97.5 percentile; WTP, water treatment plant; Jan, January; Feb, February; Mar, March; Apr, April; Aug, August; Sept, September; Oct, October; Dec, December]

Stress period	Month and year	Calibrated PCE concentration, in µg/L[1]	Range of concentrations derived from Monte Carlo simulations[2]					
			Monte Carlo simulation (Scenario 1)[3]			Monte Carlo simulation (Scenario 2)[4]		
			$P_{2.5}$, in µg/L	P_{50}, in µg/L	$P_{97.5}$, in µg/L	$P_{2.5}$, in µg/L	P_{50}, in µg/L	$P_{97.5}$, in µg/L
205	Jan 1968	58.41	38.91	55.32	76.43	40.60	63.04	98.22
206	Feb 1968	57.95	38.69	55.12	75.94	39.51	63.91	98.67
207	Mar 1968	57.43	38.44	54.74	75.51	41.62	63.54	94.21
208	Apr 1968	56.94	38.22	54.56	75.12	42.61	65.79	99.98
209	May 1968	56.45	37.99	54.20	74.61	39.39	62.35	92.79
210	June 1968	55.98	37.72	53.86	74.13	37.49	57.23	84.15
211	July 1968	55.49	37.46	53.50	73.63	37.51	56.92	83.56
212	Aug 1968	55.02	37.31	53.27	73.27	37.52	58.08	84.83
213	Sept 1968	54.58	37.16	53.00	73.05	40.06	60.24	89.84
214	Oct 1968	54.13	36.94	52.72	72.83	37.61	59.46	87.96
215	Nov 1968	53.71	36.71	52.49	72.61	42.84	64.11	96.77
216	Dec 1968	53.28	36.45	52.16	72.34	39.36	60.93	93.74
217	Jan 1969	53.07	36.40	52.03	72.40	37.42	60.60	90.38
218	Feb 1969	52.97	36.41	52.07	72.32	38.68	63.83	100.33
219	Mar 1969	52.94	36.41	52.21	72.23	40.85	62.20	90.15
220	Apr 1969	52.93	36.50	52.33	72.58	41.71	63.74	95.37
221	May 1969	52.93	36.55	52.41	72.94	40.51	60.54	94.64
222	June 1969	52.92	36.59	52.49	73.24	37.99	56.86	82.85
223	July 1969	52.90	36.61	52.54	73.52	35.02	57.32	85.75
224	Aug 1969	52.86	36.63	52.71	73.77	36.90	57.85	85.34
225	Sept 1969	52.81	36.64	52.74	73.98	39.74	59.97	89.19
226	Oct 1969	52.75	36.64	52.75	74.13	37.64	59.44	92.22
227	Nov 1969	55.19	38.34	55.24	77.72	36.74	55.89	84.87
228	Dec 1969	55.19	38.30	55.23	77.70	32.94	51.96	81.13
229	Jan 1970	55.01	38.10	55.14	77.54	32.78	50.97	81.62
230	Feb 1970	54.79	37.97	55.03	77.34	33.13	52.80	83.08
231	Mar 1970	54.49	37.71	54.76	77.08	32.85	52.72	79.35
232	Apr 1970	54.20	37.46	54.48	76.72	34.85	54.22	82.26
233	May 1970	53.90	37.21	54.17	76.27	33.91	51.26	78.11
234	June 1970	53.61	37.01	53.91	75.89	29.54	47.08	71.71
235	July 1970	53.32	36.82	53.59	75.68	28.77	46.80	72.48
236	Aug 1970	53.04	36.64	53.32	75.44	29.60	47.37	70.90
237	Sept 1970	52.78	36.47	53.06	75.25	31.55	49.00	74.82
238	Oct 1970	52.53	36.31	52.78	75.02	30.14	48.10	73.55
239	Nov 1970	52.29	36.19	52.67	74.93	32.50	53.01	81.51
240	Dec 1970	52.05	36.05	52.54	74.88	32.47	48.94	76.35
241	Jan 1971	51.96	35.96	52.53	75.02	30.00	48.86	77.29
242	Feb 1971	51.93	35.90	52.50	75.19	32.51	50.78	80.73
243	Mar 1971	51.95	35.87	52.60	75.42	32.25	49.82	78.27
244	Apr 1971	51.99	35.86	52.73	75.65	32.74	52.65	81.01
245	May 1971	52.03	35.86	52.88	75.88	30.15	49.32	76.96
246	June 1971	52.08	35.85	52.86	76.11	29.02	45.87	72.87
247	July 1971	52.12	35.92	52.88	76.35	29.03	45.64	72.37
248	Aug 1971	52.16	35.93	52.97	76.52	29.30	46.61	71.75
249	Sept 1971	52.20	35.93	53.07	76.72	30.33	48.38	74.56
250	Oct 1971	52.23	35.95	53.13	76.91	29.27	46.98	73.25
251	Nov 1971	52.26	35.98	53.25	77.05	32.40	52.55	82.47
252	Dec 1971	52.29	35.91	53.28	77.28	30.91	49.57	76.35

Appendix I5. Simulated concentrations of tetrachloroethylene in finished water at the water treatment plant, Tarawa Terrace, U.S. Marine Corps Base Camp Lejeune, North Carolina.—Continued

[PCE, tetrachloroethylene; µg/L, microgram per liter; $P_{2.5}$, Monte Carlo simulation results for the 2.5 percentile; P_{50}, Monte Carlo simulation results for the 50 percentile; $P_{97.5}$, Monte Carlo simulation results for the 97.5 percentile; WTP, water treatment plant; Jan, January; Feb, February; Mar, March; Apr, April; Aug, August; Sept, September; Oct, October; Dec, December]

Stress period	Month and year	Calibrated PCE concentration, in µg/L[1]	Range of concentrations derived from Monte Carlo simulations[2]					
			Monte Carlo simulation (Scenario 1)[3]			Monte Carlo simulation (Scenario 2)[4]		
			$P_{2.5}$, in µg/L	P_{50}, in µg/L	$P_{97.5}$, in µg/L	$P_{2.5}$, in µg/L	P_{50}, in µg/L	$P_{97.5}$, in µg/L
253	Jan 1972	49.34	33.93	50.30	73.12	29.17	48.14	77.82
254	Feb 1972	49.01	33.72	50.06	72.93	30.19	50.33	81.13
255	Mar 1972	48.68	33.47	49.71	72.72	31.69	48.44	75.80
256	Apr 1972	48.40	33.25	49.54	72.47	30.79	50.77	79.48
257	May 1972	48.14	33.10	49.27	72.26	30.44	48.53	73.97
258	June 1972	47.90	32.98	49.08	72.17	27.68	44.98	68.87
259	July 1972	47.67	32.85	48.97	72.02	27.13	43.58	66.62
260	Aug 1972	47.45	32.72	48.78	71.78	26.91	43.63	68.46
261	Sept 1972	47.25	32.60	48.69	71.47	28.10	46.38	72.80
262	Oct 1972	47.05	32.49	48.58	71.34	28.15	44.90	70.07
263	Nov 1972	46.87	32.41	48.43	71.26	30.68	49.80	78.83
264	Dec 1972	46.69	32.29	48.21	71.16	28.36	46.21	76.56
265	Jan 1973	54.28	37.52	56.04	82.79	27.54	44.70	72.51
266	Feb 1973	54.19	37.39	55.96	82.69	29.05	47.31	78.50
267	Mar 1973	53.98	37.15	55.78	82.35	28.09	46.20	73.11
268	Apr 1973	53.76	36.91	55.44	81.94	28.95	46.73	77.52
269	May 1973	53.52	36.68	55.24	81.51	26.12	45.17	70.36
270	June 1973	53.30	36.46	55.22	81.10	25.61	40.75	66.70
271	July 1973	53.08	36.24	55.12	80.74	25.25	40.82	63.84
272	Aug 1973	52.87	36.03	54.99	80.59	25.02	41.47	64.39
273	Sept 1973	52.68	35.84	54.88	80.46	26.43	43.33	68.68
274	Oct 1973	52.51	35.66	54.87	80.34	26.17	41.28	65.28
275	Nov 1973	52.35	35.49	54.80	80.25	27.77	45.41	72.92
276	Dec 1973	52.20	35.33	54.72	80.17	25.66	42.21	68.89
277	Jan 1974	52.43	35.41	54.97	80.49	25.72	42.62	69.65
278	Feb 1974	52.82	35.59	55.42	80.98	26.19	43.80	72.53
279	Mar 1974	53.39	35.86	55.92	81.66	25.08	42.86	68.49
280	Apr 1974	53.99	36.16	56.60	82.41	28.14	45.59	71.28
281	May 1974	54.63	36.49	57.21	83.20	25.84	42.70	72.49
282	June 1974	55.25	36.80	57.69	84.15	25.00	40.00	64.50
283	July 1974	55.90	37.13	58.15	85.07	24.17	40.57	65.57
284	Aug 1974	56.53	37.50	58.85	85.98	24.29	40.75	65.98
285	Sept 1974	57.10	37.85	59.43	86.86	27.22	43.16	69.98
286	Oct 1974	57.70	38.22	60.00	87.74	25.22	42.68	67.27
287	Nov 1974	58.30	38.56	60.59	88.58	28.99	47.52	76.53
288	Dec 1974	58.92	38.98	61.11	89.45	25.07	44.15	72.46
289	Jan 1975	61.00	40.30	63.17	92.62	27.61	45.83	75.73
290	Feb 1975	61.24	40.39	63.33	92.97	28.46	48.17	80.43
291	Mar 1975	61.41	40.51	63.43	93.20	28.98	46.39	77.50
292	Apr 1975	61.57	40.61	63.45	93.38	29.37	48.59	82.56
293	May 1975	61.72	40.78	63.62	93.32	28.00	46.55	76.49
294	June 1975	61.88	40.92	63.77	93.48	24.95	42.93	67.44
295	July 1975	62.05	41.05	64.04	93.91	25.59	42.20	68.93
296	Aug 1975	62.25	41.13	64.22	94.27	26.21	42.72	68.78
297	Sept 1975	62.46	41.20	64.36	94.54	25.88	44.92	73.09
298	Oct 1975	62.69	41.18	64.65	94.84	26.24	43.56	70.58
299	Nov 1975	62.92	41.12	64.91	95.15	27.40	49.02	80.06
300	Dec 1975	63.18	41.12	65.11	95.44	26.23	45.41	76.07

Appendix I5. Simulated concentrations of tetrachloroethylene in finished water at the water treatment plant, Tarawa Terrace, U.S. Marine Corps Base Camp Lejeune, North Carolina.—Continued

[PCE, tetrachloroethylene; µg/L, microgram per liter; $P_{2.5}$, Monte Carlo simulation results for the 2.5 percentile; P_{50}, Monte Carlo simulation results for the 50 percentile; $P_{97.5}$, Monte Carlo simulation results for the 97.5 percentile; WTP, water treatment plant; Jan, January; Feb, February; Mar, March; Apr, April; Aug, August; Sept, September; Oct, October; Dec, December]

Stress period	Month and year	Calibrated PCE concentration, in µg/L[1]	Range of concentrations derived from Monte Carlo simulations[2]					
			Monte Carlo simulation (Scenario 1)[3]			Monte Carlo simulation (Scenario 2)[4]		
			$P_{2.5}$, in µg/L	P_{50}, in µg/L	$P_{97.5}$, in µg/L	$P_{2.5}$, in µg/L	P_{50}, in µg/L	$P_{97.5}$, in µg/L
301	Jan 1976	73.96	48.06	76.13	111.62	27.44	47.37	78.75
302	Feb 1976	74.94	48.64	77.01	112.96	28.08	50.08	82.73
303	Mar 1976	75.97	49.28	77.88	114.29	30.00	49.48	77.65
304	Apr 1976	76.97	49.90	78.87	115.66	29.89	51.83	83.45
305	May 1976	78.00	50.66	79.94	117.25	28.96	49.32	81.75
306	June 1976	79.02	51.42	80.86	118.78	27.37	44.69	74.98
307	July 1976	80.07	52.20	81.82	120.35	28.29	45.16	75.62
308	Aug 1976	81.13	52.86	82.70	121.82	27.95	46.57	76.48
309	Sept 1976	82.17	53.51	83.71	123.46	29.17	49.14	79.62
310	Oct 1976	83.25	54.25	84.81	124.74	28.92	48.10	80.30
311	Nov 1976	84.31	55.09	85.76	126.00	31.09	53.61	90.47
312	Dec 1976	85.41	55.90	86.67	127.61	28.21	50.51	82.95
313	Jan 1977	86.61	56.70	87.66	129.36	28.88	49.71	81.57
314	Feb 1977	87.70	57.45	88.70	131.09	30.18	52.13	85.43
315	Mar 1977	88.91	58.14	89.80	133.02	29.18	51.65	83.61
316	Apr 1977	90.10	58.86	90.90	134.30	32.23	54.40	88.91
317	May 1977	91.32	59.61	91.86	135.48	30.43	50.86	86.19
318	June 1977	92.53	60.38	93.08	136.61	28.97	47.43	78.24
319	July 1977	93.75	61.24	94.29	137.80	29.03	47.45	77.48
320	Aug 1977	94.99	62.11	95.48	139.43	28.20	48.28	81.51
321	Sept 1977	96.20	62.97	96.44	140.89	30.24	50.29	85.19
322	Oct 1977	97.42	63.86	97.49	142.51	28.33	51.14	82.53
323	Nov 1977	98.62	64.58	98.62	144.08	32.33	56.02	92.86
324	Dec 1977	99.84	65.31	99.65	145.59	29.86	53.22	90.47
325	Jan 1978	101.18	66.16	101.09	147.13	44.02	75.70	120.92
326	Feb 1978	102.77	67.25	102.62	148.91	39.93	67.26	112.31
327	Mar 1978	103.04	67.39	103.04	149.08	52.50	84.64	133.87
328	Apr 1978	104.31	68.24	104.52	150.32	46.79	76.94	126.94
329	May 1978	105.19	68.81	105.34	151.12	50.49	85.95	136.76
330	June 1978	106.88	70.00	107.10	153.19	42.45	73.13	119.19
331	July 1978	107.95	70.77	108.05	154.56	45.08	75.24	121.43
332	Aug 1978	108.69	71.12	108.58	155.63	48.54	80.46	135.92
333	Sept 1978	109.61	71.68	109.40	156.91	48.81	83.51	139.85
334	Oct 1978	111.18	72.89	110.78	158.60	44.55	75.04	121.83
335	Nov 1978	111.08	72.99	110.76	158.33	59.23	100.40	162.58
336	Dec 1978	111.93	73.52	111.71	159.48	58.45	100.01	162.64
337	Jan 1979	113.14	74.30	112.93	161.01	57.81	95.20	164.77
338	Feb 1979	114.05	74.80	113.75	162.04	58.23	99.50	166.62
339	Mar 1979	114.98	75.32	114.60	163.14	59.21	101.26	162.26
340	Apr 1979	115.82	76.01	115.14	164.14	64.03	105.77	169.77
341	May 1979	116.68	76.83	115.85	165.22	60.49	104.49	166.33
342	June 1979	117.47	77.56	116.62	166.12	57.29	95.08	158.63
343	July 1979	118.29	78.22	117.32	166.52	60.76	97.83	159.43
344	Aug 1979	119.08	78.87	117.95	167.11	60.40	101.30	162.28
345	Sept 1979	119.83	79.50	118.62	167.82	67.04	105.09	167.67
346	Oct 1979	120.59	80.14	119.49	168.59	63.07	104.48	172.01
347	Nov 1979	121.31	80.74	120.12	169.34	74.24	119.14	191.45
348	Dec 1979	122.04	81.35	120.77	170.09	68.90	113.89	186.42

Appendix I5. Simulated concentrations of tetrachloroethylene in finished water at the water treatment plant, Tarawa Terrace, U.S. Marine Corps Base Camp Lejeune, North Carolina.—Continued

[PCE, tetrachloroethylene; µg/L, microgram per liter; $P_{2.5}$, Monte Carlo simulation results for the 2.5 percentile; P_{50}, Monte Carlo simulation results for the 50 percentile; $P_{97.5}$, Monte Carlo simulation results for the 97.5 percentile; WTP, water treatment plant; Jan, January; Feb, February; Mar, March; Apr, April; Aug, August; Sept, September; Oct, October; Dec, December]

Stress period	Month and year	Calibrated PCE concentration, in µg/L[1]	Range of concentrations derived from Monte Carlo simulations[2]					
			Monte Carlo simulation (Scenario 1)[3]			Monte Carlo simulation (Scenario 2)[4]		
			$P_{2.5}$, in µg/L	P_{50}, in µg/L	$P_{97.5}$, in µg/L	$P_{2.5}$, in µg/L	P_{50}, in µg/L	$P_{97.5}$, in µg/L
349	Jan 1980	123.28	82.20	122.09	171.34	61.30	101.54	159.81
350	Feb 1980	122.98	81.93	121.80	171.45	77.70	131.23	206.13
351	Mar 1980	124.03	82.63	122.99	172.63	67.73	114.94	183.21
352	Apr 1980	123.90	82.42	123.27	172.41	86.02	143.61	229.05
353	May 1980	124.69	82.89	123.73	173.81	85.23	138.95	220.28
354	June 1980	125.83	83.92	124.67	175.54	80.14	128.55	203.28
355	July 1980	0.72	0.10	0.43	1.67	0.06	0.32	1.22
356	Aug 1980	0.75	0.11	0.45	1.73	0.07	0.34	1.28
357	Sept 1980	121.36	80.64	120.61	170.25	74.54	128.20	195.86
358	Oct 1980	121.72	80.95	121.00	170.55	82.88	137.09	215.09
359	Nov 1980	122.14	81.32	121.73	171.07	89.83	145.35	231.15
360	Dec 1980	122.95	81.96	122.56	171.97	87.97	143.51	226.80
361	Jan 1981	114.05	76.20	113.83	159.33	81.35	131.65	210.19
362	Feb 1981	114.39	76.42	114.22	159.76	71.73	120.32	185.47
363	Mar 1981	115.60	77.32	115.10	161.62	65.38	104.23	164.75
364	Apr 1981	116.55	78.07	116.07	163.34	61.89	101.55	158.35
365	May 1981	117.30	78.64	116.91	164.52	63.14	99.62	156.29
366	June 1981	118.36	79.53	117.92	165.37	54.95	86.73	140.98
367	July 1981	133.29	89.77	132.96	186.08	58.22	92.47	142.21
368	Aug 1981	134.31	90.57	133.94	187.73	59.68	95.47	151.17
369	Sept 1981	120.72	81.40	120.32	168.91	58.90	98.56	150.82
370	Oct 1981	121.04	81.71	120.86	169.57	61.42	99.80	157.59
371	Nov 1981	121.41	82.04	121.17	170.30	60.76	101.36	158.08
372	Dec 1981	121.81	82.41	121.56	171.08	63.30	102.27	160.36
373	Jan 1982	103.95	70.61	103.86	145.41	55.35	91.05	141.55
374	Feb 1982	105.86	71.96	105.76	147.68	56.60	92.63	140.40
375	Mar 1982	107.52	73.05	107.51	149.67	59.57	93.91	147.10
376	Apr 1982	108.83	74.01	108.79	151.25	58.43	97.00	147.50
377	May 1982	148.50	101.45	147.91	206.23	66.65	107.89	166.05
378	June 1982	110.78	75.70	110.41	153.60	61.01	99.03	151.27
379	July 1982	111.98	76.77	111.69	154.90	62.24	97.91	154.37
380	Aug 1982	113.07	77.74	112.66	156.03	63.70	99.09	152.90
381	Sept 1982	114.04	78.49	113.60	157.00	65.21	100.91	153.98
382	Oct 1982	114.60	79.03	114.14	157.69	67.41	108.99	165.07
383	Nov 1982	113.87	78.41	113.67	157.37	88.82	142.12	223.75
384	Dec 1982	115.16	79.21	114.95	158.89	79.98	128.05	193.75
385	Jan 1983	1.25	0.25	0.75	2.48	0.17	0.61	1.90
386	Feb 1983	1.29	0.27	0.78	2.56	0.18	0.63	1.94
387	Mar 1983	111.76	77.09	112.19	156.29	78.57	123.82	194.41
388	Apr 1983	112.66	77.92	112.99	157.31	74.18	119.77	182.63
389	May 1983	113.97	79.21	114.10	158.82	70.85	117.76	174.86
390	June 1983	106.10	74.18	106.03	147.67	68.30	103.53	162.13
391	July 1983	116.70	81.48	116.62	162.17	66.41	108.10	166.88
392	Aug 1983	117.72	82.09	117.54	163.39	67.97	107.12	161.29
393	Sept 1983	117.83	82.03	117.63	163.40	76.74	120.27	183.16
394	Oct 1983	117.97	82.03	117.88	163.53	84.95	133.04	207.24
395	Nov 1983	118.63	82.60	118.70	164.81	89.04	142.71	224.56
396	Dec 1983	120.78	84.23	120.74	167.35	72.65	113.38	171.38

Appendix I5. Simulated concentrations of tetrachloroethylene in finished water at the water treatment plant, Tarawa Terrace, U.S. Marine Corps Base Camp Lejeune, North Carolina.—Continued

[PCE, tetrachloroethylene; µg/L, microgram per liter; $P_{2.5}$, Monte Carlo simulation results for the 2.5 percentile; P_{50}, Monte Carlo simulation results for the 50 percentile; $P_{97.5}$, Monte Carlo simulation results for the 97.5 percentile; WTP, water treatment plant; Jan, January; Feb, February; Mar, March; Apr, April; Aug, August; Sept, September; Oct, October; Dec, December]

Stress period	Month and year	Calibrated PCE concentration, in µg/L[1]	Range of concentrations derived from Monte Carlo simulations[2]					
			Monte Carlo simulation (Scenario 1)[3]			Monte Carlo simulation (Scenario 2)[4]		
			$P_{2.5}$, in µg/L	P_{50}, in µg/L	$P_{97.5}$, in µg/L	$P_{2.5}$, in µg/L	P_{50}, in µg/L	$P_{97.5}$, in µg/L
397	Jan 1984	132.87	92.63	133.27	185.03	103.04	159.84	247.01
398	Feb 1984	180.39	126.52	180.97	249.43	94.25	150.35	230.69
399	Mar 1984	183.02	128.61	183.55	252.50	99.38	159.70	240.42
400	Apr 1984	151.46	106.37	151.54	208.97	97.90	155.71	236.45
401	May 1984	153.42	107.63	153.20	211.58	92.85	146.63	220.85
402	June 1984	182.13	127.45	181.99	250.57	94.11	152.75	228.36
403	July 1984	156.39	109.41	156.40	214.58	101.95	160.97	234.39
404	Aug 1984	170.47	106.73	158.25	238.65	108.76	168.54	261.54
405	Sept 1984	181.22	113.28	168.51	253.93	117.53	184.30	295.64
406	Oct 1984	173.73	108.42	161.84	245.02	120.12	182.33	281.84
407	Nov 1984	173.77	108.41	161.92	245.70	124.18	187.60	287.36
408	Dec 1984	173.18	107.82	161.69	246.06	127.85	193.50	301.23
409	Jan 1985	176.12	109.98	164.71	251.48	122.98	187.00	293.19
410	Feb 1985	3.64	1.13	2.67	6.57	0.47	1.41	3.74
411	Mar 1985	8.71	3.21	6.58	14.79	8.83	20.01	41.59
412	Apr 1985	8.09	2.99	6.16	13.70	9.00	20.41	42.30
413	May 1985	4.76	1.50	3.46	8.36	0.58	1.68	4.47
414	June 1985	5.14	1.65	3.80	9.21	0.64	1.81	4.78
415	July 1985	5.54	1.80	4.12	10.04	0.69	1.96	5.12
416	Aug 1985	6.01	1.98	4.50	10.97	0.76	2.14	5.56
417	Sept 1985	6.50	2.19	4.88	11.89	0.83	2.30	6.03
418	Oct 1985	7.06	2.43	5.33	12.88	0.92	2.53	6.53
419	Nov 1985	7.64	2.68	5.78	13.90	1.02	2.76	7.07
420	Dec 1985	8.27	2.93	6.32	14.99	1.13	3.00	7.59
421	Jan 1986	8.85	3.18	6.82	15.87	1.24	3.22	8.14
422	Feb 1986	9.42	3.45	7.30	16.67	1.35	3.46	8.69
423	Mar 1986	12.14	4.55	9.43	21.18	1.85	4.67	11.50
424	Apr 1986	10.83	4.09	8.44	18.71	1.64	4.08	9.90
425	May 1986	11.56	4.42	9.06	19.63	1.79	4.41	10.49
426	June 1986	12.28	4.77	9.70	20.59	1.94	4.76	11.08
427	July 1986	13.06	5.14	10.35	21.75	2.11	5.12	11.77
428	Aug 1986	13.84	5.54	11.01	23.04	2.29	5.51	12.50
429	Sept 1986	14.61	5.90	11.70	24.30	2.49	5.89	13.19
430	Oct 1986	15.42	6.28	12.41	25.59	2.71	6.33	13.94
431	Nov 1986	16.21	6.66	13.11	26.70	2.93	6.73	14.77
432	Dec 1986	17.03	7.06	13.77	27.86	3.17	7.20	15.65
433	Jan 1987	17.85	7.47	14.46	29.04	3.41	7.66	16.46
434	Feb 1987	18.49	7.82	15.02	29.91	3.62	8.04	17.16
435	Mar 1987				WTP closed			

[1]Results from Faye (2008) and reported in Maslia et al. (2007, Appendix A2)

[2]$P_{97.5}$ and $P_{2.5}$ represent the upper and lower bound, respectively, of 95 percent of Monte Carlo simulations; for a Gaussian (normal) distribution, the median (P_{50}) should equal the mean value

[3]Scenario 1 Monte Carlo simulation is for pumping uncertainty excluded

[4]Scenario 2 Monte Carlo simulation is for pumping uncertainty included

Appendix I —Reconstructed (Simulated) Mean Monthly Concentrations of Selected Water-Supply Wells, for Tetrachloroethylene (PCE), Trichloroethylene (TCE), *trans*-1,2-Dichloroethylene (1,2-tDCE), Vinyl Chloride (VC), and Benzene, Hadnot Point-Holcomb Boulevard Study Area

Appendix A3. Reconstructed (simulated) mean concentrations in groundwater at selected water-supply wells for tetrachloroethylene (PCE), trichloroethylene (TCE), *trans*-1,2-dichloroethylene (1,2-tDCE), vinyl chloride (VC), and benzene, Hadnot Point–Holcomb Boulevard study area, U.S. Marine Corps Base Camp Lejeune, North Carolina, January 1942–June 2008.

[—, no pumping]

Stress period	Month and year	Concentration, in micrograms per liter											
		[1]PCE	[1]TCE						[2]1,2-tDCE	[2]VC	Benzene		
		HP-651	HP-651	HP-601	HP-602	HP-608	HP-634	HP-660	HP-651	HP-651	[3]HP-602	[3]HP-603	[1]HP-608
1–6	Jan. 1942–June 1942	—	—	—	—	—	—	—	—	—	—	—	—
7–114	July 1942–June 1951	—	—	0	0	0	—	—	—	—	0	0	0
115	July 1951	—	—	0	1	0	—	—	—	—	0	0	0
116	Aug. 1951	—	—	0	2	0	—	—	—	—	0	0	0
117	Sept. 1951	—	—	0	4	0	—	—	—	—	0	0	0
118	Oct. 1951	—	—	0	5	0	—	—	—	—	0	0	0
119	Nov. 1951	—	—	0	9	0	—	—	—	—	0	0	0
120	Dec. 1951	—	—	0	12	0	—	—	—	—	0	0	0
121	Jan. 1952	—	—	0	18	0	—	—	—	—	0	0	0
122	Feb. 1952	—	—	0	23	0	—	—	—	—	0	0	0
123	Mar. 1952	—	—	0	27	0	—	—	—	—	0	0	0
124	Apr. 1952	—	—	0	34	0	—	—	—	—	0	0	0
125	May 1952	—	—	0	42	0	—	—	—	—	0	0	0
126	June 1952	—	—	0	49	0	—	—	—	—	0	0	0
127	July 1952	—	—	0	58	0	—	—	—	—	0	0	0
128	Aug. 1952	—	—	0	71	0	—	—	—	—	0	0	0
129	Sept. 1952	—	—	0	81	0	—	—	—	—	0	0	0
130	Oct. 1952	—	—	0	92	0	—	—	—	—	0	0	0
131	Nov. 1952	—	—	0	106	0	—	—	—	—	0	0	0
132	Dec. 1952	—	—	0	120	0	—	—	—	—	0	0	0
133	Jan. 1953	—	—	0	136	0	—	—	—	—	0	0	0
134	Feb. 1953	—	—	0	148	0	—	—	—	—	0	0	0
135	Mar. 1953	—	—	0	157	0	—	—	—	—	0	0	0
136	Apr. 1953	—	—	0	170	0	—	—	—	—	0	0	0
137	May 1953	—	—	0	181	0	—	—	—	—	0	0	0
138	June 1953	—	—	0	191	0	—	—	—	—	0	0	0
139	July 1953	—	—	0	201	0	—	—	—	—	0	0	0
140	Aug. 1953	—	—	0	218	0	—	—	—	—	0	0	0
141	Sept. 1953	—	—	0	229	0	—	—	—	—	0	0	0
142	Oct. 1953	—	—	0	238	0	—	—	—	—	0	0	0
143	Nov. 1953	—	—	0	252	0	—	—	—	—	0	0	0
144	Dec. 1953	—	—	0	264	0	—	—	—	—	0	0	0
145	Jan. 1954	—	—	0	275	0	—	—	—	—	0	0	0
146	Feb. 1954	—	—	0	283	0	—	—	—	—	0	0	0
147	Mar. 1954	—	—	0	287	0	—	—	—	—	0	0	0
148	Apr. 1954	—	—	0	296	0	—	—	—	—	0	0	0
149	May 1954	—	—	0	303	0	—	—	—	—	0	0	0
150	June 1954	—	—	0	311	0	—	—	—	—	0	0	0

Appendix A3. Reconstructed (simulated) mean concentrations in groundwater at selected water-supply wells for tetrachloroethylene (PCE), trichloroethylene (TCE), *trans*-1,2- dichloroethylene (1,2-tDCE), vinyl chloride (VC), and benzene, Handot Point–Holcomb Boulevard study area, U.S. Marine Corps Base Camp Lejeune, North Carolina, January 1942–June 2008.—Continued

[—, no pumping]

Stress period	Month and year	Concentration, in micrograms per liter											
		[1]PCE	[1]TCE						[2]1,2-tDCE	[2]VC	Benzene		
		HP-651	HP-651	HP-601	HP-602	HP-608	HP-634	HP-660	HP-651	HP-651	[3]HP-602	[3]HP-603	[1]HP-608
151	July 1954	—	—	0	320	0	—	—	—	—	0	0	0
152	Aug. 1954	—	—	0	334	0	—	—	—	—	0	0	0
153	Sept. 1954	—	—	0	346	—	—	—	—	—	0	0	—
154	Oct. 1954	—	—	0	356	—	—	—	—	—	0	0	—
155	Nov. 1954	—	—	0	375	—	—	—	—	—	0	0	—
156	Dec. 1954	—	—	0	388	—	—	—	—	—	0	0	—
157	Jan. 1955	—	—	0	403	—	—	—	—	—	0	0	—
158	Feb. 1955	—	—	0	413	—	—	—	—	—	0	—	—
159	Mar. 1955	—	—	0	419	—	—	—	—	—	0	—	—
160	Apr. 1955	—	—	0	433	—	—	—	—	—	0	—	—
161	May 1955	—	—	0	443	—	—	—	—	—	1	—	—
162	June 1955	—	—	0	453	—	—	—	—	—	1	—	—
163	July 1955	—	—	0	464	0	—	—	—	—	1	0	0
164	Aug. 1955	—	—	0	484	0	—	—	—	—	1	0	0
165	Sept. 1955	—	—	0	514	0	—	—	—	—	1	0	0
166	Oct. 1955	—	—	0	524	0	—	—	—	—	1	0	0
167	Nov. 1955	—	—	0	532	1	—	—	—	—	1	0	0
168	Dec. 1955	—	—	0	537	1	—	—	—	—	1	0	0
169	Jan. 1956	—	—	0	543	1	—	—	—	—	1	0	0
170	Feb. 1956	—	—	0	547	1	—	—	—	—	1	0	0
171	Mar. 1956	—	—	1	547	1	—	—	—	—	1	0	0
172	Apr. 1956	—	—	1	548	1	—	—	—	—	1	0	0
173	May 1956	—	—	1	552	1	—	—	—	—	1	0	0
174	June 1956	—	—	1	554	1	—	—	—	—	1	0	0
175	July 1956	—	—	1	557	2	—	—	—	—	2	—	0
176	Aug. 1956	—	—	1	565	2	—	—	—	—	2	—	0
177	Sept. 1956	—	—	1	571	2	—	—	—	—	2	—	1
178	Oct. 1956	—	—	1	576	2	—	—	—	—	2	—	1
179	Nov. 1956	—	—	1	584	2	—	—	—	—	2	—	1
180	Dec. 1956	—	—	1	588	3	—	—	—	—	2	—	1
181	Jan. 1957	—	—	1	596	3	—	—	—	—	2	—	1
182	Feb. 1957	—	—	1	598	3	—	—	—	—	2	—	1
183	Mar. 1957	—	—	1	598	4	—	—	—	—	2	—	1
184	Apr. 1957	—	—	1	602	4	—	—	—	—	3	—	1
185	May 1957	—	—	1	605	4	—	—	—	—	3	0	1
186	June 1957	—	—	1	608	5	—	—	—	—	3	0	1
187	July 1957	—	—	1	609	5	—	—	—	—	3	0	1
188	Aug. 1957	—	—	2	613	5	—	—	—	—	3	0	1
189	Sept. 1957	—	—	2	619	6	—	—	—	—	3	0	1
190	Oct. 1957	—	—	2	619	6	—	—	—	—	3	0	1
191	Nov. 1957	—	—	2	627	7	—	—	—	—	4	0	1
192	Dec. 1957	—	—	2	631	7	—	—	—	—	4	0	1

Appendix A3. Reconstructed (simulated) mean concentrations in groundwater at selected water-supply wells for tetrachloroethylene (PCE), trichloroethylene (TCE), *trans*-1,2- dichloroethylene (1,2-tDCE), vinyl chloride (VC), and benzene, Handot Point–Holcomb Boulevard study area, U.S. Marine Corps Base Camp Lejeune, North Carolina, January 1942–June 2008.—Continued

[—, no pumping]

Stress period	Month and year	Concentration, in micrograms per liter											
		[1]PCE	[1]TCE						[2]1,2-tDCE	[2]VC	Benzene		
		HP-651	HP-651	HP-601	HP-602	HP-608	HP-634	HP-660	HP-651	HP-651	[3]HP-602	[3]HP-603	[1]HP-608
193	Jan. 1958	—	—	2	637	7	—	—	—	—	4	0	1
194	Feb. 1958	—	—	2	639	8	—	—	—	—	4	0	1
195	Mar. 1958	—	—	2	638	8	—	—	—	—	4	0	2
196	Apr. 1958	—	—	2	640	9	—	—	—	—	5	0	2
197	May 1958	—	—	2	642	10	—	—	—	—	5	0	2
198	June 1958	—	—	2	643	10	—	—	—	—	5	0	2
199	July 1958	—	—	3	644	11	—	—	—	—	5	0	2
200	Aug. 1958	—	—	3	646	11	—	—	—	—	5	0	2
201	Sept. 1958	—	—	3	650	12	—	—	—	—	6	0	2
202	Oct. 1958	—	—	3	651	13	—	—	—	—	6	0	2
203	Nov. 1958	—	—	3	656	14	—	—	—	—	6	0	2
204	Dec. 1958	—	—	3	657	14	—	—	—	—	6	0	2
205	Jan. 1959	—	—	3	658	15	—	—	—	—	7	0	2
206	Feb. 1959	—	—	3	658	15	—	—	—	—	7	0	2
207	Mar. 1959	—	—	3	655	16	—	—	—	—	7	0	2
208	Apr. 1959	—	—	3	654	17	—	—	—	—	7	0	2
209	May 1959	—	—	4	653	18	—	—	—	—	8	0	2
210	June 1959	—	—	4	650	18	—	—	—	—	8	0	2
211	July 1959	—	—	4	649	19	—	—	—	—	8	0	2
212	Aug. 1959	—	—	4	650	20	—	—	—	—	8	0	2
213	Sept. 1959	—	—	4	651	21	—	—	—	—	9	0	2
214	Oct. 1959	—	—	4	648	22	—	—	—	—	9	0	2
215	Nov. 1959	—	—	4	652	23	—	—	—	—	9	0	2
216	Dec. 1959	—	—	4	652	24	—	—	—	—	10	0	2
217	Jan. 1960	—	—	4	654	25	0	—	—	—	10	0	3
218	Feb. 1960	—	—	4	652	26	0	—	—	—	10	0	3
219	Mar. 1960	—	—	5	647	27	0	—	—	—	10	0	3
220	Apr. 1960	—	—	5	645	27	0	—	—	—	11	0	3
221	May 1960	—	—	5	643	28	1	—	—	—	11	0	3
222	June 1960	—	—	5	639	29	2	—	—	—	11	0	3
223	July 1960	—	—	5	640	30	3	—	—	—	11	0	3
224	Aug. 1960	—	—	5	638	31	6	—	—	—	12	0	3
225	Sept. 1960	—	—	5	637	32	9	—	—	—	12	0	3
226	Oct. 1960	—	—	5	632	33	14	—	—	—	12	0	3
227	Nov. 1960	—	—	5	632	33	19	—	—	—	13	0	3
228	Dec. 1960	—	—	5	630	34	25	—	—	—	13	0	3

Appendix A3. Reconstructed (simulated) mean concentrations in groundwater at selected water-supply wells for tetrachloroethylene (PCE), trichloroethylene (TCE), *trans*-1,2- dichloroethylene (1,2-tDCE), vinyl chloride (VC), and benzene, Handot Point–Holcomb Boulevard study area, U.S. Marine Corps Base Camp Lejeune, North Carolina, January 1942–June 2008.—Continued

[—, no pumping]

Stress period	Month and year	Concentration, in micrograms per liter											
		[1]PCE	[1]TCE						[2]1,2-tDCE	[2]VC	Benzene		
		HP-651	HP-651	HP-601	HP-602	HP-608	HP-634	HP-660	HP-651	HP-651	[3]HP-602	[3]HP-603	[1]HP-608
229	Jan. 1961	—	—	5	629	34	32	—	—	—	14	0	3
230	Feb. 1961	—	—	5	626	35	41	—	—	—	14	0	3
231	Mar. 1961	—	—	5	621	35	51	—	—	—	14	0	3
232	Apr. 1961	—	—	5	621	36	63	—	—	—	15	0	3
233	May 1961	—	—	6	621	37	74	—	—	—	15	0	3
234	June 1961	—	—	6	622	38	88	—	—	—	15	0	3
235	July 1961	—	—	6	620	39	102	—	—	—	16	0	3
236	Aug. 1961	—	—	6	620	40	120	—	—	—	16	0	3
237	Sept. 1961	—	—	6	620	40	133	—	—	—	16	0	3
238	Oct. 1961	—	—	6	615	41	149	—	—	—	17	0	3
239	Nov. 1961	—	—	6	614	41	161	—	—	—	17	0	3
240	Dec. 1961	—	—	6	610	41	175	—	—	—	17	0	3
241	Jan. 1962	—	—	6	607	41	188	—	—	—	18	0	3
242	Feb. 1962	—	—	6	602	41	209	—	—	—	18	0	3
243	Mar. 1962	—	—	6	594	41	226	—	—	—	18	0	3
244	Apr. 1962	—	—	6	590	41	245	—	—	—	19	0	3
245	May 1962	—	—	6	588	41	258	—	—	—	19	0	3
246	June 1962	—	—	6	587	42	279	—	—	—	19	0	4
247	July 1962	—	—	7	585	43	300	—	—	—	20	0	4
248	Aug. 1962	—	—	7	584	44	325	—	—	—	20	0	4
249	Sept. 1962	—	—	7	583	45	339	—	—	—	20	0	4
250	Oct. 1962	—	—	7	577	45	357	—	—	—	21	0	4
251	Nov. 1962	—	—	7	574	45	370	—	—	—	21	0	4
252	Dec. 1962	—	—	7	571	45	382	—	—	—	22	0	4
253	Jan. 1963	—	—	7	569	45	395	—	—	—	22	0	4
254	Feb. 1963	—	—	7	566	45	412	—	—	—	22	0	4
255	Mar. 1963	—	—	7	559	45	424	—	—	—	22	0	4
256	Apr. 1963	—	—	7	553	45	438	—	—	—	23	0	4
257	May 1963	—	—	7	550	45	448	—	—	—	23	0	4
258	June 1963	—	—	7	545	45	457	—	—	—	24	0	4
259	July 1963	—	—	7	540	45	466	—	—	—	24	0	4
260	Aug. 1963	—	—	8	538	45	483	—	—	—	25	0	4
261	Sept. 1963	—	—	8	536	45	492	—	—	—	25	0	4
262	Oct. 1963	—	—	8	532	45	504	—	—	—	25	0	4
263	Nov. 1963	—	—	8	531	45	511	—	—	—	26	0	4
264	Dec. 1963	—	—	8	529	45	517	—	—	—	26	0	4

Appendix A3. Reconstructed (simulated) mean concentrations in groundwater at selected water-supply wells for tetrachloroethylene (PCE), trichloroethylene (TCE), *trans*-1,2- dichloroethylene (1,2-tDCE), vinyl chloride (VC), and benzene, Handot Point–Holcomb Boulevard study area, U.S. Marine Corps Base Camp Lejeune, North Carolina, January 1942–June 2008.—Continued

[—, no pumping]

Stress period	Month and year	Concentration, in micrograms per liter											
		[1]PCE	[1]TCE						[2]1,2-tDCE	[2]VC	Benzene		
		HP-651	HP-651	HP-601	HP-602	HP-608	HP-634	HP-660	HP-651	HP-651	[3]HP-602	[3]HP-603	[1]HP-608
265	Jan. 1964	—	—	8	529	45	524	—	—	—	27	0	4
266	Feb. 1964	—	—	8	527	45	534	—	—	—	27	0	4
267	Mar. 1964	—	—	8	522	45	539	—	—	—	27	0	4
268	Apr. 1964	—	—	8	518	45	547	—	—	—	28	0	4
269	May 1964	—	—	8	516	45	552	—	—	—	28	0	4
270	June 1964	—	—	8	512	45	556	—	—	—	28	0	4
271	July 1964	—	—	8	510	46	563	—	—	—	29	0	4
272	Aug. 1964	—	—	8	508	46	573	—	—	—	29	0	4
273	Sept. 1964	—	—	8	507	46	580	—	—	—	30	0	5
274	Oct. 1964	—	—	8	505	47	589	—	—	—	30	0	5
275	Nov. 1964	—	—	9	503	47	589	—	—	—	31	0	5
276	Dec. 1964	—	—	9	501	46	591	—	—	—	31	0	5
277	Jan. 1965	—	—	9	499	46	588	—	—	—	31	0	5
278	Feb. 1965	—	—	9	497	46	592	—	—	—	32	0	5
279	Mar. 1965	—	—	9	492	46	594	—	—	—	32	0	5
280	Apr. 1965	—	—	9	487	45	595	—	—	—	32	0	5
281	May 1965	—	—	9	484	45	594	—	—	—	33	0	5
282	June 1965	—	—	9	483	46	597	—	—	—	33	0	5
283	July 1965	—	—	9	481	46	600	—	—	—	33	0	5
284	Aug. 1965	—	—	9	478	46	604	—	—	—	34	0	5
285	Sept. 1965	—	—	9	475	46	601	—	—	—	34	1	5
286	Oct. 1965	—	—	9	470	45	600	—	—	—	35	1	5
287	Nov. 1965	—	—	9	468	45	594	—	—	—	35	1	5
288	Dec. 1965	—	—	9	465	44	588	—	—	—	36	1	5
289	Jan. 1966	—	—	9	464	43	586	—	—	—	36	1	5
290	Feb. 1966	—	—	9	462	43	589	—	—	—	36	1	5
291	Mar. 1966	—	—	9	458	43	590	—	—	—	36	2	5
292	Apr. 1966	—	—	9	455	42	591	—	—	—	37	2	5
293	May 1966	—	—	9	454	43	591	—	—	—	37	2	5
294	June 1966	—	—	9	452	42	593	—	—	—	38	2	5
295	July 1966	—	—	9	452	43	598	—	—	—	38	3	5
296	Aug. 1966	—	—	9	453	43	610	—	—	—	39	3	5
297	Sept. 1966	—	—	10	454	44	613	—	—	—	39	3	5
298	Oct. 1966	—	—	10	450	44	615	—	—	—	39	4	5
299	Nov. 1966	—	—	10	450	43	612	—	—	—	40	4	5
300	Dec. 1966	—	—	10	451	43	613	—	—	—	41	4	5

Appendix A3. Reconstructed (simulated) mean concentrations in groundwater at selected water-supply wells for tetrachloroethylene (PCE), trichloroethylene (TCE), *trans*-1,2- dichloroethylene (1,2-tDCE), vinyl chloride (VC), and benzene, Handot Point–Holcomb Boulevard study area, U.S. Marine Corps Base Camp Lejeune, North Carolina, January 1942–June 2008.—Continued

[—, no pumping]

Stress period	Month and year	Concentration, in micrograms per liter											
		[1]PCE	[1]TCE						[2]1,2-tDCE	[2]VC	Benzene		
		HP-651	HP-651	HP-601	HP-602	HP-608	HP-634	HP-660	HP-651	HP-651	[3]HP-602	[3]HP-603	[1]HP-608
301	Jan. 1967	—	—	10	452	43	613	—	—	—	42	4	5
302	Feb. 1967	—	—	10	453	43	619	—	—	—	42	4	5
303	Mar. 1967	—	—	10	449	43	619	—	—	—	42	4	5
304	Apr. 1967	—	—	10	449	42	623	—	—	—	43	5	5
305	May 1967	—	—	10	448	42	622	—	—	—	43	5	5
306	June 1967	—	—	10	447	42	623	—	—	—	43	5	5
307	July 1967	—	—	10	448	43	630	—	—	—	44	5	5
308	Aug. 1967	—	—	11	452	43	642	—	—	—	45	5	5
309	Sept. 1967	—	—	11	454	43	646	—	—	—	45	5	6
310	Oct. 1967	—	—	11	453	43	651	—	—	—	46	5	6
311	Nov. 1967	—	—	11	457	44	652	—	—	—	47	6	6
312	Dec. 1967	—	—	11	461	44	657	—	—	—	47	6	6
313	Jan. 1968	—	—	11	463	44	656	—	—	—	48	6	6
314	Feb. 1968	—	—	11	463	44	657	—	—	—	48	6	6
315	Mar. 1968	—	—	11	459	44	654	—	—	—	48	6	6
316	Apr. 1968	—	—	11	459	44	654	—	—	—	49	6	6
317	May 1968	—	—	11	458	44	648	—	—	—	49	6	6
318	June 1968	—	—	11	456	44	646	—	—	—	49	7	6
319	July 1968	—	—	11	457	44	649	—	—	—	50	7	6
320	Aug. 1968	—	—	11	459	44	655	—	—	—	51	7	6
321	Sept. 1968	—	—	11	460	45	655	—	—	—	51	7	6
322	Oct. 1968	—	—	11	460	45	659	—	—	—	51	7	6
323	Nov. 1968	—	—	12	465	45	658	—	—	—	52	8	6
324	Dec. 1968	—	—	12	467	45	658	—	—	—	53	8	6
325	Jan. 1969	—	—	12	469	45	653	—	—	—	53	8	6
326	Feb. 1969	—	—	12	469	45	654	—	—	—	53	8	6
327	Mar. 1969	—	—	12	466	45	651	—	—	—	53	8	6
328	Apr. 1969	—	—	12	466	46	652	—	—	—	54	8	6
329	May 1969	—	—	12	466	46	647	—	—	—	55	9	6
330	June 1969	—	—	12	466	46	648	—	—	—	55	8	6
331	July 1969	—	—	12	467	47	647	—	—	—	56	8	6
332	Aug. 1969	—	—	12	467	47	636	—	—	—	56	10	6
333	Sept. 1969	—	—	12	466	48	609	—	—	—	56	11	6
334	Oct. 1969	—	—	12	459	48	582	—	—	—	55	12	6
335	Nov. 1969	—	—	12	452	48	581	—	—	—	57	13	6
336	Dec. 1969	—	—	12	452	48	576	—	—	—	58	14	6

Appendix A3. Reconstructed (simulated) mean concentrations in groundwater at selected water-supply wells for tetrachloroethylene (PCE), trichloroethylene (TCE), *trans*-1,2- dichloroethylene (1,2-tDCE), vinyl chloride (VC), and benzene, Hadnot Point–Holcomb Boulevard study area, U.S. Marine Corps Base Camp Lejeune, North Carolina, January 1942–June 2008.—Continued

[—, no pumping]

Stress period	Month and year	Concentration, in micrograms per liter											
		[1]PCE	[1]TCE						[2]1,2-tDCE	[2]VC	Benzene		
		HP-651	HP-651	HP-601	HP-602	HP-608	HP-634	HP-660	HP-651	HP-651	[3]HP-602	[3]HP-603	[1]HP-608
337	Jan. 1970	—	—	12	453	48	566	—	—	—	59	15	6
338	Feb. 1970	—	—	12	454	48	563	—	—	—	59	16	6
339	Mar. 1970	—	—	12	452	48	556	—	—	—	59	17	6
340	Apr. 1970	—	—	12	451	47	550	—	—	—	60	18	6
341	May 1970	—	—	12	452	47	540	—	—	—	61	18	6
342	June 1970	—	—	11	451	47	533	—	—	—	61	19	6
343	July 1970	—	—	11	453	47	529	—	—	—	62	20	6
344	Aug. 1970	—	—	12	457	48	529	—	—	—	63	20	6
345	Sept. 1970	—	—	11	459	49	524	—	—	—	64	21	6
346	Oct. 1970	—	—	11	459	48	519	—	—	—	64	22	6
347	Nov. 1970	—	—	11	461	48	509	—	—	—	65	23	6
348	Dec. 1970	—	—	11	463	48	502	—	—	—	66	24	6
349	Jan. 1971	—	—	11	466	48	493	—	—	—	67	25	6
350	Feb. 1971	—	—	11	468	48	490	—	—	—	67	26	6
351	Mar. 1971	—	—	11	467	48	485	—	—	—	67	26	6
352	Apr. 1971	—	—	11	466	48	481	—	—	—	68	27	6
353	May 1971	—	—	11	468	48	474	—	—	—	69	28	6
354	June 1971	—	—	11	470	48	470	—	—	—	70	29	6
355	July 1971	—	—	11	472	48	468	—	—	—	70	29	7
356	Aug. 1971	—	—	11	474	49	468	—	—	—	71	30	7
357	Sept. 1971	—	—	11	477	49	464	—	—	—	72	31	7
358	Oct. 1971	—	—	11	482	50	466	—	—	—	73	31	7
359	Nov. 1971	—	—	11	484	50	461	—	—	—	74	32	7
360	Dec. 1971	—	—	11	488	50	454	—	—	—	75	33	7
361	Jan. 1972	—	—	11	491	50	447	—	—	—	76	34	7
362	Feb. 1972	—	—	11	493	50	446	—	—	—	76	35	7
363	Mar. 1972	—	—	11	492	50	441	—	—	—	77	36	7
364	Apr. 1972	—	—	11	489	50	437	—	—	—	78	37	7
365	May 1972	—	—	10	490	50	430	—	—	—	79	38	7
366	June 1972	—	—	10	490	50	426	—	—	—	79	38	7
367	July 1972	0	1	10	490	50	422	—	69	8	80	39	7
368	Aug. 1972	0	9	10	490	50	420	—	634	16	81	40	7
369	Sept. 1972	0	27	10	490	50	415	—	1102	25	82	41	7
370	Oct. 1972	0	31	10	487	50	410	—	1491	33	82	42	7
371	Nov. 1972	1	94	10	487	50	404	—	1815	41	83	42	7
372	Dec. 1972	2	215	10	487	50	398	—	2083	49	84	43	7

Appendix A3. Reconstructed (simulated) mean concentrations in groundwater at selected water-supply wells for tetrachloroethylene (PCE), trichloroethylene (TCE), *trans*-1,2- dichloroethylene (1,2-tDCE), vinyl chloride (VC), and benzene, Handot Point–Holcomb Boulevard study area, U.S. Marine Corps Base Camp Lejeune, North Carolina, January 1942–June 2008.—Continued

[—, no pumping]

Stress period	Month and year	Concentration, in micrograms per liter											
		[1]PCE	[1]TCE						[2]1,2-tDCE	[2]VC	Benzene		
		HP-651	HP-651	HP-601	HP-602	HP-608	HP-634	HP-660	HP-651	HP-651	[3]HP-602	[3]HP-603	[1]HP-608
373	Jan. 1973	2	283	10	487	50	392	—	2,306	57	85	44	7
374	Feb. 1973	3	391	10	486	49	389	—	2,492	64	85	45	7
375	Mar. 1973	5	538	9	483	49	383	—	2,646	72	85	46	7
376	Apr. 1973	6	636	9	479	49	381	—	2,773	80	87	46	7
377	May 1973	8	771	9	477	49	374	—	2,880	87	87	48	7
378	June 1973	10	954	9	477	49	372	—	2,968	95	88	48	7
379	July 1973	13	1,187	9	474	49	367	—	3,041	102	88	49	7
380	Aug. 1973	18	1,530	9	472	49	366	—	3,102	110	89	50	8
381	Sept. 1973	22	1,761	9	471	49	362	—	3,152	117	90	51	8
382	Oct. 1973	22	1,738	9	467	48	358	—	3,194	124	91	52	8
383	Nov. 1973	31	2,209	9	465	47	348	—	3,229	131	92	52	7
384	Dec. 1973	39	2,637	9	465	47	344	—	3,258	139	92	52	8
385	Jan. 1974	43	2,776	8	465	47	339	—	3,282	146	93	52	8
386	Feb. 1974	48	2,998	8	463	46	337	—	3,302	152	93	53	8
387	Mar. 1974	54	3,234	8	461	46	332	—	3,318	159	93	53	8
388	Apr. 1974	57	3,344	8	456	46	330	—	3,332	166	95	54	8
389	May 1974	62	3,501	8	457	46	326	—	3,344	173	95	53	8
390	June 1974	68	3,711	8	455	47	324	—	3,353	179	96	54	8
391	July 1974	75	3,947	8	453	47	321	—	3,361	186	97	55	8
392	Aug. 1974	84	4,255	8	453	47	322	—	3,368	192	98	55	8
393	Sept. 1974	91	4,406	8	452	47	318	—	3,373	199	98	55	8
394	Oct. 1974	90	4,256	8	449	47	315	—	3,377	205	99	57	8
395	Nov. 1974	103	4,749	8	446	46	308	—	3,381	211	100	57	8
396	Dec. 1974	114	5,039	8	444	46	304	—	3,384	217	101	58	8
397	Jan. 1975	119	5,061	8	444	46	300	—	3,387	223	102	58	8
398	Feb. 1975	126	5,205	7	443	45	298	—	3,389	229	102	59	8
399	Mar. 1975	133	5,338	7	438	45	293	—	3,391	235	102	60	8
400	Apr. 1975	136	5,372	7	434	45	292	—	3,392	241	103	60	8
402	May 1975	141	5,425	7	433	45	288	—	3,394	247	104	60	8
402	June 1975	147	5,550	7	431	45	286	—	3,395	253	104	61	8
403	July 1975	154	5,677	7	431	45	285	—	3,395	258	105	60	9
404	Aug. 1975	163	5,840	7	429	45	285	—	3,396	264	106	61	9
405	Sept. 1975	168	5,899	7	432	46	285	—	3,397	270	107	60	9
406	Oct. 1975	165	5,647	7	430	46	283	—	3,397	275	108	62	9
407	Nov. 1975	178	6,061	7	428	46	278	—	3,398	280	109	62	9
408	Dec. 1975	188	6,208	7	427	46	274	—	3,398	286	110	63	9

Appendix A3. Reconstructed (simulated) mean concentrations in groundwater at selected water-supply wells for tetrachloroethylene (PCE), trichloroethylene (TCE), *trans*-1,2- dichloroethylene (1,2-tDCE), vinyl chloride (VC), and benzene, Handot Point–Holcomb Boulevard study area, U.S. Marine Corps Base Camp Lejeune, North Carolina, January 1942–June 2008.—Continued

[—, no pumping]

Stress period	Month and year	Concentration, in micrograms per liter											
		[1]PCE	[1]TCE						[2]1,2-tDCE	[2]VC	Benzene		
		HP-651	HP-651	HP-601	HP-602	HP-608	HP-634	HP-660	HP-651	HP-651	[3]HP-602	[3]HP-603	[1]HP-608
409	Jan. 1976	193	6,211	7	425	45	271	—	3,398	291	111	64	9
410	Feb. 1976	199	6,297	7	423	44	269	—	3,398	296	111	65	9
411	Mar. 1976	206	6,390	7	418	44	267	—	3,399	301	111	66	9
412	Apr. 1976	209	6,374	7	415	43	265	—	3,399	306	113	67	9
413	May 1976	213	6,411	6	415	43	263	—	3,399	311	113	67	9
414	June 1976	220	6,490	6	416	43	263	—	3,399	316	113	67	9
415	July 1976	226	6,574	6	415	43	263	—	3,399	321	114	67	9
416	Aug. 1976	234	6,700	6	417	43	265	—	3,399	326	116	68	9
417	Sept. 1976	239	6,724	6	419	44	265	—	3,399	331	117	68	9
418	Oct. 1976	234	6,484	6	418	44	266	—	3,399	335	117	69	9
419	Nov. 1976	247	6,792	6	419	44	263	—	3,400	340	119	70	9
420	Dec. 1976	256	6,915	6	421	43	262	—	3,400	345	120	70	9
421	Jan. 1977	258	6,860	6	422	43	259	—	3,400	349	121	71	9
422	Feb. 1977	262	6,906	6	420	43	260	—	3,400	354	121	72	9
423	Mar. 1977	267	6,933	6	418	43	258	—	3,400	358	121	72	9
424	Apr. 1977	267	6,881	6	417	42	258	—	3,399	363	122	73	9
425	May 1977	270	6,885	6	418	42	257	—	3,367	368	123	73	9
426	June 1977	274	6,917	6	417	42	257	—	3,341	372	124	74	9
427	July 1977	278	6,957	6	416	42	256	—	3,320	377	124	74	9
428	Aug. 1977	283	7,032	6	417	42	258	—	3,302	382	126	75	9
429	Sept. 1977	286	7,027	6	418	42	258	—	3,287	386	126	76	9
430	Oct. 1977	279	6,771	6	419	42	260	—	3,274	390	127	76	9
431	Nov. 1977	291	7,042	6	421	42	259	—	3,264	395	129	76	9
432	Dec. 1977	297	7,107	6	423	42	258	—	3,255	399	129	77	9
433	Jan. 1978	297	7,039	6	427	—	259	—	3,248	404	131	78	—
434	Feb. 1978	300	7,055	6	427	—	261	—	3,242	408	131	80	—
435	Mar. 1978	303	7,062	6	425	—	261	—	3,238	412	131	81	—
436	Apr. 1978	302	6,998	6	427	—	264	—	3,233	416	133	81	—
437	May 1978	303	6,982	6	428	—	264	—	3,230	420	134	82	—
438	June 1978	306	6,998	6	427	—	263	—	3,227	424	135	83	—
439	July 1978	310	7,039	6	427	—	264	—	3,225	428	136	84	—
440	Aug. 1978	314	7,095	6	430	—	268	—	3,223	432	137	85	—
441	Sept. 1978	316	7,086	6	431	—	268	—	3,222	436	138	86	—
442	Oct. 1978	308	6,849	6	431	—	270	—	3,220	440	138	87	—
443	Nov. 1978	318	7,072	6	434	—	269	—	3,219	443	140	88	—
444	Dec. 1978	323	7,135	—	438	—	269	—	3,218	447	143	90	—

Appendix A3. Reconstructed (simulated) mean concentrations in groundwater at selected water-supply wells for tetrachloroethylene (PCE), trichloroethylene (TCE), *trans*-1,2- dichloroethylene (1,2-tDCE), vinyl chloride (VC), and benzene, Handot Point–Holcomb Boulevard study area, U.S. Marine Corps Base Camp Lejeune, North Carolina, January 1942–June 2008.—Continued

[—, no pumping]

Stress period	Month and year	Concentration, in micrograms per liter											
		[1]PCE	[1]TCE						[2]1,2-tDCE	[2]VC	Benzene		
		HP-651	HP-651	HP-601	HP-602	HP-608	HP-634	HP-660	HP-651	HP-651	[3]HP-602	[3]HP-603	[1]HP-608
445	Jan. 1979	322	7,062	—	444	—	—	—	3,218	449	145	91	—
446	Feb. 1979	324	7,068	—	448	—	—	—	3,173	451	146	93	—
447	Mar. 1979	325	7,066	—	449	—	—	—	3,118	452	148	95	—
448	Apr. 1979	324	6,995	—	—	—	—	—	3,073	453	—	97	—
449	May 1979	324	6,968	—	—	—	—	—	3,035	454	—	98	—
450	June 1979	324	6,958	—	—	—	—	—	3,004	455	—	99	—
451	July 1979	326	6,969	—	—	—	212	—	2,978	456	—	100	—
452	Aug. 1979	329	7,015	—	—	—	219	—	2,956	457	—	—	—
453	Sept. 1979	330	6,989	—	—	30	224	—	2,938	459	—	100	11
454	Oct. 1979	322	6,756	—	—	29	230	—	2,923	460	—	101	10
455	Nov. 1979	329	6,934	—	357	29	229	—	2,911	461	141	102	10
456	Dec. 1979	332	6,977	—	359	29	230	—	2,901	462	145	102	10
457	Jan. 1980	331	6,915	—	363	29	231	—	2,892	463	148	103	10
458	Feb. 1980	333	6,943	—	365	28	237	—	2,885	464	150	104	10
459	Mar. 1980	335	6,964	—	366	29	243	—	2,898	466	151	104	10
460	Apr. 1980	334	6,912	—	369	28	249	—	2,921	467	154	106	10
461	May 1980	333	6,879	—	374	29	252	—	2,940	469	156	105	10
462	June 1980	334	6,888	—	376	29	255	—	2,956	471	158	106	10
463	July 1980	336	6,911	—	378	29	260	—	2,969	472	160	107	10
464	Aug. 1980	337	6,926	—	379	29	264	—	2,980	474	161	108	10
465	Sept. 1980	337	6,912	—	381	29	266	—	2,989	475	163	108	10
466	Oct. 1980	328	6,652	—	382	29	271	—	2,997	477	165	109	10
467	Nov. 1980	336	6,870	—	384	29	272	—	3,003	478	167	110	10
468	Dec. 1980	340	6,926	—	387	29	274	—	3,008	480	168	110	10
469	Jan. 1981	339	6,882	—	390	29	277	—	3,013	481	170	111	10
470	Feb. 1981	339	6,880	—	391	29	281	—	3,016	483	171	112	10
471	Mar. 1981	340	6,888	—	390	29	284	—	3,019	484	173	113	10
472	Apr. 1981	339	6,844	—	390	28	289	—	3,022	486	174	114	9
473	May 1981	339	6,844	—	393	28	294	—	3,024	487	175	114	9
474	June 1981	340	6,849	—	394	29	298	—	3,025	488	176	114	9
475	July 1981	342	6,879	—	397	29	305	—	3,027	490	178	114	10
476	Aug. 1981	344	6,930	—	403	30	314	—	3,058	495	180	113	10
477	Sept. 1981	345	6,928	—	405	30	318	—	3,206	499	182	115	10
478	Oct. 1981	337	6,730	—	—	30	327	—	3,329	504	—	116	10
479	Nov. 1981	345	6,921	—	393	30	326	—	3,431	508	182	117	10
480	Dec. 1981	348	6,984	—	394	29	327	—	3,516	513	184	117	10

Appendix A3. Reconstructed (simulated) mean concentrations in groundwater at selected water-supply wells for tetrachloroethylene (PCE), trichloroethylene (TCE), *trans*-1,2- dichloroethylene (1,2-tDCE), vinyl chloride (VC), and benzene, Handot Point–Holcomb Boulevard study area, U.S. Marine Corps Base Camp Lejeune, North Carolina, January 1942–June 2008.—Continued

[—, no pumping]

Stress period	Month and year	Concentration, in micrograms per liter											
		[1]PCE	[1]TCE						[2]1,2-tDCE	[2]VC	Benzene		
		HP-651	HP-651	HP-601	HP-602	HP-608	HP-634	HP-660	HP-651	HP-651	[3]HP-602	[3]HP-603	[1]HP-608
481	Jan. 1982	349	6,975	—	400	29	336	—	3,587	517	185	117	10
482	Feb. 1982	350	6,996	—	405	30	346	—	3,646	521	187	118	10
483	Mar. 1982	351	7,008	—	405	30	350	—	3,694	526	189	118	10
484	Apr. 1982	350	6,970	—	406	30	356	—	3,735	530	190	119	10
485	May 1982	350	6,958	—	408	30	358	—	3,769	534	191	120	10
486	June 1982	350	6,964	—	409	30	362	—	3,796	538	193	120	10
487	July 1982	351	6,975	—	410	30	364	—	3,820	542	194	120	10
488	Aug. 1982	353	7,011	—	411	30	370	—	3,839	546	196	121	10
489	Sept. 1982	353	7,017	—	414	30	376	—	3,855	550	197	121	10
490	Oct. 1982	347	6,852	—	415	31	382	—	3,868	555	199	121	10
491	Nov. 1982	352	6,976	—	419	31	384	—	3,877	559	199	121	10
492	Dec. 1982	353	7,012	—	424	31	387	—	3,884	564	201	121	10
493	Jan. 1983	352	6,975	—	427	31	387	—	3,891	568	203	121	10
494	Feb. 1983	352	6,971	—	432	32	391	—	3,896	573	205	120	10
495	Mar. 1983	352	6,972	—	435	33	396	—	3,900	577	208	120	10
496	Apr. 1983	350	6,920	—	434	33	400	—	3,904	581	208	121	10
497	May 1983	350	6,903	—	435	33	399	—	3,907	585	210	121	10
498	June 1983	350	6,923	—	435	33	399	—	3,909	590	212	122	10
499	July 1983	352	6,958	—	434	34	400	—	3,911	594	213	122	10
500	Aug. 1983	353	6,985	—	435	34	402	—	3,913	598	214	123	10
501	Sept. 1983	353	6,976	—	438	34	399	—	3,915	602	215	123	10
502	Oct. 1983	346	6,809	—	441	34	403	—	3,927	606	216	123	10
503	Nov. 1983	352	6,963	—	447	35	—	—	3,945	611	217	123	10
504	Dec. 1983	353	7,004	—	454	35	—	—	3,961	615	219	123	10
505	Jan. 1984	353	6,988	—	464	—	—	—	3,973	620	220	125	—
506	Feb. 1984	353	6,992	—	472	35	370	—	3,984	624	222	124	10
507	Mar. 1984	353	6,998	—	477	35	383	—	3,993	628	226	124	10
508	Apr. 1984	352	6,969	—	481	35	403	—	4,000	632	225	124	10
509	May 1984	352	6,975	—	490	36	420	—	4,006	637	227	124	10
510	June 1984	352	6,975	—	494	37	433	—	4,011	641	230	124	10
511	July 1984	352	6,978	—	496	38	444	1	4,015	645	231	124	10
512	Aug. 1984	352	6,983	—	495	38	456	1	4,019	649	232	124	10
513	Sept. 1984	351	6,966	—	499	40	469	1	4,022	653	233	123	10
514	Oct. 1984	342	6,721	—	495	40	480	1	4,024	656	235	124	10
515	Nov. 1984	348	6,895	—	493	41	478	1	4,027	660	236	123	10
516	Dec. 1984	337	6,583	—	—	—	—	—	4,037	653	—	125	—

Appendix A3. Reconstructed (simulated) mean concentrations in groundwater at selected water-supply wells for tetrachloroethylene (PCE), trichloroethylene (TCE), *trans*-1,2- dichloroethylene (1,2-tDCE), vinyl chloride (VC), and benzene, Handot Point–Holcomb Boulevard study area, U.S. Marine Corps Base Camp Lejeune, North Carolina, January 1942–June 2008.—Continued

[—, no pumping]

Stress period	Month and year	Concentration, in micrograms per liter											
		[1]PCE	[1]TCE						[2]1,2-tDCE	[2]VC	Benzene		
		HP-651	HP-651	HP-601	HP-602	HP-608	HP-634	HP-660	HP-651	HP-651	[3]HP-602	[3]HP-603	[1]HP-608
517	Jan. 1985	343	6,772	—	—	—	—	—	3,400	652	—	128	—
518	Feb. 1985	—	—	—	—	—	—	—	—	—	—	129	—
519	Mar. 1985	—	—	—	—	—	—	—	—	—	—	130	—
520	Apr. 1985	—	—	—	—	—	—	—	—	—	—	131	—
521	May 1985	—	—	—	—	—	—	—	—	—	—	132	—
522	June 1985	—	—	—	—	—	—	—	—	—	—	133	—
523	July 1985	—	—	—	—	—	—	—	—	—	—	133	—
524	Aug. 1985	—	—	—	—	—	—	—	—	—	—	133	—
525	Sept. 1985	—	—	—	—	—	—	—	—	—	—	133	—
526	Oct. 1985	—	—	—	—	—	—	—	—	—	—	133	—
527	Nov. 1985	—	—	—	—	—	—	—	—	—	—	133	—
528	Dec. 1985	—	—	—	—	—	—	—	—	—	—	134	—
529	Jan. 1986	—	—	—	—	—	—	—	—	—	—	135	—
530	Feb. 1986	—	—	—	—	—	—	—	—	—	—	136	—
531	Mar. 1986	—	—	—	—	—	—	—	—	—	—	136	—
532	Apr. 1986	—	—	—	—	—	—	—	—	—	—	137	—
533	May 1986	—	—	—	—	—	—	—	—	—	—	138	—
534	June 1986	—	—	—	—	—	—	—	—	—	—	138	—
535	July 1986	—	—	—	—	—	—	—	—	—	—	137	—
536	Aug. 1986	—	—	—	—	—	—	—	—	—	—	137	—
537	Sept. 1986	—	—	—	—	—	—	—	—	—	—	138	—
538	Oct. 1986	—	—	—	—	—	—	—	—	—	—	139	—
539	Nov. 1986	—	—	—	—	—	—	—	—	—	—	139	—
540	Dec. 1986	—	—	—	—	—	—	—	—	—	—	140	—
541	Jan. 1987	—	—	—	—	—	—	—	—	—	—	139	—
542	Feb. 1987	—	—	—	—	—	—	—	—	—	—	141	—
543	Mar. 1987	—	—	—	—	—	—	—	—	—	—	141	—
544	Apr. 1987	—	—	—	—	—	—	—	—	—	—	142	—
545	May 1987	—	—	—	—	—	—	—	—	—	—	142	—
546	June 1987	—	—	—	—	—	—	—	—	—	—	142	—
547	July 1987	—	—	—	—	—	—	—	—	—	—	142	—
548	Aug. 1987	—	—	—	—	—	—	—	—	—	—	143	—
549	Sept. 1987	—	—	—	—	—	—	—	—	—	—	143	—
550	Oct. 1987	—	—	—	—	—	—	—	—	—	—	145	—
551	Nov. 1987	—	—	—	—	—	—	—	—	—	—	145	—
552	Dec. 1987	—	—	—	—	—	—	—	—	—	—	146	—

Appendix A3. Reconstructed (simulated) mean concentrations in groundwater at selected water-supply wells for tetrachloroethylene (PCE), trichloroethylene (TCE), *trans*-1,2- dichloroethylene (1,2-tDCE), vinyl chloride (VC), and benzene, Handot Point–Holcomb Boulevard study area, U.S. Marine Corps Base Camp Lejeune, North Carolina, January 1942–June 2008.—Continued

[—, no pumping]

Stress period	Month and year	Concentration, in micrograms per liter											
		[1]PCE	[1]TCE						[2]1,2-tDCE	[2]VC	Benzene		
		HP-651	HP-651	HP-601	HP-602	HP-608	HP-634	HP-660	HP-651	HP-651	[3]HP-602	[3]HP-603	[1]HP-608
553	Jan. 1988	—	—	—	—	—	—	—	—	—	—	146	—
554	Feb. 1988	—	—	—	—	—	—	—	—	—	—	147	—
555	Mar. 1988	—	—	—	—	—	—	—	—	—	—	147	—
556	Apr. 1988	—	—	—	—	—	—	—	—	—	—	148	—
557	May 1988	—	—	—	—	—	—	—	—	—	—	148	—
558	June 1988	—	—	—	—	—	—	—	—	—	—	148	—
559	July 1988	—	—	—	—	—	—	—	—	—	—	148	—
560	Aug. 1988	—	—	—	—	—	—	—	—	—	—	148	—
561	Sept. 1988	—	—	—	—	—	—	—	—	—	—	149	—
562	Oct. 1988	—	—	—	—	—	—	—	—	—	—	150	—
563	Nov. 1988	—	—	—	—	—	—	—	—	—	—	150	—
564	Dec. 1988	—	—	—	—	—	—	—	—	—	—	151	—
565	Jan. 1989	—	—	—	—	—	—	—	—	—	—	151	—
566	Feb. 1989	—	—	—	—	—	—	—	—	—	—	151	—
567	Mar. 1989	—	—	—	—	—	—	—	—	—	—	152	—
568	Apr. 1989	—	—	—	—	—	—	—	—	—	—	151	—
569	May 1989	—	—	—	—	—	—	—	—	—	—	152	—
570	June 1989	—	—	—	—	—	—	—	—	—	—	152	—
571	July 1989	—	—	—	—	—	—	—	—	—	—	152	—
572	Aug. 1989	—	—	—	—	—	—	—	—	—	—	151	—
573	Sept. 1989	—	—	—	—	—	—	—	—	—	—	151	—
574	Oct. 1989	—	—	—	—	—	—	—	—	—	—	152	—
575	Nov. 1989	—	—	—	—	—	—	—	—	—	—	153	—
576	Dec. 1989	—	—	—	—	—	—	—	—	—	—	153	—
577	Jan. 1990	—	—	—	—	—	—	—	—	—	—	154	—
578	Feb. 1990	—	—	—	—	—	—	—	—	—	—	155	—
579	Mar. 1990	—	—	—	—	—	—	—	—	—	—	155	—
580	Apr. 1990	—	—	—	—	—	—	—	—	—	—	156	—
581	May 1990	—	—	—	—	—	—	—	—	—	—	156	—
582	June 1990	—	—	—	—	—	—	—	—	—	—	157	—
583	July 1990	—	—	—	—	—	—	—	—	—	—	157	—
584	Aug. 1990	—	—	—	—	—	—	—	—	—	—	157	—
585	Sept. 1990	—	—	—	—	—	—	—	—	—	—	158	—
586	Oct. 1990	—	—	—	—	—	—	—	—	—	—	159	—
587	Nov. 1990	—	—	—	—	—	—	—	—	—	—	159	—
588	Dec. 1990	—	—	—	—	—	—	—	—	—	—	160	—

Appendix A3. Reconstructed (simulated) mean concentrations in groundwater at selected water-supply wells for tetrachloroethylene (PCE), trichloroethylene (TCE), *trans*-1,2- dichloroethylene (1,2-tDCE), vinyl chloride (VC), and benzene, Handot Point–Holcomb Boulevard study area, U.S. Marine Corps Base Camp Lejeune, North Carolina, January 1942–June 2008.—Continued

[—, no pumping]

Stress period	Month and year	Concentration, in micrograms per liter											
		[1] PCE	[1] TCE						[2] 1,2-tDCE	[2] VC	Benzene		
		HP-651	HP-651	HP-601	HP-602	HP-608	HP-634	HP-660	HP-651	HP-651	[3] HP-602	[3] HP-603	[1] HP-608
589	Jan. 1991	—	—	—	—	—	—	—	—	—	—	159	—
590	Feb. 1991	—	—	—	—	—	—	—	—	—	—	160	—
591	Mar. 1991	—	—	—	—	—	—	—	—	—	—	160	—
592	Apr. 1991	—	—	—	—	—	—	—	—	—	—	160	—
593	May 1991	—	—	—	—	—	—	—	—	—	—	161	—
594	June 1991	—	—	—	—	—	—	—	—	—	—	160	—
595	July 1991	—	—	—	—	—	—	—	—	—	—	159	—
596	Aug. 1991	—	—	—	—	—	—	—	—	—	—	160	—
597	Sept. 1991	—	—	—	—	—	—	—	—	—	—	160	—
598	Oct. 1991	—	—	—	—	—	—	—	—	—	—	161	—
599	Nov. 1991	—	—	—	—	—	—	—	—	—	—	162	—
600	Dec. 1991	—	—	—	—	—	—	—	—	—	—	162	—
601	Jan. 1992	—	—	—	—	—	—	—	—	—	—	162	—
602	Feb. 1992	—	—	—	—	—	—	—	—	—	—	164	—
603	Mar. 1992	—	—	—	—	—	—	—	—	—	—	164	—
604	Apr. 1992	—	—	—	—	—	—	—	—	—	—	165	—
605	May 1992	—	—	—	—	—	—	—	—	—	—	164	—
606	June 1992	—	—	—	—	—	—	—	—	—	—	165	—
607	July 1992	—	—	—	—	—	—	—	—	—	—	165	—
608	Aug. 1992	—	—	—	—	—	—	—	—	—	—	164	—
609	Sept. 1992	—	—	—	—	—	—	—	—	—	—	165	—
610	Oct. 1992	—	—	—	—	—	—	—	—	—	—	166	—
611	Nov. 1992	—	—	—	—	—	—	—	—	—	—	166	—
612	Dec. 1992	—	—	—	—	—	—	—	—	—	—	167	—
613	Jan. 1993	—	—	—	—	—	—	—	—	—	—	167	—
614	Feb. 1993	—	—	—	—	—	—	—	—	—	—	168	—
615	Mar. 1993	—	—	—	—	—	—	—	—	—	—	168	—
616	Apr. 1993	—	—	—	—	—	—	—	—	—	—	169	—
617	May 1993	—	—	—	—	—	—	—	—	—	—	169	—
618	June 1993	—	—	—	—	—	—	—	—	—	—	170	—
619	July 1993	—	—	—	—	—	—	—	—	—	—	170	—
620	Aug. 1993	—	—	—	—	—	—	—	—	—	—	171	—
621	Sept. 1993	—	—	—	—	—	—	—	—	—	—	170	—
622	Oct. 1993	—	—	—	—	—	—	—	—	—	—	170	—
623	Nov. 1993	—	—	—	—	—	—	—	—	—	—	171	—
624	Dec. 1993	—	—	—	—	—	—	—	—	—	—	172	—

Appendix A3. Reconstructed (simulated) mean concentrations in groundwater at selected water-supply wells for tetrachloroethylene (PCE), trichloroethylene (TCE), *trans*-1,2- dichloroethylene (1,2-tDCE), vinyl chloride (VC), and benzene, Handot Point–Holcomb Boulevard study area, U.S. Marine Corps Base Camp Lejeune, North Carolina, January 1942–June 2008.—Continued

[—, no pumping]

Stress period	Month and year	Concentration, in micrograms per liter											
		[1]PCE	[1]TCE						[2]1,2-tDCE	[2]VC	Benzene		
		HP-651	HP-651	HP-601	HP-602	HP-608	HP-634	HP-660	HP-651	HP-651	[3]HP-602	[3]HP-603	[1]HP-608
625	Jan. 1994	—	—	—	—	—	—	—	—	—	—	172	—
626	Feb. 1994	—	—	—	—	—	—	—	—	—	—	172	—
627	Mar. 1994	—	—	—	—	—	—	—	—	—	—	172	—
628	Apr. 1994	—	—	—	—	—	—	—	—	—	—	173	—
629	May 1994	—	—	—	—	—	—	—	—	—	—	173	—
630	June 1994	—	—	—	—	—	—	—	—	—	—	174	—
631	July 1994	—	—	—	—	—	—	—	—	—	—	173	—
632	Aug. 1994	—	—	—	—	—	—	—	—	—	—	174	—
633	Sept. 1994	—	—	—	—	—	—	—	—	—	—	174	—
634	Oct. 1994	—	—	—	—	—	—	—	—	—	—	174	—
635	Nov. 1994	—	—	—	—	—	—	—	—	—	—	174	—
636	Dec. 1994	—	—	—	—	—	—	—	—	—	—	174	—
637	Jan. 1995	—	—	—	—	—	—	—	—	—	—	174	—
638	Feb. 1995	—	—	—	—	—	—	—	—	—	—	175	—
639	Mar. 1995	—	—	—	—	—	—	—	—	—	—	175	—
640	Apr. 1995	—	—	—	—	—	—	—	—	—	—	176	—
641	May 1995	—	—	—	—	—	—	—	—	—	—	176	—
642	June 1995	—	—	—	—	—	—	—	—	—	—	175	—
643	July 1995	—	—	—	—	—	—	—	—	—	—	176	—
644	Aug. 1995	—	—	—	—	—	—	—	—	—	—	176	—
645	Sept. 1995	—	—	—	—	—	—	—	—	—	—	177	—
646	Oct. 1995	—	—	—	—	—	—	—	—	—	—	177	—
647	Nov. 1995	—	—	—	—	—	—	—	—	—	—	177	—
648	Dec. 1995	—	—	—	—	—	—	—	—	—	—	178	—
649	Jan. 1996	—	—	—	—	—	—	—	—	—	—	177	—
650	Feb. 1996	—	—	—	—	—	—	—	—	—	—	178	—
651	Mar. 1996	—	—	—	—	—	—	—	—	—	—	178	—
652	Apr. 1996	—	—	—	—	—	—	—	—	—	—	179	—
653	May 1996	—	—	—	—	—	—	—	—	—	—	179	—
654–798	June 1996–June 2008	—	—	—	—	—	—	—	—	—	—	—	—

[1] Results obtained using MT3DMS model (Jones et al. 2013)

[2] Results obtained using linear control model, TechControl (Guan et al. 2013)

[3] Results obtained using LNAPL model, TechFlowMP (Jang et al. 2013)

Appendix J — Hadnot Point Water Treatment Plant Reconstructed (Simulated) Mean Monthly Finished Water Concentrations

Appendix A7. Reconstructed (simulated) monthly mean concentrations in finished water for tetrachloroethylene (PCE), trichloroethylene (TCE), *trans*-1,2-dichloroethylene (1,2-tDCE), and vinyl chloride (VC) at the Hadnot Point water treatment plant, Hadnot Point–Holcomb Boulevard study area, U.S. Marine Corps Base Camp Lejeune, North Carolina, January 1942–June 2008.

[Concentrations in finished water computed using mixing-model approach; —, water treatment plant not operating; *, model simulations not conducted]

Stress period	Month and year	Concentrations in finished water, in micrograms per liter				
		Tetrachloroethylene (PCE)	Trichloroethylene (TCE)	*Trans*-1,2-dichloroethylene (1,2,-tDCE)	Vinyl chloride (VC)	Benzene
1–6	Jan.–June 1942	—	—	—	—	—
7–12	July–Dec. 1942	0	0	*	*	0
13–120	Jan. 1943–Dec. 1951	0	0	0	0	0
121	Jan. 1952	0	1	0	0	0
122	Feb. 1952	0	0	0	0	0
123	Mar. 1952	0	0	0	0	0
124	Apr. 1952	0	1	0	0	0
125	May 1952	0	1	0	0	0
126	June 1952	0	1	0	0	0
127	July 1952	0	1	0	0	0
128	Aug. 1952	0	2	0	0	0
129	Sept. 1952	0	2	0	0	0
130	Oct. 1952	0	2	0	0	0
131	Nov. 1952	0	3	0	0	0
132	Dec. 1952	0	3	0	0	0
133	Jan. 1953	0	4	0	0	0
134	Feb. 1953	0	3	0	0	0
135	Mar. 1953	0	3	0	0	0
136	Apr. 1953	0	5	0	0	0
137	May 1953	0	4	0	0	0
138	June 1953	0	3	0	0	0
139	July 1953	0	4	0	0	0
140	Aug. 1953	0	6	0	0	0
141	Sept. 1953	0	5	0	0	0
142	Oct. 1953	0	4	0	0	0
143	Nov. 1953	0	7	0	0	0
144	Dec. 1953	0	6	0	0	0
145	Jan. 1954	0	6	0	0	0
146	Feb. 1954	0	5	0	0	0
147	Mar. 1954	0	4	0	0	0
148	Apr. 1954	0	7	0	0	0
149	May 1954	0	5	0	0	0
150	June 1954	0	7	0	0	0
151	July 1954	0	7	0	0	0
152	Aug. 1954	0	10	0	0	0
153	Sept. 1954	0	9	0	0	0
154	Oct. 1954	0	8	0	0	0
155	Nov. 1954	0	14	0	0	0
156	Dec. 1954	0	11	0	0	0

Appendix A7. Reconstructed (simulated) monthly mean concentrations in finished water for tetrachloroethylene (PCE), trichloroethylene (TCE), *trans*-1,2-dichloroethylene (1,2-tDCE), and vinyl chloride (VC) at the Hadnot Point water treatment plant, Hadnot Point–Holcomb Boulevard study area, U.S. Marine Corps Base Camp Lejeune, North Carolina, January 1942–June 2008.—Continued

[Concentrations in finished water computed using mixing-model approach; —, water treatment plant not operating; *, model simulations not conducted]

Stress period	Month and year	Concentrations in finished water, in micrograms per liter				
		Tetrachloroethylene (PCE)	Trichloroethylene (TCE)	*Trans*-1,2-dichloroethylene (1,2,-tDCE)	Vinyl chloride (VC)	Benzene
157	Jan. 1955	0	12	0	0	0
158	Feb. 1955	0	9	0	0	0
159	Mar. 1955	0	7	0	0	0
160	Apr. 1955	0	14	0	0	0
161	May 1955	0	11	0	0	0
162	June 1955	0	10	0	0	0
163	July 1955	0	10	0	0	0
164	Aug. 1955	0	14	0	0	0
165	Sept. 1955	0	13	0	0	0
166	Oct. 1955	0	11	0	0	0
167	Nov. 1955	0	19	0	0	0
168	Dec. 1955	0	14	0	0	0
169	Jan. 1956	0	15	0	0	0
170	Feb. 1956	0	11	0	0	0
171	Mar. 1956	0	8	0	0	0
172	Apr. 1956	0	17	0	0	0
173	May 1956	0	13	0	0	0
174	June 1956	0	11	0	0	0
175	July 1956	0	12	0	0	0
176	Aug. 1956	0	16	0	0	0
177	Sept. 1956	0	14	0	0	0
178	Oct. 1956	0	13	0	0	0
179	Nov. 1956	0	21	0	0	0
180	Dec. 1956	0	17	0	0	0
181	Jan. 1957	0	17	0	0	0
182	Feb. 1957	0	12	0	0	0
183	Mar. 1957	0	9	0	0	0
184	Apr. 1957	0	19	0	0	0
185	May 1957	0	14	0	0	0
186	June 1957	0	12	0	0	0
187	July 1957	0	12	0	0	0
188	Aug. 1957	0	16	0	0	0
189	Sept. 1957	0	14	0	0	0
190	Oct. 1957	0	12	0	0	0
191	Nov. 1957	0	20	0	0	0
192	Dec. 1957	0	16	0	0	0

Appendix A7. Reconstructed (simulated) monthly mean concentrations in finished water for tetrachloroethylene (PCE), trichloroethylene (TCE), *trans*-1,2-dichloroethylene (1,2-tDCE), and vinyl chloride (VC) at the Hadnot Point water treatment plant, Hadnot Point–Holcomb Boulevard study area, U.S. Marine Corps Base Camp Lejeune, North Carolina, January 1942–June 2008.—Continued

[Concentrations in finished water computed using mixing-model approach; —, water treatment plant not operating; *, model simulations not conducted]

Stress period	Month and year	Concentrations in finished water, in micrograms per liter				
		Tetrachloroethylene (PCE)	Trichloroethylene (TCE)	*Trans*-1,2-dichloroethylene (1,2,-tDCE)	Vinyl chloride (VC)	Benzene
193	Jan. 1958	0	17	0	0	0
194	Feb. 1958	0	12	0	0	0
195	Mar. 1958	0	9	0	0	0
196	Apr. 1958	0	18	0	0	0
197	May 1958	0	14	0	0	0
198	June 1958	0	12	0	0	0
199	July 1958	0	13	0	0	0
200	Aug. 1958	0	18	0	0	0
201	Sept. 1958	0	15	0	0	0
202	Oct. 1958	0	13	0	0	0
203	Nov. 1958	0	22	0	0	0
204	Dec. 1958	0	17	0	0	0
205	Jan. 1959	0	18	0	0	0
206	Feb. 1959	0	13	0	0	0
207	Mar. 1959	0	9	0	0	0
208	Apr. 1959	0	19	0	0	0
209	May 1959	0	14	0	0	0
210	June 1959	0	13	0	0	0
211	July 1959	0	13	0	0	0
212	Aug. 1959	0	18	0	0	0
213	Sept. 1959	0	15	0	0	0
214	Oct. 1959	0	14	0	0	0
215	Nov. 1959	0	22	0	0	0
216	Dec. 1959	0	17	0	0	0
217	Jan. 1960	0	16	0	0	0
218	Feb. 1960	0	11	0	0	0
219	Mar. 1960	0	9	0	0	0
220	Apr. 1960	0	16	0	0	0
221	May 1960	0	13	0	0	0
222	June 1960	0	12	0	0	0
223	July 1960	0	12	0	0	0
224	Aug. 1960	0	15	0	0	0
225	Sept. 1960	0	14	0	0	0
226	Oct. 1960	0	13	0	0	0
227	Nov. 1960	0	18	0	0	0
228	Dec. 1960	0	14	0	0	0

Appendix A7. Reconstructed (simulated) monthly mean concentrations in finished water for tetrachloroethylene (PCE), trichloroethylene (TCE), *trans*-1,2-dichloroethylene (1,2-tDCE), and vinyl chloride (VC) at the Hadnot Point water treatment plant, Hadnot Point–Holcomb Boulevard study area, U.S. Marine Corps Base Camp Lejeune, North Carolina, January 1942–June 2008.—Continued

[Concentrations in finished water computed using mixing-model approach; —, water treatment plant not operating; *, model simulations not conducted]

Stress period	Month and year	Concentrations in finished water, in micrograms per liter				
		Tetrachloroethylene (PCE)	Trichloroethylene (TCE)	*Trans*-1,2-dichloroethylene (1,2,-tDCE)	Vinyl chloride (VC)	Benzene
229	Jan. 1961	0	16	0	0	0
230	Feb. 1961	0	12	0	0	0
231	Mar. 1961	0	10	0	0	0
232	Apr. 1961	0	18	0	0	0
233	May 1961	0	15	0	0	0
234	June 1961	0	14	0	0	0
235	July 1961	0	14	0	0	0
236	Aug. 1961	0	19	0	0	0
237	Sept. 1961	0	17	0	0	0
238	Oct. 1961	0	17	0	0	0
239	Nov. 1961	0	19	0	0	0
240	Dec. 1961	0	15	0	0	0
241	Jan. 1962	0	16	0	0	0
242	Feb. 1962	0	14	0	0	0
243	Mar. 1962	0	12	0	0	0
244	Apr. 1962	0	19	0	0	0
245	May 1962	0	16	0	0	0
246	June 1962	0	15	0	0	0
247	July 1962	0	16	0	0	0
248	Aug. 1962	0	21	0	0	0
249	Sept. 1962	0	18	0	0	0
250	Oct. 1962	0	19	0	0	0
251	Nov. 1962	0	22	0	0	1
252	Dec. 1962	0	20	0	0	0
253	Jan. 1963	0	20	0	0	0
254	Feb. 1963	0	20	0	0	0
255	Mar. 1963	0	17	0	0	0
256	Apr. 1963	0	24	0	0	1
257	May 1963	0	19	0	0	0
258	June 1963	0	19	0	0	0
259	July 1963	0	19	0	0	0
260	Aug. 1963	0	24	0	0	1
261	Sept. 1963	0	21	0	0	0
262	Oct. 1963	0	22	0	0	0
263	Nov. 1963	0	24	0	0	1
264	Dec. 1963	0	21	0	0	1

Appendix A7. Reconstructed (simulated) monthly mean concentrations in finished water for tetrachloroethylene (PCE), trichloroethylene (TCE), *trans*-1,2-dichloroethylene (1,2-tDCE), and vinyl chloride (VC) at the Hadnot Point water treatment plant, Hadnot Point–Holcomb Boulevard study area, U.S. Marine Corps Base Camp Lejeune, North Carolina, January 1942–June 2008.—Continued

[Concentrations in finished water computed using mixing-model approach; —, water treatment plant not operating; *, model simulations not conducted]

Stress period	Month and year	Concentrations in finished water, in micrograms per liter				
		Tetrachloroethylene (PCE)	Trichloroethylene (TCE)	*Trans*-1,2-dichloroethylene (1,2,-tDCE)	Vinyl chloride (VC)	Benzene
265	Jan. 1964	0	22	0	0	1
266	Feb. 1964	0	21	0	0	0
267	Mar. 1964	0	18	0	0	0
268	Apr. 1964	0	25	0	0	1
269	May 1964	0	21	0	0	1
270	June 1964	0	20	0	0	0
271	July 1964	0	21	0	0	0
272	Aug. 1964	0	25	0	0	1
273	Sept. 1964	0	22	0	0	1
274	Oct. 1964	0	24	0	0	1
275	Nov. 1964	0	25	0	0	1
276	Dec. 1964	0	23	0	0	1
277	Jan. 1965	0	22	0	0	1
278	Feb. 1965	0	23	0	0	1
279	Mar. 1965	0	19	0	0	0
280	Apr. 1965	0	26	0	0	1
281	May 1965	0	21	0	0	1
282	June 1965	0	21	0	0	1
283	July 1965	0	21	0	0	1
284	Aug. 1965	0	25	0	0	1
285	Sept. 1965	0	22	0	0	1
286	Oct. 1965	0	23	0	0	1
287	Nov. 1965	0	23	0	0	1
288	Dec. 1965	0	21	0	0	1
289	Jan. 1966	0	21	0	0	1
290	Feb. 1966	0	22	0	0	1
291	Mar. 1966	0	19	0	0	0
292	Apr. 1966	0	26	0	0	1
293	May 1966	0	21	0	0	1
294	June 1966	0	21	0	0	1
295	July 1966	0	21	0	0	1
296	Aug. 1966	0	26	0	0	1
297	Sept. 1966	0	23	0	0	1
298	Oct. 1966	0	25	0	0	1
299	Nov. 1966	0	26	0	0	1
300	Dec. 1966	0	26	0	0	1

Appendix A7. Reconstructed (simulated) monthly mean concentrations in finished water for tetrachloroethylene (PCE), trichloroethylene (TCE), *trans*-1,2-dichloroethylene (1,2-tDCE), and vinyl chloride (VC) at the Hadnot Point water treatment plant, Hadnot Point–Holcomb Boulevard study area, U.S. Marine Corps Base Camp Lejeune, North Carolina, January 1942–June 2008.—Continued

[Concentrations in finished water computed using mixing-model approach; —, water treatment plant not operating; *, model simulations not conducted]

Stress period	Month and year	Concentrations in finished water, in micrograms per liter				
		Tetrachloroethylene (PCE)	Trichloroethylene (TCE)	*Trans*-1,2-dichloroethylene (1,2,-tDCE)	Vinyl chloride (VC)	Benzene
301	Jan. 1967	0	25	0	0	1
302	Feb. 1967	0	26	0	0	1
303	Mar. 1967	0	23	0	0	1
304	Apr. 1967	0	30	0	0	1
305	May 1967	0	24	0	0	1
306	June 1967	0	24	0	0	1
307	July 1967	0	25	0	0	1
308	Aug. 1967	0	31	0	0	1
309	Sept. 1967	0	26	0	0	1
310	Oct. 1967	0	29	0	0	1
311	Nov. 1967	0	29	0	0	1
312	Dec. 1967	0	28	0	0	1
313	Jan. 1968	0	27	0	0	1
314	Feb. 1968	0	26	0	0	1
315	Mar. 1968	0	23	0	0	1
316	Apr. 1968	0	30	0	0	1
317	May 1968	0	24	0	0	1
318	June 1968	0	24	0	0	1
319	July 1968	0	25	0	0	1
320	Aug. 1968	0	32	0	0	1
321	Sept. 1968	0	28	0	0	1
322	Oct. 1968	0	31	0	0	1
323	Nov. 1968	0	31	0	0	2
324	Dec. 1968	0	29	0	0	1
325	Jan. 1969	0	28	0	0	1
326	Feb. 1969	0	28	0	0	1
327	Mar. 1969	0	23	0	0	1
328	Apr. 1969	0	32	0	0	2
329	May 1969	0	26	0	0	1
330	June 1969	0	26	0	0	1
331	July 1969	0	24	0	0	1
332	Aug. 1969	0	18	0	0	1
333	Sept. 1969	0	8	0	0	1
334	Oct. 1969	0	8	0	0	1
335	Nov. 1969	0	24	0	0	2
336	Dec. 1969	0	24	0	0	2

Appendix A7. Reconstructed (simulated) monthly mean concentrations in finished water for tetrachloroethylene (PCE), trichloroethylene (TCE), *trans*-1,2-dichloroethylene (1,2-tDCE), and vinyl chloride (VC) at the Hadnot Point water treatment plant, Hadnot Point–Holcomb Boulevard study area, U.S. Marine Corps Base Camp Lejeune, North Carolina, January 1942–June 2008.—Continued

[Concentrations in finished water computed using mixing-model approach; —, water treatment plant not operating; *, model simulations not conducted]

Stress period	Month and year	Concentrations in finished water, in micrograms per liter				
		Tetrachloroethylene (PCE)	Trichloroethylene (TCE)	*Trans*-1,2-dichloroethylene (1,2,-tDCE)	Vinyl chloride (VC)	Benzene
337	Jan. 1970	0	23	0	0	2
338	Feb. 1970	0	23	0	0	2
339	Mar. 1970	0	19	0	0	1
340	Apr. 1970	0	26	0	0	2
341	May 1970	0	20	0	0	2
342	June 1970	0	20	0	0	2
343	July 1970	0	20	0	0	2
344	Aug. 1970	0	24	0	0	2
345	Sept. 1970	0	21	0	0	2
346	Oct. 1970	0	23	0	0	2
347	Nov. 1970	0	25	0	0	3
348	Dec. 1970	0	22	0	0	2
349	Jan. 1971	0	22	0	0	2
350	Feb. 1971	0	21	0	0	2
351	Mar. 1971	0	17	0	0	2
352	Apr. 1971	0	24	0	0	3
353	May 1971	0	19	0	0	2
354	June 1971	0	19	0	0	2
355	July 1971	0	19	0	0	2
356	Aug. 1971	0	24	0	0	3
357	Sept. 1971	0	21	0	0	2
358	Oct. 1971	0	22	0	0	2
359	Nov. 1971	0	25	0	0	3
360	Dec. 1971	0	22	0	0	3
361	Jan. 1972	0	22	0	0	3
362	Feb. 1972	0	21	0	0	2
363	Mar. 1972	0	17	0	0	2
364	Apr. 1972	0	24	0	0	3
365	May 1972	0	19	0	0	3
366	June 1972	0	19	0	0	3
367	July 1972	0	16	3	0	2
368	Aug. 1972	0	20	38	1	3
369	Sept. 1972	0	18	50	1	2
370	Oct. 1972	0	18	12	0	3
371	Nov. 1972	0	25	133	3	3
372	Dec. 1972	0	32	146	3	2

Appendix A7. Reconstructed (simulated) monthly mean concentrations in finished water for tetrachloroethylene (PCE), trichloroethylene (TCE), *trans*-1,2-dichloroethylene (1,2-tDCE), and vinyl chloride (VC) at the Hadnot Point water treatment plant, Hadnot Point–Holcomb Boulevard study area, U.S. Marine Corps Base Camp Lejeune, North Carolina, January 1942–June 2008.—Continued

[Concentrations in finished water computed using mixing-model approach; —, water treatment plant not operating; *, model simulations not conducted]

Stress period	Month and year	Concentrations in finished water, in micrograms per liter				
		Tetrachloroethylene (PCE)	Trichloroethylene (TCE)	*Trans*-1,2-dichloroethylene (1,2,-tDCE)	Vinyl chloride (VC)	Benzene
373	Jan. 1973	0	27	74	2	3
374	Feb. 1973	0	34	113	3	2
375	Mar. 1973	0	38	123	3	2
376	Apr. 1973	0	38	80	2	3
377	May 1973	0	43	104	3	3
378	June 1973	0	57	131	4	3
379	July 1973	1	73	149	5	3
380	Aug. 1973	1	109	184	7	3
381	Sept. 1973	1	96	143	5	3
382	Oct. 1973	0	31	26	1	3
383	Nov. 1973	2	187	249	10	3
384	Dec. 1973	3	201	230	10	2
385	Jan. 1974	1	106	106	5	3
386	Feb. 1974	2	152	151	7	2
387	Mar. 1974	3	163	155	7	2
388	Apr. 1974	2	116	97	5	3
389	May 1974	2	142	122	6	2
390	June 1974	3	179	149	8	2
391	July 1974	4	209	166	9	2
392	Aug. 1974	5	274	203	12	3
393	Sept. 1974	4	217	155	9	3
394	Oct. 1974	1	50	28	2	3
395	Nov. 1974	8	399	273	17	3
396	Dec. 1974	8	369	239	15	3
397	Jan. 1975	4	179	109	7	3
398	Feb. 1975	6	252	155	11	3
399	Mar. 1975	6	261	159	11	2
400	Apr. 1975	4	174	99	7	3
401	May 1975	5	211	124	9	3
402	June 1975	7	260	151	11	2
403	July 1975	8	294	168	13	3
404	Aug. 1975	10	368	205	16	3
405	Sept. 1975	8	285	156	12	3
406	Oct. 1975	1	61	28	2	3
407	Nov. 1975	14	503	274	23	3
408	Dec. 1975	13	451	240	20	3

Appendix A7. Reconstructed (simulated) monthly mean concentrations in finished water for tetrachloroethylene (PCE), trichloroethylene (TCE), *trans*-1,2-dichloroethylene (1,2-tDCE), and vinyl chloride (VC) at the Hadnot Point water treatment plant, Hadnot Point–Holcomb Boulevard study area, U.S. Marine Corps Base Camp Lejeune, North Carolina, January 1942–June 2008.—Continued

[Concentrations in finished water computed using mixing-model approach; —, water treatment plant not operating; *, model simulations not conducted]

Stress period	Month and year	Concentrations in finished water, in micrograms per liter				
		Tetrachloroethylene (PCE)	Trichloroethylene (TCE)	*Trans*-1,2-dichloroethylene (1,2,-tDCE)	Vinyl chloride (VC)	Benzene
409	Jan. 1976	7	227	116	10	3
410	Feb. 1976	10	317	164	14	3
411	Mar. 1976	10	323	166	15	2
412	Apr. 1976	6	212	104	9	4
413	May 1976	8	257	130	12	3
414	June 1976	10	314	158	15	3
415	July 1976	12	348	174	16	3
416	Aug. 1976	15	436	214	20	4
417	Sept. 1976	11	336	163	16	3
418	Oct. 1976	2	70	29	3	3
419	Nov. 1976	19	543	264	26	4
420	Dec. 1976	19	520	249	25	3
421	Jan. 1977	9	249	116	12	4
422	Feb. 1977	13	346	164	17	3
423	Mar. 1977	13	342	162	17	2
424	Apr. 1977	8	218	99	11	4
425	May 1977	10	264	123	13	3
426	June 1977	12	320	149	17	3
427	July 1977	14	355	164	19	3
428	Aug. 1977	17	440	199	23	4
429	Sept. 1977	13	338	152	18	4
430	Oct. 1977	2	69	27	3	4
431	Nov. 1977	22	544	245	30	4
432	Dec. 1977	21	513	229	28	4
433	Jan. 1978	10	250	109	14	4
434	Feb. 1978	14	348	154	19	3
435	Mar. 1978	15	352	157	20	3
436	Apr. 1978	9	231	99	13	5
437	May 1978	12	278	123	16	4
438	June 1978	14	333	148	19	3
439	July 1978	17	388	172	23	3
440	Aug. 1978	20	475	209	28	4
441	Sept. 1978	16	364	159	22	4
442	Oct. 1978	3	74	28	4	4
443	Nov. 1978	24	544	240	33	5
444	Dec. 1978	24	546	240	33	4

Appendix A7. Reconstructed (simulated) monthly mean concentrations in finished water for tetrachloroethylene (PCE), trichloroethylene (TCE), *trans*-1,2-dichloroethylene (1,2-tDCE), and vinyl chloride (VC) at the Hadnot Point water treatment plant, Hadnot Point–Holcomb Boulevard study area, U.S. Marine Corps Base Camp Lejeune, North Carolina, January 1942–June 2008.—Continued

[Concentrations in finished water computed using mixing-model approach; —, water treatment plant not operating; *, model simulations not conducted]

Stress period	Month and year	Concentrations in finished water, in micrograms per liter				
		Tetrachloroethylene (PCE)	Trichloroethylene (TCE)	*Trans*-1,2-dichloroethylene (1,2,-tDCE)	Vinyl chloride (VC)	Benzene
445	Jan. 1979	12	268	117	16	6
446	Feb. 1979	17	370	163	23	5
447	Mar. 1979	17	378	165	24	5
448	Apr. 1979	11	230	101	15	4
449	May 1979	13	274	119	18	3
450	June 1979	15	320	138	21	3
451	July 1979	17	361	152	23	3
452	Aug. 1979	22	483	201	31	0
453	Sept. 1979	17	358	148	23	3
454	Oct. 1979	3	71	27	4	4
455	Nov. 1979	23	507	207	33	6
456	Dec. 1979	23	504	205	33	6
457	Jan. 1980	12	264	104	17	7
458	Feb. 1980	17	378	152	24	6
459	Mar. 1980	20	433	175	28	6
460	Apr. 1980	12	273	108	17	8
461	May 1980	15	322	131	21	6
462	June 1980	18	394	163	26	6
463	July 1980	20	415	173	27	6
464	Aug. 1980	23	496	206	33	7
465	Sept. 1980	18	388	162	26	7
466	Oct. 1980	3	88	32	5	8
467	Nov. 1980	25	524	222	35	7
468	Dec. 1980	26	541	229	37	6
469	Jan. 1981	14	295	122	19	8
470	Feb. 1981	18	387	163	26	7
471	Mar. 1981	19	397	169	27	6
472	Apr. 1981	12	266	109	17	9
473	May 1981	15	322	135	22	7
474	June 1981	18	380	161	26	7
475	July 1981	21	436	185	30	6
476	Aug. 1981	30	631	270	44	8
477	Sept. 1981	25	516	231	36	7
478	Oct. 1981	5	115	50	8	5
479	Nov. 1981	36	748	362	54	8
480	Dec. 1981	37	753	370	54	8

Appendix A7. Reconstructed (simulated) monthly mean concentrations in finished water for tetrachloroethylene (PCE), trichloroethylene (TCE), *trans*-1,2-dichloroethylene (1,2-tDCE), and vinyl chloride (VC) at the Hadnot Point water treatment plant, Hadnot Point–Holcomb Boulevard study area, U.S. Marine Corps Base Camp Lejeune, North Carolina, January 1942–June 2008.—Continued

[Concentrations in finished water computed using mixing-model approach; —, water treatment plant not operating; *, model simulations not conducted]

Stress period	Month and year	Concentrations in finished water, in micrograms per liter				
		Tetrachloroethylene (PCE)	Trichloroethylene (TCE)	*Trans*-1,2-dichloroethylene (1,2,-tDCE)	Vinyl chloride (VC)	Benzene
481	Jan. 1982	19	406	199	29	9
482	Feb. 1982	26	529	266	38	7
483	Mar. 1982	27	556	285	41	6
484	Apr. 1982	18	376	189	27	10
485	May 1982	21	438	227	32	8
486	June 1982	25	505	266	38	7
487	July 1982	27	551	293	42	7
488	Aug. 1982	33	670	355	51	9
489	Sept. 1982	29	588	311	44	9
490	Oct. 1982	6	138	64	9	9
491	Nov. 1982	34	706	379	55	10
492	Dec. 1982	35	721	388	56	8
493	Jan. 1983	19	389	206	30	8
494	Feb. 1983	26	526	284	42	7
495	Mar. 1983	29	588	319	47	6
496	Apr. 1983	18	372	196	29	10
497	May 1983	22	449	243	36	8
498	June 1983	27	546	298	45	7
499	July 1983	30	618	337	51	7
500	Aug. 1983	32	659	357	54	9
501	Sept. 1983	26	543	292	45	9
502	Oct. 1983	5	134	61	9	10
503	Nov. 1983	39	783	435	67	10
504	Dec. 1983	34	688	381	59	9
505	Jan. 1984	21	427	233	36	11
506	Feb. 1984	27	560	303	47	8
507	Mar. 1984	28	587	320	50	7
508	Apr. 1984	18	400	206	33	12
509	May 1984	23	491	262	42	10
510	June 1984	22	471	256	41	7
511	July 1984	24	507	278	45	7
512	Aug. 1984	26	539	295	48	8
513	Sept. 1984	21	443	241	39	8
514	Oct. 1984	3	94	40	6	8
515	Nov. 1984	31	639	358	59	8
516	Dec. 1984	2	43	26	4	2

Appendix A7. Reconstructed (simulated) monthly mean concentrations in finished water for tetrachloroethylene (PCE), trichloroethylene (TCE), *trans*-1,2-dichloroethylene (1,2-tDCE), and vinyl chloride (VC) at the Hadnot Point water treatment plant, Hadnot Point–Holcomb Boulevard study area, U.S. Marine Corps Base Camp Lejeune, North Carolina, January 1942–June 2008.—Continued

[Concentrations in finished water computed using mixing-model approach; —, water treatment plant not operating; *, model simulations not conducted]

Stress period	Month and year	Concentrations in finished water, in micrograms per liter				
		Tetrachloroethylene (PCE)	Trichloroethylene (TCE)	*Trans*-1,2-dichloroethylene (1,2,-tDCE)	Vinyl chloride (VC)	Benzene
517	Jan. 1985	16	324	163	31	4
518	Feb. 1985	0	0	0	0	3
519	Mar. 1985	0	0	0	0	3
520	Apr. 1985	0	0	0	0	4
521	May 1985	0	0	0	0	3
522	June 1985	0	0	0	0	3
523	July 1985	0	0	0	0	3
524	Aug. 1985	0	0	0	0	3
525	Sept. 1985	0	0	0	0	3
526	Oct. 1985	0	0	0	0	3
527	Nov. 1985	0	0	0	0	3
528	Dec. 1985	0	0	0	0	3
529	Jan. 1986	0	0	0	0	3
530	Feb. 1986	0	0	0	0	3
531	Mar. 1986	0	0	0	0	3
532	Apr. 1986	0	0	0	0	4
533	May 1986	0	0	0	0	3
534	June 1986	0	0	0	0	3
535	July 1986	0	0	0	0	3
536	Aug. 1986	0	0	0	0	3
537	Sept. 1986	0	0	0	0	3
538	Oct. 1986	0	0	0	0	3
539	Nov. 1986	0	0	0	0	3
540	Dec. 1986	0	0	0	0	3
541	Jan. 1987	0	0	0	0	2
542	Feb. 1987	0	0	0	0	3
543	Mar. 1987	0	0	0	0	2
544	Apr. 1987	0	0	0	0	3
545	May 1987	0	0	0	0	2
546	June 1987	0	0	0	0	2
547	July 1987	0	0	0	0	3
548	Aug. 1987	0	0	0	0	3
549	Sept. 1987	0	0	0	0	3
550	Oct. 1987	0	0	0	0	3
551	Nov. 1987	0	0	0	0	2
552	Dec. 1987	0	0	0	0	2

Appendix A7. Reconstructed (simulated) monthly mean concentrations in finished water for tetrachloroethylene (PCE), trichloroethylene (TCE), *trans*-1,2-dichloroethylene (1,2-tDCE), and vinyl chloride (VC) at the Hadnot Point water treatment plant, Hadnot Point–Holcomb Boulevard study area, U.S. Marine Corps Base Camp Lejeune, North Carolina, January 1942–June 2008.—Continued

[Concentrations in finished water computed using mixing-model approach; —, water treatment plant not operating; *, model simulations not conducted]

Stress period	Month and year	Concentrations in finished water, in micrograms per liter				
		Tetrachloroethylene (PCE)	Trichloroethylene (TCE)	*Trans*-1,2-dichloroethylene (1,2,-tDCE)	Vinyl chloride (VC)	Benzene
553	Jan. 1988	0	0	0	0	3
554	Feb. 1988	0	0	0	0	3
555	Mar. 1988	0	0	0	0	3
556	Apr. 1988	0	0	0	0	4
557	May 1988	0	0	0	0	3
558	June 1988	0	0	0	0	3
559	July 1988	0	0	0	0	3
560	Aug. 1988	0	0	0	0	3
561	Sept. 1988	0	0	0	0	3
562	Oct. 1988	0	0	0	0	3
563	Nov. 1988	0	0	0	0	3
564	Dec. 1988	0	0	0	0	3
565	Jan. 1989	0	0	0	0	3
566	Feb. 1989	0	0	0	0	3
567	Mar. 1989	0	0	0	0	3
568	Apr. 1989	0	0	0	0	3
569	May 1989	0	0	0	0	3
570	June 1989	0	0	0	0	3
571	July 1989	0	0	0	0	3
572	Aug. 1989	0	0	0	0	3
573	Sept. 1989	0	0	0	0	3
574	Oct. 1989	0	0	0	0	3
575	Nov. 1989	0	0	0	0	3
576	Dec. 1989	0	0	0	0	3
577	Jan. 1990	0	0	0	0	3
578	Feb. 1990	0	0	0	0	3
579	Mar. 1990	0	0	0	0	3
580	Apr. 1990	0	0	0	0	3
581	May 1990	0	0	0	0	3
582	June 1990	0	0	0	0	3
583	July 1990	0	0	0	0	3
584	Aug. 1990	0	0	0	0	3
585	Sept. 1990	0	0	0	0	3
586	Oct. 1990	0	0	0	0	3
587	Nov. 1990	0	0	0	0	2
588	Dec. 1990	0	0	0	0	3

Appendix A7. Reconstructed (simulated) monthly mean concentrations in finished water for tetrachloroethylene (PCE), trichloroethylene (TCE), *trans*-1,2-dichloroethylene (1,2-tDCE), and vinyl chloride (VC) at the Hadnot Point water treatment plant, Hadnot Point–Holcomb Boulevard study area, U.S. Marine Corps Base Camp Lejeune, North Carolina, January 1942–June 2008.—Continued

[Concentrations in finished water computed using mixing-model approach; —, water treatment plant not operating; *, model simulations not conducted]

Stress period	Month and year	Concentrations in finished water, in micrograms per liter				
		Tetrachloroethylene (PCE)	Trichloroethylene (TCE)	*Trans*-1,2-dichloroethylene (1,2,-tDCE)	Vinyl chloride (VC)	Benzene
589	Jan. 1991	0	0	0	0	2
590	Feb. 1991	0	0	0	0	3
591	Mar. 1991	0	0	0	0	3
592	Apr. 1991	0	0	0	0	3
593	May 1991	0	0	0	0	3
594	June 1991	0	0	0	0	3
595	July 1991	0	0	0	0	3
596	Aug. 1991	0	0	0	0	3
597	Sept. 1991	0	0	0	0	3
598	Oct. 1991	0	0	0	0	3
599	Nov. 1991	0	0	0	0	2
600	Dec. 1991	0	0	0	0	3
601	Jan. 1992	0	0	*	0	2
602	Feb. 1992	0	0	*	0	3
603	Mar. 1992	0	0	*	0	3
604	Apr. 1992	0	0	*	0	3
605	May 1992	0	0	*	0	3
606	June 1992	0	0	*	0	3
607	July 1992	0	0	*	0	3
608	Aug. 1992	0	0	*	0	3
609	Sept. 1992	0	0	*	0	3
610	Oct. 1992	0	0	*	0	3
611	Nov. 1992	0	0	*	0	3
612	Dec. 1992	0	0	*	0	3
613	Jan. 1993	0	0	*	0	3
614	Feb. 1993	0	0	*	0	3
615	Mar. 1993	0	0	*	0	3
616	Apr. 1993	0	0	*	0	4
617	May 1993	0	0	*	0	3
618	June 1993	0	0	*	0	3
619	July 1993	0	0	*	0	3
620	Aug. 1993	0	0	*	0	4
621	Sept. 1993	0	0	*	0	3
622	Oct. 1993	0	0	*	0	4
623	Nov. 1993	0	0	*	0	3
624	Dec. 1993	0	0	*	0	3

Appendix A7. Reconstructed (simulated) monthly mean concentrations in finished water for tetrachloroethylene (PCE), trichloroethylene (TCE), *trans*-1,2-dichloroethylene (1,2-tDCE), and vinyl chloride (VC) at the Hadnot Point water treatment plant, Hadnot Point–Holcomb Boulevard study area, U.S. Marine Corps Base Camp Lejeune, North Carolina, January 1942–June 2008.—Continued

[Concentrations in finished water computed using mixing-model approach; —, water treatment plant not operating; *, model simulations not conducted]

Stress period	Month and year	Concentrations in finished water, in micrograms per liter				
		Tetrachloroethylene (PCE)	Trichloroethylene (TCE)	*Trans*-1,2-dichloroethylene (1,2,-tDCE)	Vinyl chloride (VC)	Benzene
625	Jan. 1994	0	0	*	0	3
626	Feb. 1994	0	0	*	0	4
627	Mar. 1994	0	0	*	0	3
628	Apr. 1994	0	0	*	0	4
629	May 1994	0	0	*	0	3
630	June 1994	0	0	*	0	4
631	July 1994	0	0	*	0	4
632	Aug. 1994	0	0	*	0	4
633	Sept. 1994	0	0	*	0	4
634	Oct. 1994	0	0	*	0	4
635	Nov. 1994	0	0	*	0	3
636	Dec. 1994	0	0	*	0	4
637	Jan. 1995	0	0	*	0	3
638	Feb. 1995	0	0	*	0	4
639	Mar. 1995	0	0	*	0	4
640	Apr. 1995	0	0	*	0	4
641	May 1995	0	0	*	0	3
642	June 1995	0	0	*	0	4
643	July 1995	0	0	*	0	4
644	Aug. 1995	0	0	*	0	4
645	Sept. 1995	0	0	*	0	4
646	Oct. 1995	0	0	*	0	4
647	Nov. 1995	0	0	*	0	3
648	Dec. 1995	0	0	*	0	3
649	Jan. 1996	0	0	*	0	3
650	Feb. 1996	0	0	*	0	4
651	Mar. 1996	0	0	*	0	3
652	Apr. 1996	0	0	*	0	4
653	May 1996	0	0	*	0	3
654–798	June 1996–June 2008	0	0	*	0	0

Appendix K — Holcomb Boulevard Water-Distribution System Reconstructed (Simulated) Mean Monthly Finished Water Concentrations

Table A8.1. Reconstructed (simulated) monthly mean tetrachloroethylene (PCE) concentrations in finished water distributed to Holcomb Boulevard family housing areas for interconnection events, Hadnot Point–Holcomb Boulevard study area, U.S. Marine Corps Base Camp Lejeune, North Carolina, 1972–1985.[1]

[PP, Paradise Point; MP, Midway Park; BM, Berkeley Manor; WV, Watkins Village; —, not applicable; concentration in micrograms per liter (µg/L)]

Month	[2]1972				1973				1974				1975				1976			
	PP	MP	BM	[3]WV	PP	MP	BM	[3]WV	PP	MP	BM	[3]WV	PP	MP	BM	[3]WV	PP	MP	BM	[3]WV
Jan.	0	0	0	—	0	0	0	—	0	0	0	—	0	0	0	—	0	0	0	—
Feb.	0	0	0	—	0	0	0	—	0	0	0	—	0	0	0	—	0	0	0	—
Mar.	0	0	0	—	0	0	0	—	0	0	0	—	0	0	0	—	0	0	0	—
Apr.	0	0	0	—	0	0	0	—	0	0	0	—	0	0	0	—	0	0	0	—
May	0	0	0	—	0	0	0	—	0	0	0	—	0	0	0	—	0	0	0	—
June	0	0	0	—	0	0	0	—	0	0	0	—	0	0	0	—	0	0	0	—
July	0	0	0	—	0	0	0	—	0	0	0	—	0	0	0	—	0	0	0	—
Aug.	0	0	0	—	0	0	0	—	0	0	0	—	0	0	0	—	0	0	0	—
Sept.	0	0	0	—	0	0	0	—	0	0	0	—	0	0	0	—	0	0	0	—
Oct.	0	0	0	—	0	0	0	—	0	0	0	—	0	0	0	—	0	0	0	—
Nov.	0	0	0	—	0	0	0	—	0	0	0	—	0	0	0	—	0	0	0	—
Dec.	0	0	0	—	0	0	0	—	0	0	0	—	0	0	0	—	0	0	0	—
Month	**1977**				**1978**				**1979**				**1980**				**1981**			
	PP	MP	BM	[3]WV	PP	MP	BM	[3]WV	PP	MP	BM	WV	PP	MP	BM	WV	PP	MP	BM	WV
Jan.	0	0	0	—	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Feb.	0	0	0	—	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Mar.	0	0	0	—	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Apr.	0	0	0	—	0	0	0	0	0	0	0	0	0	0	0	0	0	0	2	1
May	0	0	0	—	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0
June	0	0	0	—	0	1	2	2	0	0	0	0	0	0	1	1	0	0	0	0
July	0	0	0	—	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Aug.	0	0	0	—	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Sept.	0	0	0	—	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Oct.	0	0	0	—	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Nov.	0	0	0	—	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Dec.	0	0	0	—	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Month	**1982**				**1983**				**1984**				**[4]1985**				**1986**			
	PP	MP	BM	WV	PP	MP	BM	WV	PP	MP	BM	WV	PP	MP	BM	WV	PP	MP	BM	WV
Jan.	0	0	0	0	0	0	0	0	0	0	0	0	2	2	2	2				
Feb.	0	0	0	0	0	0	0	0	0	0	0	0	3	3	3	3				
Mar.	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0				
Apr.	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0				
May	0	0	1	1	0	0	1	0	0	0	0	0	0	0	0	0				
June	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0				
July	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0				
Aug.	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0				
Sept.	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0				
Oct.	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0				
Nov.	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0				
Dec.	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0				

[1]Derived from multiplying monthly mean concentrations in finished water from the Hadnot Point water treatment plant (Appendix A7) by average percentage (unrounded) of Hadnot Point water distributed through Booster Pump 742 (Table A20); current maximum contaminant level (MCL) for PCE is 5 µg/L

[2]Prior to June 1972 when Holcomb Boulevard water treatment plant came online, 100 percent of Hadnot Point water was delivered to Holcomb Boulevard family housing areas (see Appendix A7 for January–May 1972)

[3]Watkins Village housing was not built and occupied until about 1978 (Faye et al. 2010), and the first documented interconnection occurs during May 1978 (U.S. Marine Corps Camp Lejeune Water Documents CLW #7023, #7031, and #7033)

[4]For period of January 28–February 4, 1985, booster pump 742 operated continuously due to shutdown of Holcomb Boulevard water treatment plant; this continuous event is not included in the Markov Chain analysis

Table A8.2. Reconstructed (simulated) monthly mean trichloroethylene (TCE) concentrations in finished water distributed to Holcomb Boulevard family housing areas for interconnection events, Hadnot Point–Holcomb Boulevard study area, U.S. Marine Corps Base Camp Lejeune, North Carolina, 1972–1985.[1]

[PP, Paradise Point; MP, Midway Park; BM, Berkeley Manor; WV, Watkins Village; —, not applicable; concentration in micrograms per liter (µg/L)]

Month	[2]1972				1973				1974				1975				1976			
	PP	MP	BM	[3]WV	PP	MP	BM	[3]WV	PP	MP	BM	[3]WV	PP	MP	BM	[3]WV	PP	MP	BM	[3]WV
Jan.	22	22	22	—	0	0	0	—	0	0	0	—	0	0	0	—	0	0	0	—
Feb.	21	21	21	—	0	0	0	—	0	0	0	—	0	0	0	—	0	0	0	—
Mar.	17	17	17	—	0	0	0	—	0	0	0	—	0	0	0	—	0	0	0	—
Apr.	24	24	24	—	0	0	0	—	0	0	0	—	0	0	0	—	0	0	0	—
May	19	19	19	—	0	0	0	—	0	0	0	—	0	0	0	—	0	0	0	—
June	19	19	19	—	0	0	1	—	0	0	0	—	0	0	0	—	1	2	3	—
July	1	0	0	—	0	0	0	—	0	0	0	—	0	0	0	—	0	0	0	—
Aug.	0	0	0	—	0	0	0	—	0	0	0	—	0	0	0	—	0	0	0	—
Sept.	0	0	0	—	0	0	0	—	0	0	0	—	0	0	0	—	0	0	0	—
Oct.	0	0	0	—	0	0	0	—	0	0	0	—	0	0	0	—	0	0	0	—
Nov.	0	0	0	—	0	0	0	—	0	0	0	—	0	0	0	—	0	0	0	—
Dec.	0	0	0	—	0	0	0	—	0	0	0	—	0	0	0	—	0	0	0	—
Month	**1977**				**1978**				**1979**				**1980**				**1981**			
	PP	MP	BM	[3]WV	PP	MP	BM	[3]WV	PP	MP	BM	WV	PP	MP	BM	WV	PP	MP	BM	WV
Jan.	0	0	0	—	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Feb.	0	0	0	—	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Mar.	0	0	0	—	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Apr.	0	1	2	—	0	0	0	0	0	1	2	1	0	0	0	0	0	4	39	28
May	1	1	3	—	0	2	6	4	0	1	3	2	0	0	0	0	0	4	13	10
June	1	2	3	—	3	23	51	38	0	2	6	4	2	8	17	13	0	4	10	7
July	1	2	3	—	0	0	1	1	0	1	4	2	0	0	0	0	0	2	4	3
Aug.	1	2	4	—	0	0	0	0	0	2	5	3	0	0	0	0	0	2	6	4
Sept.	0	0	0	—	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Oct.	0	0	0	—	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Nov.	0	0	0	—	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Dec.	0	0	0	—	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Month	**1982**				**1983**				**1984**				**[4]1985**				**1986**			
	PP	MP	BM	WV	PP	MP	BM	WV	PP	MP	BM	WV	PP	MP	BM	WV	PP	MP	BM	WV
Jan.	0	0	0	0	0	0	0	0	0	0	0	0	34	31	32	34				
Feb.	0	0	0	0	0	0	0	0	0	0	0	0	66	53	54	56				
Mar.	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0				
Apr.	0	3	9	7	0	0	0	0	0	2	5	3	0	0	0	0				
May	1	6	20	13	1	5	14	10	0	0	0	0	0	0	0	0				
June	0	4	10	7	0	0	2	2	0	0	0	0	0	0	0	0				
July	0	4	12	8	0	0	3	2	0	0	0	0	0	0	0	0				
Aug.	1	3	6	4	0	2	5	3	0	0	0	0	0	0	0	0				
Sept.	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0				
Oct.	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0				
Nov.	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0				
Dec.	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0				

[1] Derived from multiplying monthly mean concentrations in finished water from the Hadnot Point water treatment plant (Appendix A7) by average percentage (unrounded) of Hadnot Point water distributed through Booster Pump 742 (Table A20); current maximum contaminant level (MCL) for PCE is 5 µg/L

[2] Prior to June 1972 when Holcomb Boulevard water treatment plant came online, 100 percent of Hadnot Point water was delivered to Holcomb Boulevard family housing areas (see Appendix A7 for January–May 1972)

[3] Watkins Village housing was not built and occupied until about 1978 (Faye et al. 2010), and the first documented interconnection occurs during May 1978 (U.S. Marine Corps Camp Lejeune Water Documents CLW #7023, #7031, and #7033)

[4] For period of January 28–February 4, 1985, booster pump 742 operated continuously due to shutdown of Holcomb Boulevard water treatment plant; this continuous event is not included in the Markov Chain analysis

Table A8.3. Reconstructed (simulated) monthly mean *trans*-1,2-dichloroethylene (1,2-tDCE) concentrations in finished water distributed to Holcomb Boulevard family housing areas for interconnection events, Hadnot Point–Holcomb Boulevard study area, U.S. Marine Corps Base Camp Lejeune, North Carolina, 1972–1985.[1]

[PP, Paradise Point; MP, Midway Park; BM, Berkeley Manor; WV, Watkins Village; —, not applicable; concentration in micrograms per liter (µg/L)]

Month	[2]1972				1973				1974				1975				1976			
	PP	MP	BM	[3]WV	PP	MP	BM	[3]WV	PP	MP	BM	[3]WV	PP	MP	BM	[3]WV	PP	MP	BM	[3]WV
Jan.	0	0	0	—	0	0	0	—	0	0	0	—	0	0	0	—	0	0	0	—
Feb.	0	0	0	—	0	0	0	—	0	0	0	—	0	0	0	—	0	0	0	—
Mar.	0	0	0	—	0	0	0	—	0	0	0	—	0	0	0	—	0	0	0	—
Apr.	0	0	0	—	0	0	0	—	0	0	0	—	0	0	0	—	0	0	0	—
May	0	0	0	—	0	0	0	—	0	0	0	—	0	0	0	—	0	0	0	—
June	0	0	0	—	0	1	1	—	0	0	0	—	0	0	0	—	0	1	2	—
July	0	0	0	—	0	0	0	—	0	0	0	—	0	0	0	—	0	0	0	—
Aug.	0	0	0	—	0	0	0	—	0	0	0	—	0	0	0	—	0	0	0	—
Sept.	0	0	0	—	0	0	0	—	0	0	0	—	0	0	0	—	0	0	0	—
Oct.	0	0	0	—	0	0	0	—	0	0	0	—	0	0	0	—	0	0	0	—
Nov.	0	0	0	—	0	0	0	—	0	0	0	—	0	0	0	—	0	0	0	—
Dec.	0	0	0	—	0	0	0	—	0	0	0	—	0	0	0	—	0	0	0	—

Month	1977				1978				1979				1980				1981			
	PP	MP	BM	[3]WV	PP	MP	BM	[3]WV	PP	MP	BM	WV	PP	MP	BM	WV	PP	MP	BM	WV
Jan.	0	0	0	—	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Feb.	0	0	0	—	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Mar.	0	0	0	—	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Apr.	0	1	1	—	0	0	0	0	0	1	1	1	0	0	0	0	0	2	16	12
May	0	1	1	—	0	1	3	2	0	0	1	1	0	0	0	0	0	2	6	4
June	0	1	1	—	2	10	22	17	0	1	3	2	1	3	7	5	0	2	4	3
July	0	1	2	—	0	0	0	0	0	0	1	1	0	0	0	0	0	1	2	1
Aug.	0	1	2	—	0	0	0	0	0	1	2	1	0	0	0	0	0	1	3	2
Sept.	0	0	0	—	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Oct.	0	0	0	—	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Nov.	0	0	0	—	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Dec.	0	0	0	—	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

Month	1982				1983				1984				[4]1985				1986			
	PP	MP	BM	WV	PP	MP	BM	WV	PP	MP	BM	WV	PP	MP	BM	WV	PP	MP	BM	WV
Jan.	0	0	0	0	0	0	0	0	0	0	0	0	17	16	16	17				
Feb.	0	0	0	0	0	0	0	0	0	0	0	0	33	27	27	28				
Mar.	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0				
Apr.	0	2	4	3	0	0	0	0	0	1	2	2	0	0	0	0				
May	0	3	10	7	0	3	8	5	0	0	0	0	0	0	0	0				
June	0	2	6	4	0	0	1	1	0	0	0	0	0	0	0	0				
July	0	2	6	4	0	0	2	1	0	0	0	0	0	0	0	0				
Aug.	0	2	3	2	0	1	3	2	0	0	0	0	0	0	0	0				
Sept.	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0				
Oct.	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0				
Nov.	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0				
Dec.	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0				

[1]Derived from multiplying monthly mean concentrations in finished water from the Hadnot Point water treatment plant (Appendix A7) by average percentage (unrounded) of Hadnot Point water distributed through Booster Pump 742 (Table A20); current maximum contaminant level (MCL) for PCE is 5 µg/L

[2]Prior to June 1972 when Holcomb Boulevard water treatment plant came online, 100 percent of Hadnot Point water was delivered to Holcomb Boulevard family housing areas (see Appendix A7 for January–May 1972)

[3]Watkins Village housing was not built and occupied until about 1978 (Faye et al. 2010), and the first documented interconnection occurs during May 1978 (U.S. Marine Corps Camp Lejeune Water Documents CLW #7023, #7031, and #7033)

[4]For period of January 28–February 4, 1985, booster pump 742 operated continuously due to shutdown of Holcomb Boulevard water treatment plant; this continuous event is not included in the Markov Chain analysis

Table A8.4. Reconstructed (simulated) monthly mean vinyl chloride (VC) concentrations in finished water distributed to Holcomb Boulevard family housing areas for interconnection events, Hadnot Point–Holcomb Boulevard study area, U.S. Marine Corps Base Camp Lejeune, North Carolina, 1972–1985.[1]

[PP, Paradise Point; MP, Midway Park; BM, Berkeley Manor; WV, Watkins Village; —, not applicable; concentration in micrograms per liter (µg/L)]

Month	[2]1972				1973				1974				1975				1976			
	PP	MP	BM	[3]WV	PP	MP	BM	[3]WV	PP	MP	BM	[3]WV	PP	MP	BM	[3]WV	PP	MP	BM	[3]WV
Jan.	0	0	0	—	0	0	0	—	0	0	0	—	0	0	0	—	0	0	0	—
Feb.	0	0	0	—	0	0	0	—	0	0	0	—	0	0	0	—	0	0	0	—
Mar.	0	0	0	—	0	0	0	—	0	0	0	—	0	0	0	—	0	0	0	—
Apr.	0	0	0	—	0	0	0	—	0	0	0	—	0	0	0	—	0	0	0	—
May	0	0	0	—	0	0	0	—	0	0	0	—	0	0	0	—	0	0	0	—
June	0	0	0	—	0	0	0	—	0	0	0	—	0	0	0	—	0	0	0	—
July	0	0	0	—	0	0	0	—	0	0	0	—	0	0	0	—	0	0	0	—
Aug.	0	0	0	—	0	0	0	—	0	0	0	—	0	0	0	—	0	0	0	—
Sept.	0	0	0	—	0	0	0	—	0	0	0	—	0	0	0	—	0	0	0	—
Oct.	0	0	0	—	0	0	0	—	0	0	0	—	0	0	0	—	0	0	0	—
Nov.	0	0	0	—	0	0	0	—	0	0	0	—	0	0	0	—	0	0	0	—
Dec.	0	0	0	—	0	0	0	—	0	0	0	—	0	0	0	—	0	0	0	—

Month	1977				1978				1979				1980				1981			
	PP	MP	BM	[3]WV	PP	MP	BM	[3]WV	PP	MP	BM	WV	PP	MP	BM	WV	PP	MP	BM	WV
Jan.	0	0	0	—	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Feb.	0	0	0	—	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Mar.	0	0	0	—	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Apr.	0	0	0	—	0	0	0	0	0	0	0	0	0	0	0	0	0	0	3	2
May	0	0	0	—	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	1
June	0	0	0	—	0	1	3	2	0	0	0	0	0	1	1	1	0	0	1	0
July	0	0	0	—	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Aug.	0	0	0	—	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Sept.	0	0	0	—	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Oct.	0	0	0	—	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Nov.	0	0	0	—	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Dec.	0	0	0	—	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

Month	1982				1983				1984				[4]1985				1986			
	PP	MP	BM	WV	PP	MP	BM	WV	PP	MP	BM	WV	PP	MP	BM	WV	PP	MP	BM	WV
Jan.	0	0	0	0	0	0	0	0	0	0	0	0	3	3	3	3				
Feb.	0	0	0	0	0	0	0	0	0	0	0	0	6	5	5	5				
Mar.	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0				
Apr.	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0				
May	0	0	1	1	0	0	1	1	0	0	0	0	0	0	0	0				
June	0	0	1	1	0	0	0	0	0	0	0	0	0	0	0	0				
July	0	0	1	1	0	0	0	0	0	0	0	0	0	0	0	0				
Aug.	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0				
Sept.	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0				
Oct.	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0				
Nov.	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0				
Dec.	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0				

[1] Derived from multiplying monthly mean concentrations in finished water from the Hadnot Point water treatment plant (Appendix A7) by average percentage (unrounded) of Hadnot Point water distributed through Booster Pump 742 (Table A20); current maximum contaminant level (MCL) for PCE is 5 µg/L

[2] Prior to June 1972 when Holcomb Boulevard water treatment plant came online, 100 percent of Hadnot Point water was delivered to Holcomb Boulevard family housing areas (see Appendix A7 for January–May 1972)

[3] Watkins Village housing was not built and occupied until about 1978 (Faye et al. 2010), and the first documented interconnection occurs during May 1978 (U.S. Marine Corps Camp Lejeune Water Documents CLW #7023, #7031, and #7033)

[4] For period of January 28–February 4, 1985, booster pump 742 operated continuously due to shutdown of Holcomb Boulevard water treatment plant; this continuous event is not included in the Markov Chain analysis

Table A8.5. Reconstructed (simulated) monthly mean benzene concentrations in finished water distributed to Holcomb Boulevard family housing areas for interconnection events, Hadnot Point–Holcomb Boulevard study area, U.S. Marine Corps Base Camp Lejeune, North Carolina, 1972–1985.[1]

[PP, Paradise Point; MP, Midway Park; BM, Berkeley Manor; WV, Watkins Village; —, not applicable; concentration in micrograms per liter (μg/L)]

Month	[2]1972				1973				1974				1975				1976			
	PP	MP	BM	[3]WV	PP	MP	BM	[3]WV	PP	MP	BM	[3]WV	PP	MP	BM	[3]WV	PP	MP	BM	[3]WV
Jan.	3	3	3	—	0	0	0	—	0	0	0	—	0	0	0	—	0	0	0	—
Feb.	3	3	3	—	0	0	0	—	0	0	0	—	0	0	0	—	0	0	0	—
Mar.	2	2	2	—	0	0	0	—	0	0	0	—	0	0	0	—	0	0	0	—
Apr.	3	3	3	—	0	0	0	—	0	0	0	—	0	0	0	—	0	0	0	—
May	3	3	3	—	0	0	0	—	0	0	0	—	0	0	0	—	0	0	0	—
June	3	3	3	—	0	0	0	—	0	0	0	—	0	0	0	—	0	0	0	—
July	0	0	0	—	0	0	0	—	0	0	0	—	0	0	0	—	0	0	0	—
Aug.	0	0	0	—	0	0	0	—	0	0	0	—	0	0	0	—	0	0	0	—
Sept.	0	0	0	—	0	0	0	—	0	0	0	—	0	0	0	—	0	0	0	—
Oct.	0	0	0	—	0	0	0	—	0	0	0	—	0	0	0	—	0	0	0	—
Nov.	0	0	0	—	0	0	0	—	0	0	0	—	0	0	0	—	0	0	0	—
Dec.	0	0	0	—	0	0	0	—	0	0	0	—	0	0	0	—	0	0	0	—

Month	1977				1978				1979				1980				1981			
	PP	MP	BM	[3]WV	PP	MP	BM	[3]WV	PP	MP	BM	WV	PP	MP	BM	WV	PP	MP	BM	WV
Jan.	0	0	0	—	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Feb.	0	0	0	—	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Mar.	0	0	0	—	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Apr.	0	0	0	—	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	1
May	0	0	0	—	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
June	0	0	0	—	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0
July	0	0	0	—	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Aug.	0	0	0	—	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Sept.	0	0	0	—	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Oct.	0	0	0	—	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Nov.	0	0	0	—	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Dec.	0	0	0	—	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

Month	1982				1983				1984				[4]1985				1986			
	PP	MP	BM	WV	PP	MP	BM	WV	PP	MP	BM	WV	PP	MP	BM	WV	PP	MP	BM	WV
Jan.	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0				
Feb.	0	0	0	0	0	0	0	0	0	0	0	0	1	1	1	1				
Mar.	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0				
Apr.	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0				
May	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0				
June	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0				
July	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0				
Aug.	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0				
Sept.	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0				
Oct.	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0				
Nov.	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0				
Dec.	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0				

[1]Derived from multiplying monthly mean concentrations in finished water from the Hadnot Point water treatment plant (Appendix A7) by average percentage (unrounded) of Hadnot Point water distributed through Booster Pump 742 (Table A20); current maximum contaminant level (MCL) for PCE is 5 μg/L

[2]Prior to June 1972 when Holcomb Boulevard water treatment plant came online, 100 percent of Hadnot Point water was delivered to Holcomb Boulevard family housing areas (see Appendix A7 for January–May 1972)

[3]Watkins Village housing was not built and occupied until about 1978 (Faye et al. 2010), and the first documented interconnection occurs during May 1978 (U.S. Marine Corps Camp Lejeune Water Documents CLW #7023, #7031, and #7033)

[4]For period of January 28–February 4, 1985, booster pump 742 operated continuously due to shutdown of Holcomb Boulevard water treatment plant; this continuous event is not included in the Markov Chain analysis

Appendix L — ATSDR Response to Department of the Navy's Letter on: Assessment of ATSDTR Water Modeling for Tarawa Terrace (ATSDR 2009)

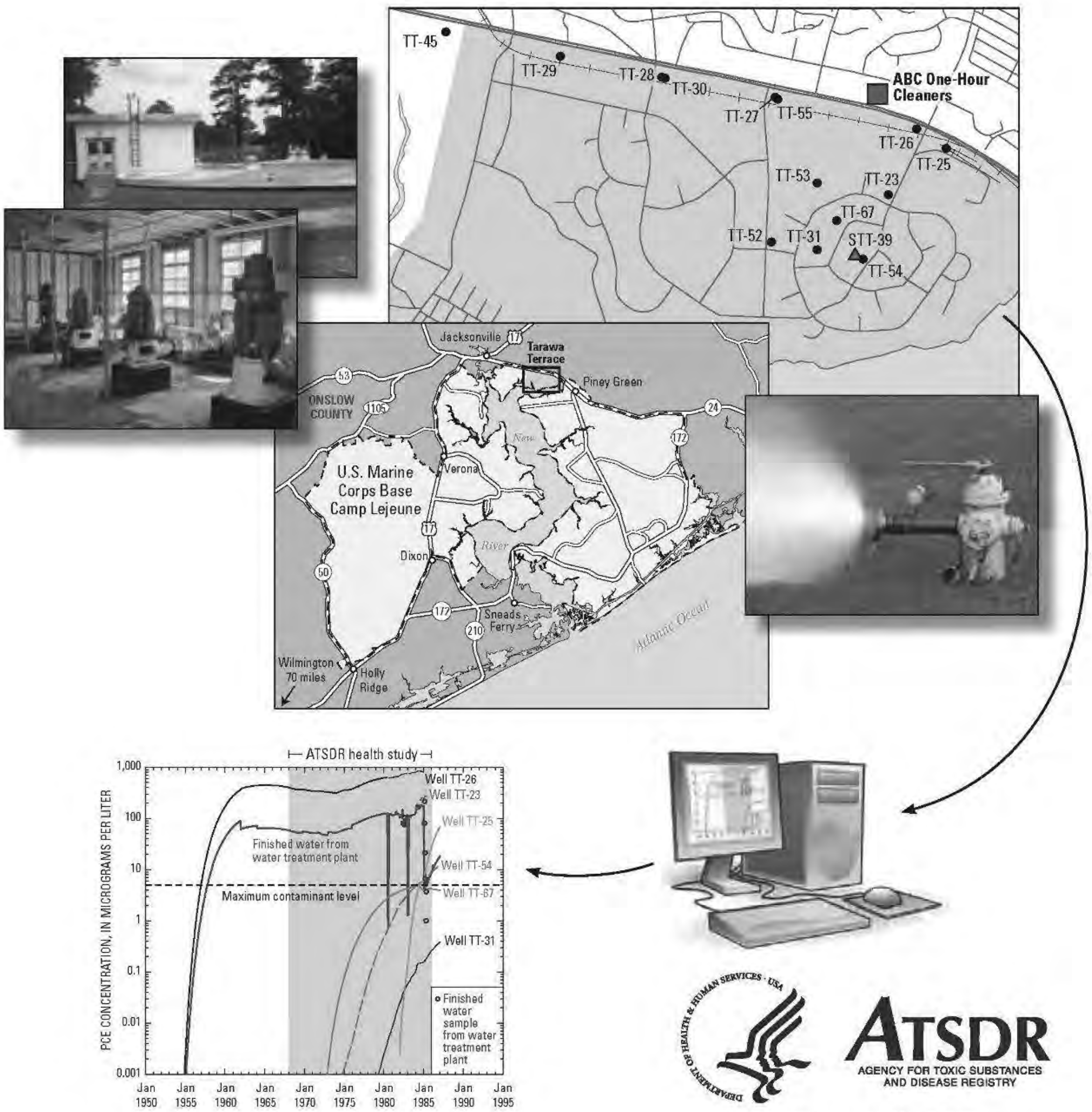
The ATSDR Response to Department of Navy's Letter is publicly available on the ATSDR website at:

ATSDR_Response2DON_10Mar09.pdf (cdc.gov)

References to "Attachment 2 – Attachment 8" in the text portion of the response included with this Appendix K are found in the publicly available report on ATSDR's website. Attachment 1 is included with this Appendix

Analyses of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water at Tarawa Terrace and Vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina: Historical Reconstruction and Present-Day Conditions

Response to the Department of the Navy's Letter on: Assessment of ATSDR Water Modeling for Tarawa Terrace



Atlanta, Georgia–March 2009

DEPARTMENT OF HEALTH & HUMAN SERVICES

Public Health Service

Agency for Toxic Substances
and Disease Registry
Atlanta GA 30333

March 10, 2009

Brian P. Harrison, M.P.A., P.E.
Department of the Navy
Naval Facilities Engineering Command
1322 Patterson Avenue, SE
Suite 1000
Washington Navy Yard, D.C. 20374-5065

Dear Mr. Harrison:

I am writing this letter in response to the Department of Navy's (DON) letter dated June 19, 2008. In that letter you reiterated the DON's continued support for working with the Agency for Toxic Substances and Disease Registry (ATSDR) and brought to my attention issues of concern to the DON regarding ATSDR's current health study. This health study uses results of water-modeling analyses to reconstruct historical levels of contaminants in base housing drinking-water supplies during the health study period of 1968–1985.

I have requested ATSDR technical staff working on the current health study at Camp Lejeune to compile responses to the scientific and technical issues you describe in your letter. These responses are enclosed. As a particular response warrants, the response is supported with additional technical and scientific documentation. Technical points of contact for responses to the DON letter are listed below:

Health study/epidemiology, Dr. Frank J. Bove, (770) 488-3809, fbove@cdc.gov
Historical reconstruction/modeling, Mr. Morris L. Maslia, (770) 488-3842, mmaslia@cdc.gov.

ATSDR appreciates the DON's support and commitment to working with us on this scientifically complex and technically challenging project. One of the benefits to the public from a complex project of this type is a demonstration of how two independent Federal Government agencies can work together for the betterment of public health.

Sincerely,

Thomas Sinks

Thomas H. Sinks, Ph.D.
Deputy Director
National Center for Environmental Health/
Agency for Toxic Substances and Disease Registry

Enclosure

cc:
H. Frumkin, NCEH/ATSDR/OD
C. Aloisio, NCEH/ATSDR/OFAS
M. Campbell, NCEH/ATSDR/OFAS
J. Masone, NCEH/ATSDR/OFAS
G. David Williamson, ATSDR/DHS
Bill Cibulas, ATSDR/DHAC
Susan Moore, ATSDR/DHAC
F. J. Bove, ATSDR/DHS
P. Z. Ruckart, ATSDR/DHS
M. L. Maslia, ATSDR/DHAC
R. Mach, DON/ASN(E)
K. Brown, DON/NAVFACHQ
D. Waddill, DON/NAVFAC ATLANTIC
M. Simmons, DON/NMCPHC
C. Rennix, DON/NMCPHC
C. Sakai, USMCHQ
S. Williams, USMCHQ

RESPONSE TO THE DEPARTMENT OF THE NAVY'S LETTER ON ASSESSMENT OF ATSDR WATER MODELING FOR TARAWA TERRACE

INTRODUCTION

The Agency for Toxic Substances and Disease Registry (ATSDR) has used the following referencing format in responding to the Department of the Navy (DON) comments contained in their letter of June 19, 2008. A comment is identified in the DON letter by a number (e.g., 1.1, 2.1, 3.1, etc.), and the ATSDR response to that particular comment is identified with a sequential number (e.g., 1.2, 2.2, 3.2, etc.). To facilitate comparison of DON comments with ATSDR responses, DON comment identifiers (e.g., 1.1, 2.1, 3.1, etc.) have been placed in the margins of the DON letter. This "marked up" letter is provided as a reference and is identified herein as Attachment 1.

BACKGROUND

This ATSDR response and related attachments are part of a continuing effort on the part of ATSDR to maintain a high level of communication between ATSDR and other agencies responsible for the current health study at Camp Lejeune. To reiterate those efforts, Attachment 2 presents information pertinent to previous meetings, presentations, and conversations between ATSDR and the Department of Defense (DOD), the DON, and the U.S. Marine Corps (USMC). Since ATSDR proposed using the historical reconstruction approach as part of the current health study during October 2003, ATSDR staff have kept the DOD, DON, and USMC fully informed, at the highest levels of command, regarding ATSDR's work plans, activities, progress, and results. Attachment 2 provides a complete chronology of meetings, presentations, and publications related to the historical reconstruction of contaminated drinking water at Tarawa Terrace and vicinity. Three examples, we believe, are noteworthy:

(1) On October 8, 2003, ATSDR presented its proposed modeling approach to support the current health study—historical reconstruction—during a meeting at ATSDR headquarters. Attending the meeting were representatives from the DOD, DON, and USMC (headquarters and Camp Lejeune). A copy of the meeting sign-in sheet and sample presentation slides also are provided in Attachment 2.

(2) On August 26, 2005, ATSDR health study and water-modeling staff met with Lt. General Kelly and his staff at USMC headquarters and presented initial water-modeling results indicating tetrachloroethylene (PCE) had reached Tarawa Terrace water-supply wells as early as 1960.

(3) On June 11, 2007, ATSDR health study and water-modeling staff met with Lt. General Kramlich and his staff at USMC headquarters and presented final water-modeling results. These results indicated that PCE dissolved in groundwater had reached Tarawa Terrace water-supply wells as early as November 1957. ATSDR also presented Lt. General Kramlich and his staff with printed copies of the Executive Summary report (Maslia et al. 2007a) that would be publicly released the following day (June 12, 2007).

RESPONSE TO SPECIFIC COMMENTS

1.1 DON Comment/Statement

During a Technical Information Meeting with the Marine Corps and Navy on March 26, 2008, the ATSDR presented their water modeling efforts in a summary report entitled "Exposure to Volatile Organic Compounds in Drinking Water and Specific Birth Defects and Childhood Cancer at U.S. Marine Corps Base Camp Lejeune, North Carolina."

1.2 ATSDR Response

During the aforementioned meeting on March 26, 2008, in Atlanta, ATSDR presented water-modeling results for Tarawa Terrace and vicinity. Staff and technical representatives from ATSDR, DON, and USMC headquarters attended the meeting. ATSDR presented a summary of published results and a list of Tarawa Terrace chapter reports to be completed. Attendees were provided with a copy of the ATSDR PowerPoint® presentation that was used during the meeting.

Note that all reports of technical analyses and water-modeling results pertinent to historical reconstruction of exposure to volatile organic compounds (VOCs) at Tarawa Terrace and vicinity published to date by ATSDR have been available on the agency's Camp Lejeune Web site (http://www.atsdr.cdc.gov/sites/lejeune/watermodeling.html) since June 2007. For example, the Executive Summary (Maslia et al. 2007a) and Chapter A (Maslia et al. 2007b) reports were released publicly during June and July 2007, respectively. As agreed upon with USMC headquarters staff, ATSDR provided Camp Lejeune and USMC headquarters staff with advanced electronic copies (508-compliant PDF® files) of the aforementioned reports 24 hours prior to their public release.

2.1 DON Comment/Statement

Monthly PCE concentrations are required for the ATSDR health study, which will examine births that occurred from 1968 (when North Carolina computerized its birth certificates) to 1985 (when the contaminated water supply wells were removed from service).

2. 2 ATSDR Response

In general, ATSDR is in agreement with this statement. Specifically, however, historical and water treatment plant (WTP) operations records indicate that only the most contaminated wells were removed from continuous service during 1985. For example, water-supply wells TT-26 and TT-23 were removed from continuous service during February and May 1985, respectively.
Remaining Tarawa Terrace water-supply wells continued to operate continuously and intermittently until the Tarawa Terrace WTP was permanently shut down during March 1987 (Maslia et al. 2007b, Table A6). Thus, ATSDR is not in agreement with the DON statement in parentheses that incorrectly describes the schedule for the removal of water-supply wells from service at Tarawa Terrace.

3.1 DON Comment/Statement

Due to lack of measured concentrations, the ATSDR used groundwater flow and contaminant transport modeling in a historical reconstruction process to simulate PCE concentrations in the drinking water on a monthly basis from 1952 to 1987.

3.2 ATSDR Response

To reconstruct monthly concentrations of PCE in drinking water, ATSDR used three types of models: (1) groundwater flow, (2) contaminant fate and transport, and (3) simple mixing based on the concepts of continuity and mass balance. The mixing model was necessary to account for the mixing of uncontaminated and contaminated water-supply wells contributing to the water supply at the Tarawa Terrace WTP. The mixing model provided the final "mixed" drinking- water concentrations on a monthly basis, and these are the values that are available on the ATSDR Web site and published in the Chapter A report (Maslia et al. 2007b).

4.1 DON Comment/Statement

Figure 1 shows the simulated concentrations of PCE versus measured concentrations in finished water from the WTP. Significantly, measured concentrations of PCE are available only in 1982 and 1985, near the end of the overall time period. Thus, the majority of the simulated concentrations cannot be compared to measured data.

4.2 ATSDR Response

ATSDR agrees that there is a lack of historical contaminant concentration data. That is why ATSDR applied the historical reconstruction process to reconstruct (or synthesize) water levels, groundwater concentrations, and drinking-water concentrations of PCE for historical periods (months) when data were not available. Note that data used to calibrate the model(s) in the historical reconstruction process can either be historical data (as was the situation for Tarawa Terrace), or present-day data obtained through a field-test program—as was the case for the water-distribution system model developed by ATSDR for the Dover Township (Toms River), New Jersey, childhood cancer cluster investigation (Maslia et al. 2000).

5.1 DON Comment/Statement

Furthermore, all of the measured concentrations were used during model calibration, leaving no data available for model validation. As a result, the Tarawa Terrace model was not validated.

5.2 ATSDR Response

A number of terms have been used throughout the published literature that reference the adequacy of model simulation to reliably reproduce real-world conditions based on the fidelity of the model and its intended use. Many groundwater modelers and hydrologists have abandoned the use of terms such as model verification and validation for the terms of history matching and post audits (Bredehoeft and Konikow 1993, Oreskes et al. 1994). However, ATSDR understands that the DON comment was intended to express the DON's concern that the calibrated Tarawa Terrace models were not compared to multiple independent sets of measured data (water levels and concentrations) as part of ATSDR's model calibration process and strategy. To address this concern, definitions of terms such as "verification" and "validation" should be agreed upon, and the consequences of undertaking a useful "validation" program for Tarawa Terrace should be completely understood by ATSDR and the DON. Model verification requires that multiple sets of field data be available for model calibration. These sets of field data should be sufficiently large in quantity and distribution and of sufficient quality to provide at least two equally useful calibration data sets. Each data set also should be sufficiently separated in time so as to represent significantly different water-level and contaminant conditions within the model domain. The field data set at Tarawa Terrace used for model calibration was not of sufficient quantity and was too compressed in time to implement a verification procedure. To appropriately calibrate the Tarawa Terrace models, all available field data were required for a single calibration data set and effort. This is consistent with and follows ASTM D5981-96, Standard Guide for Calibrating a Ground-Water Flow Model Application (1996, Note 4), that states: *"When only one data set is available, it is inadvisable to artificially split it into separate 'calibration' and 'verification' data sets. It is usually more important to calibrate to data spanning as much of the modeled domain as possible."*

To meaningfully validate the Tarawa Terrace models (or more appropriately, to conduct a post audit), sufficient time should elapse between individual sets of field data to ensure that significant changes in field conditions have occurred compared to calibrated conditions. At Tarawa Terrace, such changes, by necessity, would require the migration of the contaminant mass to a completely new location and for contaminant concentrations to change significantly when compared to calibrated conditions. Additionally, at Tarawa Terrace, validation (a post audit) would require the collection and analyses of substantial quantities of additional field data, similar to Weston's Operational Units 1 and 2 (Roy F. Weston, Inc. 1992, 1994).

Note, once an acceptable calibration was achieved (using a four-stage calibration strategy described in Maslia et al. [2007a], Faye and Valenzuela [2007], and Faye [2008]), the calibrated models were used to reconstruct historical monthly PCE and PCE degradation by-product concentrations in groundwater and drinking water (Jang and Aral 2008). This is standard practice in the modeling community—using a calibrated model to "predict" (in ATSDR's situation, "reconstruct") results for a period of time when data are not available or cannot be obtained. An example using this same approach is the application of fate and transport modeling to chlorinated organic compounds at Operable Unit 1, U.S. Naval Air Station, Jacksonville, Florida (NASJF), conducted by Davis (2007, Figures 28–31). At this site, the earliest water-quality data that are available were collected during 1992, but the fate and transport model simulations reconstruct concentrations as far back as 1945.

6.1 DON Comment/Statement

For PCE detections, the ATSDR chose the calibration standard to be "±1/2-order of magnitude of the observed valued," such that the higher value in the calibration target range is 10 times greater than the lower value …. In other words, a model-derived PCE concentration can be approximately 3 times higher or 3 times lower than the measured concentration and still fall within the calibration range.

6.2 ATSDR Response

ATSDR generally is in agreement with this statement. For model calibration, ATSDR established, *a priori*, calibration "targets" that were based on the reported accuracy of the available water-level and water-quality measurements. This is in keeping with, and following, the ASTM Standard Guide for Calibrating a Ground-Water Flow Model Application (ASTM 1996). Note, however, that published or accepted groundwater-flow or contaminant fate and transport model calibration standards are currently not established. The lack of model calibration standards is further emphasized by Anderson and Woessner (1992) who state: *"To date, there is no standard protocol for evaluating the calibration process, although the need for a standard methodology is recognized as an important part of the quality assurance in code application (National Research Council 1990)."* In thoroughly reviewing the published literature for contaminant fate and transport model applications, ATSDR did not find any examples wherein calibration targets were established *a priori* and then were followed by a comparison of model simulation results to the calibration targets, as was done in the ATSDR analyses (Maslia et al. 2007b, Faye 2008). For example, at another DON site—the NASJF—contaminant fate and transport simulations of selected chlorinated organic solvents were accepted by the DON, but the simulations did not include any *a priori* contaminant fate and transport calibration targets (Davis 2003, 2007).

7.1 DON Comment/Statement

However, all comparisons did not fall within the calibration range. At the WTP, 12% of the simulated PCE concentrations failed the calibration standard …. at the water supply wells, a majority (53%) of the simulated concentrations fell outside the calibration standard….

7.2 ATSDR Response

ATSDR will address three issues pertinent to the aforementioned DON statement:

(1) ATSDR acknowledges that several simulated head and concentration data fall outside of the range of the ATSDR established calibration targets. As discussed above, ATSDR used available data provided by the U.S. Environmental Protection Agency (USEPA), U.S. Geological Survey (USGS), USMC, and DON, and based on these data, established calibration targets *a priori*, as prescribed in ASTM D5981-96 (1996, Section 6). Furthermore, ATSDR clearly identified and conveyed to the reader (and the public) those data that met and did not meet calibration targets by providing illustrations comparing observed (measured) data, nondetect data, and simulated results with calibration targets for water-supply wells and the Tarawa Terrace WTP. These illustrations are designated as Figures A11 for water-supply wells and A12 for the WTP of the Chapter A report and are located on pages A30 and A31, respectively (Maslia et al. 2007b).

(2) Note, as well, that ATSDR did not discard any nondetect data, as is done in many environmental analyses (Helsel 2005). Rather, ATSDR clearly identified the nondetect data on the aforementioned illustrations so the reader could judge for themselves the usefulness of these data and their relation to the calibration targets. This is very much in keeping with the approach stated by Helsel (2005): "*Deleting nondetects, concentrations*

below a measured threshold, obscures the information in graphs and numerical summaries."

(3) ATSDR maintains that the models (flow, transport, and mixing) are sufficiently calibrated, given the quantity and accuracy of data provided and the intended use of the simulated historically reconstructed concentrations. Although the DON is correct in pointing out that some simulated results did not meet the calibration target, ATSDR believes that the DON should assess these results in terms of: (1) similar peer-reviewed reports, (2) currently established model calibration practices, and (3) the intended use of the modeling results by the epidemiological study. That is, are the ATSDR analyses within the accepted norm of current-day modeling practices, are the ATSDR analyses an exception to this norm, and will there be sufficient reliability for an epidemiological study?

To possibly answer the first two questions, ATSDR looks forward to discussing with the DON the results of other modeling studies of contaminant fate and transport similar to the ATSDR study at Tarawa Terrace and comparing the results of other studies to the calibration targets used by ATSDR at Tarawa Terrace. For example, the results of the ATSDR fate and transport simulations at Tarawa Terrace were compared to results of a similar study of the fate and transport modeling of chlorinated solvents at the NASJF, reported by Davis (2003). The report by Davis (2003) was peer reviewed and published by the USGS, and the published results were subsequently deemed totally acceptable to the DON. No calibration targets for contaminant concentrations were established during the NASJF study. Therefore, to directly compare Tarawa Terrace and NASJF simulation results, the ATSDR calibration targets of ±1/2-order of magnitude were applied to data and simulation results reported in Davis (2003, Figure 34). Attachment 3 shows this comparison along with similar results reported by Maslia et al. (2007b, Tables A9 and A10). The percentage of NASJF simulation results that fell within the calibration target range (passed the calibration target test) is 56% compared with 59% for the ATSDR study (44% of the NASJF results failed the calibration test compared with a failure rate of 41% for ATSDR results). Furthermore, the root-mean-square of concentration difference for the NASJF analysis is 329 μg/L compared with 337 μg/L for the ATSDR analysis. (Data used to conduct these comparisons also are included in Attachment 3.) Thus, one can conclude that the ATSDR analysis is comparable to and of the same order of accuracy and quality as the NASJF analysis that was accepted by the DON.

To address the issue of the intended use of the water-modeling results by the current ATSDR epidemiological study, the DON should be advised that a successful epidemiological study places little emphasis on the actual (absolute) estimate of concentration and, rather, emphasizes the <u>relative</u> level of exposure. That is, exposed individuals are, in effect, ranked by exposure level and maintain their rank order of exposure level regardless of how far off the estimated concentration is to the "true" (measured) PCE concentration. This rank order of exposure level is preserved regardless of whether the mean or the upper or lower 95% of simulated levels are used to estimate the monthly average contaminant levels. It is **not** the goal of the ATSDR health study to infer which health effects occur at specific PCE concentrations—this is a task for risk assessment utilizing approaches such as meta-analysis to summarize evidence from several epidemiological studies because a single epidemiological study is generally insufficient to make this determination. The goal of the ATSDR epidemiological analysis is to evaluate exposure-response relationships to determine whether the risk for a specific disease increases as the level of the contaminant (either as a categorical variable or continuous variable) increases.

8.1 DON Comment/Statement

It seems reasonable to conclude that the accuracy of the historically reconstructed PCE concentrations would be less than the calibration standard of ±1/2-order of magnitude. Thus, the historical reconstructions may be viewed as rough estimates of actual exposure concentrations, with model-derived PCE concentrations representing a relatively wide range of possible exposures. It is essential that this concept be expressed clearly and consistently to all stakeholders.

8.2 ATSDR Response

ATSDR is in disagreement with DON's assessment and interpretation as expressed in the first two sentences above. As previously discussed, there are no established calibration targets or standards that are universally accepted or used by the contaminant fate and transport modeling community. With respect to the Tarawa Terrace models, the failure of a percentage of data to conform to a designated calibration target is more a commentary on the accuracy and variability of field data used for model calibration than the model's ability to accurately simulate true field conditions. These issues are thoroughly discussed in the "Discussion" sections of the Tarawa Terrace Chapter C and F reports (Faye and Valenzuela 2007, Faye 2008) For example, note on Attachment 3 of this letter the radical changes in PCE concentration at well TT-26 during the approximately 1-month period between January 16 and February 19, 1985. Of the four comparisons of measured PCE concentrations with simulated PCE concentrations, three comparisons failed the calibration target test of ±1/2-order of magnitude while the field data varied by as much as 2.5 orders of magnitude. The two analyses recorded for February 19, 1985, are duplicative but were nonetheless counted as two failures with respect to computing a percentage of comparisons that failed the calibration target test. Furthermore, ATSDR is not aware of any other published report that establishes, *a priori*, contaminant fate and transport calibration targets. ATSDR based its calibration target of ±1/2-order of magnitude on the assumption that very restrictive or "tight" control on model calibration was desired. With 59% of the water-supply well and water treatment plant paired data points meeting these targets, ATSDR believes it met its model calibration goals.

ATSDR is in disagreement with the DON statement that the historical reconstruction results of PCE concentrations are "*rough estimates*" and represent a "*relatively wide range of possible exposures*." Results presented in the Chapter A report (Maslia et al. 2007b) demonstrate just the opposite. ATSDR meticulously followed accepted modeling standards (ASTM 1996, Hill and Tiedeman 2007) for both deterministic (single-valued input and output) and probabilistic (distributed-value input and output) modeling analyses. Results obtained are accurate on a monthly basis within the variability bands indicated, given the quality and quantity of available

data, and the uncertainty and variability of input data, pumping and water treatment plant operations, and quantity of mass released. The monthly resolutions of simulated PCE concentrations are sufficiently refined for the intended use of the epidemiological case-control study. Furthermore, as shown in Figures A25 and A26 (Maslia et al. 2007b), ATSDR clearly described and communicated that reconstructed (simulated) PCE concentrations for a specified month do have a range of values. A tabular listing of these values is provided in the Chapter I report (Maslia et al. 2009) and will be made available to the public on the ATSDR Web site.
These tabular values also are provided herein as Attachment 4. A review of Attachment 4 indicates that during the period of interest to the epidemiological study (1968–1985), when water-supply well TT-26 was pumping, the range of 95% of the Monte Carlo simulated PCE concentration values differ by a factor of about 2 when pumping uncertainty is not considered (e.g., for January 1968, $P_{97.5}$ = 76.43 μg/L and $P_{2.5}$ = 38.91 μg/L). PCE concentration values differ by a factor of about 2.5 when pumping uncertainty is considered (e.g., for January 1968, $P_{97.5}$ = 98.22 μg/L and $P_{2.5}$ = 40.60 μg/L). These ranges are, in fact, very <u>narrow</u> and provide both quantitative and qualitative indications of the precision of the ATSDR historically reconstructed PCE concentrations in drinking water.

ATSDR is in agreement with the DON statement that "*It is essential that this concept be expressed clearly and consistently to all stakeholders.*" Upon the release of the Chapter I report (Maslia et al. 2009), ATSDR intends to revise the Camp Lejeune water-modeling Web site to include a listing of ranges of PCE concentrations for a given month and year of interest. When a person queries the ATSDR Web site, they will be provided with a mean exposure concentration and the 95% Monte Carlo simulated range of values.

9.1 DON Comment/Statement

For example, the public needs to understand that the model-derived PCE concentrations represent a range of possible exposures.............................. The usefulness of the website would be enhanced if it accurately conveyed the degree of uncertainty in the model-derived concentrations.

9.2 ATSDR Response

ATSDR is in agreement with this DON statement. As stated above, ATSDR has revised the Camp Lejeune water-modeling Web site to include a listing of ranges of PCE concentrations for a given month and year of interest. When a person links to the ATSDR Web site, they will be provided with a mean exposure concentration and the 95% Monte Carlo simulated range of values.

10.1 DON Comment/Statement

Other concerns with model calibration include the simulation of contaminant mass loading and groundwater flow. With Dense, Non-Aqueous Phase Liquids (DNAPLs) such as PCE, mass estimation is always quite difficult and subject to very high uncertainty due to irregular movement and distribution of DNAPL in the subsurface.

10.2 ATSDR Response

In principle, ATSDR is in agreement with the DON statement that DNAPL movement and distribution makes it difficult to estimate contaminant mass. However, water-quality data obtained from the USEPA for the unsaturated zone in the vicinity of ABC One-Hour Cleaners and in the Upper Castle Hayne aquifer at Tarawa Terrace (Roy F. Weston, Inc. 1992, 1994; Faye and Green 2007) indicated that measured PCE concentrations in water-quality samples were significantly below the solubility limit of PCE in water. Typical solubility limits for PCE in water reported in the scientific literature range from 150–210 mg/L (Schwille 1988, Pankow and Cherry 1996, ATSDR 1997, Lawrence 2007). Reported concentrations of PCE in all water- quality samples made available to ATSDR were less than 20% of the solubility limit and most concentrations were in the range of less than 1% to 5% of the solubility limit (Faye and Green 2007). Thus, with PCE concentrations well below their solubility limit, the movement of PCE- contaminated groundwater would not be subjected to the complexities and difficulties encountered with estimating mass of density-driven flows. This concept is further borne out by Schwille (1988) who states, in referring to chlorinated hydrocarbons (CHCs): "*In most cases, the concentrations near all CHC spill sites are very low—usually far below the saturation values.*
This indicates that it may be assumed that density-affected flow will be the exception in real- world situations."

In addition, mass computations similar to those described in Pankow and Cherry (1996) were accomplished for the saturated and unsaturated zones in the vicinity of ABC One-Hour Cleaners, using hydrocone and well data made available to ATSDR by USEPA and USMC (Roy F. Weston, Inc. 1992, 1994; Faye and Green 2007). These mass computations provided a lower- limit estimate for dissolved PCE mass in groundwater needed for simulating the contaminant fate and transport of PCE at Tarawa Terrace. Furthermore, the calibration of the Tarawa Terrace fate and transport model is additionally corroborated by comparing the computed mass residing in the saturated zone from December 1991 to April 1992 (1.5×10^6 grams) to the simulated mass residing in the saturated zone during February 1992 (1.0×10^6 grams) (Faye 2008). The mass computation method described in Pankow and Cherry (1996) and similar to that used by Faye and Green (2007) has been further refined. As explained in Ricker (2008): "*this method is applicable to any contaminant dissolved in ground water.*" A copy of the paper by Ricker (2008) is provided as Attachment 5.

11.1 DON Comment/Statement

For Tarawa Terrace groundwater, the difference between observed and simulated elevations is 5 to 10 feet at many times during the 1970's and 1980's. This is a significant disparity because the total change in groundwater elevation from the source area to the receptor wells is approximately 10 to 12 feet.

11.2 ATSDR Response

This DON approach to evaluating model calibration applies a generalized "rule of thumb" to the Tarawa Terrace groundwater-flow models and is possibly based on wording found in ASTM Guide D5981-96, Standard Guide for Calibrating a Ground-Water Flow Model Application, (ASTM 1996, section 6.4.1): *"the acceptable residual should be a small fraction of the difference between the highest and lowest heads across the site."* ATSDR is not in agreement with this approach to evaluate model calibration. A careful review of ASTM D5981-96 in its entirety indicates that the DON's comment, as stated, is totally removed from the context of Section 6 of the ASTM Standard Guide as well as the context of the accuracy of field data used to calibrate the Tarawa Terrace groundwater-flow model, as described in the Chapter C report (Faye and Valenzuela 2007). For example, in Section 6.4, ASTM D5981-96 states: *"the magnitude of the acceptable residual depends partly upon the magnitude of the error of the measurement or the estimate of the calibration target and partly upon the degree of accuracy and precision required of the model's prediction."* Furthermore, Note 2 of ASTM D5981-96 states: "*Acceptable residuals may differ for different hydraulic head calibration targets within a particular model. This may be due to different errors in measurement."* The Tarawa Terrace Chapter C report (Faye and Valenzuela 2007, p. C24) provides a comprehensive discussion of water-level measurement errors arising from the use of airlines and pressure gages to measure water levels. Faye and Valenzuela also point out that this is consistent with the discussions of LeGrand (1959) who described problems associated with the use of airlines to measure water levels at Camp Lejeune as far back as 1959. As pointed out in Faye and Valenzuela (2007, p.
C24): *"Typically, reported water levels* [at supply wells] *vary in excess of 20 ft during the period of measurement, and frequently 10 ft or more from month to month…. Such variability also may indicate leaking or damaged airlines or pressure gages."*

Faye and Valenzuela (2007, p. C24) also provide detailed discussions as to the rationale for selecting two calibration target ranges for the transient groundwater-flow model. At wells where water-level measurements were obtained using airlines and pressure gages, the calibration target was selected as an absolute difference of 12 ft between simulated and measured water levels. This target was based on well-known disadvantages of using pressure gages and airlines to obtain accurate water-level measurements. Where water-level measurements were obtained using the more highly accurate tapes and similar devices at monitor wells, the calibration target was selected as an absolute difference of 3 ft between simulated and measured water levels. This target was based on the least accurate of these water-level measurements where topographic maps were used to estimate the altitude of a measuring point.

Evaluating model calibration using the "rule of thumb," as the DON has suggested, also assumes that no other information is available to determine calibration targets. When information is available, such as direct knowledge of methods of water-level measurements and information characterizing the measurement device(s), the calibration targets should be based on these data, not on a "rule of thumb." Faye and Valenzuela (2007) provide detailed listings of measured water levels in supply and monitor wells throughout Tarawa Terrace (Appendix C5).

The calibration of the Tarawa Terrace groundwater-flow and contaminant fate and transport models and the computation of related calibration metrics are described in great detail in published ATSDR reports (Faye and Valenzuela 2007, Maslia et al. 2007b, Faye 2008). The calibration approach used by ATSDR closely follows published guidelines for model calibration (National Research Council 1990;Anderson and Woessner 1992; ASTM 2004, 2006, 2008). Nowhere in these publications could we find any reference to the “rule of thumb” for model calibration found in ASTM (1996) and subsequently promoted by the DON. The use of hydraulic head change over a model domain to define an acceptable residual for groundwater model calibration is not found or discussed in any of the aforementioned references. Anderson and Woessner (1992) and ASTM D5940-93 (2008) provide several metrics for evaluating the calibration process and comparing groundwater-flow model simulation to site-specific information. Among these metrics are the use of a scatter diagram and the computation of the mean error, the mean absolute error, the root-mean-square (*RMS*) of error, and standard deviation of error.[1] In conformance with these metrics, the calibration of the ATSDR groundwater-flow models was evaluated using scatter diagrams (Figures C9 and C20 in Faye and Valenzuela [2007] and Figure A10 in Maslia et al. [2007b]) and by computing the mean absolute error of the differences between simulated and observed head at all known observation and water-supply wells within the model domain as well as the *RMS* and standard deviation of these differences (Table C10 in Faye and Valenzuela [2007] and Table A8 in Maslia et al. [2007b]). Attachment 6 to this letter, the scatter diagram from Maslia et al. (2007b), and Attachment 7, Table A8 from Maslia et al. 2007b, describe the computation of the absolute error (head difference) and related *RMS* and standard deviation. The calibration of the ATSDR Tarawa Terrace groundwater-flow and contaminant fate and transport models was based on available water-level and water-quality data to determine calibration targets and closely adheres to accepted model calibration standards and evaluation procedures, such as those described in the aforementioned publications.

12.1 DON Comment/Statement

In addition, model results suggest that the simulated PCE concentrations at the WTP depend significantly on the pumping rates at the various water supply wells. The degree to which simulated well operations match actual operations is a concern. The Navy/Marine Corps would welcome the opportunity for further technical discussion with ATSDR on these issues.

12.2 ATSDR Response

ATSDR is in agreement with the DON that PCE concentrations at the WTP are dependent on the pumping rates assigned to water-supply wells. This dependency is based on the principles of continuity and conservation of mass. The PCE concentration in finished water at the WTP is a function of individual water-supply well pumping rates and their simulated PCE concentrations for a given historical month (stress period)—also referred to as a flow-weighted average PCE concentration (Faye 2008). ATSDR shares the DON’s concern that simulated operations may not match historical operations. Thus, when monthly pumpage data were available, ATSDR used these data in the transient groundwater-flow model (for example, Table C8 in Faye and Valenzuela [2007] and Table I16 in Maslia et al. [2009]). To address issues of missing pumping operational data and the effect of uncertain pumping rates on simulated PCE concentrations, ATSDR conducted additional and complex analyses that described in detail: (1) issues of

[1]The term “error” as used in Anderson and Woessner (1992) and some other references is defined in the ATSDR analyses as “head difference” and refers to the difference between measured and simulated potentiometric heads or water levels.

pumping schedule variation on the arrival of PCE at water-supply wells and the WTP (Wang and Aral 2008) and (2) assessment of uncertain pumping rates by conducting a probabilistic analysis wherein pumping rate was defined as an uncertain model parameter (Maslia et al. 2009, Figure I25).

13.1 DON Comment/Statement

. . . certain combinations of input parameters resulted in wells drying out, so only 510 physically viable realizations were produced. Thus, 330 out of 840 realizations were not viable, raising concerns about the representativeness of the input parameter distributions.

13.2 ATSDR Response

The issue that should be addressed is not how many realizations produced physically plausible solutions, but rather, are the 510 realizations that were successfully produced sufficient to represent an infinite number of random solutions? The metric that determines whether or not this question is answered in the affirmative is the relative change in stopping criteria between successive model simulations. If this relative change is small within a predetermined range, then additional simulations are redundant and do not statistically contribute to an improvement of the representativeness of the overall results with respect to the statistical distributions. The Chapter I report (Maslia et al. 2009) describes in detail the criteria used to determine when a sufficient number of realizations have been achieved. Three stopping criteria were used to halt the Monte Carlo simulation: (1) relative change in the arithmetic mean of PCE concentration in finished water at the Tarawa Terrace WTP, $\Delta \overline{C}$; (2) relative change in the standard deviation of PCE concentration in finished water at the Tarawa Terrace WTP, $\Delta \sigma_C$; and (3) relative change in the coefficient of variation of PCE concentration in finished water at the Tarawa Terrace WTP, ΔC_v. Mathematical formulae and definitions of the aforementioned stopping criteria metrics are listed in Table I13 of the Chapter I report (Maslia et al. 2009). In applying the stopping criteria to the Monte Carlo simulations, an upper and lower bound of ±0.25% was used for each metric. When the computed relative change ($\Delta \overline{C}$, $\Delta \sigma_C$, and ΔC_v) was within the aforementioned bounds and the total number of realizations was 500 or more, the Monte Carlo simulation process was halted. Examples of the stopping criteria for each metric are shown graphically in Attachment 8 (Maslia et al. 2009, Figure I26). As can be seen from the stopping criteria, insignificant change (much less than 2.5%) occurs after 300 realizations. Therefore, 510 realizations were more than sufficient to represent an infinite number of random solutions.

14.1 DON Comment/Statement

Although a summary of the probabilistic analysis is presented in Chapter A of the ATSDR modeling report, the details will be in Chapter I, which is not yet available. The Navy/Marine Corps feels that additional information on this matter would likely help our understanding.

14.2 ATSDR Response

An electronic version (508-compliant PDF®) of the Chapter I report (Maslia et al. 2009) was provided to the DON and USMC on February 13, 2009, and is now available on the ATSDR Web site. Printed copies of the report are expected to be available around March 20, 2009. The

Chapter I report describes in detail the Monte Carlo simulation process and how this process was incorporated into Tarawa Terrace groundwater-flow and contaminant fate and transport models. Additionally, details pertaining to generating uncertain parameter distributions using Monte Carlo and sequential Gaussian simulation are discussed. Note, however, results presented in the Chapter I report do not change or alter results and interpretations presented in the Chapter A report.

15.1 DON Comment/Statement

The usefulness and applicability of the model-derived PCE concentrations for Tarawa Terrace are affected by the following ….

15.2 ATSDR Response

ATSDR has responded in detail to the items numbered in the Summary Section of the DON letter of June 19, 2008. To summarize, ATSDR used data and information that were provided by the USEPA and the USMC. In addition, other data sources from the USGS also were used. This formed the basis for the conceptual models of groundwater flow and contaminant fate and transport applied to the Tarawa Terrace area.

Calibration targets were selected based on the quality and availability of water-level and water-quality data provided to ATSDR. Model analyses and calibrations were conducted by following accepted and published standards for groundwater-flow and contaminant fate and transport models (ASTM 1996, 2004, 2006). It must be emphasized, however, that model calibration standards or targets for groundwater-flow and contaminant fate and transport modeling analyses do not exist, as stated in Anderson and Woessner (1992): *"To date, there is no standard protocol for evaluating the calibration process, although the need for a standard methodology is recognized as an important part of the quality assurance in code application (National Research Council 1990)."* Thus, ATSDR maintains that the models (flow, transport, and mixing) are sufficiently calibrated, given the quantity and accuracy of data provided and the intended use of the simulated historically reconstructed concentrations for the epidemiological study, previously discussed above in the last paragraph of section 7.2.

The concept behind the historical reconstruction process is as follows: (1) when data are limited or unavailable for a certain time period, the data that are available are used to calibrate a model (or models), and (2) the missing data are "reconstructed" or "synthesized" using the calibrated model(s).

16.1 DON Comment/Statement

Groundwater modeling studies are always subject to a high degree of uncertainty, and in this sense, the Tarawa Terrace water model is no exception …. Any use of reconstructed concentrations must take into account the inherent uncertainty in the model results.

16.2 ATSDR Response

ATSDR is not in agreement with the DON that there is a *"high degree of uncertainty"* associated with the Tarawa Terrace models. ATSDR acknowledges that uncertainty and variability exist in model input parameter values and in model output (simulated water levels and PCE concentrations). However, ATSDR has quantified the uncertainty and variability through the use of probabilistic analyses that apply Monte Carlo and sequential Gaussian simulation methods to the Tarawa Terrace groundwater-flow and contaminant fate and transport models. The probabilistic analyses, summarized in Chapter A and described in detail in Chapter I, indicate that for 95% of the Monte Carlo simulations, there is a PCE-concentration range of about 2 when pumping is not an uncertain input parameter and a factor of about 2.5 when pumping is an uncertain parameter. This is well within acceptable confidence limits for the intended use of the reconstructed PCE concentrations needed by the epidemiological case-control study. As previously discussed in section 7.2 of ATSDR's response, the ATSDR health study is not trying to infer at what <u>specific</u> PCE concentration effects are seen. Instead, the epidemiological analysis is trying to evaluate an exposure-response relationship in which the exposures are categorized levels, <u>not</u> absolute values.

17.1 DON Comment/Statement

Recommendations
1. Improve communication …, 2. Convene an expert panel …, 3. Finalize remaining sections…,
4. Apply all lessons learned from the Tarawa Terrace modeling efforts to the scoping of the approach for Hadnot Point.

17.2 ATSDR Response

1. ATSDR water-modeling and health study staff will be meeting with the ATSDR Office of Communications to develop effective methods to communicate results of the historical reconstruction analyses and the uncertainty associated with reconstructed concentrations. ATSDR has removed the Web application that provides a "single" value estimate of historical PCE concentration in Tarawa Terrace drinking water. This Web application has been replaced with Figure I29 and Appendix I5 (Maslia et al. 2009).

2. ATSDR is in the process of organizing an Expert Panel for the Hadnot Point and Holcomb Boulevard areas. The panel is scheduled to meet on April 29 and 30 at ATSDR headquarters. Initial information packets have been mailed to the 13 panel members and panel chair, and a courtesy packet has also been provided to USMC headquarters staff.

3. Chapter I is complete and was released to the DON and USMC on February 13, 2009. Printed copies should be available after March 20. Chapters J (water-distribution modeling) and K (Supplemental Information) are anticipated to be final during June 2009.

4. ATSDR agrees and is in the process of applying lessons learned from the Tarawa Terrace analyses as work progresses on the Hadnot Point and Holcomb Boulevard areas.

CONCLUSIONS

ATSDR appreciates the DON's continued support for the agency's current health study and completion of water-modeling activities. The issues of concern and recommendations contained in the DON's assessment of water-modeling analyses at Tarawa Terrace and vicinity have been carefully considered and fully addressed in ATSDR's responses. The online release of Tarawa Terrace Chapter I report (Maslia et al. 2009) on February 13, 2009, provides additional confidence that the historically reconstructed PCE concentrations determined by Faye (2008) are reasonable, conform well to field observations, and are reliable for their intended use in the epidemiological study.

REFERENCES

Agency for Toxic Substances and Disease Registry. Toxicological Profile for Tetrachloroethylene. Atlanta, GA: U.S. Department of Health and Human Services; 1997.

Anderson MP, and Woessner WW. Applied Groundwater Modeling: Simulation of Flow and Advective Transport. Academic Press, Inc.; 1992.

ASTM. Standard Guide for Calibrating a Ground-Water Flow Model Application. D5981–96 (Reapproved 2002). West Conshohocken, PA: ASTM International; 1996.

ASTM. Standard Guide for Application of a Ground-Water Flow Model to a Site-Specific Problem. D55447–04. West Conshohocken, PA: ASTM International; 2004.

ASTM. Standard Guide for Subsurface Flow and Transport Modeling. D5880–95 (Reapproved 2006). West Conshohocken, PA: ASTM International; 2006.

ASTM. Standard Guide for Comparing Ground-Water Flow Model Simulations to Site-Specific Information. D5940-93. West Conshohocken, PA: ASTM International; 2008.

Bredehoeft JD, and Konikow LF. Ground-Water Models: Validate or Invalidate. Ground Water. 1993; 31(2):178–179.

Davis JH. Fate and Transport Modeling of Selected Chlorinated Organic Compounds at Hangar 1000, U.S. Naval Air Station, Jacksonville, Florida. Tallahassee, FL: U.S. Geological Survey Water-Resources Investigations Report 03-4089; 2003.

Davis JH. Fate and Transport Modeling of Selected Chlorinated Organic Compounds at Operable Unit 1, U.S. Naval Air Station, Jacksonville, Florida. Tallahassee, FL: U.S. Geological Survey Scientific Investigations Report 2007-5043; 2007.

Faye RE. Analyses of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water at Tarawa Terrace and Vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina: Historical Reconstruction and Present-Day Conditions—Chapter F: Simulation of the Fate and Transport of Tetrachloroethylene (PCE). Atlanta, GA: Agency for Toxic Substances and Disease Registry; 2008.

Faye RE, and Green JW Jr. Analyses of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water at Tarawa Terrace and Vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina: Historical Reconstruction and Present-Day Conditions— Chapter E: Occurrence of Contaminants in Groundwater. Atlanta, GA: Agency for Toxic Substances and Disease Registry; 2007.

Faye RE, and Valenzuela C. Analyses of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water at Tarawa Terrace and Vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina: Historical Reconstruction and Present-Day Conditions— Chapter C: Simulation of Groundwater Flow. Atlanta, GA: Agency for Toxic Substances and Disease Registry; 2007.

Helsel DR. Nondetects and Data Analysis: Statistics for Censored Environmental Data. Hoboken, NJ: John Wiley & Sons; 2005.

Hill MC, and Tiedeman CR. Effective Groundwater Model Calibration. Hoboken, NJ: John Wiley & Sons; 2007.

Jang W, and Aral MM. Analyses of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water at Tarawa Terrace and Vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina: Historical Reconstruction and Present-Day Conditions— Chapter G: Simulation of Three-Dimensional Multispecies, Multiphase Mass Transport of Tetrachloroethylene (PCE) and Associated Degradation By-Products. Atlanta, GA: Agency for Toxic Substances and Disease Registry; 2008.

Lawrence SJ. Analyses of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water at Tarawa Terrace and Vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina: Historical Reconstruction and Present-Day Conditions—Chapter D: Properties of Degradation Pathways of Common Organic Compounds in Groundwater. Atlanta, GA: Agency for Toxic Substances and Disease Registry; 2007.

LeGrand HE. Evaluation of Well-Water Supply, Marine Corps Base, Camp Lejeune, North Carolina: Project Report, Contract NBy-7595; 1959.

Maslia ML. Expert Peer Review Panel Evaluating ATSDR's Water-Modeling Activities in Support of the Current Study of Childhood Birth Defects and Cancer at the U.S. Marine Corps Base Camp Lejeune, North Carolina: Atlanta, GA: Agency for Toxic Substances and Disease Registry; 2005.

Maslia ML, Sautner JB, Aral MM, Reyes JJ, Abraham JE, and Williams RC. Using Water-Distribution System Modeling to Assist Epidemiologic Investigations. Journal of Water Resources Planning and Management. 2000; 126(4):180-198.

Maslia ML, Sautner JB, Faye RE, Suárez-Soto RJ, Aral MM, Grayman WM, Jang W, Wang J, Bove FJ, Ruckart PZ, Valenzuela C, Green JW Jr, and Krueger AL. Analyses of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water at Tarawa Terrace and Vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina: Historical Reconstruction and Present-Day Conditions—Executive Summary. Atlanta, GA: Agency for Toxic Substances and Disease Registry; 2007a.

Maslia ML, Sautner JB, Faye RE, Suárez-Soto RJ, Aral MM, Grayman WM, Jang W, Wang J, Bove FJ, Ruckart PZ, Valenzuela C, Green JW Jr, and Krueger AL. Analyses of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water at Tarawa Terrace and Vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina: Historical Reconstruction and Present-Day Conditions—Chapter A: Summary of Findings. Atlanta, GA: Agency for Toxic Substances and Disease Registry; 2007b.

Maslia ML, Suárez-Soto RJ, Wang J, Aral MM, Faye RE, Sautner JB, Valenzuela C, and Grayman WM. Analyses of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water at Tarawa Terrace and Vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina: Historical Reconstruction and Present-Day Conditions— Chapter I: Parameter Sensitivity, Uncertainty, and Variability Associated with Model Simulations of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water. Atlanta, GA: Agency for Toxic Substances and Disease Registry; 2009.

National Research Council. Ground Water Models: Scientific and Regulatory Applications. Washington, DC: National Academy of Sciences; 1990.

Oreskes N, Shrader-Frechette K, and Belitz K. Verification, Validation, and Confirmation of Numerical Models in the Earth Sciences. Science. 1994; 263:641–646.

Pankow JF, and Cherry JA. Dense Chlorinated Solvents and Other DNAPLs in Groundwater: History, Behavior, and Remediation. Portland, OR: Waterloo Press; 1996.

Ricker JA. A Practical Method to Evaluate Ground Water Contaminant Plume Stability. Ground Water Monitoring & Remediation. 2008; 28(4):85–94.

Roy F. Weston, Inc. Remedial Investigation Report, ABC One-Hour Cleaners, Jacksonville, North Carolina: Roy F. Weston, Inc.; 1992.

Roy F. Weston, Inc. Remedial Investigation Report, ABC One-Hour Cleaners, Operable Unit 2, Jacksonville, North Carolina: Roy F. Weston, Inc.; 1994.

Schwille F. Dense Chlorinated Solvents in Porous and Fractured Media. Translated by Pankow, JF. Boca Raton: Lewis Publishers (CRC Press); 1988.

Wang J, and Aral MM. Analyses of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water at Tarawa Terrace and Vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina: Historical Reconstruction and Present-Day Conditions— Chapter H: Effect of Groundwater Pumping Schedule Variation on Arrival of Tetrachloroethylene (PCE) at Water-Supply Wells and the Water Treatment Plant. Atlanta, GA: Agency for Toxic Substances and Disease Registry; 2008.

Response to the Department of the Navy's Letter on Assessment of ATSDR Water Modeling for Tarawa Terrace

Attachment 1: Department of Navy Comments, June 19, 2008

Assessment of
ATSDR Water Modeling for Tarawa Terrace

The purpose of this assessment is (1) to document the Navy/Marine Corps' current understanding of the ATSDR water modeling for Tarawa Terrace and (2) to serve as a basis for additional technical discussions between the Navy/Marine Corps and ATSDR.

Background

1.1 During a Technical Information Meeting with the Marine Corps and Navy on March 26, 2008, the ATSDR presented their water modeling efforts in a summary report entitled "Exposure to Volatile Organic Compounds in Drinking Water and Specific Birth Defects and Childhood Cancer at U.S. Marine Corps Base Camp Lejeune, North Carolina," (March 26, 2008). The report indicates that the following specific information is needed in order to conduct a health study on these birth defects:

1. When did contaminated groundwater reach water supply wells? **month and year**
2. What was the timing, level, and duration of maternal or infant exposure to contaminated drinking water:
    a. In which **months** did exposure occur?
    b. What was the **monthly** average level of contamination?
    c. For how many **months** did exposure occur?

Thus, extensive data are required in order to conduct the proposed health study. Since no measured concentrations of PCE (perchloroethylene) are available prior to 1982, the ATSDR has used modeling to simulate these concentrations at Tarawa Terrace, and proposes a similar modeling approach for Hadnot Point. The results of the Tarawa Terrace modeling are being documented in the ATSDR modeling report entitled "Analysis of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water at Tarawa Terrace and Vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina: Historical Reconstruction and Present-Day Conditions" (ongoing, but initial chapters published in 2007 and 2008).

In general, the usefulness of a groundwater flow and contaminant transport model depends on an accurate estimate of numerous model parameters that describe site geology, groundwater velocity, well pumping rates, and contaminant properties. Many of these parameters are highly variable and difficult to estimate directly. Therefore, model calibration and validation are essential steps in the modeling process. Model calibration involves adjusting the initial parameter values until simulated model concentrations match measured concentrations. In a second step, the calibrated model is validated by comparing simulated concentrations to additional measured concentrations that were not used during calibration. During validation, the model is "put at risk," and it may be judged unsuccessful if the simulated and measured concentrations do not match.

Tarawa Terrace Water Modeling

The Tarawa Terrace housing development at Camp Lejeune was constructed in 1951, and the Tarawa Terrace Water Treatment Plant (WTP) began to distribute drinking water during 1952-1953. The only documented source of contamination at Tarawa Terrace is ABC One-Hour

Cleaners, which began operations during 1953, using the chlorinated solvent PCE in its dry cleaning process. PCE concentrations were measured at the WTP in 1982 and 1985, and no measured concentrations of PCE are available prior to 1982.

Monthly PCE concentrations are required for the ATSDR health study, which will examine
2.1 births that occurred from 1968 (when North Carolina computerized its birth certificates) to 1985
(when the contaminated water supply wells were removed from service). Due to lack of
measured concentrations, the ATSDR used groundwater flow and contaminant transport
modeling in a historical reconstruction process to simulate PCE concentrations in the drinking 3.1
water on a monthly basis from 1952 to 1987.

Figure 1 shows the simulated concentrations of PCE versus measured concentrations in finished
4.1 water from the WTP. Significantly, measured concentrations of PCE are available only in 1982
and 1985, near the end of the overall time period. Thus, the majority of the simulated
concentrations cannot be compared to measured data. Furthermore, all of the measured
concentrations were used during model calibration, leaving no data available for model 5.1
validation. As a result, the Tarawa Terrace model was not validated.

During calibration, model parameters were adjusted to cause the simulated concentrations at the Water Treatment Plant (WTP) to meet the calibration standard to the degree possible. For PCE detections, the ATSDR chose the calibration standard to be "± 1/2-order of magnitude of the observed valued," such that the higher value in the calibration target range is 10 times greater than the lower value. For example, at the WTP in May 1982, the calibration target range was 25 to 253 ug/L, based on the measured PCE concentration of 80 ug/L. The simulated concentration of 148 ug/L fell within this range. As another example, at supply well TT-26 in January 1985, the calibration target range was 500 to 5,000 ug/L based on the measured PCE concentration of 6.1
1,580 ug/L. In this case, the range was quite large because it was calculated from a relatively high measured concentration. The simulated concentration of 804 fell within the range, near the lower end. In summary, based on the chosen calibration standard, the calibration process was viewed as "successful" over a range that spanned a factor of 10. In other words, a model-derived PCE concentration can be approximately 3 times higher or 3 times lower than the measured concentration and still fall within the calibration range.

Thus, if all comparisons had fallen within the calibration range, the chosen calibration standard would give an idea of the accuracy, or degree of fit, between simulated and measured
concentrations. However, all comparisons did not fall within the calibration range. At the WTP,
12% of the simulated PCE concentrations failed the calibration standard (p. F42 in the ATSDR
7.1 modeling report). It should be noted that these failures involved non-detects or very low
concentrations. More significantly, at the water supply wells, a majority (53%) of the simulated
concentrations fell outside the calibration standard **(p. F33 in the ATSDR modeling report).**
Graphs of simulated versus observed concentrations of PCE in water supply wells RW2, TT-23, TT-25, TT-26, and TT-54 are shown below in Figures F13 through F17 (p. F34 and F35 of the ATSDR modeling report). The graphs show that only a few observed PCE concentrations are available, and there are substantial differences between observed and simulated concentrations. Model performance at the supply wells raises concerns about the degree to which the model calibration was successful. It seems reasonable to conclude that the accuracy of historically
8.1

8.1 reconstructed PCE concentrations would be less than the calibration standard of ± 1/2-order of magnitude. Thus, the historical reconstructions may be viewed as rough estimates of actual exposure concentrations, with model-derived PCE concentrations representing a relatively wide range of possible exposures. It is essential that this concept be expressed clearly and consistently to all stakeholders.

9.1 For example, the public needs to understand that the model-derived PCE concentrations represent a range of possible exposures. This concept should be expressed more clearly on the Camp Lejeune website (http://www.atsdr.cdc.gov/sites/lejeune/watermodeling.html). Currently the website has a section that says: "Find Out PCE Levels During Your Tour; Find out the levels of PCE and PCE degradation by-products in the drinking water serving your home in Tarawa Terrace by entering the dates you lived in Tarawa Terrace housing from 1952 to 1987." Following a disclaimer, a search engine produces contaminant concentrations, reported to 4 significant digits, for any or all months between January 1952 and February 1987. With no error bars or ranges included, this webpage conveys a sense of certainty that is not justified. The usefulness of the website would be enhanced if it accurately conveyed the degree of uncertainty in the model-derived concentrations.

10.1 Other concerns with model calibration include the simulation of contaminant mass loading and groundwater flow. With Dense, Non-Aqueous Phase Liquids (DNAPLs) such as PCE, mass estimation is always quite difficult and subject to very high uncertainty due to irregular movement and distribution of DNAPL in the subsurface. For Tarawa Terrace groundwater, the difference between observed and simulated elevations is 5 to 10 feet at many times during the 1970's and 1980's. This is a significant disparity because the total change in groundwater elevation from the source area to the receptor wells is approximately 10 to 12 feet. 11.1 In addition, 12.1 model results suggest that the simulated PCE concentrations at the WTP depend significantly on the pumping rates at the various water supply wells. The degree to which simulated well operations match actual operations is a concern. The Navy/Marine Corps would welcome the opportunity for further technical discussion with ATSDR on these issues.

The ATSDR performed a sensitivity analysis to determine the relative importance of individual model parameters. In addition, a probabilistic analysis was performed to assess variability and uncertainty associated with the model results. Both approaches are standard practice. Chapter A of the ATSDR modeling report describes the probabilistic analysis, during which input parameters such as hydraulic conductivity, recharge, and dispersivity were chosen from distributions of possible values. The model was run 840 times to produce "realizations" that form a distribution of simulated PCE concentrations, rather than a single result (pp. A52 – A61 of the ATSDR modeling report). However, 13.1 certain combinations of input parameters resulted in wells drying out, so only 510 physically viable realizations were produced. Thus, 330 out of 840 realizations were not viable, raising concerns about the representativeness of the input parameter distributions. 14.1 Although a summary of the probabilistic analysis is presented in Chapter A of the ATSDR modeling report, the details will be in Chapter I, which is not yet available. The Navy/Marine Corps feels that additional information on this matter would likely help our understanding.

Overall, it is important to keep in mind that both the sensitivity analysis and the probabilistic analysis were performed entirely within the "model world," not the "real world." These methods provide valuable insight into the behavior of the model, but they are not a substitute for real, measured PCE concentrations. Again, the Navy/Marine Corps looks forward to additional discussion and clarification of our understanding of these issues.

Summary

15.1 The usefulness and applicability of the model-derived PCE concentrations for Tarawa Terrace are affected by the following:

1. Model simulations provide monthly concentrations from 1952 to 1987, but measured concentrations for model calibration are available only in 1982 and 1985. Thus, the majority of the simulated concentrations cannot be compared to measured data.
2. Simulated concentrations did not fall within calibration targets for a majority of the measured PCE concentrations at the water supply wells, suggesting that the "accuracy" of the model is less than the chosen calibration standard of ± 1/2-order of magnitude.
3. Due to lack of measured PCE concentrations, the Tarawa Terrace model was not validated. Therefore, the model was not "put at risk," and it is difficult to judge the accuracy of the simulated PCE concentrations beyond the limited times when calibration data are available.

16.1 Groundwater modeling studies are always subject to a high degree of uncertainty, and in this sense, the Tarawa Terrace water model is no exception. However, the goal of the Tarawa Terrace model is to reconstruct PCE concentrations on a monthly basis over approximately 30 years in order to conduct a health study. This is an extremely difficult goal since measured PCE concentrations are not available prior to 1982, and the historical reconstruction of monthly exposure concentrations must go back to the 1950's. Any use of reconstructed concentrations must take into account the inherent uncertainty in the model results.

Recommendations

17.1 As a starting point for further discussions, the Navy/Marine Corps proposes the following recommendations:

1. Improve communication with the public and other stakeholders by developing a method for presenting the uncertainty in the model-derived PCE concentrations. The method should be clear and readily understood, perhaps using error bars or presenting a concentration range rather than a single number. The method should be applied consistently whenever concentrations are discussed or presented in model reports, websites, public meetings, etc.
2. Convene an expert panel to examine the model results and determine the best use for the data. Overall, the panel should develop a path forward that is scientifically sound and will best meet the critical concerns of the public.
3. Finalize the remaining sections of the Tarawa Terrace water modeling report.
4. Apply all lessons learned from the Tarawa Terrace modeling efforts to the scoping of the approach for Hadnot Point.

Appendix M — ATSDR Response to National Research Council Report on Contaminated Water-Supplies at Camp Lejeune: Assessing Potential Health Effects (NRC 2009)

Agency for Toxic Substances and Disease Registry (ATSDR)

Response to the National Research Council (NRC) Report
Contaminated Water Supplies at Camp Lejeune—Assessing Potential Health Effects

By: The ATSDR Exposure-Dose Reconstruction Program Staff

July 1, 2009

INTRODUCTION

The Agency for Toxic Substances and Disease Registry's (ATSDR) Exposure-Dose Reconstruction Program staff has reviewed the National Research Council (NRC) report titled, "*Contaminated Water Supplies at Camp Lejeune—Assessing Potential Health Effects.*" Specifically, our review focused on Section 2 of the report (p. 28–66), "Exposure to Contaminants in Water Supplies at Camp Lejeune." Based on our review of Section 2, we conclude the following:

> The National Research Committee report (NRC 2009) contains numerous misrepresentations and distortions of ATSDR water-modeling analyses, field data and related interpretations and conclusions that are clearly contradicted by findings in ATSDR technical reports. Those ATSDR reports that describe groundwater contamination and the results of model studies related to contamination of drinking water at the Tarawa Terrace base housing area, Camp Lejeune, North Carolina, along with additional supporting information from the Department of Navy, the U.S. Marine Corps, and other sources were provided to the NRC committee during the course of their deliberations. Because the NRC report contains many errors and misrepresentations with respect to the findings of the ATSDR water-modeling analyses and because conclusions and recommendations contained in the NRC report are at such odds with recommendations rendered by several review panels consisting of national and international experts in water modeling and epidemiology, the NRC report cannot be considered an authoritative interpretation or guidance document related to the historical exposure assessment of contaminated drinking water at Camp Lejeune.

We base the aforementioned statements on four overarching issues discussed below. In addition, we present specific examples wherein the NRC committee arrived at erroneous conclusions by using incorrect data and otherwise misrepresenting data and information contained in reports that summarize ATSDR investigations at Tarawa Terrace and vicinity. Additional supporting documentation and in-depth technical reviews related to specific NRC report comments are provided in Appendix I and II of this document.

ISSUE 1: USE OF HISTORICAL RECONSTRUCTION FOR EXPOSURE ASSESSMENT

Models must be used and have been successfully used to reconstruct historical contaminant concentrations when pertinent data are limited or unavailable (Rodenbeck and Maslia 1998, McLaren/Hart-ChemRisk 2000, Maslia et al. 2001, Reif et al. 2003, Kopecky et al 2004). If models cannot be used to reconstruct historical exposure to contaminants, then models also should not be used for predictive analyses such as planning for remediation strategies or the management of future water supplies. Furthermore, the NRC report (2009) erroneously states that "cutting-edge" models used by ATSDR were not in the public domain and were not documented, and, as such, falsely claims that ATSDR simulation results are invalid and unacceptable.

ISSUE 2: CHARACTERIZATION OF PCE AS A DENSE NON-AQUEOUS PHASE LIQUID (DNAPL)

Characterizing tetrachloroethylene (PCE) contamination in groundwater at the ABC One-Hour Cleaners site and at Tarawa Terrace base housing as a "free-phase" or "pure-phase" DNAPL (NRC 2009, p. 38) contradicts and misrepresents concentration data presented in ATSDR and in other reports and documents. Those reports and documents unequivocally describe the PCE in groundwater in the vicinity of ABC One-Hour Cleaners as "dissolved-phase" PCE (Shiver 1985, Roy F. Weston, Inc. 1992, 1994, Faye and Green 2007). The solubility limit of PCE in water occurs at a concentration of at least 210,000 micrograms per liter (µg/L) (Pankow and Cherry 1996, Lawrence 2007). PCE in groundwater that occurs at concentrations much less than the solubility limit is, by definition, dissolved-phase PCE. The ATSDR conceptualization of groundwater flow and of dissolved-phase PCE conditions at ABC One-Hour Cleaners and the Tarawa Terrace base housing area is shown below in Figure 1. PCE-concentration data presented in ATSDR reports (Faye and Green 2007, Tables E5 and E7) indicate that concentrations of PCE in groundwater at Tarawa Terrace and vicinity occur at much less than 10% of the solubility limit. The NRC characterization of PCE in the vicinity of ABC One-Hour Cleaners as DNAPL PCE is further discredited by the process selected to remediate the PCE contamination in groundwater at Tarawa Terrace and vicinity, as described below.

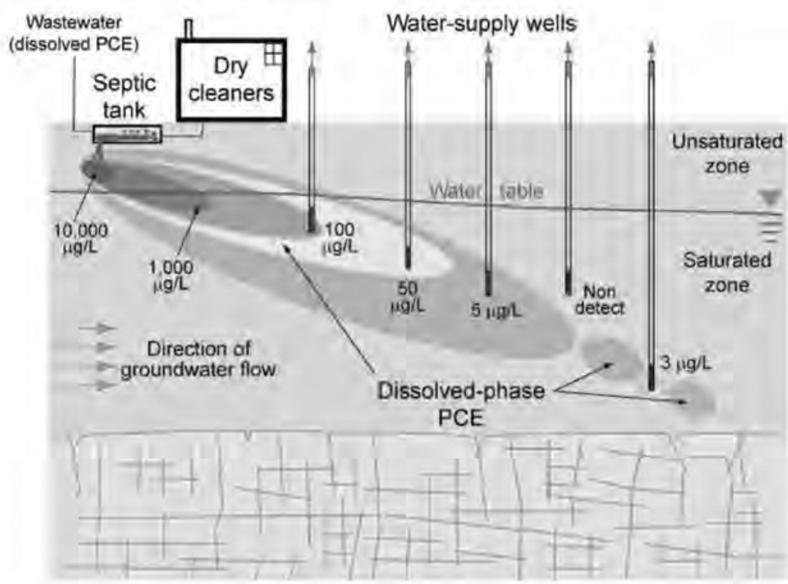


Figure 1. Conceptual model of groundwater flow and dissolved-phase PCE transport at, and in the vicinity of, ABC One-Hour Cleaners (solubility of PCE is at least 210,000 µg/L [Pankow and Cherry 1996, Lawrence 2007])

Processes selected to remediate free-phase DNAPL PCE in groundwater are totally different from processes used to remediate dissolved-phase PCE in groundwater. The remediation process currently in progress at the ABC One-Hour Cleaners and at Tarawa Terrace is conducted under the auspices of the U.S. Environmental Protection Agency (USEPA). This remediation process was approved by the North Carolina Department of Environment and Natural Resources (NCDENR) and is correctly described as "groundwater extraction by wells and treatment by air stripping" (i.e., pump-and-treat). This remediation process is appropriate only for dissolved-phase PCE—not DNAPL PCE (NCDENR 2003, Weston Solutions Inc. 2005, 2007).

ISSUE 3: EVALUATION OF UNCERTAINTY

Uncertainties with respect to model input parameters and field data accuracy are common to all model investigations and are particularly evident when models are used to reconstruct historical groundwater conditions and contaminant concentrations. Uncertainties related to model studies at Tarawa Terrace and vicinity were largely the result of imperfect knowledge regarding the parameters input to equations solved as part of the historical reconstruction process. To quantify uncertainty, ATSDR systematically applied well-established, scientifically accepted techniques to analyze field data and simulation results (McLaren/Hart-ChemRisk 2000, Wang and Aral 2008, Maslia et al. 2009). For example, model parameters based on field data were characterized by a range of values that described what was known about each parameter's uncertainty and variability. The uncertainty and variability were then described using statistical determinations of probability and confidence limits. The uncertainty techniques developed and applied by ATSDR were never intended to provide "accurate" answers, as implied in the NRC report (NRC 2009, p. 16). Rather, ATSDR's uncertainty analyses outcome indicate the possible range of concentrations at a given historical time, which is the intended purpose of an uncertainty analysis.

ISSUE 4: RELIABILITY OF RECONSTRUCTED HISTORICAL CONCENTRATIONS

ATSDR's analyses presented in the water-modeling reports indicate that reconstructed historical contaminant concentrations in drinking water (finished water delivered from the Tarawa Terrace water treatment plant) provide reliable and acceptable comparisons with measured PCE-concentrations in drinking water samples collected at the water treatment plant. Twenty-five water-quality samples obtained from the Tarawa Terrace water treatment plant during May 1982–October 1985 contained PCE concentrations ranging form 215 µg/L to non-detect (detection limits of 2–10 µg/L). For the same period, model predictions of PCE concentrations at the water treatment plant ranged from 176 µg/L to 3.6 µg/L (Maslia et al. 2007, Table A10). Reconstructed PCE concentrations in drinking water vary by a factor of 2-3 from measured concentrations at specific times, which is within acceptable limits for model studies and also within limits required by the epidemiological study. These data and findings are never presented or discussed in the NRC report (NRC 2009).

EXAMPLES OF MISREPRESENTATION OF DATA AND INCORRECT INFORMATION IN THE NRC REPORT

Listed below are specific examples wherein the NRC committee scientists used incorrect data and misrepresented data and information contained in ATSDR Tarawa Terrace reports to come to erroneous conclusions. All report statements and page numbers refer to the referenced NRC report (NRC 2009).

- NRC Report, p. 33: *"Figure 2-3 illustrates various possible pathways for groundwater contamination from a DNAPL source"*

  Figure 2-3 in the NRC report grossly misrepresents the migration and transport of PCE-contaminated groundwater away from the source area at ABC One-Hour Cleaners toward the Tarawa Terrace base housing area. All relevant field data indicate that dissolved-phase PCE—not DNAPL PCE—was transported along groundwater pathways, probably within one or several contaminant plumes, as illustrated in the conceptual drawing shown in Figure 1 above.

- NRC Report, p. 38: *"A shallow monitoring well installed close to the cleaners detected an extremely high PCE concentration of 12,000 μg/L (Faye and Green 2007). Such a high concentration is an indication of a source region that contains pure-phase PCE (the highest possible concentration PCE in water is about 110,000 μg/L)"*

  These statements from the NRC report not only incorrectly define the solubility limit of PCE in water but conclude incorrectly that a single PCE concentration in groundwater is indicative of a "pure-phase" PCE source at ABC One-Hour Cleaners. Pankow and Cherry (1996) and Lawrence (2007) report the highest possible concentration of PCE in water (also known as the solubility limit of PCE) is 237,000 μg/L and 210,000 μg/L at 25° C, respectively. The NRC report does not provide a reference for the solubility limit of 110,000 μg/L noted above. The "extremely high concentration of 12,000 μg/L" is less than 6% of the PCE solubility in water (12,000/210,000 = 5.7%). Thus, the location of this high PCE concentration sample can only be used to identify the source location, but is not a guarantee or confirmation that "free-phase" or "pure-phase" PCE exists at this sample location, at the ABC One-Hour Cleaners site, or within the Tarawa Terrace base housing area.

- NRC Report, pgs. 38-39: *"The gasoline contamination was traced to various spills and leaks from 12 underground storage tanks (USTs) associated with various buildings in the Tarawa Terrace shopping center."*

  The contamination referred to above is a "gasoline-type odor" noted at supply well TT-53 and described in Chapter E of the Tarawa Terrace series of reports (Faye and Green, p. 14). No effort is made in Chapter E or any other report of the Tarawa Terrace series to link the gasoline odor at well TT-53 to any source. The statement to the contrary quoted above from the NRC report is totally false.

- NRC Report, p. 43: "*. . . and the U.S. Environmental Protection Agency (EPA) model MT3DMS to simulate PCE transport . . .*"

The model MT3DMS is the second generation of the modular three-dimensional transport model MT3D. The model MT3D was developed by Zheng (1990) and released as a public domain code by EPA during 1990. MT3DMS was developed by Zheng and Wang (1999) on behalf of the U.S. Army Engineer Research and Development Center.

- NRC Report, p. 43: "*For example, MT3DMS can predict transport only of dissolved contaminants, so a key approximation was made to represent the mass dissolved from the DNAPL source. To apply MT3DMS, ATSDR replaced the highly complex DNAPL contaminated source zone with a hypothetical model node where PCE was injected directly into the saturated aquifer formation at a constant rate (1.2 kg/day).*"

  The NRC report misrepresents the characterization of PCE contamination as a DNAPL or pure-phase source. The fact is that ATSDR and other reports and documents unequivocally describe the PCE in groundwater in the vicinity of ABC One-Hour Cleaners as dissolved-phase PCE (see Figure 1, above). Therefore, MT3DMS or any other model capable of simulating dissolved-phase contaminants in groundwater is an appropriate model choice and no approximation is needed (with respect to dissolved-phase PCE) to correctly characterize the occurrence of PCE in the source area at ABC One-Hour Cleaners.

- NRC Report, p. 43: "*Unlike the MODFLOW and MT3DMS codes, the PSOpS and TechFlowMP codes lack validation by a broad spectrum of practicing geoscientist in an open-source environment.*"

  The NRC report misrepresents the PSOpS and TechFlowMP codes as not validated and not in the public domain. Model validation is not determined by the number of "practicing geoscientists" that use and apply a particular model; rather, numerical models are validated by comparing model predictions to known mathematical (analytical) solutions and site-specific field data when available—this was done with TechFlowMP. Both PSOpS and TechFlowMP are open source and the source codes are available by contacting the principal investigator of the ATSDR-Georgia Tech Research Program on Exposure-Dose Reconstruction Program, Dr. M.M. Aral (email: maral@ce.gatech.edu). These codes can also be accessed through the website of the Multimedia Environmental Simulations Laboratory at Georgia Tech (http://mesl.ce.gatech.edu/).

  It is equally important to note, however, that the use and application of specialized codes to address specific problems that routinely used codes, such as MODFLOW and MT3DMS, cannot address, is not shunned by government-based scientific organizations, but rather, it is recognized and encouraged. As stated in the U.S. Environmental Protection Agency report, "Guidance on the Development, Evaluation, and Application of Environmental Models" (USEPA 2009, p. 31):

  > "However, the Agency acknowledges there will be times when the use of proprietary models provide the most reliable and best-accepted characterization of a system."

  The point being made in this statement is that the most appropriate model should be applied to characterize a system, not necessarily, the most popular or often-used model; and this is the exact modeling philosophy and approach that ATSDR took when applying the TechFlowMP and PSOpS models at ABC One-Hour Cleaners and Tarawa Terrace and vicinity.

- NRC Report, p. 48: "*. . ., spatial variations in concentration are averaged over a relatively large control volume represented by the model grid cells (the typical volume of a computational cell in layer 1 is about 100,000 ft^3), whereas the water-quality data represent spatial variations on the scale of the control volume represented by the well (which we estimate at about 10-100 ft^3).*"

  This statement from the NRC report completely and falsely misrepresents the application of field water-quality data applied to the calibration of the Tarawa Terrace fate and transport model. Chapter F of the Tarawa Terrace series of reports states clearly and unambiguously that scale effects were taken into account when selecting field water-quality data for model calibration and, as such, only data collected at supply wells were used (Faye 2008, p. 31). Control volumes related to operating water-supply wells at Tarawa Terrace are of the same order of magnitude represented by grid cells in model layer 1.

- NRC Report p. 48: "*Because insufficient historical pumping data were available to constrain the model predictions form 1953 to 1980, the ability of the advanced optimization models to estimate the dates accurately is questionable.*"

  In this statement, the NRC report misrepresents the rationale behind the development, use, and application of the PSOpS optimization model. The PSOpS model was not developed and applied to "estimate dates accurately"—scientifically, this is not possible. Rather, ATSDR's optimization model was developed and applied to Tarawa Terrace calibrated groundwater flow and contaminant fate and transport models to derive alternate pumping scenarios by systematically and objectively varying the on-off cycling of water-supply wells. In doing so, the 5 μg/L PCE concentration front arrived at water-supply wells at times that differed from the calibrated arrival date. This approach provided an "envelope" or range of arrival times. Uncertainty and variability issues related to modeling can never be answered with exactitude as use of the term "accuracy" implies.

- NRC Report p. 49: "*Constant values of dispersivity (longitudinal dispersivity of 25 ft and transverse of 2.5 ft) were used in the transport model. There is insufficient information available on the nature and amount of heterogeneity to use these fixed values with a sufficient level of confidence in predictive simulations.*"

  Constant values of dispersivity were used in the calibrated, deterministic fate and transport model (Faye 2008). However, for the uncertainty analyses using Monte Carlo simulation, disersivity values were assigned on a cell-by-cell basis, as discussed in Chapter I of the Tarawa Terrace report series (Maslia et al. 2008, Table I15, and p. I42) Furthermore, the NRC report fails to discuss that although assigned dispersivity values were constant for the deterministic modeling approach, the resulting dispersion matrix values (in the fate and transport equation) were not constant because specific discharge (Darcy velocities) and groundwater velocities vary cell-by-cell. Assigning constant dispersivity values to model arrays is a commonly used approach, especially when pertinent site-specific field data, such as the results of tracer tests, are unavailable. Furthermore, in the absence of site-specific field data the longitudinal dispesivity of 25 ft was chosen based on: (1) literature values for similar aquifer materials, and (2) numerical requirements for Peclet and Courant numbers that minimize numerical dispersion and oscillation.

- NRC Report p. 49: "*Review of water-quality monitoring data indicates substantial temporal variability even at a single well. For example, seven measurements taken on well TT-26 from January to September 1985 indicates that the concentration at this well varied from 3.8 to 1,580 µg/L (see Table 2-3). The model predictions for the same timeframe ranged from 804 to 788 µg/L.*"

  The NRC report fails to mention that the "monitoring data" are from a single water-supply well (TT-26) and not a properly constructed monitor well. Thus, the temporal variation of PCE concentration could equally be caused by errors in, and different methods of, water-sample collection and analysis. These issues are thoroughly discussed in Chapter F of the Tarawa Terrace series of reports (Fay 2008, p. 45) and largely rebut the NRC example of "substantial temporal variability" of contaminant concentrations at wells. Additionally, the NRC report does not list or discuss the 25 water-quality samples obtained from the Tarawa Terrace water treatment plant from May 1982–October 1985 that range in value from 215 µg/L to non-detect (detection limits of 2–10 µg/L) nor does it compare these data with model predictions of 176 to 3.6 µg/L at the water treatment plant for the same timeframe (Maslia et al. 2007, Table A10).

- NRC Report p. 49: "*The TechFlowMP model predicted very high vapor concentrations. For example, TechFlowMP predicted that the PCE vapor concentration in the top 10 ft of soil beneath the Tarawa Terrace elementary school should be 1,418 µg/L. Studies of PCE vapor concentrations in buildings that house or are near a dry-cleaning facility have reported measured concentrations around 55 µg/L.*"

  The NRC report grossly misrepresents the aforementioned model predicted values. The fact is, as specifically discussed in Chapter A of the Tarawa Terrace report series, the value "1,418 µg/L" refers to the maximum simulated PCE concentration in <u>groundwater</u> (model layer 1) at the Tarawa Terrace elementary school during December 1984. The maximum simulated <u>vapor-phase</u> PCE concentration in the top 10 ft of soil was 137 µg/L during December 1984 (Maslia et al. 2007, p. A44). The aforementioned measured PCE-vapor concentration referred to in the NRC report (55 µg/L) was obtained from buildings that house or are near a residential dry cleaning facility in New York City during 2001–2003 (McDermott et al. 2005). There is absolutely no basis, rationale, or scientific justification for comparing ATSDR model simulations of vapor concentration in the pore space of soils beneath the Tarawa Terrace elementary school area for December 1984 with dry-cleaner PCE-vapor measurements made in a building in New York City during 2001–2003.

- NRC Report p. 49: "*The biodegradation model used within the TechFlowMP code is based on an untested preliminary research model. . . The simple first-order modeling framework that also used a single decay coefficient for the entire modeling domain may not capture those biologic complexities . . .* "

  The TechFlowMP code represents a series of processes such as vapor migration, unsaturated flow, saturated groundwater flow, multiphase fate and transport of a contaminant, decay, and biodegradation. Thus, biodegradation is just one of a number of hydrologic and geochemical processes that are contained within the TechFlowMP modeling framework. The NRC report is incorrect in implying that the TechFlowMP code and the aforementioned process are an "untested preliminary research model." To the contrary, processes within the TechFlowMP model were tested against known analytical solutions and available field data provided to ATSDR by the Department of the Navy and the U.S. Marine Corps. The TechFlowMP code is a public domain code, so anyone who wants to further test the code, can do so by contacting the principal investigator of the ATSDR-Georgia Tech Research Program on Exposure-Dose Reconstruction Program, Dr. M.M. Aral (email: maral@ce.gatech.edu) or they can access the code through the website of the Multimedia Environmental Simulations Laboratory at Georgia Tech (http://mesl.ce.gatech.edu/).

Manipulating the constant decay coefficient value during the model calibration process to arrive at non-constant decay coefficient values (i.e., spatial variation) in the absence of site-specific field data, is not a defensible technical or scientific approach to model simulation and calibration. The decay coefficient assigned to ATSDR fate and transport models was derived from limited field data and literature reported values. For example, ATSDR used a mean value for decay coefficient (reaction rate) of 5.0×10^{-4} day^{-1} with a range of 2.3×10^{-4} to 7.7×10^{-4} d^{-1} (Maslia et al. 2007, 2009).

- <u>NRC Report p. 50</u>: "*The TechFlowMP simulations assumed that the biodegradation byproduct of TCE is trans-1,2-DCE. However, the scientific literature indicates that cis-1,2-DCE is the predominant product of TCE reduction under in situ groundwater conditions*"

The primary byproduct of the TCE bioreaction (biodegradation) highly depends on the chemical-biological conditions (especially, microorganisms and nutrients) at contaminated sites (Bradley 2003), meaning that the biological reaction of TCE is highly site-specific. For example, Christiansen et al. (1997) and Miller et al. (2005) reported the anaerobic biological degradation of TCE produced more *trans*-1,2-DCE than *cis*-1,2-DCE. At the TCE-contaminated site in Key West, Florida, the ratio of *trans*-1,2-DCE to *cis*-1,2-DCE was greater than 2 (SWMU9 2002). Griffin (2004) reported that the ratio could reach up to 3.5, based on field data for several sites, including Tahquamenon River, MI; Red Cedar River, MI; Pine River, MI; and Perfume River, Vietnam.

In the modeling of contaminant transport at a contaminated site, the field measurement data at the site are very important in validating the numerical models and in obtaining more accurate simulation results. For the numerical study at the Tarawa Terrace area, we had limited field data regarding the concentrations of PCE, TCE, and *trans*-1,2-DCE. Review of degradation byproduct data analyses, provided to ATSDR by the Department of the Navy, U.S. Marine Crops, the North Carolina Department of Environment and Natural Resources, and others indicated that the predominant degradation byproduct of TCE at Tarawa Terrace and vicinity was *trans*-1,2-DCE (Faye and Green 2007, Tables E2 and E7). As mentioned above, since the primary byproduct of the biological degradation of TCE depends on site-specific conditions, it is more reasonable to select *trans*-1,2-DCE instead of *cis*-1,2-DCE as a primary TCE-bioreaction-byproduct in the study on the groundwater contamination at the Tarawa Terrace area. This NRC critique, therefore, ignores site-specific TCE degradation byproduct data pertinent to Tarawa Terrace and vicinity, listed in Chapter E of the Tarawa Terrace report series.

- NRC Report p. 50: "*The inherent and, in this case, profound limitations of historical modeling due to uncertainties in various model parameters and pumping stresses should be communicated along with modeling prediction.*"

  All modeling analyses have "inherent" uncertainties. ATSDR openly acknowledges that concept. Uncertainty is not limited solely to historical reconstruction modeling as represented by this NRC report statement but is an inherent feature of all models when useful data are absent or sparse. The "profound limitation" that seems to so concern the NRC committee should not be that uncertainties exist with respect to model results but that no effort is made to explain and quantify those uncertainties. In this respect, ATSDR has provided very detailed analyses of uncertainty pertinent to the Tarawa Terrace models (Maslia et al. 2007, 2009, Wang and Aral 2008).

  ATSDR agrees with the last part of the aforementioned NRC report statement that uncertainties should be communicated along with model predictions. ATSDR has done exactly that as explained in detail in Chapters A and I of the Tarawa Terrace report series (Maslia et al. 2007, p. A47-A61, Maslia et al. 2009) as well as on ATSDR's website, which can be found at the following internet addresses:

  http://www.atsdr.cdc.gov/sites/lejeune/cljweb/disclaimer_ChapterIgraph.html and
  http://www.atsdr.cdc.gov/sites/lejeune/cljweb/disclaimer_ChapterItable.html.

CONCLUSIONS AND RECOMMENDATIONS IN THE NRC REPORT (P. 65–66)

As articulated in the paragraphs above and in detail in Appendices I and II, Section 2 of the NRC report "Contaminated Water Supplies at Camp Lejeune-Assessing Potential Health Effects" (NRC 2009) substantially lacks the scientific credibility and attention to technical details one has come to expect from and indeed appreciates in other scientific reports published by the NRC. Section 2 of the NRC report contains technical errors, misrepresentations of data, and erroneous interpretations of published information. Because of these deficiencies, ATSDR believes conclusions contained in Section 2 of the NRC report must be discredited. In addition, most of the conclusions and recommendations in Section 2 of the NRC report are substantially at odds with recommendations rendered by several review panels consisting of national and international experts in water modeling and epidemiology. For these reasons, ATSDR concludes that Section 2 of the NRC report cannot be considered an authoritative, scientifically valid interpretation or guidance document related to the historical exposure assessment of contaminated drinking water at Camp Lejeune.

The NRC committee "concluded that ATSDR applied scientifically rigorous approaches to address the complex groundwater-contamination scenario at Tarawa Terrace." ATSDR does agree with the NRC report that simpler methods to model Hadnot Point should be considered, recognizing, though, that simpler models will be characterized by greater uncertainty because of simplifying and limiting assumptions. ATSDR strongly disagrees, however, with the NRC report's recommendation that monthly estimates of contaminants levels not be used on the epidemiological studies. Therefore, to complete historical reconstruction of contaminant levels for the Hadnot Point area of Camp Lejeune, ATSDR recommends the following approach:

- Application of simpler modeling approaches,
- Application of "locally-refined-grid" numerical models for selected sites,
- Development of algorithms to reconstruct water-supply well on-off cycling patterns,
- Application of sensitivity and uncertainty analyses to further refine estimates of model parameters based on data for Hadnot Point and vicinity, and
- Address and pursue recommendations made by water-modeling expert panels.

REFERENCES

Bradley PM. History and Ecology of chloroethene biodegradation: A Review. Bioremediation Journal. 2003; 7(2): 81–109.

Christiansen N, Christensen SR, Arvin E, and Ahring BK. Transformation of Tetrachloroethene in an Upflow Anaerobic Sludgeblanket Reactor. Applied Microbiology and Technology.1997;47(1):91-94.

Faye RE. Analyses of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water at Tarawa Terrace and Vicinity, U.S. Marine corps Base Camp Lejeune, North Carolina: Historical Reconstruction and Present-Day Conditions—Chapter F: Occurrence of Contaminants in Groundwater. Atlanta, GA: Agency for Toxic Substances and Disease Registry; 2008.

Faye RE, and Green JW Jr. Analyses of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water at Tarawa Terrace and Vicinity, U.S. Marine corps Base Camp Lejeune, North Carolina: Historical Reconstruction and Present-Day Conditions—Chapter E: Occurrence of Contaminants in Groundwater. Atlanta, GA: Agency for Toxic Substances and Disease Registry; 2007.

Griffin BM, Tiedje JM, and Loffler FE. Anaerobic Microbial Reductive Dechlorination of Tetrachloroethene to Predominately trans-1,2-Dichloroethene. Environmental Science and Technology. 2004; 38(16): 4300-4303.

Kopecky KJ, Davis S, Hamilton TE, Saporito MS, and Onstad LE. Estimation of Thyroid Radiation Doses for the Hanford Thyroid Disease Study: Results and Implications for Statistical Power of the Epidemiological Analyses. Health Physics. 2004; 87(1):15–32.

Lawrence SJ. Analyses of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water at Tarawa Terrace and Vicinity, U.S. Marine corps Base camp Lejeune, North Carolina: Historical Reconstruction and Present-Day Conditions—Chapter D: Properties and Degradation Pathways of Common Organic Compounds in Groundwater. Atlanta, GA: Agency for Toxic Substances and Disease Registry; 2007.

Maslia ML, Sautner JB, Aral MM, Gillig RE, Reyes JJ, and Williams RC. Historical Reconstruction of the Water-Distribution System Serving the Dover Township Area, New Jersey: January 1962–December 1996. Atlanta, GA: Agency for Toxic Substances and Disease Registry; 2001 October.

Maslia ML, Sautner JB, Faye RE, Suárez--Soto RJ, Aral MM, Grayman WM, Jang W, Wang J, Bove FJ, Ruckart PZ, Valenzuela C, Green JW Jr, and Krueger AL. Analyses of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water at Tarawa Terrace and Vicinity, U.S. Marine corps Base camp Lejeune, North Carolina: Historical Reconstruction and Present-Day Conditions—Chapter A: Summary of Findings. Atlanta, GA: Agency for Toxic Substances and Disease Registry; 2007.

Maslia ML, Suárez-Soto RJ, Wang J, Aral MM, Faye RE, Sautner JB, Valenzuela C, and Grayman WM. Analyses of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water at Tarawa Terrace and Vicinity, U.S. Marine corps Base camp Lejeune, North Carolina: Historical Reconstruction and Present-Day Conditions—Chapter I: Parameter Sensitivity, Uncertainty, and Variability Associated with Model Simulations of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water. Atlanta, GA: Agency for Toxic Substances and Disease Registry; 2008.

McDermott MJ, Mazor KA, Shost SJ, Narang RS, Aldous KM, and Storm JE. Tetrachloroethylene (PCE, Perc) Levels in Residential Dry Cleaner Buildings in Diverse Communities in New York City. Environmental Health Perspectives. 2005; 113(1):1336–1343.

McLaren/Hart-ChemRisk. Oak Ridge Dose Reconstruction Project Summary Report. Alameda, CA: McLaren/Hart-ChemRisk; 2000 March.

Melts VJ. Deposition, in the General Court of Justice, Superior Court Division; 2001 April 12. Report No.: 01-CVS-566.

Miller GS, Milliken CE, Sowers KR, and May HD. Reductive Dechlorination of Tetrachloroethene to trans-Dichloroethene and cis-Dichloroethene by PCB-Dechlorinating Bacterium DF-1; 2005:2631-2635.

National Research Council (NRC). Contaminated Water Supplies at Camp Lejeune—Assessing Potential Health Effects. Washington, DC: The National Academies Press; 2009 June.

North Carolina Department of Environment and Natural Resources (NCDENR). Superfund Five-Year Review Report, ABC One Hour Cleaners, Jacksonville, Onslow County, North Carolina, EPA ID: NCD 024644494. Raleigh, NC: North Carolina Department of Environment and Natural Resources; 2003 August.

Pankow JF, and Cherry JA. Dense Chlorinated Solvents and Other DNAPLs in Groundwater: History, Behavior, and Remediation: Waterloo Press; 1996.

Reif JS, Burch JB, Nuckols JR, Metzger L, Ellington D, and Anger KW. Neurobehavioral Effects of Exposure to Trichloroethylene Through a Municipal Water Supply. Environmental Research. 2003; 93:248–258.

Rodenbeck SE, and Maslia ML. Groundwater Modeling and GIS to Determine Exposure to TCE at Tucson. Practice Periodical of Hazardous, Toxic, and Radioactive Waste Management. 1998; 2(2):53–61.

Roy F. Weston, Inc. Remedial Investigation Report, ABC One-Hour Cleaners, Operable Unit 2, Jacksonville, North Carolina: Roy F. Weston, Inc.; 1994.

Roy F. Weston, Inc. Remedial Investigation Report, ABC One-Hour Cleaners, Jacksonville, North Carolina: Roy F. Weston, Inc.; 1992.

Shiver R. Groundwater Investigation to Define the Source(s) of Tetrachloroethylene that Have Contaminated Three Community Water Supply Wells at Tarawa Terrace I, Camp Lejeune Marine Cops Base, Onslow County: North Carolina Department of Natural Resources and Community Development; 1985.

SWMU9. Treatability Study Annual Monitoring Report, Naval Air Facility: Key West, Florida. Norfolk, VA: Southern Division Naval Facilities Engineering Command, Tetra Tech. NUS, Inc.; 2002.

USEPA. Guidance on the Development, Evaluation, and Application of Environmental Models. Washington, DC: U.S. Environmental Protection Agency, Office of the Science Advisor, Council for Regulatory Environmental Modeling; 2009 March. Report No.: EPA/100/K-09/003. [cited 2009 July 1]; Available from *http://www.epa.gov/crem/cremlib.html*

Weston Solutions, Inc. ABC One-Hour Cleaners Groundwater Remediation Project Update. West Chester, PA; Weston Solutions, Inc.; 2005 August 31.

Weston Solutions, Inc. ABC One-Hour Cleaners Groundwater Remediation Project Summary. West Chester, PA; Weston Solutions, Inc.; 2007 March 30.

Wang J, and Aral MM. Analyses of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water at Tarawa Terrace and Vicinity, U.S. Marine corps Base camp Lejeune, North Carolina: Historical Reconstruction and Present-Day Conditions—Chapter H: Effect of Groundwater Pumping Schedule Variation on Arrival of Tetrachlorothylene (PCE) at Water-Supply Wells and the Water Treatment Plant. Atlanta, GA: Agency for Toxic Substances and Disease Registry; 2008.

Zheng C. MT3D. A Modular Three-Dimensional Transport Model for Simulation of Advection, Dispersion, and Chemical Reaction of Contaminants in Groundwater Systems. Rockville, MD: S.S. Papadopulos & Associates, Inc.; 1990.

Zheng C, and Wang PP. MT3DMS: A Modular Three-Dimensional Multi-Species Model for Simulation of Advection, Dispersion, and Chemical Reactions of Contaminants in Groundwater Systems: Documentation and User's Guide. Vicksburg, MS: U.S. Army Engineer Research and Development Center; 1999. Report No.: SERDP-99.

APPENDIX I: RESPONSE TO SPECIFIC NRC REPORT COMMENTS BY R.E. FAYE, CONSULTANT TO EASTERN RSEARCH GROUP, INC.

1. DNAPL (PCE) SOURCE

The National Research Council (NRC) report implicitly characterizes the source area for PCE contamination at Tarawa Terrace as containing a free-phase DNAPL mass (NRC 2009, p. 33, 38, 43, and 49). Extensive field data collection and analyses of soil and groundwater samples in the immediate vicinity of ABC One-Hour Cleaners, the source of PCE to the subsurface and to groundwater, and subsequently within the center of mass of the PCE plume as it migrated downgradient from ABC One-Hour Cleaners substantially contradict the NRC's characterization of the PCE source as a free-phase DNAPL mass. These data indicate conclusively that the source area was characterized solely by PCE dissolved in groundwater at concentrations ranging from about 15 percent to less than 1 percent of PCE solubility in water (210,000 µg/L) (Roy F. Weston, Inc. 1992, 1994, Weston Solutions, Inc. 2005). The earliest of these data are published and described in detail in Chapter E of the Tarawa Terrace series of reports (Faye and Green 2007). The maximum simulated PCE concentration in the source area was about 88,000 µg/L, which is less than 42 percent of water solubility. Multi-phase flow as described in the NRC report (NRC 2009) was never observed during the collection and analyses of numerous soil and groundwater samples and most probably never occurred within the domain of the Tarawa Terrace models.

A floor drain at ABC One-Hour Cleaners transferred waste from the dry cleaning processes, including PCE waste or spillage, to a septic tank which in turn transferred liquid wastes to a drain field where PCE was introduced into the subsurface. This septic tank was the major source of PCE to groundwater at ABC None-Hour Cleaners and also received waste water from several bathrooms and washing machines at the dry cleaners (Shiver 1985; Meltz 2001). Use of the floor drain and septic system was terminated in 1985 or early in 1986. Concentrations of PCE in the liquid phase of the septic tank used by ABC One-Hour Cleaners were determined in 1991 and equaled 6,800 µg/L. Samples of the liquid phase collected in 1986 contained PCE concentrations of 1,040 µg/L (Roy F. Weston, Inc. 1992, 1994). Substantial dilution of free phase PCE undoubtedly occurred continuously within the septic tank at ABC One-Hour Cleaners prior to the introduction of the septic waste to the drain field and subsequently to groundwater where additional dilution occurred. A similar characterization of the PCE source at ABC One-Hour Cleaners is described in Chapter F of the Tarawa Terrace series of reports (Faye 2008).

With the exception of a passing reference to a PCE concentration of 12,000 µg/L determined in groundwater in the vicinity of ABC One-Hour Cleaners, no basis is provided in the NRC report (NRC 2009) for a free-phase characterization of DNAPLs in the PCE source area and no technical or scientific rationale for such a characterization is otherwise provided. Such omissions are professionally and scientifically irresponsible and seriously diminish the credibility of NRC's findings and conclusions with respect to the PCE source characterization.

2. CALIBRATION TARGETS

Assigning calibration targets prior to the beginning of model simulations is an accepted and well-recognized adjunct to trial-and-error model calibration (Anderson and Woessner 1992; van der Heijde and Elnawawy 1993, ASTM 2002). The determination of calibration targets is, by definition, somewhat to highly subjective and is dependent on the desired degree of fidelity or

APPENDIX I: RESPONSE TO SPECIFIC NRC REPORT COMMENTS BY R.E. FAYE, CONSULTANT TO EASTERN RSEARCH GROUP, INC.—continued

correspondence to the hydrogeologic environment accorded to the model simulations. For the Tarawa Terrace models, a high degree of fidelity was anticipated and calibration targets were assigned accordingly in conjunction with the estimated accuracies of field data. For example, the calibration target for field potentionmetric levels determined by a tape down method was ± 3.0 ft.This target was derived from the least accurate water-level measurements at locations where land-surface altitude was determined using topographic maps. Similarly, the calibration target for water-level measurements determined by airline measurements was ± 12 ft and was based on the presumed resolution of airline pressure gages. These approaches are described in detail in Chapter C of the Tarawa Terrace series of reports (Faye and Valenzuela 2007, p. 24) and, as such, partly contradict the finding of the NRC report that "the basis used for setting the values of the 'calibration target range' was unclear" (Faye and Valenzuela 2007, p. 49). Assignment of a calibration target to contaminant concentration data was more subjective than the methods used for water-level measurements. Expected guidance from literature sources was not forthcoming as, apparently, calibration targets are not widely used as adjuncts to fate and transport model calibration. Nevertheless, simulation results and related residuals were examined in the few reports that summarized results of investigations similar to those undertaken at Tarawa Terrace and a half-order of magnitude range was decided upon as a reasonable and rigorous calibration target for the fate and transport simulations.

REFERENCES—APPENDX I

Anderson MP, and Woessner WW. Applied Groundwater Modeling: Simulation of Flow and Advective Transport. Academic Press, Inc.; 1992.

ASTM. Standard Guide for Calibrating a Ground-Water Flow Model Application. D5981–96 (Reapproved 2002). West Conshohocken, PA: ASTM International; 2002.

Faye RE. Analyses of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water at Tarawa Terrace and Vicinity, U.S. Marine corps Base Camp Lejeune, North Carolina: Historical Reconstruction and Present-Day Conditions—Chapter F: Occurrence of Contaminants in Groundwater. Atlanta, GA: Agency for Toxic Substances and Disease Registry; 2008.

Faye RE, and Green JW Jr. Analyses of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water at Tarawa Terrace and Vicinity, U.S. Marine corps Base Camp Lejeune, North Carolina: Historical Reconstruction and Present-Day Conditions—Chapter E: Occurrence of Contaminants in Groundwater. Atlanta, GA: Agency for Toxic Substances and Disease Registry; 2007.

Faye RE, and Valenzuela C. Analyses of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water at Tarawa Terrace and Vicinity, U.S. Marine corps Base Camp Lejeune, North Carolina: Historical Reconstruction and Present-Day Conditions—Chapter C: Simulation of Groundwater Flow. Atlanta, GA: Agency for Toxic Substances and Disease Registry; 2007.

Melts VJ. Deposition, in the General Court of Justice, Superior Court Division; 2001 April 12. Report No.: 01-CVS-566.

National Research Council (NRC). Contaminated Water Supplies at Camp Lejeune—Assessing Potential Health Effects. Washington, DC: The National Academies Press; 2009 June.

Roy F. Weston, Inc. Remedial Investigation Report, ABC One-Hour Cleaners, Operable Unit 2, Jacksonville, North Carolina: Roy F. Weston, Inc.; 1994.

APPENDIX I: RESPONSE TO SPECIFIC NRC REPORT COMMENTS BY R.E. FAYE, CONSULTANT TO EASTERN RSEARCH GROUP, INC.—continued

Roy F. Weston, Inc. Remedial Investigation Report, ABC One-Hour Cleaners, Jacksonville, North Carolina: Roy F. Weston, Inc.; 1992.

Shiver R. Groundwater Investigation to Define the Source(s) of Tetrachloroethylene that Have Contaminated Three Community Water Supply Wells at Tarawa Terrace I, Camp Lejeune Marine Cops Base, Onslow County: North Carolina Department of Natural Resources and Community Development; 1985.

van der Heijde PKM, and Elnawawy OA. Quality Assurance and Quality Control in the Development and Application of Ground-Water Models. Ada, OK: U.S. Environmental Protection Agency, Research and Development, EPA/600/SR-93/001; 1993 May.

Weston Solutions, Inc. ABC One-Hour Cleaners Groundwater Remediation Project Update. West Chester, PA; Weston Solutions, Inc.; 2005 August 31.

APPENDIX II: RESPONSE TO SPECIFIC NRC REPORT COMMENTS BY M.M. ARAL, PRINCIPAL INVESTIGATOR, ATSDR-GEORGIA TECH RESEARCH PROGRAM ON EXPOSURE-DOSE RECONSTRUCTION

MEMORANDUM

To: Morris Maslia, PE
Project Manager
Exposure-Dose Reconstruction Program
ATSDR, CDC

From: Prof. Mustafa M. Aral
Director, Multimedia Environmental Simulations Laboratory
School of Civil and Environmental Engineering
Georgia Institute of Technology
Atlanta, Georgia 30332-0355
Phone: 404 · 894 · 2243
Fax: 404 · 894 · 5111
E-mail: maral@ce.gatech.edu
WWW: http://mesl.ce.gatech.edu/

Date: June 27, 2009

Subject: **Response to Comments of the NRC Report on ATSDR Water Modeling Study.**

The National Research Council (NRC) was requested to conduct a review by the Department of Navy (DON), under a mandate by the U.S. Congress (Public Law 109-364, Section 318). The U.S. Navy requested the NRC review to address whether adverse health outcomes are associated with past drinking-water contamination at U.S. Marine Corps (USMC) Base Camp Lejeune, North Carolina. The NRC review included an assessment of the Agency for Toxic Substances and Disease Registry's (ATSDR) current health study on birth defects and specific childhood cancers at Camp Lejeune and in particular, water-modeling analyses and findings to date. The NRC report released on Saturday July 13, 2009 (NRC 2009) covers a wide range of topics that include: (i) conceptual topics of exposure analysis and source characterization that are based on expert opinions of NRC committee members; (ii) water modeling based on observations of the NRC committee and the critique of the science-based tools and analyses that are described in ATSDR technical reports on Tarawa Terrace and vicinity (Maslia et al. 2007); and, (iii) the critique of findings and interpretation of water-modeling study results that were completed by ATSDR at Tarawa Terrace and vicinity at Camp Lejeune.

To accurately respond to the comments made under each category that I have identified above, the review comments I am providing below are grouped under two specific headings. This is in an effort so as not to confuse the reader and mix-and-match the review comments reported by the NRC committee which range from "conceptual topics" to the "actual data reported" in the ATSDR water-modeling study. I hope this approach will provide ATSDR with a clear picture of a range of erroneous statements and mischaracterizations made in the NRC report which are very puzzling. Accordingly, the discussion included in my review comments will cover the range

APPENDIX II: RESPONSE TO SPECIFIC NRC REPORT COMMENTS BY M.M. ARAL, PRINCIPAL INVESTIGATOR, ATSDR-GEORGIA TECH RESEARCH PROGRAM ON EXPOSURE-DOSE RECONSTRUCTION—continued

from "conceptual" perspectives on exposure analysis to "water-modeling analysis" and "application specific" topics that are addressed in the NRC report.

It is important to note that the review comments I am providing below are only associated with the water-modeling aspects of the current ATSDR health study and the NRC report and do not cover any epidemiological aspects. All references to the "NRC report" refer to the recently released NRC report titled, "*Contaminated Water Supplies at Camp Lejeune—Assessing Potential Health Effects*" and cited as NRC (2009) in the Reference section of this memorandum. Furthermore, the reader should recognize that sentences in *italic font* are extracted verbatim from the NRC report and statements in "regular" font are my responses to those specific NRC report statements.

A. REVIEW COMMENTS ASSOCIATED WITH CONCEPTUAL TOPICS OF EXPOSURE ANALYSIS AND SITE CHARACTERIZATION:

1. **Comment on p. 29:** *Exposure assessment for epidemiologic studies of the effects of water-supply contamination includes two components. The first is estimation of the magnitude, duration, and variability of contaminant concentrations in water supplied to consumers. An important consideration is hydrogeologic plausibility: an association between a contaminant source and exposure of an individual or population cannot exist unless there is a plausible hydrogeologic route of transport for the contaminant between the source and the receptor (Nuckols et al., 2004). The second component is information on individual water use patterns and other water-related behaviors that affect the degree to which exposures occur, including drinking-water consumption (ingestion) and dermal contact and inhalation related to the duration and frequency of showering, bathing, and other water-use activities. Water use is an important determinant of variability of exposure to water-supply contaminants, particularly if it varies widely in the study population. Ideally, exposure-assessment strategies include both components, but in practice it may be difficult to obtain either adequately.*

   Response: In this comment, which also includes a reference to the work of one of the committee members (Nuckols et al. 2004), the NRC committee is providing the reader with their understanding of the components of an exposure study that is associated with pollutants that may exist in an aquatic pathway at a contaminated site. The aquatic exposure analysis framework described in this statement is a conceptual statement and represents a very restrictive view of the exposure pathway analysis that needs to be considered at contaminated sites given the current understanding of the interaction between environmental pathways and the behavior of chemicals along those pathways.

   Current knowledge in this scientific field recognizes that in an aquatic exposure study the environment must be considered as a whole and scientific and regulatory approaches alike must take into account complex interactions between multimedia and intermedia interactions that exist in a multitude of potential environmental pathways at a site. In my opinion one should not emphasize only the concept of a "**hydrogeologic** connection" between the contaminant source and the exposure point as put forth by the NRC

APPENDIX II: RESPONSE TO SPECIFIC NRC REPORT COMMENTS BY M.M. ARAL, PRINCIPAL INVESTIGATOR, ATSDR-GEORGIA TECH RESEARCH PROGRAM ON EXPOSURE-DOSE RECONSTRUCTION—continued

committee. This conceptual suggestion made by the NRC committee would be a very elementary and a restrictive exposure analysis framework.

As specialists in this field, we are well aware of the fact that pollutants released to an aquatic environment are distributed among environmental media such as air, water, soil, vegetation etc., as a result of complex physical, chemical and biological processes. Thus, environmental pollution is a **multi-pathway problem** and environmental exposure assessment methods require that we carefully consider the transport, fate and accumulation of pollutants in the environment as a whole, (Cohen 1986). Methods that are proposed to evaluate environmental migration or exposure characterization in this envirosphere must consider all potential pathways and also the interactions between these pathways. In the scientific literature, the multi-pathway approach to environmental exposure analysis is identified as Total Exposure Characterization (TEC).

Elements of this multi-pathway analysis for an aquatic contamination source are imbedded in the ATSDR water-modeling study that is being conducted for the Tarawa Terrace area of the Camp Lejeune site as much as possible given the data restrictions. The specific pathways and processes considered in the ATSDR water-modeling study are: (i) saturated groundwater; (ii) unsaturated groundwater; (iii) vapor emissions; (iv) multispecies analysis of contaminants in these three pathways; (v) mixing in the water treatment system; and, (vi) water-distribution system estimates.

In this analysis framework it is also important to recognize that one should not try to fit a physical problem to a model that may be readily available for use. Instead, appropriate models should be selected or developed that would fit the characterization of the physical problem at hand. Thus, selection of appropriate modeling tools to complete such an analysis is very important and is considered in sufficient detail in the ATSDR study. This is a very important point, which was either completely ignored in the NRC report or, steps taken by the ATSDR water-modeling team to address these issues in a sound scientific manner were considered scientifically not credible without the NRC committee providing any supporting evidence. I will revisit this issue in more detail in my comments below while providing case-specific public domain data and public domain information.

2. **Comment on p. 33:** *At a typical waste site, spent VOCs are present in the unsaturated zone (a partially saturated soil layer above the water table) in the form of dense nonaqueous-phase liquids (DNAPLs)*....... (after a lengthy discussion of what DNAPL is and how DNAPL-based contaminants behave in the subsurface and what the consequences of such a source are, the NRC report continues in this section with the following remarks linking DNAPL presence to the aquifers at Camp Lejeune.) ..... *The presence of low-permeability units (such as the Castle Hayne confining unit or any clay units) would limit vertical migration of both DNAPL and dissolved contaminants.....*

Response: The NRC report does not provide any information for the **justification** of this conceptualization of the contamination source at the ABC One-Hour Cleaners site and

APPENDIX II: RESPONSE TO SPECIFIC NRC REPORT COMMENTS BY M.M. ARAL, PRINCIPAL INVESTIGATOR, ATSDR-GEORGIA TECH RESEARCH PROGRAM ON EXPOSURE-DOSE RECONSTRUCTION—continued

Tarawa Terrace and vicinity other than providing a reference to a source concentration of 12,000 μg/L, reported in Chapter E of the ATSDR Tarawa Terrace report series (Faye and Green 2007, p. 38). This is followed by a reference to a number of 110,000 μg/L (p. 38 of the NRC report, second paragraph from bottom of page). As indicated in the NRC report, this is the highest possible concentration of tetrachloroethylene (PCE) in water. Because this reference number is given in the NRC report **without a reference citation, I question the credibility of this reference number. The NRC report also does not discuss the importance of this number in their conceptualization of the contaminant source as a DNAPL**. Furthermore, the NRC report does not refer to a data source on the solubility levels of PCE in water like those data sources reported in Chapter D of the ATSDR Tarawa Terrace report series (Lawrence 2007). The NRC report does not refer to or cite a database that may exist in USMC files at Camp Lejeune, unknown to the ATSDR water-modeling team, that NRC committee members may have had access to that would indicate the presence of DNAPL-phase PCE at the site. The NRC report also does not refer to a systematic dry-cleaner disposal procedure that is reported in the documents they have reviewed for handling the disposal of the chemical PCE as a pure-phase PCE at the ABC One-Hour Cleaners site.

In the NRC report, the highest concentration of dissolved PCE, 110,000 μg/L, must imply the NRC committee understanding of the solubility level of PCE in water. Because a reference is not provided, I could not confirm this number. However, our references indicate that the solubility of PCE in water is around 200,000 μg/L (= 200 mg/L) at 15°C or higher. In Chapter D of the ATSDR Tarawa Terrace report series (Lawrence 2007, p. D12, Table D9), solubility of PCE is reported to be 210, 000 μg/L (=210 mg/L) at 25°C, which is the solubility number I would like to work with for my analysis below. There are other references in the literature that report the solubility of PCE at much higher concentrations as well, which are not referenced here. This is because I would like to focus on what is reported in the ATSDR Tarawa Terrace series of reports.

The 12,000 μg/L concentration reported in NRC report (and also in Chapter E of the ATSDR Tarawa Terrace report series [Faye and Green 2007]) as a justification for the presence of a DNAPL phase is about 5.7% to 6% of the solubility level of PCE (12,000/200,000 = 6% or 12,000/210,000 = 5.7%). The 12,000 μg/L concentration is the dissolved-phase PCE concentration in the groundwater at ABC One-Hour Cleaners as reported by ATSDR (Faye and Green 2007). Although this is a high concentration, this value is much less than PCE's solubility limit in water (200,000 μg/L at 15°C or 210,000 μg/L at 25°C). The location of the highest concentration sample within Tarawa Terrace and vicinity can be used to identify the source location at the site. High concentrations at a site may suggest the possibility of non-aqueous phase (NAPL) PCE (PCE in form of NAPL) presence but this does not guarantee a NAPL presence at the site, because in this case, 12,000 μg/L is 6% or less of the solubility limit of PCE.

Thus, the conceptual DNAPL contaminant source characterization that is provided in the NRC report without any justification and without any field data support is both extremely bothersome and irresponsible. This reference to the presence of a DNAPL-phase

APPENDIX II: RESPONSE TO SPECIFIC NRC REPORT COMMENTS BY M.M. ARAL, PRINCIPAL INVESTIGATOR, ATSDR-GEORGIA TECH RESEARCH PROGRAM ON EXPOSURE-DOSE RECONSTRUCTION—continued

contaminant source at the site not only appears in the aforementioned comment on NRC report page 33, but it is repeatedly referred to in other pages of the NRC report which is an attempt to discredit the ATSDR analysis and its findings from its source conceptualization origins. As a member of the ATSDR water-modeling team, I respectfully request that, through ATSDR, I should be provided with the recorded field data evidence that the NRC committee was privy to that would support the DNAPL conceptualization. Also reporting the solubility of PCE in water at about **half the value of the data reported in the ATSDR Chapter D report** (Lawrence 2007) **without providing a reference** (page 38 of the NRC report) is a scientifically unacceptable practice. Short of citing field data evidence and an appropriate reference for the solubility level of PCE as reported in the NRC report, I would question the scientific basis of the complete NRC report that relies on the accuracy of this erroneous conceptualization. Without field data evidence, the NRC review is based on hypothetical conditions and assumptions that are extracted from the scientific work of others (Figure 2-3 of the NRC report) which is based on studies that are conducted at other sites—and these sites have no relevance to the ABC One-Hour Cleaners site or Tarawa Terrace and vicinity. The purpose of this assertion (PCE DNAPL source conceptualization) and misrepresentation of data and site-specific conditions by the NRC committee is not clear to me.

During the NRC committee review process, the question of the characterization of the source was brought to the attention of ATSDR water-modeling team members in a request for information by an NRC committee member (Email communication from P. Clement to M.L. Maslia, ATSDR, May 5-11, 2008). During that time, ATSDR water-modeling team members provided the NRC with data ATSDR had on the subject matter clearly showing why we selected to simulate the PCE source as a dissolved-phase source. Furthermore, we clearly identified why the dissolved-phase injection procedure applied in the models used for the ATSDR water-modeling analyses. The information that was provided to the NRC was based on data from several remedial investigation reports, site reports, and other DON and USMC files (Shiver 1985, Roy F. Weston 1992, 1994). In these field study reports, there is no recorded data reported by DON and USMC consultants that would provide evidence of, or substantiate the existence of, the presence of a DNAPL source at ABC One-Hour Cleaners or Tarawa Terrace. If the DNAPL source conceptualization that appears in the NRC report is based solely on the data source and information we provided to the NRC committee, then I do not agree with the NRC's source characterization. I, therefore, consider this to be a misrepresentation of the conditions at the site. If this conceptualization is based on any other information or data that we are not aware of, and if this information was provided to NRC by DON, the USMC, or their consultants, we need to be provided with that information and data. Because the reference to a DNAPL-phase in the aquifers underlying ABC One-Hour Cleansers and Tarawa Terrace and vicinity appears in several places within the NRC report, I will revisit this topic again in my discussion below.

In the aforementioned statement on page 33 of the NRC report, I also noticed that the NRC committee acknowledged that the PCE source was discharged to the unsaturated zone of the aquifer underlying ABC One-Hour Cleaners and Tarawa Terrace and vicinity.

APPENDIX II: RESPONSE TO SPECIFIC NRC REPORT COMMENTS BY M.M. ARAL, PRINCIPAL INVESTIGATOR, ATSDR-GEORGIA TECH RESEARCH PROGRAM ON EXPOSURE-DOSE RECONSTRUCTION—continued

However, given that observation, the NRC committee fails to provide a justifiable critique of the use of the MODFLOW family of codes that only considers a saturated groundwater zone by which analyze the physical problem at the site. On the contrary, the NRC committee considers the MODFLOW family of codes to be an acceptable modeling choice. This is probably because the NRC committee considers these MODFLOW codes as accepted state-of-the-art tools for typical groundwater pathway modeling. This is an example of a typical case of fitting a physical problem to a code "concept" I referenced in my response statement "A-1" above, which the ATSDR water-modeling team tried to avoid as much as possible.

In recognition of this problem and also in recognition of the general perception that prevails in the scientific community that the MODFLOW family of codes is an accepted procedure, the ATSDR water-modeling team first utilized the MODFLOW and MT3DMS codes in their simulations. In addition, to enhance our understanding of conditions at the site, ATSDR has and extended their analyses. The ATSDR water-modeling team applied the TechFLOW^{MP} software to understand and evaluate the unsaturated zone injection conditions that are implemented at the site. TechFLOW^{MP} is a public domain code that can be accessed from the Georgia Tech website for individual use without a fee (http://mesl.ce.gatech.edu/). The NRC report attempts to discredit this extra effort and the steps taken by the ATSDR water-modeling team to simulate the proper source disposal conditions at the ABC One-Hour Cleaners site by classifying: (i) the TechFLOW^{MP} code as a research tool; and, (ii) a proprietary code that is not verified. Again, this is very puzzling and a misrepresentation of the scientific and public domain facts of this case by the NRC committee. These NRC statements that appear in several places in the NRC report ignore a scientifically sound attempt by the ATSDR water-modeling team to properly solve a physical problem, above and beyond a traditional MODFLOW and MT3DMS application which the NRC review committee accepts (NRC 2009, p. 43). Additionally, these NRC statements misrepresent the public domain information of the status of a model used in the analysis. NRC committee remarks in this regard misrepresent a public domain code as a proprietary code without checking with the authors of the code or the web site where this code can be accessed freely by anybody without a fee. Further, the NRC committee failed to check current technical literature and scientific publications containing substantial evidence of publications involving the TechFLOW^{MP}. Contained in this technical literature and scientific publications is evidence where the TechFLOW^{MP} code has been tested and verified against other applications. (see web site : http://mesl.ce.gatech.edu/PUBLICATIONS/Publications.html) This lack of due diligence by the NRC committee is also very puzzling.

I am very familiar with the expertise of the scientists who prepared the NRC report, many of whom I know personally and respect. What I do not understand is how they reached these puzzling and in some cases erroneous conclusions, which are not justified in the NRC report they prepared. Misrepresentation of these scientific and public domain facts is extremely bothersome and, in my opinion, sheds a dark cloud over the scientific credibility and integrity of the overall NRC report.

APPENDIX II: RESPONSE TO SPECIFIC NRC REPORT COMMENTS BY M.M. ARAL, PRINCIPAL INVESTIGATOR, ATSDR-GEORGIA TECH RESEARCH PROGRAM ON EXPOSURE-DOSE RECONSTRUCTION—continued

B. REVIEW COMMENTS ASSOCIATED WITH SCIENCE-BASED TOOLS, ANALYSES, AND INTERPRETATION OF STUDY RESULTS:

1. **Comment on p. 43:** *For example, MT3DMS can predict the transport only of dissolved contaminants, so a key approximation was made to represent the mass dissolved from the DNAPL source. To apply MT3DMS, ATSDR replaced the highly complex DNAPL contaminated source zone with a hypothetical model node where PCE was injected directly into the saturated aquifer formation at a constant rate (1.2 kg/day).*

   Response: This NRC report statement relies on their unsubstantiated and undocumented source characterization concept (see my review comment "A-2"). Using this conceptualization as an undisputable fact, the NRC committee then attempts to discredit the groundwater-modeling study conducted by ATSDR at the ABC One-Hour Dry Cleansers site and Tarawa Terrace and vicinity. This statement is a hyperbole, wherein first an "assumption" is made and then that "assumption" is considered to be a "fact" to critique the findings of a study. This approach in a critique does not even deserve a scientific response; and again, brings about more questions as to the scientific credibility and integrity of the NRC report.

2. **Comment on p. 43:** *Unlike the MODFLOW and MT3DMS codes, the PSOpS and TechFlowMP codes lack validation by a broad spectrum of practicing geoscientists in an open-source environment.*

   Response: I have addressed the path the NRC committee chose in reference to the misrepresentation of TechFLOW^{MP} as a proprietary code in my aforementioned response A-2. I will not repeat that here again. In reference to the PSOpS model developed by the Georgia Tech group, I would like to enquire of the NRC committee the following: Can a reference to a public domain code be provided by the NRC that is available through the published literature? Has such a public domain code been developed for, and applied to, any study that they are aware of to manage pumping-schedule operations in an optimal manner for a complex system such as the one at Tarawa Terrace? The answer to these questions is obvious and the answer is: "This type of public domain model does not exist."

   PSOpS is an optimization application that was developed by the Georgia Tech group participating in the ATSDR water-modeling analysis to yield answers to specialized uncertainty-related questions pertinent to the current health study at Camp Lejeune. The analysis is based on the MODFLOW family of codes in the generation of the database used to solve an optimization problem. The development of this optimization model was necessary to respond to scientific questions raised by the ATSDR Expert Panel (March 2005) whose members guided our study and contributed significantly to its quality. The members of this ATSDR Expert Panel are well known and respected scientists in the field and their names are listed in the Expert Panel report (Maslia 2005) that also is available on the ATSDR website. The question ATSDR Expert Panel members raised in this case

APPENDIX II: RESPONSE TO SPECIFIC NRC REPORT COMMENTS BY M.M. ARAL, PRINCIPAL INVESTIGATOR, ATSDR-GEORGIA TECH RESEARCH PROGRAM ON EXPOSURE-DOSE RECONSTRUCTION—continued

was related to the uncertainty of a pumping-schedule operation that may be implemented at the site and the characterization of its effects on the study outcome. The PSOpS model that was developed for the purposes of this analysis and used in the ATSDR water-modeling analyses to address this question became part of the PhD thesis of a graduate student at Georgia Tech. In that sense, the theoretical background of the model is reviewed and accepted by an independent PhD thesis committee at Georgia Tech and the detailed documentation of this model can be found in the PhD thesis of Dr. J. Wang, which is public domain information (Wang 2008)

In conclusion, the NRC committee is most likely aware of the following: (1) specialized models such as PSOpS are not available in the technical public-domain literature; and, (2) codes such as PSOps only are developed for the specialized purposes of the current study to find answers to specialized questions that are raised by the current water-modeling analysis. The concept of using an optimization algorithm that is fed by a database through the MODFLOW family of models, which is a common and routine procedure, is both scientifically sound and scientifically necessary in a study such as the one ATSDR is conducting at Camp Lejeune. If the NRC committee can provide us with a reference to another public domain model that can be used for our study and that would serve the same purpose, instead of the PSOpS model, we would be glad to use that model instead of the PSOpS model. To my knowledge, such a model is not available. In my opinion, the NRC committee also should recognize that the ATSDR water-modeling effort is not a run-of-the-mill work product and the problem at hand is not a routine problem that can be or should be analyzed using routine models. In such cases it is expected that specialized methods can be developed and implemented—this should not be shunned by the NRC, but instead, it should be applauded. It is most puzzling to see, that under the name "NRC," this approach is not encouraged, but instead, it is criticized.

3. **Comment on p. 44:** *The DNAPL source zone was represented by using a model node where PCE was injected continuously into the unconfined model layer-1 of the saturated zone at a constant rate of 1.2 kg/day (Faye 2008).*

Response: Again, in this statement, the NRC committee is asserting that the DNAPL source zone was misrepresented in the current study. I refer the reader to my previous comments in my response A-2 in reference to the DNAPL source mischaracterization by the NRC committee.

To reiterate, we have not represented a DNAPL source zone as an injection point in our models because there is no DNAPL source zone in the aquifer underlying the ABC One-Hour Dry Cleaners site and Tarawa Terrace and vicinity. If the claim of the NRC committee can be substantiated by any field data, not only we will modify our modeling study efforts, **but also we would strongly recommend that the U.S. Environmental Protection Agency (USEPA), their consultants, and the North Carolina Department of Environment and Natural Resources (NCDENR) should immediately abandon their current remediation efforts at the ABC One-Hour Dry Cleaners site and Tarawa Terrace and vicinity and adopt remediation strategies that would yield**

APPENDIX II: RESPONSE TO SPECIFIC NRC REPORT COMMENTS BY M.M. ARAL, PRINCIPAL INVESTIGATOR, ATSDR-GEORGIA TECH RESEARCH PROGRAM ON EXPOSURE-DOSE RECONSTRUCTION—continued

more effective results for a DNAPL source contaminant. USEPA and NCDENR field consultants who are currently not implementing DNAPL remediation technologies at the site is additional evidence that these agencies and their consultants also does not agree with the NRC committee as to the characterization of the contamination source as DNPL-phase PCE.

4. **Comment on p. 48:** *Because insufficient historical pumping data were available to constrain the model predictions from 1953 to 1980, the ability of the advanced optimization models to estimate the dates* ***accurately*** *is questionable.*

Response: There are obvious uncertainties in the physical problem being studied at ABC One-Hour Dry Cleaners and Tarawa Terrace and vicinity. The NRC committee would most likely agree with this statement. If we accept this statement, then the question becomes, should one completely ignore uncertainty in the analysis or, should one try to develop techniques that would provide an estimate of the effects of the uncertainty on the solution in a systematic way? We have chosen the second route.

The NRC committee should accept the fact that answers to uncertainty questions cannot be answered "**accurately**" as the report states in the above statement. Expecting that from an uncertainty analysis outcome would be scientifically irresponsible. Our uncertainty analyses are not provided to give "**accurate**" answers to the problem studied. Instead, our uncertainty analyses are used as estimates that would indicate the variability range of deterministic results provided earlier. The domain of uncertainty analysis is a scientific field which is not in the realm of the traditional groundwater fate and transport analysis expertise and should be viewed using a different microscope and expertise.

5. **Comment on p. 48:** *(5) there is no spatial variation in the microbiologic or geochemical characteristics.*

Response: The NRC committee correctly identified that in the application of the TechFLOW^{MP} model to the aquifers underlying the ABC One-Hour Dry Cleaners site and Tarawa Terrace and vicinity, we assumed no spatial variation of microbiologic characteristics. If the NRC committee is familiar with the finite element procedures used in the TechFLOW^{MP} model, they would acknowledge that this is not a restriction of the model but a restriction of the available field data for the site. If the microbial distribution in an aquifer can be accurately characterized, which we doubt can be accomplished in this case or any case, we can certainly include that heterogeneity in our modeling effort.

Having pointed out this fact, I would also like to question issues pertaining to levels of acceptable homogeneity considered in our modeling effort and compare it with levels of unacceptable homogeneity that are shunned in our modeling analysis based on the critique presented in the NRC report. For example the assumption of uniform infiltration across the model domain when the MODFLOW family of model codes is utilized was not critiqued in the NRC report, but the assumption of uniform microbial distribution in the multilayer aquifer domain is critiqued. Between these two processes, which would be the

APPENDIX II: RESPONSE TO SPECIFIC NRC REPORT COMMENTS BY M.M. ARAL, PRINCIPAL INVESTIGATOR, ATSDR-GEORGIA TECH RESEARCH PROGRAM ON EXPOSURE-DOSE RECONSTRUCTION—continued

easier process to characterize? I think the answer to this question is obvious—the infiltration process. Thus, although both processes are characterized by heterogeneity in the aquifer, accepting the homogeneity assumption for the infiltration case but not accepting homogeneity assumption for the microbial distribution case would be setting the bar too high and would be scientifically irresponsible considering the levels of data that may be available to characterize either process. A scientific review committee should be able to make these distinctions easily and come up with appropriate conclusions in their prepared review comments.

6. **Comment on p. 49:** *However, there are some important limitations in ATSDR's modeling efforts because of the sparse set of water quality measurements, the need to make unverifiable assumptions, and the complex nature of the PCE source contamination.*

   Response: There are limitations of the modeling analyses conducted by ATSDR water-modeling team. We would be the first to acknowledge these limitations. This is evident by the level of detail of the uncertainty analysis conducted as part of the water-modeling analysis to envelope the effect of those uncertainties on the outcome presented. However, in my opinion, characterizing the uncertainty analysis outcome as not "**accurate**" as previously stated (see response B-4) or, that uncertainty analysis only should be conducted in "**verifiable**" cases as stated above is not a scientifically sound assessment or procedure. An uncertainty that can be verified is no longer uncertain.

7. **Comment on p. 49 first bullet:** *The effects of the DNAPL in both unsaturated and saturated zones have not been included in the studies.*

   Response: The NRC report brings back the DNAPL issue here again. Please see my response in A-2 and other comments above.

8. **Comment on p. 49 second bullet:** *Constant values of dispersivity (longitudinal dispersivity of 25 ft and transverse 2.5 ft) were used in the transport model.*

   Response: Although dispersivity is considered to be constant, based on the definition of the hydrodynamic diffusion coefficient, the hydrodynamic diffusion coefficients are variable because they depend on the velocity field at the site. This is a common assumption in most studies where field data are not available to support spatially variable dispersion coefficients. This comment again is related to my discussion of acceptable homogeneity and unacceptable homogeneity conditions at a site study (see my response B-5).

9. **Comment on p. 49 bullet four:** *The numerical codes TechFLowMP and PSOpS used in the modeling are research tools and are not widely accepted public-domain codes, such as MODFLOW and MT3DMS, so their validation is important.*

APPENDIX II: RESPONSE TO SPECIFIC NRC REPORT COMMENTS BY M.M. ARAL, PRINCIPAL INVESTIGATOR, ATSDR-GEORGIA TECH RESEARCH PROGRAM ON EXPOSURE-DOSE RECONSTRUCTION—continued

Response: This characterization is a misrepresentation of the aforementioned models, clearly identified in my response A-2. As the NRC committee may acknowledge, the availability of codes with the capabilities of these models are very limited (see my response A-2 and B-2). In my opinion the use of these models in complex analysis should not be shunned by NRC, but instead, it should be encouraged since they are providing supplemental information beyond MODFLOW family of code applications (see my response in B-2).

10. **Comment on p. 49 bullet five:** *The PSOpS modeling study is based on the premise that an optimization model can be used to evaluate pumping stresses. Without site-specific pumping and water-quality data, the results will be nonunique and uncertain.*

Response: PSOpS modeling concept is based on the effort of estimating the effects of uncertainty on the modeling outcome. This analysis is approached in a systematic manner following a well accepted process such as an optimization analysis based on some constraints to satisfy the demands. The PSOpS model uses the MODFLOW family of codes as its database engine. We are not claiming that the outcome provides the exact conditions representing the problem at the site. But the outcome of the analysis provides us with an envelope which bounds our deterministic analysis. This is a standard uncertainty analysis procedure similar to, for example, Monte Carlo analysis that is routinely used in uncertainty analysis. Monte Carlo analysis, according to a well established procedure, systematically evaluates the effects of uncertainty on the problem solution. In such an application, it is not **certain** that the random numbers generated would **exactly** represent the actual conditions for the problem at the site. However, the bounding limits of the analysis are the ultimate goal. The application of PSOpS, in essence, is very similar to that analogy.

As I have stated earlier, this goes back to the NRC report statement about the "**accuracy**" of the uncertainty analysis results that cannot be justified scientifically. Please see my response in B-4. Also, I have to emphasize again what I stated earlier: The domain of uncertainty analysis is a scientific field which is not in the realm of the traditional groundwater fate and transport analysis expertise and should be viewed using a different microscope and expertise.

11. **Comment on p. 49 bullet seven:** *The TechFlowMP model predicted very high vapor concentrations. For example, TechFlowMP predicted that the PCE vapor concentration in the top 10 ft of soil beneath the Tarawa Terrace elementary school should be 1,418 µg/L. Studies of PCE vapor concentrations in buildings that house or are near a dry-cleaning facility have reported measured concentrations around 55 µg/L.*

Response: This reference to a vapor concentration at 1,418 µg/L is another example of misrepresentation of the results of the modeling analyses by the ATSDR water-modeling team. This aforementioned information was taken from Chapter A of the ATSDR Tarawa Terrace report series (Maslia et al. 2007, p. A44). The statement provided in the ATSDR report reads as follows:

APPENDIX II: RESPONSE TO SPECIFIC NRC REPORT COMMENTS BY M.M. ARAL, PRINCIPAL INVESTIGATOR, ATSDR-GEORGIA TECH RESEARCH PROGRAM ON EXPOSURE-DOSE RECONSTRUCTION—continued

"b. the maximum simulated PCE concentration in groundwater (model layer 1) at the Tarawa Terrace elementary school was 1,418 µg/L (Figure A15b), whereas the maximum simulated vapor-phase PCE (in the top 10 ft of soil) was 137 µg/L (Figure A20a)"

The above sentence, taken directly from the ATSDR report submitted to NRC, clearly states that the groundwater (not vapor) concentration of PCE in layer "1" is 1,418 µg/L concentration. Vapor concentration is given separately in the paragraph towards the end of that sentence. For the NRC report to represent this number (1,418 µg/L) as the vapor concentration that is simulated at the site in order to discredit a study does not fit into any norm of a scientific review. I will provide a more detailed analysis of this case using simulation results to bring clarity to the concern raised in the NRC report.

In this case, the work product referred to are the TechFLOW^{MP} modeling results and the particular analysis mentioned was conducted by the Georgia Tech group participating in the ATSDR water-modeling analysis of the ABC One-Hour Cleaners site and Tarawa Terrace and vicinity (Jang and Aral 2007). In order to provide the reader with clear evidence of scientific misrepresentation of the facts which seem to appear too frequently in the NRC report, the actual data reported in our report is presented below in sufficient detail—unlike the other responses I have provided to other comments in this document.

In the numerical study of the multispecies, multiphase groundwater contamination at ABC One-Hour Dry Cleaners and Tarawa Terrace and vicinity, TechFLOW^{MP} simulations used two boundary-conditions to characterize the ground surface under the original pumping schedule: (1) GSBC = 0.01 and (2) GSBC = 1.0 (Jang and Aral 2007, p. G15). Here the acronym "GSBC" stands for the Ground Surface Boundary Condition. For the in-/out-flux of gas between the atmosphere and the unsaturated zone, if the ground surface does not have low-permeable zones or hindrances due to pavement, lakes, or buildings, the GSBC value is set to be 1.0. This implies that the soil gas can be freely released into the atmosphere from the unsaturated zone. However, when some objects, including roads, buildings, ponds, or highly water-saturated areas, are present at the ground surface, the soil gas can not be released into the atmosphere freely. Under such a condition, GSBC is set to be 0.01 in the current study. Actually any number between these two extremes can be considered in the analysis. However, just to show the bounds of the results, the discussion here will be confined to these two extreme cases.

In order to analyze the concentration distribution around the school area as it is referred to in the aforementioned NRC report comment, the location of the school at Tarawa Terrace has to be identified, and it shown in Figure 1.

APPENDIX II: RESPONSE TO SPECIFIC NRC REPORT COMMENTS BY M.M. ARAL, PRINCIPAL INVESTIGATOR, ATSDR-GEORGIA TECH RESEARCH PROGRAM ON EXPOSURE-DOSE RECONSTRUCTION—continued

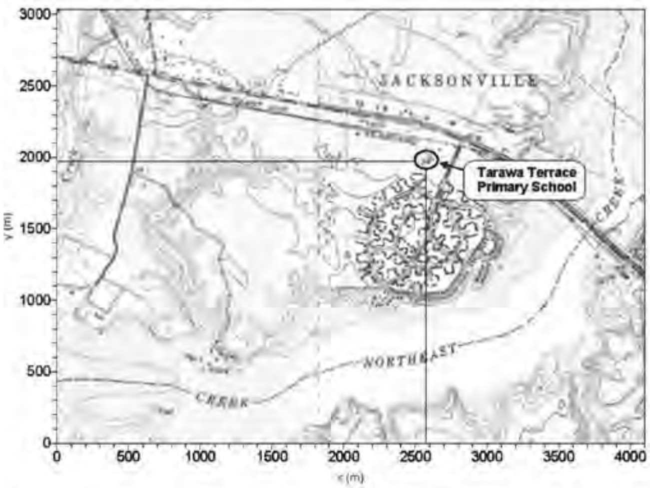


Figure 1. Location of the Tarawa Terrace Elementary School

In the school area, the groundwater table is near the ground surface (CH2MHILL 2007). In this study, the ground surface is at z = 7.6 meters (m, z = 25 ft), and the groundwater table is around z = 2.4 – 4 m (z = 8 – 13 ft) (Jang and Aral 2007, Figure G3, p. G10). Thus, the concentration distributions of the vaporized PCE at z = 6 m are presented below, where the unsaturated zone is at this location.

As shown in Figure 2, under GSBC = 0.01, which is more representative of an area where there are buildings and pavements, the predicted vaporized PCE concentrations in the pore space of the soil at the center of the school area (x = 2,580 m, y = 1,975 m) are about 15.5 µg/L during December 1984 (Figure 2a) and 3.7 µg/L during December 1994 (Figure 2b). Within the school area (marked with the circle in this figure), the PCE concentration ranges 0.1-100 µg/L during December 1984 (Figure 2a) and 0.1-50 µg/L during December 1994 (Figure 2b).

APPENDIX II: RESPONSE TO SPECIFIC NRC REPORT COMMENTS BY M.M. ARAL, PRINCIPAL INVESTIGATOR, ATSDR-GEORGIA TECH RESEARCH PROGRAM ON EXPOSURE-DOSE RECONSTRUCTION—continued

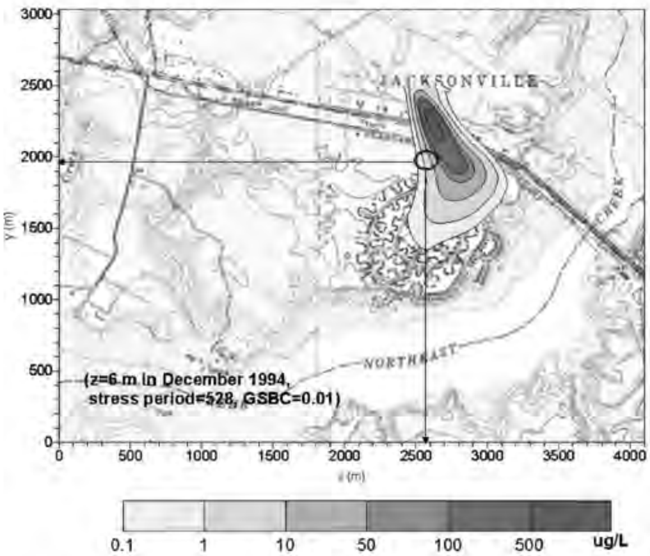


Figure 2b. Vaporized PCE concentrations in the gas phase under the original pumping schedule (PS-O) with GSBC=0.01, at z=6, December 1994.

Having provided this comparison, I also question the source of the reference number, 55 μg/L, that is used in the NRC report. The NRC report provides a reference in this case and this reference is McDermott et al. (2005). I was curious about this reference; therefore, I located and obtained a copy of the referenced paper. In the McDermott et al. (2005) study, the authors are analyzing and reporting data on the PCE vapor concentrations in a building where dry-cleaner operations are housed in New York City. Does the NRC committee expect us to accept the concept that what is observed (measured) as vapor concentration in a building that houses a dry-cleaner facility in New York City should also apply to the pore space of the soils at the site of an elementary school area in Camp Lejeune, North Carolina? Or do they expect that what we have simulated in the pore space of the soils at a site in North Carolina should also confirm the observations made in New York City, 17–20 years beyond our final simulation date (2001–2003), in some dry-cleaner facility building? In my opinion, these types of comparisons, expectations, and assertions are scientifically not acceptable and credible; they discredit the NRC report in its entirety.

In the groundwater contamination study that utilized TechFlow^{MP} (Jang and Aral 2007), the local equilibrium of contaminant partitioning between the water and gas phases is

APPENDIX II: RESPONSE TO SPECIFIC NRC REPORT COMMENTS BY M.M. ARAL, PRINCIPAL INVESTIGATOR, ATSDR-GEORGIA TECH RESEARCH PROGRAM ON EXPOSURE-DOSE RECONSTRUCTION—continued

implemented while calculating the contaminant distribution between the two phases (gas and liquid). Thus, we can use the Henry coefficient, *H*, in estimating PCE concentration in the gas phase from the concentration in the groundwater phase as follows:

$$C_{Vapor,PCE} = HC_{GroundWate,PCE}$$

For PCE, *H* is 0.35 (Jang and Aral 2007, Table G2). Using the dissolved PCE concentration in the groundwater shown in Figure G5 of Jang and Aral (2007) (in the unsaturated and saturated zones), the overall concentration distribution of the vaporized PCE within the gas phase in the unsaturated zone can also be estimated. This simple calculation could have been done by the NRC committee to confirm the vapor concentration numbers they are reporting in their statement. In Figure G5 of Jang and Aral (2007), the dissolved PCE concentration in the groundwater is 100-500 μg/L near the ground surface at the location of the elementary school ($x = 2{,}580$ m, $y = 1{,}975$ m). Therefore, the vaporized PCE concentration will be approximately 35-175 μg/L in the unsaturated zone near the school area. The cross section line A-A' in Figure G5 is located at $x = 2{,}606$ m.

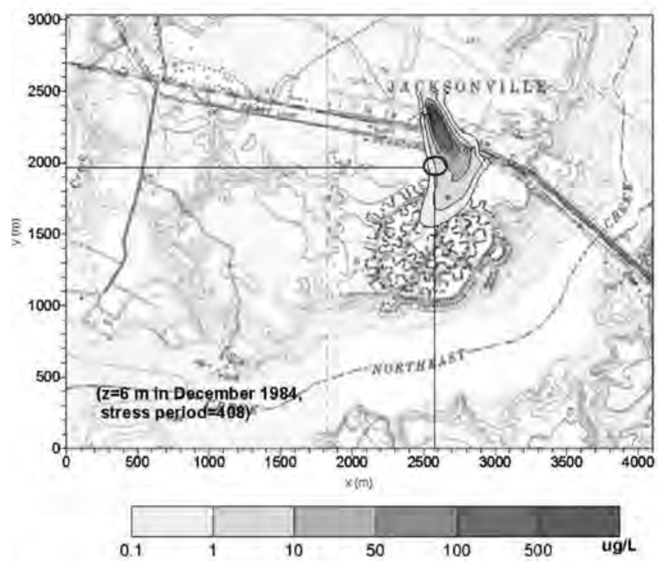


Figure 3a. Vaporized PCE concentrations in the gas phase under the original pumping schedule (PS-O) with GSBC=0.01, z=6, December 1984.

APPENDIX II: RESPONSE TO SPECIFIC NRC REPORT COMMENTS BY M.M. ARAL, PRINCIPAL INVESTIGATOR, ATSDR-GEORGIA TECH RESEARCH PROGRAM ON EXPOSURE-DOSE RECONSTRUCTION—continued

Let us also analyze the results of the other boundary condition that is used in the TechFLOW^{MP} model out of curiosity and see if the vapor concentration value of 1,418 µg/L reported in the NRC report was referring to that case. The results reported in (Jang and Aral 2007) under the condition GSBC = 1 are shown in Figure 3. The predicted vaporized PCE concentrations at the center of the school area ($x = 2580$ m, $y = 1975$m) are about 0.99 during December 1984 (Figure 3a) and 0.1 µg/L during December 1994 (Figure 3b) (i.e. more PCE vapor is released to the atmosphere and less is remaining in the pore space when compared to the previous results). Within the school area (marked with the circle in the figure), the concentration ranges 0.1-10 µg/L in December 1984 (Figure 3a) and less than 5 µg/L in December 1994 (Figure 3b).

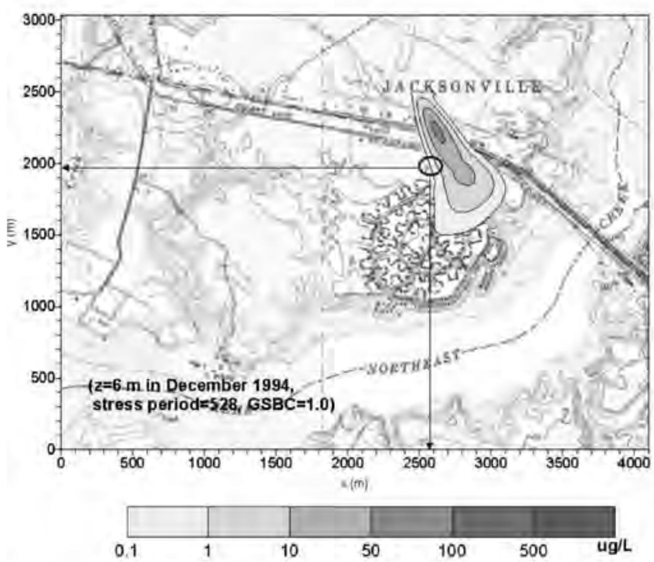


Figure 3b. Vaporized PCE concentrations in the gas phase under the original pumping schedule (PS-O) with GSBC=0.01, z=6, December 1994.

As can be seen from these results the number reported in the NRC report does not exist in the ATSDR water-modeling analysis as vapor concentration. This is a clear misrepresentation of the ATSDR water-modeling results. The purpose of this misrepresentation is not clear to us.

The field investigation during 2007 (CH2MHILL 2007) it was reported that the vaporized concentrations of PCE near the ground surface were below detection limits or very low,

APPENDIX II: RESPONSE TO SPECIFIC NRC REPORT COMMENTS BY M.M. ARAL, PRINCIPAL INVESTIGATOR, ATSDR-GEORGIA TECH RESEARCH PROGRAM ON EXPOSURE-DOSE RECONSTRUCTION—continued

3.9 ppbv (parts per billion volume), which is equivalent to 0.028 µg/L. Considering the time gap between the end of the historical simulation time (December 1994) and the field investigation time (July 2007), the simulation results that are provided in the Chapter G report of the ATSDR Tarawa Terrace report series (Jang and Aral 2007) provide reasonable modeling results and represent acceptable levels of expected vapor concentration near the Tarawa Terrace elementary school. Are we asserting that this is absolutely the case? The answer to that question is absolutely "No." This outcome is only an estimate based on the assumptions and limitations of the models considered in the ATSDR water-modeling analyses and the assumptions and limitations are based on our best judgment of the conditions that may exist at the ABC One-Hour Dry Cleaners site and Tarawa Terrace and vicinity.

The ATSDR water-modeling reports do not report such high concentration of vaporized PCE concentration in the gas phase. The vaporized PCE concentration of 1,418 µg/L is equivalent to a dissolved PCE concentration of 4,051 µg/L, in the groundwater:

$$C_{Vapor,PCE} = HC_{GroundWate,PCE}$$
$$C_{GroundWate,PCE} = 1418 / 0.35 = 4051.4$$

I also note that the unsaturated zone is located at a very thin layer near the ground surface (z = 7.6 m (25 ft)) in Jang and Aral (2007, Figure G5) which is characterized in terms of several layers in water-modeling analysis. The maximum thickness of the unsaturated zone is about 7.6 m.

In conclusion the data, the associated discussion of the vapor levels near the Tarawa Terrace elementary school area, and also the reference provided in the NRC report (McDermott et al. 2005) are far from the facts of the case and the results that are presented by the ATSDR water-modeling team. Again I see here a misrepresentation of the data reported in a study to discredit a study. The purpose of that approach is not clear to me. However, I can declare without hesitation that this approach does not have any scientific credibility and place in any scientific document.

12. **Comment on p. 49 bullet eight:** *The biodegradation model used within the TechFlowMP code is based on an untested preliminary research model.*

and also,

> **Comment on p. 50:** *The TechFlowMP simulations assumed that the biodegradation byproduct of TCE is trans-1,2-DCE. However, the scientific literature indicates that cis-1,2-DCE is the predominant product of TCE reduction under in situ groundwater conditions.*

Response: The detailed description of "why *trans*-1,2-dichloroethylene is chosen as the representative byproduct of TCE bioreaction at the Tarawa Terrace area instead of *cis*-

APPENDIX II: RESPONSE TO SPECIFIC NRC REPORT COMMENTS BY M.M. ARAL, PRINCIPAL INVESTIGATOR, ATSDR-GEORGIA TECH RESEARCH PROGRAM ON EXPOSURE-DOSE RECONSTRUCTION—continued

1,2-DCE" is given in page G4 of the report, Chapter G (Jang and Aral 2007). Additional explanation regarding this issue is given below.

As shown in Figure G2 of the report (Jang and Aral 2007), the anaerobic biological degradation of trichloroethylene (TCE) generates three isomers, *cis*-1,2-dichloroethylene (*cis*-1,2-DCE), *trans*-1,2-dichloroethylene (*trans*-1,2-DCE), and 1,1-dichloroethylene (1,1-DCE). As discussed in the report (Jang and Aral 2007), *cis*-1,2-DCE (1,2-cDCE) is the most common byproduct among the three DCE isomers produced theoretically (Wiedemeier 1998). Even though *cis*-1,2-DCE has been often used as a primary byproduct of TCE-biodegradation under the anaerobic conditions in contaminant-transport modeling of chlorinated ethenes (Clement et al. 2000; Jang and Aral 2008), but the primary byproduct of the TCE bioreaction highly depends on the chemical-biological conditions (especially, microorganisms and nutrients) at the contaminated sites (Bradley 2003), implying that the biological reaction of TCE is highly site-specific. For example, Christiansen et al. (1997) and Miller et al. (2005) reported the anaerobic biological degradation of TCE produced more *trans*-1,2-DCE than *cis*-1,2-DCE. At the TCE-contaminated site in Key West, Florida, the ratio of *trans*-1,2-DCE to *cis*-1,2-DCE was greater than 2 (SWMU9 2002). Griffin (2004) reported that the ratio could reach up to 3.5, based on field data for several sites, including Tahquamenon River, MI; Red Cedar River, MI; Pine River, MI; and Perfume River, Vietnam.

In the modeling of contaminant transport at a contaminated site, the field measurement data at the site are very important in validating the numerical models and in obtaining more accurate simulation results. For the numerical study at the Tarawa Terrace area, we had limited field data regarding the concentrations of PCE, TCE, and *trans*-1,2-DCE. This is indicated in the following statement of the ATSDR report: Review of degradation byproduct data analyses, provided to ATSDR by the Department of the Navy, U.S. Marine Crops, the North Carolina Department of Environment and Natural Resources, and others indicated that the predominant degradation byproduct of TCE at Tarawa Terrace and vicinity was *trans*-1,2-DCE (Faye and Green 2007, Tables E2 and E7).

As mentioned above, since the primary byproduct of the biological degradation of TCE depends on site-specific conditions, it is more reasonable to select *trans*-1,2-DCE instead of *cis*-1,2-DCE as a primary TCE-bioreaction-byproduct in the study on the groundwater contamination at the Tarawa Terrace area.

The NRC critique, therefore, ignores site-specific TCE degradation byproduct data pertinent to Tarawa Terrace and vicinity, listed in Chapter E of the Tarawa Terrace report series. This statement again clearly demonstrates the lack of due diligence by the NRC review committee in their review of the data that exists at the Tarawa Terrace, Camp Lejeune site and their lack of understanding of the facts of the site specific case based on this data. This is very bothersome.

APPENDIX II: RESPONSE TO SPECIFIC NRC REPORT COMMENTS BY M.M. ARAL, PRINCIPAL INVESTIGATOR, ATSDR-GEORGIA TECH RESEARCH PROGRAM ON EXPOSURE-DOSE RECONSTRUCTION—continued

13. **Comment on p. 50 next to last bullet:** *In the absence of data, historical reconstruction efforts that use groundwater models can only provide a general conceptual framework for what happened at the site and why.*

    Response: Historical reconstruction is a procedure that is accepted in the literature. It uses models to predict the past in a conceptually similar manner the models are routinely used to predict the future in engineering studies. The ATSDR response document provides references to such historical reconstruction applications.

14. **Comment on p. 65:** *Therefore, the committee recommends the use of simpler approaches (such as analytic models, average estimates based on monitoring data, mass-balance calculations, and conceptually simpler MODFLOW/MT3DMS models) that use available data to rapidly reconstruct and characterize the historical contamination of the Hadnot Point water-supply system. Simpler approaches may yield the same kind of uncertain results as complex models but are a better alternative because they can be performed more quickly and with relatively less resources, which would help to speed-up the decision-making process.*

    Response: Use of simpler models may be easier to implement. We are already proceeding in that direction for the Hadnot point study. However, how the detailed questions that are raised in the NRC report could be answered using simpler models is not clear to me.

CONCLUSIONS:

Examples of the scientific evidence presented in this response statement and the discussion of this evidence herein clearly indicate that the data and the analysis presented in the NRC report (NRC 2009) are misrepresentations and mischaracterizations of the findings of the ATSDR water-modeling analyses conducted at the ABC One-Hour Cleaners site and Tarawa Terrace and vicinity. The conceptual characterizations made by the NRC committee also do not fit available field data or reported field conditions by the USEPA, their consultants, or the NCDENR which are guiding current remediation efforts at ABC One-Hour Cleaners and Tarawa Terrace and vicinity. Thus, what is in question here is the credibility of the complete contents of the NRC report as a scientific document of any value.

As I have said earlier, I know and respect many of the NRC committee members. What I do not understand is, how they reached these puzzling and in some cases erroneous conclusions in their review.

Thus, I believe, due to the presence of numerous errors, misrepresentations and mischaracterization of the scientific facts of the ATSDR water-modeling analyses, the NRC report cannot be used as a guidance document in its entirety. In light of the concerns that I have raised in this response statement, I recommend that the NRC should be asked to: (i) prepare a supplemental document in which detailed correction of all the facts of the case would be

APPENDIX II: RESPONSE TO SPECIFIC NRC REPORT COMMENTS BY M.M. ARAL, PRINCIPAL INVESTIGATOR, ATSDR-GEORGIA TECH RESEARCH PROGRAM ON EXPOSURE-DOSE RECONSTRUCTION—continued

included without misrepresentation or mischaracterization; (ii) based on these facts a reanalysis and reinterpretation of the ATSDR water-modeling analysis should be conducted and documented; and, (iii) the outcome be reissued in a report immediately to serve the public health concern of the former Marines at Camp Lejeune, North Carolina. Otherwise, in the opinion of many scientists who will review the contents of the NRC report and the responses to the report such as this one, what is in question is the credibility of the NRC as an institution.

This response statement is respectfully submitted to ATSDR to document my scientific evaluation of the findings of the NCR report.

REFERENCES

Bradley, PM. History and Ecology of Chloroethene Biodegradation: A Review. Bioremediation Journal. 2003;7(2): 81-109.

CH2MHILL. Field Sampling Plan, Tarawa Terrace Elementary School, Marine Corps Base Camp Lejeune, North Carolina. Raleigh, NC: CH2MHILL; 2007 July.

Christiansen N, Christensen SR, Arvin E, and Ahring BK. Transformation of Tetrachloroethene in an Upflow Anaerobic Sludgeblanket Reactor. 1997;47(1):91-94.

Clement, TP, Johnson, CD, Sun, YW, Klecka, GM, and Bartlett, C. Natural Attenuation of Chlorinated Ethene Compounds: Model Development and Field-Scale Application at the Dover Site. Journal of Contaminant Hydrology. 2000; 42(2-4):113-140.

Cohen, Y. Pollutants in a Multimedia Environment. New York: Plenum Publication Corp.; 1986.

Faye RE, and Green JW Jr. Analyses of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water at Tarawa Terrace and Vicinity, U.S. Marine corps Base Camp Lejeune, North Carolina: Historical Reconstruction and Present-Day Conditions—Chapter E: Occurrence of Contaminants in Groundwater. Atlanta, GA: Agency for Toxic Substances and Disease Registry; 2007.

Griffin BM, Tiedje JM, and Loffler FE. Anaerobic Microbial Reductive Dechlorination of Tetrachloroethene to Predominately trans-1,2-Dichloroethene. Environmental Science and Technology. 2004; 38(16): 4300-4303.

Jang W, and Aral MM. Analyses of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water at Tarawa Terrace and Vicinity, U.S. Marine corps Base camp Lejeune, North Carolina: Historical Reconstruction and Present-Day Conditions—Chapter G: Simulation of Three-Dimensional Multispecies, Multiphase Mass Transport of Tetrachloroethylene (PCE) and Associated Degradation By-Products. Atlanta, GA: Agency for Toxic Substances and Disease Registry; 2007.

Jang WY, and Aral MM. Effect of Biotransformation on Multispecies Plume Evolution and Natural Attenuation. Transport in Porous Media. 2008; 72(2): 207-226.

Lawrence SJ. Analyses of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water at Tarawa Terrace and Vicinity, U.S. Marine corps Base camp Lejeune, North Carolina: Historical Reconstruction and Present-Day Conditions—Chapter D: Properties and Degradation Pathways of Common Organic Compounds in Groundwater. Atlanta, GA: Agency for Toxic Substances and Disease Registry; 2007.

APPENDIX II: RESPONSE TO SPECIFIC NRC REPORT COMMENTS BY M.M. ARAL, PRINCIPAL INVESTIGATOR, ATSDR-GEORGIA TECH RESEARCH PROGRAM ON EXPOSURE-DOSE RECONSTRUCTION—continued

Maslia ML. Expert Peer Review Panel Evaluating ATSDR's Water-Modeling Activities in SUpport of the Current Study of Childhood Birth Defects and Cancer at U.S. Marine Corps Base Camp Lejeune, North Carolina: Atlanta, GA: Agency for Toxic Substances and Disease Registry; 2005.

Maslia ML, Sautner JB, Faye RE, Suárez-Soto RJ, Aral MM, Grayman WM, Jang W, Wang J, Bove FJ, Ruckart PZ, Valenzuela C, Green JW Jr., and Krieger AL. Analyses of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water at Tarawa Terrace and Vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina: Historical Reconstruction and Present-Day Conditions Chapter A: Summary of Findings. Atlanta, GA: Agency for Toxic Substances and Disease Registry; 2007.

McDermott MJ, Mazor KA, Shost SJ, Narang RS, Aldous KM, and Storm JE. Tetrachloroethylene (PCE, Perc) Levels in Residential Dry Cleaner Buildings in Diverse Communities in New York City. Environmental Health Perspectives. 2005; 113(1):1336–1343.

Miller GS, Milliken CE, Sowers KR, and May HD. Reductive Dechlorination of Tetrachloroethene to trans-Dichloroethene and cis-Dichloroethene by PCB-Dechlorinating Bacterium DF-1; Environmental Science and Technology. 2005:2631-2635.

National Research Council (NRC). Contaminated Water Supplies at Camp Lejeune—Assessing Potential Health Effects. Washington, DC: The National Academies Press; 2009 June.

Nuckols, JR., Wared MH, and Jarup L. Using Geographic Information Systems for Exposure Assessment in Environmental Epidemiology Studies. Environmental Health Perspectives. 2004; 112(9):1007-1015.

Roy F. Weston, Inc. Remedial Investigation Report, ABC One-Hour Cleaners, Operable Unit 2, Jacksonville, North Carolina: Roy F. Weston, Inc.; 1994.

Roy F. Weston, Inc. Remedial Investigation Report, ABC One-Hour Cleaners, Jacksonville, North Carolina: Roy F. Weston, Inc.; 1992.

Shiver R. Groundwater Investigation to Define the Source(s) of Tetrachloroethylene that Have Contaminated Three Community Water Supply Wells at Tarawa Terrace I, Camp Lejeune Marine Cops Base, Onslow County: North Carolina Department of Natural Resources and Community Development; 1985.

SWMU 9. Treatability Study Annual Monitoring Report, Naval Air Facility, Key West, Florida. Norfolk, VA: Southern Division Naval Facilities Engineering Command, Tetra Tech. NUS, Inc.; 2002.

Wang J. Sensitivity and Uncertainty Analyses of Contaminant Fate and Transport in a Field-Scale Subsurface System. Ph.D. Dissertation. Atlanta, GA: Georgia Institute of Technology, School of Civil and Environmental Engineering; 2008 April.

Wiedemeier TH. Technical Protocol for Evaluating Natural Attenuation of Chlorinated Solvents in Ground Water. Cincinnati, OH: National Risk Management Research Laboratory Office of Research and Development; 1998.

Appendix N — ATSDR Editorial Response in Ground Water Journal (Maslia et al. 2012) to the Article, "*Complexities in Hindcasting Models—When Should We Say Enough Is Enough*?" by T. P. Clement (2010)

Journal/ Volume 50, No. 1 pp. 1–166
January–February 2012

ground water

VOLUME 50

Serving Groundwater Professionals Since 1963

national ground water association

Journal of the Scientists and Engineers Division of NGWA
A National Ground Water Association Publication

B. Sautner[7], Barbara A. Anderson[8], Frank J. Bove[9], Perri Z. Ruckart[10], and Susan M. Moore[11]
[1]Corresponding author: Agency for Toxic Substances and Disease Registry, Division of Health Assessment and Consultation (ATSDR/DHAC), 4770 Buford Highway, N.E., Mail Stop F-59, Atlanta, GA; (770) 488-3842; mmaslia@cdc.gov
[2]Multimedia Environmental Simulations Laboratory, School of Civil and Environmental Engineering, Georgia Institute of Technology, Atlanta, GA; (404) 894-2243; maral@ce.gatech.edu
[3]R.E. Faye and Associates, Inc., Blairsville, GA; (706) 745-4048; refaye@windstream.net
[4]Eastern Research Group, Inc., Lexington, MA.
[5]W.M. Grayman Consulting Engineer, Cincinnati, OH; (513) 761-1722; grayman@fuse.net
[6]Agency for Toxic Substances and Disease Registry, Division of Health Assessment and Consultation, Atlanta, GA; rsuarezsoto@cdc.gov
[7]Agency for Toxic Substances and Disease Registry, Division of Health Assessment and Consultation, Atlanta, GA; (770) 488-0667; jsautner@cdc.gov
[8]Agency for Toxic Substances and Disease Registry, Division of Health Assessment and Consultation, Atlanta, GA; (770) 488-0710; baanderson@cdc.gov
[9]Agency for Toxic Substances and Disease Registry, Division of Health Studies (DHS), Atlanta, GA; (770) 488-3809; fbove@cdc.gov
[10]Agency for Toxic Substances and Disease Registry, Division of Health Assessment and Consultation, Atlanta, GA; (770) 488-3808; pruckart@cdc.gov
[11]Agency for Toxic Substances and Disease Registry, Division of Health Assessment and Consultation, Atlanta, GA; (770) 488-3667; smoore1@cdc.gov

"*Complexities in Hindcasting Models—When Should We Say Enough Is Enough*," by T. Prabhakar Clement, v. 49, no. 5: 620–629.

Comment by Morris L. Maslia[1], Mustafa M. Aral[2], Robert E. Faye[3,4], Walter M. Grayman[5], René J. Suárez-Soto[6], Jason

In a recent article, T.P. Clement (2010, hereafter referred to as TPC) discusses the complexities and limitations of "hindcasting" models and criticizes the use of complex models when undertaking investigations of subsurface reactive transport processes. TPC implies that complex numerical models that simulate reactive transport processes in groundwater are likely if not always an inappropriate tool to apply to "hindcasting" investigations and that scientists and engineers who implement these investigations using such models are somehow not aware of the technical and scientific complexities and limitations of such methods and approaches (p. 625). To illustrate his point of view, TPC uses a case study of an ongoing health study of exposure to volatile organic compounds (VOCs) in drinking water at U.S. Marine Corps Base Camp Lejeune, North Carolina (hereafter referred to as the case-control health study at Camp Lejeune). The article presents some thought-provoking points-of-view. However, we believe there is a lack of detail on several key issues that require specificity and clarification, particularly with respect to modeling approaches and methods, the physics of contaminant occurrence and reactive transport in the subsurface, and agency policies for the review and dissemination of data and reports. We thank the editors of *Ground Water* for allowing a multidisciplinary team

s

of scientists and engineers working on the Camp Lejeune case-control health study the opportunity to discuss and respond to the TPC *Ground Water* Issue Paper.

"Hindcasting" vs. Historical Reconstruction

TPC defines "hindcasting" as the use of models for predicting the past to understand and resolve historical problems (p. 621). This definition, we believe, is extremely narrow and does not address the significantly broader and multidisciplinary area of exposure assessment, which includes a variety of scientific disciplines such as environmental science, epidemiology, and toxicology. Rather, we believe a more correct term than "hindcasting" is that of *historical reconstruction*, which seeks to provide estimates of contaminant concentrations in drinking water (or other environmental media) when direct, past knowledge of contaminant concentrations is limited or unavailable. Characteristically, historical reconstruction includes the application of simulation tools, such as models, to re-create or represent past conditions. A plethora of examples that describe successful historical reconstruction analyses exist in the published literature (Rodenbeck and Maslia 1998; McLaren/Hart-ChemRisk 2000; Costas et al. 2002; Reif et al. 2003; Kopecky et al. 2004; Maslia et al. 2005; Sahmel et al. 2010). Application of historical reconstruction methods and approaches to the case-control health study at Camp Lejeune recognized and required the collective expertise of team members with diverse skills and knowledge and did not focus on one discipline, such as groundwater modeling, as implied in the TPC article.

Historical reconstruction, by definition, does not preclude the use of current or present-day sources of information. In fact, successful historical reconstruction utilizes all pertinent sources of information, historical, and present-day (Maslia et al. 2000; Sahmel et al. 2010). TPC also states there are unique issues and challenges related to "hindcasting efforts that use complex models" (p. 621), apparently because no present opportunity exists to collect historical data. He fails to mention that a calibrated "hindcasting" model can just as easily be applied to the simulation of future events as well as past conditions. In fact, whether a particular model simulates past events ("hindcasting") or future events (forecasting), generic issues related to model development, calibration, and analyses of uncertainty of results are similar for both models. The calibration of a model must either stand or fall on its own merits, without the benefit of future data collection that may be accomplished later in time or the lost opportunity for data collection previously foregone. At the time of calibration, when model results are provided to policy makers, a "hindcasting" model is *not* uniquely disadvantaged compared with a forecasting model just because model predictions are historical rather than latter in time. Few, if any, policy makers or the public would accept the premise that policy decisions must be delayed for several years or several decades to further validate an existing model when a decision must be forthcoming.

Application of "Complex" Models vs. "Simple" Models to Simulate Subsurface Reactive Processes

The Agency for Toxic Substances and Disease Registry (ATSDR) is directed by congressional mandate to perform specific functions concerning the effect on public health of hazardous substances in the environment—health studies being a specific example of this mandate (http://www.atsdr.cdc.gov/about/index.html). ATSDR seeks to advance the science of environmental public health by: (1) collecting, analyzing, and summarizing data related to environmental exposures and health and (2) conducting research to identify associations between environmental exposures and health risk. ATSDR's case-control health study and water-modeling investigations at Camp Lejeune include major components of data collection and analysis as well as research. To complete the health study at Camp Lejeune, ATSDR water-modeling investigations were tasked to determine (1) arrival date(s) of contaminants at water-supply wells; (2) mean monthly concentrations of contaminants arriving at base water treatment plants (WTPs) from individual wells; (3) mean monthly concentration of contaminants distributed to base housing areas; and (4) the reliability of and confidence in the simulated results (Maslia et al. 2007, 2009a, 2009b). ATSDR completed these tasks by applying the concept and methodology of *historical reconstruction*. These results are designed to provide epidemiologists with historical monthly concentrations of contaminants in drinking water at Camp Lejeune to evaluate the effects of exposure to contaminated water supplies with respect to specific birth defects (neural tube defects, cleft lip, and cleft palate) and childhood cancers (leukemia and non-Hodgkin's lymphoma).

TPC suggests that because of limited information and data and the complex nature of reactive transport processes in the subsurface, simpler models should be used. We point out, however, that simpler models will not necessarily reduce the level of uncertainty or meet project needs. It is our view that the most *appropriate* model(s) that can provide the needed information, rather than the simplest model, should be used. Thus, if a conceptually simpler model is an *appropriate* model that can meet the requirements of the Camp Lejeune case-control health study, we are in agreement that it should be applied during the historical reconstruction process. This approach is applied to all ATSDR water-modeling investigations. TPC further suggests that model complexity should be limited to a level consistent with a level of available data and invokes the notion of model parsimony or "Occam's razor" to support this point of view (p. 625). TPC's statement contradicts the fundamental precept of "Occam's razor" which, with respect to scientific thought and reasoning, requires that explanatory factors are not to be multiplied beyond necessity. Thus, selection of a "simple" or "complex" model to simulate reactive transport processes in groundwater, according to "Occam's razor," should be based on study objectives, not the "level" or availability of supporting data. Whether or not sufficient data are available to completely complement model development and calibration becomes apparent when a degree of uncertainty is assigned to simulation results.

With respect to reconstructing historical groundwater VOC concentrations at Camp Lejeune, "simple" models, by definition, probably imply the application of analytical fate and transport codes. Such "simple" models are limited to—among other limiting assumptions—uniform flow fields and constant velocities. Consequently, these analytical ("simple") models neither assess the transient aspects of water-supply well operations nor determine consecutive monthly contaminant concentrations in these wells—a goal and requirement of the case-control health study at Camp Lejeune.

While questioning ATSDR's historical reconstruction approach for not using "simple" models, TPC appears to contradict himself by implying that ATSDR's historical reconstruction analyses were not sufficiently complex to account for multiple competing biological-chemical processes (p. 625). After describing various complex research models that may address these complexities (e.g., incorporation of carbon limitations, modeling interactions between carbon and terminal electron acceptors), TPC concludes that such research models require extensive biochemical field data (p. 625). Thus, using "simple" models would probably always preclude consideration and simulation of complex biochemical degradation processes.

Correction and Clarification of Specific Contaminant Data Analyses and Modeling Issues

Objective of the Water-Modeling Effort

The TPC article implies that the objective for water modeling supporting the case-control health study at Camp Lejeune was for "policy-making" purposes, to advance the research interests (and funding) of the water modelers, or to satisfy politicians and citizens groups (p. 626). This is *not* the case. The water modeling was requested by ATSDR epidemiologists who required monthly drinking water contamination estimates to assess associations between in utero exposures by month and trimester and specific birth defects and childhood cancers. It is standard practice in epidemiological studies of adverse reproductive outcomes to assess exposures (whether environmental, occupational, or diet risk factors) at the monthly or trimester level (Rothman et al. 2008, 602-603).

Characterization of the Contaminant Source

TPC characterizes tetrachloroethylene (PCE) contamination in groundwater at the ABC One-Hour Cleaners site and at Tarawa Terrace base housing as a "free-phase" or "pure-phase" dense, nonaqueous-phase liquid [DNAPL (p. 5)]. This characterization directly contradicts and misrepresents field concentration data presented by Faye and Green (2007) and in other reports and documents (Shiver 1985; Weston 1992, 1994) that describe PCE and other contaminants in the subsurface in the vicinity of Tarawa Terrace and ABC One-Hour Cleaners. Those reports and documents unequivocally describe the PCE in groundwater in the vicinity of ABC One-Hour Cleaners as "dissolved-phase" PCE. As noted by Keuper and Davies (2009), assessing for the presence of DNAPL must be made using a weight-of-evidence approach with multiple lines of evidence combining to form either a positive or a negative determination. Using one groundwater sample point with a concentration of 12,000 μg/L (as TPC apparently does) and a solubility in excess of 150,000 μg/L (Pankow and Cherry 1996; Lawrence 2007; Clement 2011), does *not* constitute a weight-of-evidence approach for a positive determination for the presence of DNAPL in soil or groundwater at Tarawa Terrace and vicinity. Rather, the weight-of-evidence approach using all site data results in a negative determination for the presence of DNAPL. It is noteworthy that more than 100 soil-boring and 140 groundwater samples were collected in the immediate vicinity of the ABC One-Hour Cleaners at depths ranging from a few feet to more than 60 feet below land surface. These data, which were tabulated and described in detail by Faye and Green (2007, Figure E2, Tables E5 and E7), did not indicate any free-phase DNAPL. Thus, while the one data value cited by TPC (12,000 μg/L) may be indicative of a contaminant source, it is definitely not indicative of free-phase DNAPL at ABC One-Hour Cleaners and Tarawa Terrace and vicinity. Furthermore, in describing the disposal practices from the ABC One-Hour Cleaners, TPC states that free-phase PCE (DNAPL) was disposed into a septic tank (p. 624). What TPC did not state is that the cleaners also continuously discharged wash and wastewater to the septic tank, thereby continuously diluting the PCE (Faye and Green 2007).

The characterization by TPC of PCE in the vicinity of ABC One-Hour Cleaners as a DNAPL is further discredited by the process selected by government agencies to remediate the PCE contamination in the groundwater. Processes selected to remediate free-phase (DNAPL) PCE in groundwater are totally different from processes used to remediate dissolved-phase PCE in groundwater. The remediation process currently in progress at the ABC One-Hour Cleaners and at Tarawa Terrace is conducted under the auspices of the U.S. Environmental Protection Agency (USEPA) and was approved by the North Carolina Department of Environment and Natural Resources (NCDENR). This process is correctly described as "groundwater extraction by wells and treatment by air stripping"—pump-and-treat (NCDENR 2003; Weston Solutions Inc. 2005, 2007). This remediation process is appropriate only for dissolved-phase PCE—not for DNAPL PCE.

Degradation Products of PCE

The biodegradation products of PCE are trichloroethylene (TCE), 1,1-dichloroethylene (1,1-DCE), *trans*- and *cis*-1,2-DCE, vinyl chloride, and ethene (Lawrence 2007; Wang and Aral 2008). As pointed out by TPC, our multispecies simulations using the TechFlowMP code did not consider *cis*-1,2-DCE as a degradation product. Although some scientific literature indicates that *cis*-1,2-DCE is the predominant product of TCE reduction under in situ groundwater conditions (NRC 2009, 49), the primary byproduct of the TCE bioreaction (biodegradation) highly depends on the chemical-biological conditions (especially microorganisms and nutrients) at contaminated sites (Bradley 2003), meaning that the biological degradation of TCE in the subsurface is highly site-specific. For example, Christiansen et al. (1997) and Miller et al. (2005) reported that the anaerobic biological degradation of TCE produced more *trans*-1,2-DCE than *cis*-1,2-DCE. At the TCE-contaminated site in Key West, Florida, the ratio of *trans*-1,2-DCE to *cis*-1,2-DCE was greater than 2 (SWMU9 2002). Griffin (2004) reported that the ratio could reach up to 3.5, based on field data for several sites, including Tahquamenon River, MI; Red Cedar River, MI; Pine River, MI; and Perfume River, Vietnam.

To calibrate reactive transport models at Tarawa Terrace and vicinity, limited field data regarding the concentrations of PCE, TCE, and *trans*-1,2-DCE were available and provided by Faye and Green (2007). TPC apparently ignored or was not aware of these data, although he frequently cites the reference by Faye and Green (2007) in the *Ground Water* article. Review of degradation byproduct data analyses, provided to ATSDR by the Department of the Navy, U.S. Marine Corps, the NCDENR, and others indicated that the predominant degradation byproduct of TCE at Tarawa Terrace and vicinity was *trans*-1,2-DCE (Faye and Green 2007, Tables E2 and E7). Because the primary byproduct of the biological degradation of TCE depends on site-specific conditions, selecting *trans*-1,2-DCE instead of *cis*-1,2-DCE as the primary TCE-bioreaction-byproduct in the study area was clearly the appropriate choice.

Model Calibration

The TPC article states that the Tarawa Terrace groundwater fate and transport model were calibrated to a limited number of data points, which are PCE levels measured in finished water samples collected in the early 1980s (p. 622). The fact is that a four-stage calibration process was used and compared with published field data at every calibration stage. Specifically, these four stages are (Maslia et al. 2007)

- Stage 1: a predevelopment calibration of the groundwater flow model, which compared simulated and measured predevelopment water levels in monitor wells (Faye and Valenzuela 2007, Figure C9),
- Stage 2: a transient calibration of the groundwater flow model, which compared simulated and transient water levels in monitor and supply wells (Faye and Valenzuela, Figures C10 through C17 and C20),
- Stage 3: a groundwater fate and transport model, which compared simulated and measured PCE concentrations in water-supply wells (Faye 2008, Table F13 and Figures F12 through F17), and
- Stage 4: a mixing model calibration, which compared computed and measured PCE concentrations in finished water at the Tarawa Terrace WTP (Maslia et al. 2007, Table A10 and Figure A12).

TPC also implies that reactive transport model results were presented without calibrating to degradation product field data (p. 622). Calibration field data were not presented by TPC in his Figure 3 (taken from Maslia et al. 2007, Figure A19). However, available field data used for calibration were presented by Faye and Green (2007) and were compared with simulation results in Jang and Aral (2008, Figures G6 and G10).

Research Models vs. Public Domain Codes

TPC (p. 622) states that ATSDR used an advanced research code TechFlowMP (Jang and Aral 2008) to predict (simulate) the concentration of PCE along with degradation products TCE, *trans*-1,2-DCE, and vinyl chloride and that applying research codes on high-visibility projects is not a good idea (p. 626). It is important to note that public-domain/open-source codes such as MODFLOW and MT3DMS were developed under the auspices of U.S. government-sponsored research programs and were once classified as "research codes." What then constitutes an acceptable model code, be it applied to a site of interest or a "high-profile site"? The answer may be found in Jakeman et al. (2006) who propose and describe 10 iterative steps in development and evaluation of environmental models. Thus, model validation (verification) should not be determined by the number of practitioners that use and apply a particular model (e.g., "consulting companies"), as implied by TPC (p. 626). Rather, models should be validated (verified) by following a consistent and defensible development protocol and comparing model predictions to known mathematical (analytical) solutions and site-specific field data when available. The TechFlowMP code was validated using just such a process. TechFlowMP is open-source and can be accessed through the website of the Multimedia Environmental Simulations Laboratory at Georgia Tech (http://mesl.ce.gatech.edu/). Additional application and testing of the code is welcomed and encouraged.

Note as well the use and application of specialized codes to address specific problems, including problems that routinely or commonly used codes do not or cannot address are not shunned by government-based scientific organizations, but rather it is recognized and encouraged (USEPA 2009). The point being that the most *appropriate* model should be applied to characterize a system, not necessarily, the most popular or frequently used model. This is the modeling philosophy and approach that

ATSDR used when applying any of the models (including the TechFlowMP model) to simulate subsurface conditions at ABC One-Hour Cleaners and Tarawa Terrace and vicinity.

Uncertainty and Variability of Simulation Results

All modeling analyses have "inherent" uncertainties. ATSDR openly acknowledges this concept. Uncertainty is not limited solely to the historical reconstruction analyses of Tarawa Terrace as critiqued by the TPC article. Uncertainty is an inherent feature of all models even when useful data are plentiful. The "profound limitation" that seemed to so concern some in evaluating the ATSDR historical reconstruction analyses (NRC 2009, 50), should not be that uncertainties exist with respect to model results but that no effort is made to explain and quantify those uncertainties. In this respect, ATSDR has provided very detailed analyses of uncertainty pertinent to the Tarawa Terrace models (Maslia et al. 2007, 2009; Wang and Aral 2008).

Review and Dissemination of Water-Modeling Results

The TPC article implies that results of ATSDR's modeling analyses were going to be used in a decision-making process by the Department of Navy (DON). Therefore, some outside body [e.g., National Research Council (NRC)] had to be assigned the responsibility to assess the complexity of analyses being used and the impact of this complexity on time and resources. This premise is incorrect. ATSDR is a *public* health agency and part of our responsibility is the dissemination of information—technical and nontechnical—using a variety of communication methods (e.g., websites, reports, and meetings) to all interested parties and stakeholders, such as those listed by TPC (p. 622). The TPC article further states that reconstructed historical concentrations were "widely disseminated to various groups" (former Camp Lejeune residents, health scientists, and congressional committees) via websites, public meetings, and reports (p. 622). These statements imply that ATSDR somehow intentionally or unintentionally avoided a rigorous external peer review of its modeling approach, methodology, and results. The facts are that every chapter report published in the Tarawa Terrace historical reconstruction report series (available at http://www.atsdr.cdc.gov/sites/lejeune/index.html) underwent extensive external peer review (review comments and ATSDR responses can be produced by the project officer if needed). Authors completely addressed all external peer review comments; the majority of which were accepted by the authors and included in the final published reports.

In passing, we point out that the reference to Faye and Green (2007) cited by TPC (p. 622 and p. 628) is incorrect. Faye (2007) describes the geohydrologic framework and Faye and Green (2007) describe the occurrence of contaminants in groundwater. We provide the correct citations in the References section.

Concluding Remarks

In the *Ground Water* article, TPC proposes the following idea: Should we go with a complex model or the expert opinion (simple model)? This implies there is no option but to choose one approach or the other. As engineers and scientists, we propose that applying and evaluating the results of several different approaches and types of models is often the best path. A good model will inherently include expert opinion because models are typically developed beginning with a simple conceptual model that is then transformed into a more complex model. We agree with Bredehoeft's opinion (2010) in that the model (simple or complex) is not an end in itself, but a tool by which to organize one's thinking and engineering judgment. In the case of the case-control health study at Camp Lejeune, models are powerful tools used to assist epidemiologists in facilitating the estimation of historical exposures during each month of the mother's pregnancy.

Finally, the *Ground Water* article states (p. 627) that the overall reaction to the NRC report (2009) was mixed. Similar to the TPC article, the NRC report contained numerous factual errors, incorrectly characterized the contaminant PCE source, and overlooked data (that ATSDR had inventoried, compiled, and published) and other pertinent epidemiological and toxicological issues that are beyond the scope of this discussion. Although the case-control health study at Camp Lejeune is a complex endeavor, ATSDR continues to maintain the scientific credibility and thoroughness of its analyses—from both the water-modeling and epidemiological perspectives—through the use of expert panels and external peer review. It is our aim that by addressing the complex issues associated with the process of historical reconstruction in this discussion, our colleagues who have developed and applied models solely in the groundwater modeling and remediation fields, will broaden their horizons and come to appreciate the need and usefulness of extending and incorporating modeling into the multidisciplinary field of exposure assessment science.

Disclaimers

The findings and conclusions in this Discussion article are those of the authors and do not necessarily represent the views of the ATSDR.

The use of trade names and commercial sources is for identification only and does not imply endorsement by the ATSDR.

References

Bradley, P.M. 2003. History and ecology of chloroethene biodegradation: A review. *Bioremediation Journal* 7, no. 2: 81–109.

Bredehoeft, J. 2010. Models and model analysis. *Ground Water* 48: 328.

Christiansen, N., S.R. Christense, E. Arvin, and B.K. Ahring. 1997. Transformation of tetrachloroethene in an upflow

anaerobic sludgeblanket reactor. *Applied Microbiology and Technology* 47, no. 1: 91–94.
Clement, T.P. 2010. Complexities in hindcasting models — When should we say enough is enough. *Ground Water* 49, no. 5: 620–629.
Clement, T.P. 2011. Bioremediation of contaminated groundwater systems. In *Groundwater Quality and Quantity Management*, ed. M.M. Aral and S.W. Taylor, Chapter 13, 563. Reston, Virginia: ASCE Publication.
Costas, K., R.S. Knorr, and S.K. Condon. 2002. A case-control study of childhood leukemia in Woburn, Massachusetts: The relationship between leukemia incidence and exposure to public drinking water. *The Science of the Total Environment* 300: 23–35.
Faye, R.E. 2007. Analyses of groundwater flow, contaminant fate and transport, and distribution of drinking water at Tarawa Terrace and vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina: Historical reconstruction and present-day conditions. In *Geohydrologic Framework of the Castle Hayne Aquifer System*, Chapter B. Atlanta, Georgia: Agency for Toxic Substances and Disease Registry.
Faye, R.E. 2008. Analyses of groundwater flow, contaminant fate and transport, and distribution of drinking water at Tarawa Terrace and vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina: Historical reconstruction and present-day conditions. *Simulation of the Fate and Transport of Tetrachloroethylene (PCE)*, Chapter F. Atlanta, Georgia: Agency for Toxic Substances and Disease Registry.
Faye, R.E., and J.W. Green Jr. 2007. Analyses of groundwater flow, contaminant fate and transport, and distribution of drinking water at Tarawa Terrace and vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina: Historical reconstruction and present-day conditions. *Occurrence of Contaminants in Groundwater*, Chapter E. Atlanta, Georgia: Agency for Toxic Substances and Disease Registry.
Faye, R.E., and C. Valenzuela. 2007. Analyses of groundwater flow, contaminant fate and transport, and distribution of drinking water at Tarawa Terrace and vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina: Historical reconstruction and present-day conditions. *Simulation of Groundwater Flow*, Chapter C. Atlanta, Georgia: Agency for Toxic Substances and Disease Registry.
Griffin, B.M., J.M. Tiedje, and F.E. Loffler. 2004. Anaerobic microbial reductive dechlorination of tetrachloroethene to predominately trans-1,2-dichloroethene. *Environmental Science and Technology* 38, no. 16: 4300–4303.
Jakeman, A.J., R.A. Letcher, and J.P. Norton. 2006. Ten iterative steps in development and evaluation of environmental models. *Environmental Modeling & Software* 21: 602–614.
Jang, W., and M.M. Aral. 2008. Analyses of groundwater flow, contaminant fate and transport, and distribution of drinking water at Tarawa Terrace and vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina: Historical reconstruction and present-day conditions. *Simulation of Three-Dimensional Multispecies, Multiphase Mass Transport of Tetrachloroethylene (PCE) and Associated Degradation By-Products*, Chapter G. Atlanta, Georgia: Agency for Toxic Substances and Disease Registry.
Keuper, B.H., and K.L. Davies. 2009. *Assessment and Delineation of DNAPL Source Zones at Hazardous Waste Sites*. Cincinnati, Ohio: U.S. Environmental Protection Agency, National Risk Management Research Laboratory; EPA/600/R-09/119.
Kopecky, K.J., S. Davis, T.E. Hamilton, M.S. Saporito, and L.E. Onstad. 2004. Estimation of thyroid radiation doses for the hanford thyroid disease study: Results and implications for statistical power of the epidemiological analyses. *Health Physics* 87, no. 1: 15–32.
Lawrence, S.J. 2007. Analyses of groundwater flow, contaminant fate and transport, and distribution of drinking water at Tarawa Terrace and vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina: Historical reconstruction and present-day conditions. *Properties and Degradation Pathways of Common Organic Compounds in Groundwater*, Chapter D. Atlanta, Georgia: Agency for Toxic Substances and Disease Registry.
Maslia, M.L., M.M. Aral, J.J. Reyes, J.E. Abraham, and R.C. Williams. 2000. Using water-distribution system modeling to assist epidemiologic investigations. *ASCE Journal of Water Resources Planning and Management* 126, no. 4: 180–198.
Maslia, M.L., R.J. Reyes, R.E. Gillig, J.B. Sautner, J.B. Fagliano, and M.M. Aral. 2005. Public health partnerships addressing childhood cancer investigations: Case study of Toms River, Dover Township, New Jersey, USA. *International Journal of Hygiene and Environmental Health* 208: 45–54.
Maslia, M.L., J.B. Sautner, R.E. Faye, R.J. Suárez-Soto, M.M. Aral, W.M. Grayman, W. Jang, J. Wang, F.J. Bove, P.Z. Ruckart, C. Valenzuela, J.W. Green Jr., and A.L. Krueger. 2007. Analyses of groundwater flow, contaminant fate and transport, and distribution of drinking water at Tarawa Terrace and vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina: Historical reconstruction and present-day conditions. *Summary of Findings*, Chapter A. Atlanta, Georgia: Agency for Toxic Substances and Disease Registry.
Maslia, M.L., M.M. Aral, R.E. Faye, R.J. Suárez-Soto, J.B. Sautner, J. Wang, W. Jang, F.J. Bove, and P.Z. Ruckart. 2009a. Reconstructing historical exposures to volatile organic compound-contaminated drinking water at a U.S. military base. *Water Quality, Exposure and Health* 1: 49–68.
Maslia, M.L., R.J. Suárez-Soto, J. Wang, M.M. Aral, R.E. Faye, J.B. Sautner, C. Valenzuela, and W.M. Grayman. 2009b. Analyses of groundwater flow, contaminant fate and transport, and distribution of drinking water at Tarawa Terrace and vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina: Historical reconstruction and present-day conditions. *Parameter Sensitivity, Uncertainty, and Variability Associated with Model Simulations of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water*, Chapter I. Atlanta, Georgia: Agency for Toxic Substances and Disease Registry.
McLaren/Hart-ChemRisk. 2000. *Oak Ridge Dose Reconstruction Project Summary Report*. Alameda, California: McLaren/Hart-ChemRisk.
Miller, G.S., C.E. Milliken, K.R. Sowers, and H.D. May. 2005. Reductive dechlorination of tetrachloroethene to trans-dichloroethene and cis-dichloroethene by PCB-dechlorinating bacterium DF-1. *Environmental Science and Technology* 39, no. 8: 2631–2635.
National Research Council (NRC). 2009. Contaminated water supplies at Camp Lejeune: Assessing potential health effects. In *Board on Environmental Studies and Toxicology*, 328. Washington, D.C.: National Academies Press.
North Carolina Department of Environment and Natural Resources (NCDENR). 2003. *Superfund Five-year Review Report, ABC One Hour Cleaners, Jacksonville, Onslow County, North Carolina, EPA ID: NCD 024644494*. Raleigh, North Carolina: North Carolina Department of Environment and Natural Resources.
Pankow, J.F., and J.A. Cherry. 1996. Dense chlorinated solvents and other DNAPLs in groundwater. In *History, Behavior, and Remediation*. Portland, Oregon: Waterloo Press.
Reif, J.S., J.B. Burch, J.R. Nuckols, L. Metzger, D. Ellington, and K.W. Anger. 2003. Neurobehavioral effects of exposure to trichloroethylene through a municipal water supply. *Environmental Research* 93: 248–258.
Rodenbeck, S.E., and M.L. Maslia. 1998. Groundwater modeling and GIS to determine exposure to TCE at Tucson.

Practice Periodical of Hazardous, Toxic, and Radioactive Waste Management* 2, no. 2: 53–61.
Rossman, L.A. 2000. *EPANET 2 User's Manual.* Cincinnati, Ohio: U.S. Environmental Protection Agency, National Risk Management Research Laboratory; EPA/600-R-00/57.
Rothman, K.J., S. Greenland, and T.L. Lash. 2008. *Modern Epidemiology*, 3rd ed. Philadelphia, Pennsylvania: Lippincott Williams.
Roy F. Weston, Inc. 1992. *Remedial Investigation Report, ABC One-Hour Cleaners.* Jacksonville, North Carolina: Roy F. Weston, Inc.
Roy F. Weston, Inc. 1994. *Remedial Investigation Report, ABC One-Hour Cleaners, Operable*, Unit 2, Jacksonville, North Carolina: Roy F. Weston, Inc.
Sahmel, J., K. Devlin, D. Paustenbach, D. Hollins, and S. Gaffney. 2010. The role of exposure reconstruction in occupational human health risk assessment: Current methods and a recommended framework. *Critical Reviews in Toxicology* 40, no. 9: 799–843.
Shiver, R. 1985. *Groundwater Investigation to Define the Source(s) of Tetrachloroethylene that Have Contaminated Three Community Water Supply Wells at Tarawa Terrace I, Camp Lejeune Marine Corps Base, Onslow County.* Onslow County, North Carolina: North Carolina Department of Natural Resources and Community Development.
SWMU9. 2002. *Treatability Study Annual Monitoring Report, Naval Air Facility: Key West, Florida.* Norfolk, Virginia: Southern Division Naval Facilities Engineering Command, Tetra Tech. NUS, Inc.
USEPA. 2009. *Guidance on the Development, Evaluation, and Application of Environmental Models.* Washington, DC: U.S. Environmental Protection Agency, Office of the Science Advisor, Council for Regulatory Environmental Modeling; EPA/100/K-09/003. http://www.epa.gov/crem/cremlib.html.
Wang, J., and M.M. Aral. 2008. Analyses of groundwater flow, contaminant fate and transport, and distribution of drinking water at Tarawa Terrace and vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina: Historical reconstruction and present-day conditions. *Effect of Groundwater Pumping Schedule Variation on Arrival of Tetrachlorothylene (PCE) at Water-Supply Wells and the Water Treatment Plant.* Chapter H. Atlanta, Georgia: Agency for Toxic Substances and Disease Registry.
Weston Solutions, Inc. 2005. *ABC One-Hour Cleaners Groundwater Remediation Project Update.* West Chester, Pennsylvania: Weston Solutions, Inc.
Weston Solutions, Inc. 2007. *ABC One-Hour Cleaners Groundwater Remediation Project Summary.* West Chester, Pennsylvania: Weston Solutions, Inc.

Note: Comment received May 3, 2011, accepted May 18, 2011.

Appendix O — Post-Audit of the Tarawa Terrace Flow and Transport Model, N. L. Jones and R. Jeffrey Davis, Integral Consulting, Inc., October 25, 2024

Tarawa Terrace Flow and Transport Model Post-Audit

Prepared for
Bell Legal Group
219 Ridge Street
Georgetown, SC 29440

Prepared by

Norman L. Jones
Norm Jones Consulting LLC
4174 N 430 E
Provo, UT 84604

R. Jeffrey Davis
integral
Integral Consulting Inc.
2231 E Murray Holladay Road
Suite 201
Salt Lake City, UT 84117

October 25, 2024

CONTENTS

LIST OF FIGURES

LIST OF TABLES

ACRONYMS AND ABBREVIATIONS

ATSDR	Agency for Toxic Substances and Disease Registry
PCE	tetrachloroethylene
GMS	Groundwater Modeling System
MAE	mean absolute error
ME	mean error
NGWA	National Groundwater Association

EXECUTIVE SUMMARY

This post-audit report evaluates the performance of groundwater flow and transport models developed for the Tarawa Terrace region of Camp Lejeune by the Agency for Toxic Substances and Disease Registry (ATSDR). The models were originally designed to simulate the migration of tetrachloroethylene (PCE) contamination from the ABC Cleaners site, located adjacent to the northern boundary of Tarawa Terrace. The audit extends the original model's simulation period from 1995 to 2008 and assesses the accuracy of its predictions by comparing simulated PCE concentrations to actual concentrations measured at monitoring wells during this extended period.

The first step of the audit involved updating the original models, which were created using MODFLOW 96 and MT3DMS software. Both models covered a period between 1951 and 1994. These were successfully updated to MODFLOW 2000 and MT3DMS v5.3, ensuring compatibility with current software versions. Importantly, no significant discrepancies were detected between the original and updated models, confirming that the update process did not alter the results.

The simulation period was then extended to cover the years from 1995 through 2008. During this update, new rainfall and recharge data were incorporated in the MODFLOW model based on nearby weather stations, as the original station's data was incomplete. Additionally, the pumping rates for a set of remediation wells were included, as these wells played a role in altering groundwater flow during this period. The PCE source, which originated from ABC Cleaners and was terminated in the original model at the end of 1984, was left unchanged.

The extended MT3DMS model was found to perform well in simulating PCE concentrations at monitoring wells across the study area. The errors are remarkably well balanced, indicating a good overall fit between simulated and observed concentrations. There were localized discrepancies in error magnitude, particularly in areas where monitoring wells showed significant temporal and spatial variability. Some wells exhibited large fluctuations in measured concentrations over time, which likely resulted from natural subsurface variability, sampling errors, or differences in analytical methods. In other cases, wells showed significant differences in the magnitude of measured concentrations despite being adjacent to one another.

Despite these localized anomalies, the extended MT3DMS model captured the broader patterns of PCE plume migration with reasonable accuracy, particularly during the later years of the simulation. The largest errors were concentrated in a few monitoring wells that were already noted for irregularities in the observed data, but the model's predictions were generally consistent with observed concentrations at most well locations.

In summary, this post-audit found that the original Tarawa Terrace groundwater flow and transport models were developed using sound methodology and continue to provide reliable insights into the migration of PCE contamination. Despite the inherent challenges in simulating complex subsurface conditions and dealing with incomplete data, the model effectively simulates long-term trends in contaminant migration. Based on this post-audit, we can find no significant evidence that would invalidate the analyses performed by ATSDR with the original model.

1 INTRODUCTION

Our names are Norman L. Jones and R. Jeffrey Davis, and we have been asked to provide a post-audit of groundwater flow and transport models originally developed by the Agency for Toxic Substances and Disease Registry (ATSDR). This post-audit included extending both models from 1995 through 2008. Based on this review, effort, and analysis, as more fully described herein, we have reached the conclusions and opinions set forth below. A complete list of all materials relied upon to form the opinions in the report will be produced within seven days of the report's submittal. Our conclusions are subject to any new materials, data, or other information provided to us prior to depositions or trial at which time our opinions and conclusions may be updated.

In July 2007, the ATSDR, U.S. Department of Health and Human Services, published a report on a groundwater flow and transport model of the Tarawa Terrace region of the Camp Lejeune military base (Maslia et al. 2007; Faye and Valenzuela 2008; Faye 2008). The model was developed to simulate groundwater flow in the aquifers beneath Tarawa Terrace and to simulate the migration of tetrachloroethylene (PCE)[1] in the aquifers resulting from the release of PCE by ABC Cleaners, which is directly adjacent to the northern boundary of the Tarawa Terrace property. The original model was developed using the MODFLOW 96 software (USGS 1996) to simulate groundwater flow and the MT3DMS software (Zheng and Wang 1999) to simulate contaminant transport. MODFLOW and MT3DMS are companion programs where the groundwater flow field computed by MODFLOW is used by MT3DMS to simulate the fate and transport of PCE.

The original Tarawa Terrace flow model was designed to simulate flow conditions over a period from 1951 to 1994. The computation grid used by the model consisted of 270 rows and 200 columns, resulting in a uniform grid cell size of 50 ft x 50 ft. In the vertical direction, the model contained seven layers corresponding to a series of hydrogeologic units, including the Tarawa Terrace aquifer and the underlying Castle Hayne aquifer system. Model features include recharge resulting from vertical percolation of water from rainfall, general head boundary conditions on the north simulating exchange (primarily inflow) of water with the aquifer north of Tarawa Terrace, no-flow boundary conditions on the west representing a no-flow boundary along a topographic divide, and specified head boundary conditions on the south and east representing Northeast Creek. The model also included the withdrawal of groundwater via pumping wells and a drain representing potential discharge of groundwater to the channel of Frenchmans Creek on the west side of the model.

For the transport model, PCE was introduced through a single cell corresponding to the ABC Cleaners spill location at a mass loading rate of 1,200 g/day for a period from January 1953 to December 1984, and the resulting plume migration was simulated through the end of the flow

[1] PCE is also known by other names, including tetrachloroethene. In this report we refer to it as tetrachloroethylene.

and transport simulation period in December of 1994. Transport processes simulated include advection, dispersion, sorption, and biodegradation.

The original flow and transport models were calibrated using a multi-stage process. In the first stage, the flow model was calibrated to steady state flow conditions representing a pre-development state prior to the introduction of groundwater extraction wells. It was then converted to a transient model with pumping wells and time-varying recharge over the period of 1951 to 1994. The transient model was calibrated to transient water levels measured at monitoring wells in the region. In the final stage, the MT3DMS transport model was included, and the parameters of both the flow and transport model were adjusted until both the heads simulated by MODFLOW and the concentrations simulated by MT3DMS matched the field-observed heads, flows, and PCE concentrations within a reasonable range.

The objective of the post-audit is to extend the range of the groundwater flow and transport models from 1995 to 2008 and compare the output of the transport model with concentrations sampled at monitoring wells in Tarawa Terrace during the 1995–2008 period to assess the performance of the model as an interpretive and predictive tool. This comparison involved both a quantitative analysis of simulated versus observed concentrations and a qualitative analysis of the shape and migration of the simulated PCE plume over that period.

In the following sections, we described the steps we took to a) import the original model and update it to work with recent versions of MODLOW and MT3DMS, b) extend the flow model to 1995–2008 conditions, c) extend the transport model to 1995–2008 conditions, and d) compare the simulated PCE concentrations to field-observed PCE concentrations over the extended simulation period.

2 IMPORTING AND RUNNING THE ORIGINAL MODEL

To begin the post-audit, we were provided with a copy of the MODFLOW96 and MT3DMS input files used in the original model. We elected to use the Groundwater Modeling System (GMS) software, version 10.8 (Aquaveo LLC 2024) to perform the model updates. The GMS software is developed and distributed by Aquaveo LLC in Provo, Utah. GMS is a graphical user interface for the MODFLOW and MT3DMS codes and works as a pre- and post-processor (Owens et al. 1996). GMS can be used to build new models from scratch, or to import and modify existing models. The model data are then saved by GMS to input files that can be read by MODFLOW/MT3DMS. The model results output by MODFLOW/MT3DMS are then read by GMS where they can be displayed graphically and analyzed numerically.

We began by attempting to import the MODFLOW 96 files. MODFLOW has been continuously updated and improved since it was initially launched in 1984 (McDonald and Harbaugh 1984), resulting in numerous versions. MODFLOW 96 was released in 1996 and was widely used but was updated to MODFLOW 2000 (Harbaugh et al. 2000) and MODFLOW 2005 (Harbaugh 2005) in 2000 and 2005, respectively. More recent versions include MODFLOW-USG (Panday et al. 2013) and MODFLOW 6 (Langevin et al. 2017). While newer versions provide some new capabilities, both MODFLOW 2000 and MODFLOW 2005 are widely used and provide access to all of the model features used in the original Tarawa Terrace model. However, MODFLOW 96 has been mostly discontinued and is not supported by the GMS software. GMS does provide the capability to import MODFLOW 96 files and convert them to newer versions. When we attempted to import the original MODFLOW 96 files to GMS, we discovered that the files would not import properly, and GMS displayed an error message. After some exploration, we determined that we had to make a minor edit to the original WEL (wel.dat). Lines 4 through 13 were changed from a "-1" value to a value of "0." Once the model was imported, we saved a copy of the model in MODFLOW 2000 format. To import the MT3DMS files, we had to manually update the mass loading of 1,200 g/day in GMS from January 1953 through December 1984. This was due to an outdated version of the Source Sink Mixing (SSM) package used in the original simulation. The MT3DMS files were saved in an updated format compatible with the current version of MT3DMS (v5.3) used by GMS.

After importing and converting the MODFLOW and MT3DMS files and saving them to the newer formats, we re-ran the flow and transport simulations and imported the solutions to GMS. At this point, we performed a qualitative analysis to ensure that the process of converting the files and updating to the newer versions did not change the model outputs. First, the simulated head contours from the updated flow model were compared to the head contours described in the ATSDR modeling report (Faye and Valenzuela 2008) as shown in Figure 1. The results of the updated model seem to match the results of the original model. Next, we compared PCE concentrations simulated by the updated MT3DMS model and to the concentrations simulated by the original MT3DMS model (Figure 2). Once again, the results seem to match well, indicating that no errors were introduced to the model in the conversion process.

3 EXTENDING THE FLOW MODEL

After confirming that the flow and transport simulations were properly imported and updated, we proceeded to modify both the flow and transport simulations for the post-audit. The changes made to the MODFLOW model are described in this section. The only changes made to the MODFLOW model were to extend the simulation period, update recharge values over the new period, and modify the pumping rates at remediation wells. No other changes were made to simulation settings or boundary conditions and sources/sinks.

3.1 SIMULATION PERIOD

The original simulation was from January 1951 through December 1994. We extended the simulation period through December 2008 so that the simulation included the period from 1995 to 2008. For the new simulation, no changes were made to the inputs for the original 1951–1994 period and thus the model solution for that period remained unchanged in the new model. For 1995–2008, we used the same stress period interval used in the original model, with monthly stress periods and one time step per stress period.

3.2 RAINFALL-RECHARGE

For the original flow model, the primary source of water to the aquifer was input from precipitation that infiltrated to the water table, which is simulated in MODFLOW as recharge where the units are length/time (feet/day). In the original model, a single annual recharge rate was used for each year of the simulation as illustrated in Table C7 of Faye and Valenzuela (2008). The recharge rate was found by applying a recharge coefficient of 0.235 to the annual precipitation to find an effective recharge rate representing the fraction of rainfall that percolates to the water table. This recharge rate is then entered into the Recharge Package in MODFLOW, and the package applies water to the top active cell during each stress period.

The precipitation values used in the original simulation were obtained from the Maysville-Hofman Forest station, which is north of Tarawa Terrace. For the post-audit, we attempted to obtain precipitation data from the same station. We found three different precipitation data sets that were purported to be from the Hofman Forest station, but each of these data sets was determined to be unusable. None of the data sets had a complete set of precipitation data for the 1995 to 2008 period. Furthermore, for the partial data during the period of interest, one of the data sets contained some extreme anomalies in monthly precipitation that did not appear in neighboring rain gauge stations. As a result, we elected to use rain gauge data from other stations in the vicinity of Tarawa Terrace. Using the National Oceanic and Atmospheric Administration National Weather Service website (National Weather Service 2024), we located three rain gauges near Tarawa Terrace that had a complete set of rainfall measurements during the period 1995 to 2008. The locations of these gauges relative to Tarawa Terrace are shown in

Figure 3. The mean rainfall for each of these gauges over the 1951 to 1994 period is similar to the mean rainfall for the Hofman Forest station over the same period, and the annual variations were in a consistent range. Thus, we took a simple average of each of the three stations over the 1995 to 2008 period to estimate the average annual rainfall at Tarawa Terrace and multiplied these averages by 0.235 to get the effective recharge rate and converted it to units of feet/day for use in the extended MODFLOW simulation. The rainfall values, averages, and effective recharge rates are summarized in Table 1.

3.3 PUMPING AT WELLS

Another change to the MODFLOW model over the extended simulation period was related to pumping associated with a set of remediation wells. These wells withdraw water from the aquifer, thus impacting both the flow field and the subsequent movement of contaminants simulated by the MT3DMS simulation. We were provided with a list of remediation wells and their pumping history for a period beginning in 1999 and continuing through the end of 2008. The well names, coordinates, model layers, and pumping histories over the period of interest are shown in Table 2. In each case, the pumping rates were turned on for each well at the rates shown on the corresponding dates and held constant at that rate until the next rate change or until the wells were turned off. All the other pumping wells in the model had zero pumping rates during the extended simulation period. The locations of the remediation wells are shown in Figure 4.

4 EXTENDING THE TRANSPORT MODEL

For the transport model, no changes were required to the MT3DMS inputs for the extended simulation period, except for enabling the Transport Observation package. The same dynamic transport step options used in the original model were applied to the new stress periods from 1995 to 2008. The PCE source at the location of the ABC Cleaners facility was turned off at the end of 1983, matching the original model.

4.1 OBSERVED CONCENTRATIONS

The main objective of extending the flow and transport simulation was to assess the performance of the model in simulating the migration of the PCE plume over the extended period and to compare the simulated PCE concentrations to PCE concentrations observed at monitoring wells during the 1995–2008 period. A list of the monitoring wells is shown in Table 3, the PCE concentrations observed at the wells in Table 4, and the locations of the wells in Figure 5. As presented in Table 4, the samples were all taken at 12 distinct dates beginning in 1997 and ending in 2008. The model layers associated with each well were determined by comparing the well screen depths with the grid cell top and bottom elevations for the grid cells containing the monitoring well locations and confirmed by documents provided by counsel (Weston ABC One-Hour Cleaners Dataset).

The monitoring well locations and the observed concentrations were imported as observation points in an "observation" coverage (spatial features layer) in the Map Module of the GMS software. This information was then linked by GMS to the MT3DMS Transport Observation package, which was turned on and used in the simulation. This allows MT3DMS to calculate the simulated PCE concentrations at the cells containing the observation wells and output the results in a format that we could easily access and use in our analysis.

4.2 TEMPORTAL AND SPATIAL ANOMALIES

While the observed concentrations at each monitoring well listed in Table 4 are generally consistent over time, there are some exceptions that should be noted. For Well C13 in Model Layer 3, the observed concentration of 5,400 μg/L in 2002 is an order of magnitude higher than any subsequent concentrations observed at the same well and is substantially higher than all other concentrations but one. The highest concentration of 6,900 μg/L was measured at Well RWS-4A in Layer 1. The observed concentrations at this well showed extreme fluctuations over time. The observed concentration of 280 μg/L in January 2002 was followed only 3 months later by an observed concentration of 6,900 μg/L—the highest value measured. Then for the sequence of observations from 2003 to 2007, the concentrations oscillated from 1,100 → 0 → 1,000 → 92 → 1,600. This high degree of fluctuation could be due to sampling errors, differences in analytical techniques, and/or extreme heterogeneity in aquifer properties near the well.

In addition to variations over time, there are spatial variations in the observed concentrations. Well FWS-13 has zero or low (<5 μg/L) observed concentrations over the entire range of sampling dates. However, as shown in Figure 5, it is immediately adjacent to FWS-12, RWS-3A, and RWS-4A, all of which show high concentrations over the entire range of sampling dates. Likewise, in Model Layer 3, monitoring well C12 has low observed concentrations despite being adjacent to RWC-2, which has high concentrations. Furthermore, Wells FWC-11 and C5 have zero or low (<5 μg/L) observed concentrations over all sampling dates and are relatively close to C3, which has high concentrations over most dates. C14 has high concentrations over the four dates sampled despite being directly adjacent to C13, C15-S, C15-D, and C16, all of which have low concentrations on those dates.

This temporal and spatial variability in concentrations at selected wells illustrates the extreme variability often seen when dealing with concentration data from monitoring wells. It highlights why focusing on absolute concentrations at specific dates and locations when analyzing the performance of a flow and transport model is less important than assessing the overall distribution of simulated concentrations and comparing the shape of the simulated plume with the general spatial distribution of observed concentrations. Each of these sites with high variability is generally correlated with higher model error, as shown below in the Results section.

5 RESULTS

The main objective of this post-audit is to assess the performance of the flow and transport model over the extended period of 1995 to 2008 using PCE concentrations observed in monitoring wells over that period. Before presenting the results, it is helpful to remember that when simulating the migration of a PCE contaminant plume using MODFLOW and MT3DMS, achieving a close match between simulated and observed concentrations can be challenging for several reasons:

1. **Complex Subsurface Conditions**: The subsurface environment is inherently complex, with variations in soil heterogeneity, permeability, porosity, and hydraulic conductivity. These properties vary spatially in ways that are not fully captured in the model, affecting how the contaminant plume moves through the groundwater system.
2. **Temporal Variability**: The concentration of contaminants can change over time due to factors like seasonal variations in groundwater flow, biodegradation, and chemical reactions. Simulating these dynamic processes accurately over the entire simulation period is challenging.
3. **Limitations in Model Resolution**: MODFLOW and MT3DMS rely on discretizing the subsurface into numerical grids consisting of cells that represent a subset of the aquifer. The resolution of these grids can limit the model's ability to capture fine-scale variations in plume behavior, particularly in areas with sharp concentration gradients, small-scale heterogeneities, or preferential pathways.
4. **Measurement Variability**: The observed concentrations at observation wells may contain some degree of measurement error or uncertainty. Field data collection is subject to variability, which adds another layer of complexity when trying to match it closely with model outputs. As outlined above in Section 4.2, extreme variations were observed in some of the measured concentrations used in this post-audit.

Each of these challenges was highlighted in the Faye (2008) report on pp. F44–45. It was reported that at several sites, measured concentrations varied by several orders of magnitude over a few feet of depth.

Given these challenges, it is important to qualitatively assess the overall behavior of the simulated plume in addition to quantitatively analyzing the differences in simulated and observed concentrations at specific times and locations. A qualitative evaluation helps ensure that the model captures the key processes governing plume migration, such as its general direction, spread, and interaction with sources, sinks, and aquifer boundaries. This broader perspective can offer valuable insights into the overall value of the model as an interpretive or predictive tool.

After running both the extended MODFLOW and MT3DMS simulations, we analyzed the resulting PCE concentrations at a set of monitoring well locations and compared them to the observed concentrations. In the MT3DMS simulation, the spill at ABC Cleaners was simulated using a mass loading rate of 1,200 g/day at a single cell from January 1953 to December 1983 as described in Faye (2008). We did not alter this mass loading rate for the extended simulation. The resulting concentrations computed by the MT3DMS model are in units of grams/cubic foot. We converted these concentrations to units of micrograms/liter by multiplying the MT3DMS concentrations by a conversion factor of 35,314.7. We chose to present the simulated concentrations in micrograms/liter to match the units used in the original Faye (2008) report. This was applied to both the simulated concentrations at monitoring well locations and to the gridded data used to display the migration of the PCE plume.

5.1 MONITORING WELLS

A complete list of the observed and simulated concentrations at the monitoring well locations is shown in Table 5. The "Error" column represents the difference between the simulated and observed concentrations, and the "Abs(Error)" column is the absolute value of the error. These observations were sampled at a unique set of time periods as shown in Table 4. Taking all values into consideration, the mean error (ME) = 21 μg/L, indicating that the positive and negative errors are well balanced. The mean absolute error (MAE) = 334 μg/L.

These concentration values are displayed on a scatter plot of simulated concentrations versus observed concentrations in Figure 6. Because this is a log-log plot, it does not show values where either the simulated or observed concentrations are zero. The results are similar to the results for the original model shown in Figure F12 on p. F33 of the Faye (2008) report; although in this case, there are far more samples to compare. The dashed line in Figure 6 indicates a perfect match between the simulated and observed values. The points on the plot are mostly centered on the line, but as was the case with the original model, the simulated values appear to be biased on the high side, with the simulated values greater than the observed values. However, when the sites with zero observed or simulated concentrations (not shown on Figure 6) are factored in, the errors are balanced, as indicated by the low ME (21 μg/L) reported above.

We calculated a scatter plot of simulated versus observed concentrations for each monitoring well location where both the simulated and observed concentrations are non-zero, and the plots are shown in Figure 7. While there is high variability at some sites, most of the sites show good agreement.

Next, we generated time series plots of simulated versus observed concentrations at monitoring well locations. The results are shown in Figure 8. For Sites C1, S8, and S11, both simulated and observed concentrations were zero for all measurement dates. In general, the simulated and observed curves become closer as the simulation progresses. It should be noted that the vertical scale on each plot is variable, and the magnitude of the differences between simulated and observed concentrations can vary greatly from one plot to the next.

5.2 MIGRATION OF PCE PLUME

To get a qualitative understanding of the of the spatial distribution of the simulated PCE plume versus time and how it correlates with the temporal and spatial distribution of the observed PCE concentrations, we next generated a series of maps showing the simulated PCE plume in Model Layers 1, 3, and 5 at selected sampling dates (Figures 9–13). For each date, we overlaid the monitoring wells that were sampled on that date in each layer. The intervals and colors for the simulated PCE plume contours were selected to match those used in Figures F18–F25 in the Faye (2008) report. The monitoring well symbols are colored based on the relative magnitude of the absolute error at that date.

The results for each of the sampling dates are generally consistent. The spatial distribution of green and yellow symbols at monitoring well locations shows good overall fit of the simulated plume relative to observed concentrations, especially at the later sampling dates. The larger errors tend to be concentrated in the center of the plume where the simulated concentrations are greater. This is somewhat expected because comparing larger numbers will organically result in larger differences. Furthermore, the high errors generally coincide with the monitoring wells exhibiting high temporal and spatial variation, as described in Section 4.2. The wells identified in that section with extreme variability include FWS-13, RWS-4A, RWC-2, FWC-11, C5, and C14, all of which exhibit high errors. Other wells, such as S3 and S5, have high errors in the earlier dates but are in better agreement at later dates when the high simulated concentrations in the center of the plume dissipate over time.

To further compare the spatial distribution of the PCE plume with the PCE concentrations observed at monitoring wells, we took the errors and absolute errors from Table 5 and calculated the ME and MAE at each monitoring well location. The results are tabulated in Table 6. These MAE values were then used to create the maps shown in Figures 14–16. There is a separate map for each of the Model Layers 1, 3, and 5. In each figure, the MAE magnitudes for each monitoring well are displayed at the monitoring well locations and are superimposed on contour plots of the simulated PCE plume. The MAE error norm represents errors from multiple sampling dates, and the footprint of the plume migrated over time as illustrated previously in Figures 9–13. However, the intent here is to illustrate the spatial distribution of the error relative to the overall plume footprint, and the plume footprint is at the largest state at this point in the simulation, so it represents a useful basis of comparison.

The PCE plume for December 2008 for Model Layer 1 and the MAE at monitoring wells located in Layer 1 are shown in Figure 14. The errors at the wells are color-coded for three ranges, as shown in the figure legend. The spatial distribution of the errors indicates that there is a good overall agreement between the shape of the plume and the observed PCE concentrations at the monitoring wells. The wells with the highest errors are Wells FWS-13 and RWS-4A, which were noted in Section 4.2 as having high temporal and spatial anomalies. The simulated PCE plume for Layer 3 for the same date and the errors for monitoring wells in Layer 3 are shown in Figure 15. Once again, most of the wells on the fringes of the plume are in good agreement.

The highest errors are at Wells FWC-11, C5, C13, C14, and RWC-2, which were identified in Section 4.2 as having high anomalies. The simulated PCE plume and errors for Layer 5 are shown in Figure 16. This layer contained only two monitoring wells, and the errors are low.

In summary, the 7 wells identified as having anomalies in the observed data have high errors while the remaining 30 wells exhibit low or moderate errors, indicating good overall agreement between the simulated PCE plume and the observed concentrations over the range of the extended simulation.

6 CONCLUSIONS

Our conclusions from the post-audit analysis are as follows:

1. **Model Import and Update**: The original MODFLOW and MT3DMS models were successfully imported and updated to modern versions (MODFLOW 2000 and MT3DMS v5.3), ensuring compatibility with current software. The updated models matched the original model outputs, validating the update process.

2. **Extended Simulation Period**: The flow and transport models were extended from the original period (1951–1994) to cover the period from 1995 to 2008. Modifications included updating the recharge data based on new precipitation data and incorporating pumping rates for the remediation wells. The PCE source at ABC Cleaners was left unchanged, consistent with the original simulation ending in 1984.

3. **Observed vs. Simulated Concentrations**: The post-audit revealed that the updated MT3DMS model adequately simulated PCE concentrations at monitoring wells over the extended period. While there was a high variability at some monitoring well locations, the errors are remarkably well balanced, indicating a good overall fit between simulated and observed concentrations.

4. **PCE Plume Migration**: The extended model captured the overall migration of the PCE plume between 1995 and 2008. Simulated plumes were consistent with observed concentrations at most monitoring wells, especially during the latter stages of the simulation. The largest discrepancies occurred at a relatively small subset of wells that exhibited high temporal and spatial variability in observed concentrations. This variability may be due to sampling errors, aquifer heterogeneity, or variations in analytical methods.

5. **Model Performance**: The model performance was evaluated using both qualitative and quantitative methods. Despite challenges inherent in simulating subsurface flow and transport, such as soil heterogeneity, data uncertainty, and model resolution limits, the model reasonably captured the key behaviors of the PCE plume. The high variability in certain well measurements introduced some error but did not significantly undermine the model's overall accuracy.

In summary, the extended model demonstrates that the original model was developed using sound methods, and the model remains a reliable tool for understanding the general trends of contaminant migration in the Tarawa Terrace region. Based on this post-audit, we can find no significant evidence that would invalidate the analyses performed by ATSDR with the original model.

7 REFERENCES

Aquaveo LLC. 2024. Groundwater Modeling System, Aquaveo LLC, Provo, UT.

Faye, R.E., and C. Valenzuela. 2008. Analyses of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water at Tarawa Terrace and Vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina: Historical Reconstruction and Present-Day Conditions – Chapter C: Simulation of Groundwater Flow. Agency for Toxic Substances and Disease Registry U.S. Department of Health and Human Services, Atlanta, GA.

Faye, R.E. 2008, Analyses of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water at Tarawa Terrace and Vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina: Historical Reconstruction and Present-Day Conditions – Chapter F: Simulation of the Fate and Transport of Tetrachloroethylene (PCE). Agency for Toxic Substances and Disease Registry, U.S. Department of Health and Human Services, Atlanta, GA.

Harbaugh, A.W. 2005. MODFLOW-2005: The U.S. Geological Survey Modular Ground-Water Model—the Ground-Water Flow Process; Techniques and Methods. U.S. Geological Survey.

Harbaugh, A.W., E.R. Banta, M.C. Hill, and M.G McDonald. 2000. MODFLOW-2000, the U.S. Geological Survey Modular Ground-Water Model—User Guide to Modularization Concepts and the Ground-Water Flow Process. U.S. Geological Survey Open-File Report 00-92 2000. U.S. Geological Survey.

Langevin, C.D., J.D. Hughes, E.R. Banta, R.G. Niswonger, S. Panday, and A.M. Provost. 2017. Documentation for the MODFLOW 6 Groundwater Flow Model. U.S. Geological Survey.

Maslia, M.L., J.B. Sautner, R.E. Faye, R.J. Saurez-Soto, M.M. Aral, et al. 2007. Analyses of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water at Tarawa Terrace and Vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina: Historical Reconstruction and Present-Day Conditions – Chapter A: Summary of Findings. Agency for Toxic Substances and Disease Registry U.S. Department of Health and Human Services, Atlanta, GA.

McDonald, M.G., and A.W. Harbaugh. 1984. A Modular Three-Dimensional Finite-Difference Ground-Water Flow Model. Open-File Report.

National Weather Service. 2024. Home page. https://www.weather.gov/. Accessed on October 19, 2024. U.S. Department of Commerce and National Weather Service.

Owen, S.J., N.L. Jones, and J.P. Holland. 1996. A Comprehensive Modeling Environment for the Simulation of Groundwater Flow and Transport. *Eng. Comput.* 12:235–242.

Panday, S., C.D. Langevin, R.G. Niswonger, M. Ibaraki, and J.D. Hughes. 2013. MODFLOW–USG Version 1: An Unstructured Grid Version of MODFLOW for Simulating Groundwater Flow and Tightly Coupled Processes Using a Control Volume Finite-Difference Formulation. U.S. Geological Survey.

USGS. 1996. USGS MODFLOW-96: MODular Three-Dimensional Finite-Difference Ground-Water FLOW Model with the Hydrograph Package. https://water.usgs.gov/nrp/gwsoftware/modflow/modflow-96h.htm Accessed on October 13, 2024. Available online: https://water.usgs.gov/nrp/gwsoftware/modflow/modflow-96h.htm. (Accessed on October 13, 2024). U.S. Geologic Survey.

Weston ABC One-Hour Cleaners Dataset[2]

Zheng, C., and P.P. Wang. 1999. MT3DMS, A Modular Three-Dimensional Multi-Species Transport Model for Simulation of Advection, Dispersion and Chemical Reactions of Contaminants in Groundwater Systems; Documentation and User's Guide. U.S. Army Engineer Research and Development Center Contract Report SERDP-99-1. Vicksburg, MS. 202 pp.

[2] Reference will be updated.

8 QUALIFICATIONS

I, **R. Jeffrey Davis**, P.E., CGWP, have almost 30 years of experience with civil and environmental engineering, hydrogeology, groundwater fate and transport modeling, and software and model development. I have both undergraduate and graduate degrees from Brigham Young University in civil engineering. I currently serve on the board of directors for the National Ground Water Association (NGWA), as well as on NGWA's per- and polyfluoroalkyl substances and Managed Aquifer Recharge advisory groups. I was one of the leads for NGWA's Groundwater Modeling Advisory Panel. I have developed and used numerous groundwater models for the agricultural industry and the mining industry, including projects involving environmental impact statements, environmental assessments, water management, groundwater–surface water interaction and contamination, dewatering, and water treatment. I also have extensive experience with the oil and gas industry, including water supply, hydraulic fracturing, and groundwater protection for the upstream market, and worked on a variety of oil release projects. I have extensive knowledge of groundwater flow-and-transport principles and have led numerous workshops and classes in the United States and around the world. I have taught several classes and workshops in association with NGWA and other professional organizations and universities for the past 3 decades. I also share my research and project work regularly with the professional societies with which I am affiliated. I frequently use groundwater models to explain fate and transport of contaminants or groundwater supplies and availability. Recent such examples include groundwater impacts from agricultural activities in Minnesota; aqueous film-forming foam contamination impacts to groundwater in Martin County, Florida; a pipeline of produced water spill in North Dakota; and groundwater availability and surface water impacts in Ventura County, California. I am regularly asked to provide opinions or participate on panels to discuss groundwater, water supply, or contaminated groundwater issues.

I, **Norman L. Jones**, Ph.D., have 33 years of experience in civil and environmental engineering. I graduated with a B.S. degree in civil engineering from Brigham Young University and with M.S. and Ph.D. degrees in civil engineering from the University of Texas at Austin. I have been a faculty member in the Civil and Construction Engineering Department at Brigham Young University since January 1991 where I currently hold the rank of Professor. I have taught university courses in a variety of subjects, including computer programming, soil mechanics, seepage and slope stability analysis, and groundwater modeling. The primary focus of my research has been groundwater flow and transport modeling, software development, remote sensing, groundwater sustainability analysis, and hydroinformatics. I was the original developer of the GMS software, which is a graphical user interface for MODFLOW and MT3DMS and is used by thousands of organizations all over the world. GMS is now developed and maintained by Aquaveo, LLC in Provo, Utah, a company that I helped found in 2007. I have taught numerous short courses on groundwater flow and transport modeling over my career. I am a member of the Hydroinformatics Research Laboratory at Brigham Young University. I have been the principal or co-investigator on more than $20M of externally funded research. I have authored 179 technical publications, including 88 peer-reviewed journal articles, and 1 book. I am a recipient of the Walter L. Huber Civil Engineering Research Prize from the American Society of Civil Engineers and the John Hem Award for Science and Engineering from NGWA. I have been involved in a number of consulting projects, including work as a technical expert in litigation cases. I am an active member of the American Water Resources Association, the NGWA, the American Geophysical Union, and the American Society of Civil Engineers.

9 COMPENSATION

My, **R. Jeffrey Davis**, experience is summarized in my resume, which is included as Exhibit 1. I am being compensated at a rate of $498 an hour for my time in preparation of this report and $498 an hour for my deposition and trial testimony, if necessary. My compensation is not contingent upon the opinions I developed or the outcome of this litigation case.

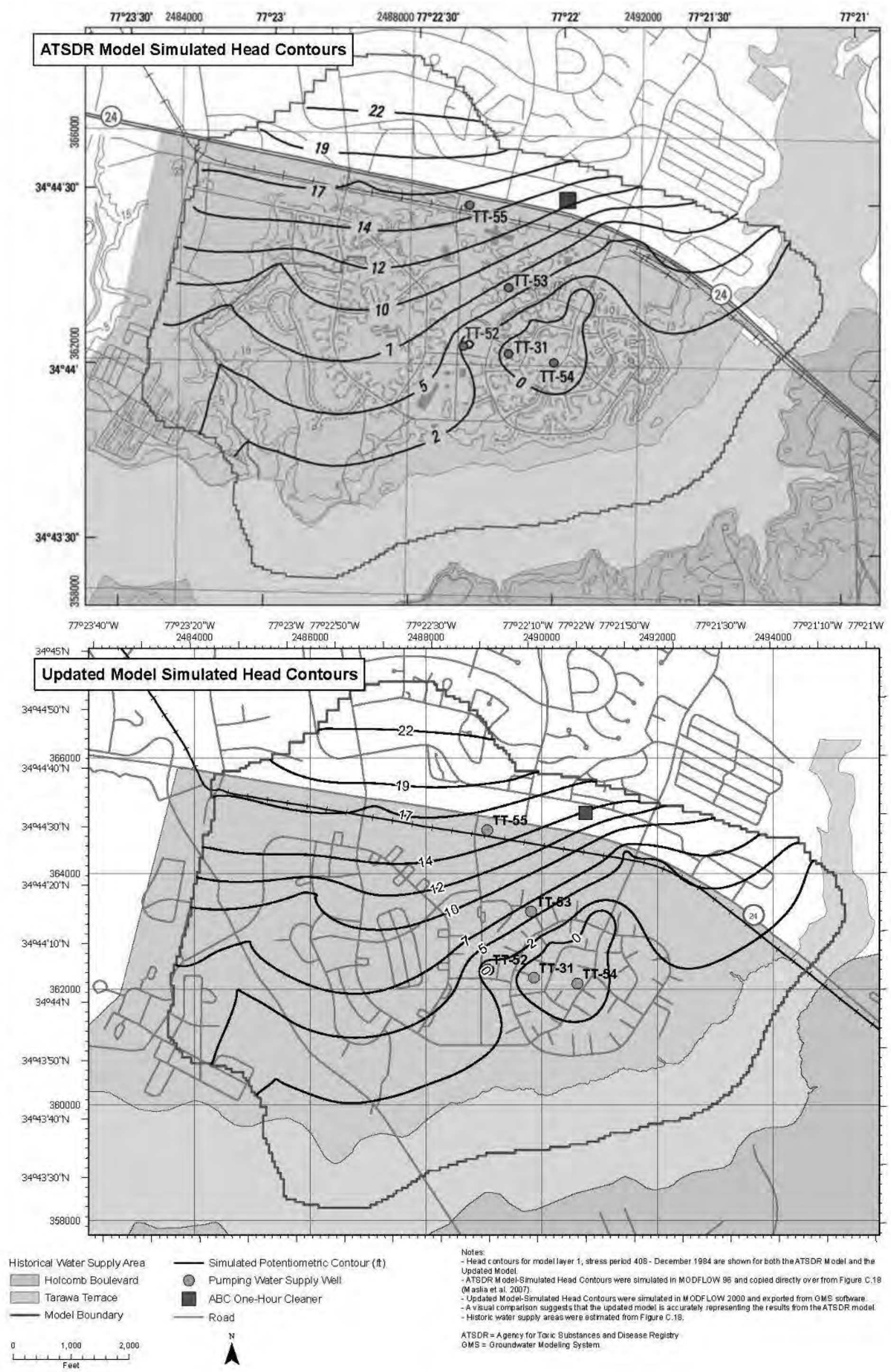
My, **Norman L. Jones**, experience is summarized in my resume, which is included as Exhibit 2. I am being compensated at a rate of $500 an hour for my time in preparation of this report and $1,000 an hour for my deposition and trial testimony, if necessary. My compensation is not contingent upon the opinions I developed or the outcome of this litigation case.

10 PREVIOUS TESTIMONY

I, **R. Jeffrey Davis**, have not given any deposition or trial testimony in the last 4 years.

I, **Norman L. Jones**, gave deposition testimony on October 20, 2021, in MICHAEL YATES and NORMAN L. JONES vs TRAEGER PELLET GRILLS LLC, in the United States District Court for the District of Utah Central Division, Case No. 2:19-cv-00723-BSJ. With the exception of this case, I have not given any deposition or trial testimony in the last 4 years.

Figures

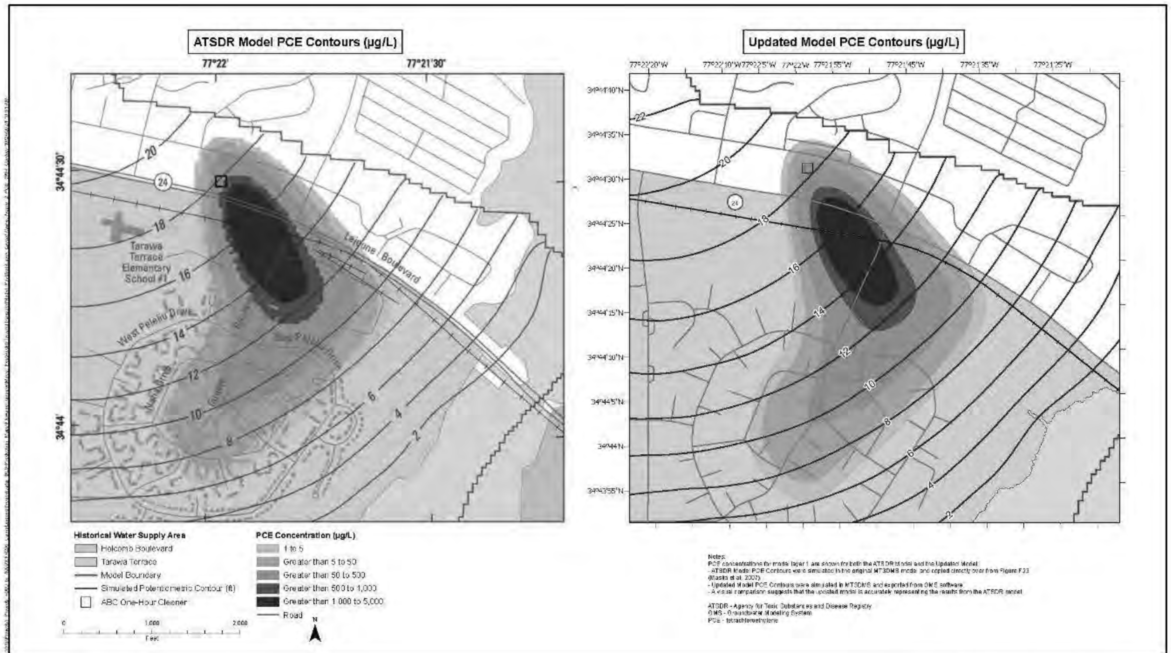


Notes:
- Head contours for model layer 1, stress period 408 - December 1984 are shown for both the ATSDR Model and the Updated Model.
- ATSDR Model-Simulated Head Contours were simulated in MODFLOW 96 and copied directly over from Figure C.18 (Maslia et al. 2007).
- Updated Model-Simulated Head Contours were simulated in MODFLOW 2000 and exported from GMS software.
- A visual comparison suggests that the updated model is accurately representing the results from the ATSDR model.
- Historic water supply areas were estimated from Figure C.18.

ATSDR = Agency for Toxic Substances and Disease Registry
GMS = Groundwater Modeling System

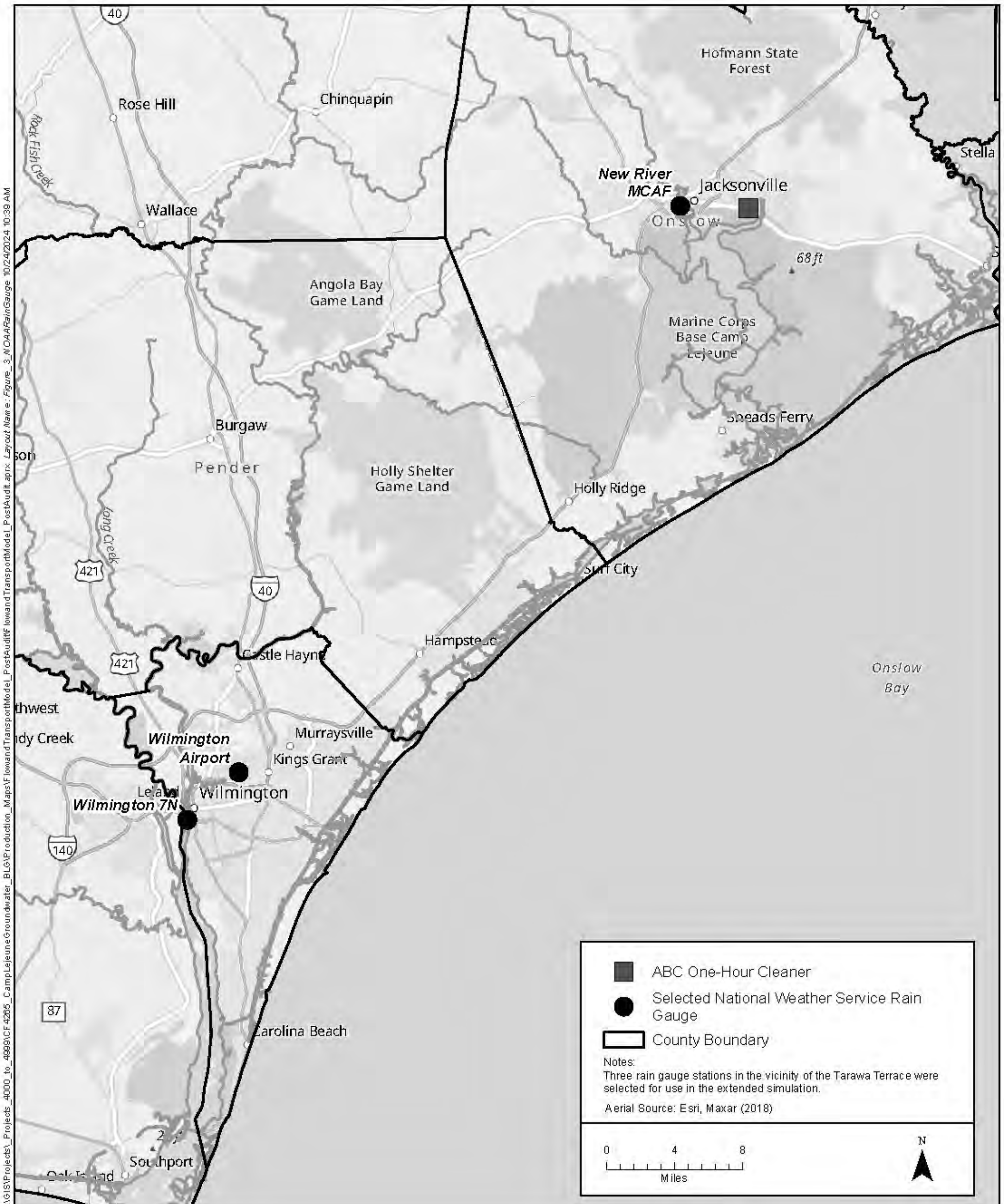
integral consulting inc.

Figure 1.
Comparison of Original Model-Simulated Head Contours to Updated Model-Simulated Head Contours
Tarawa Terrace Flow and Transport Model Post-Audit



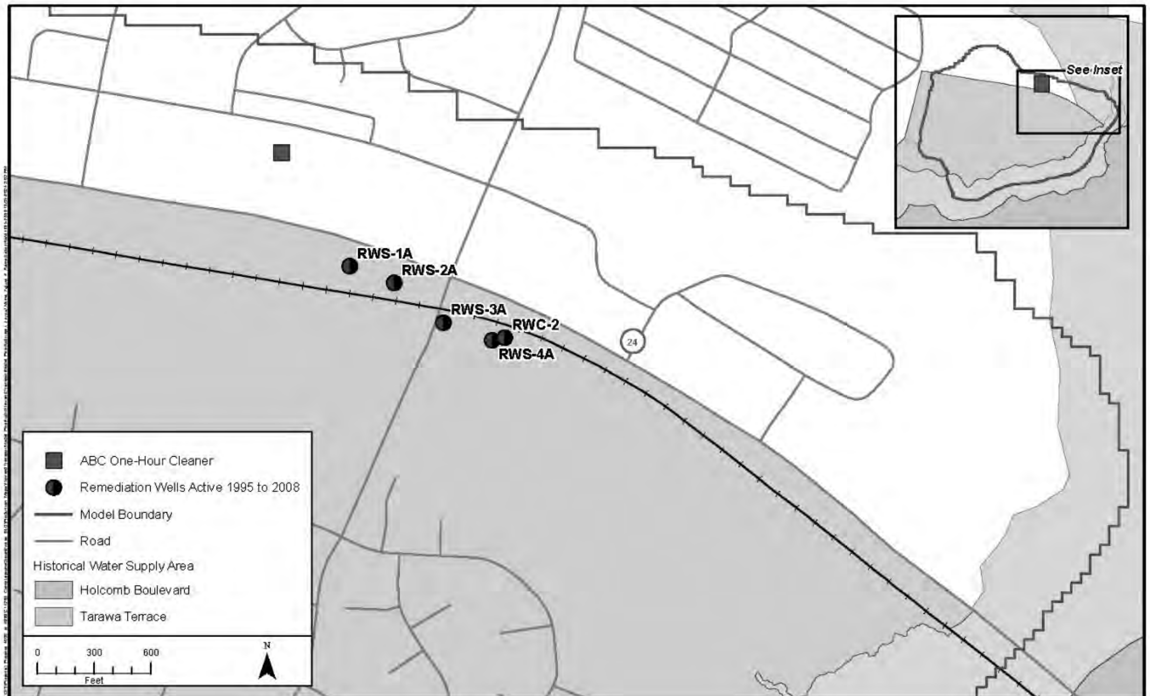
integral

Figure 2.
Comparison of Original Model-Simulated PCE Concentrations to Updated Model-Simulated PCE Concentrations
Tarawa Terrace Flow and Transport Model Post-Audit



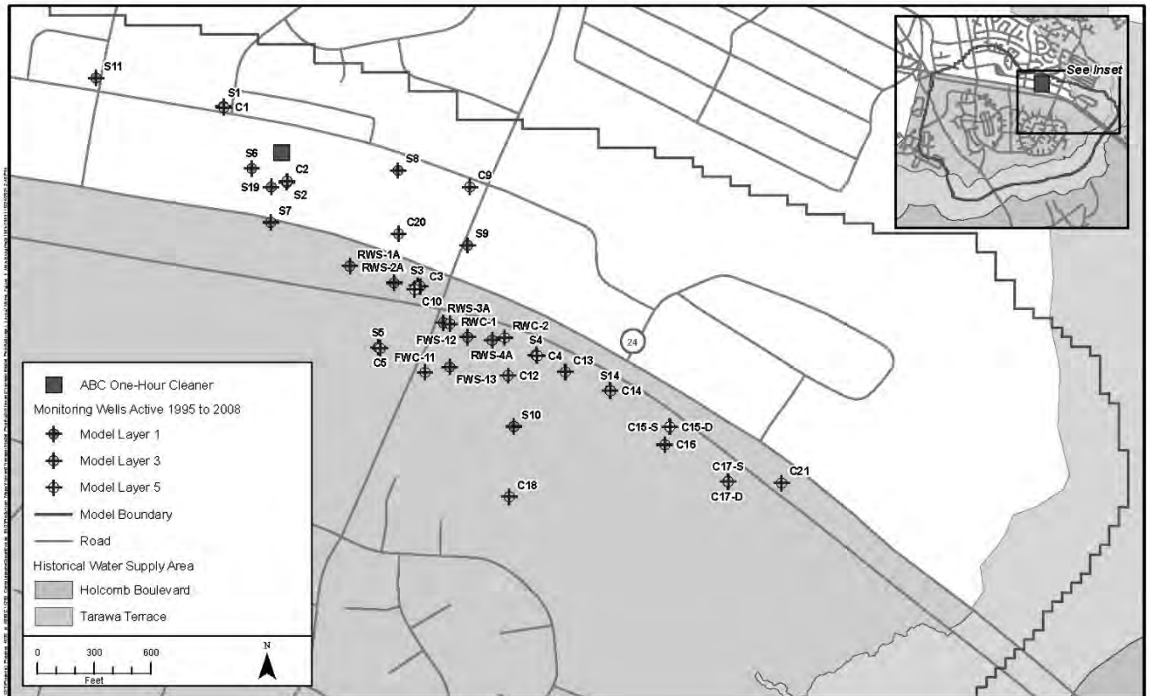
integral consulting inc.

Figure 3.
National Weather Service Rain Gauge Locations Selected for Extended Simulation
Tarawa Terrace Flow and Transport Model Post-Audit



integral consulting inc.

Figure 4.
Location of Remediation Wells Active During the 1995 to 2008 Period
Tarawa Terrace Flow and Transport Model Post-Audit



integral consulting inc.

Figure 5.
Location of Monitoring Wells Active During the 1995 to 2008 Period
Tarawa Terrace Flow and Transport Model Post-Audit

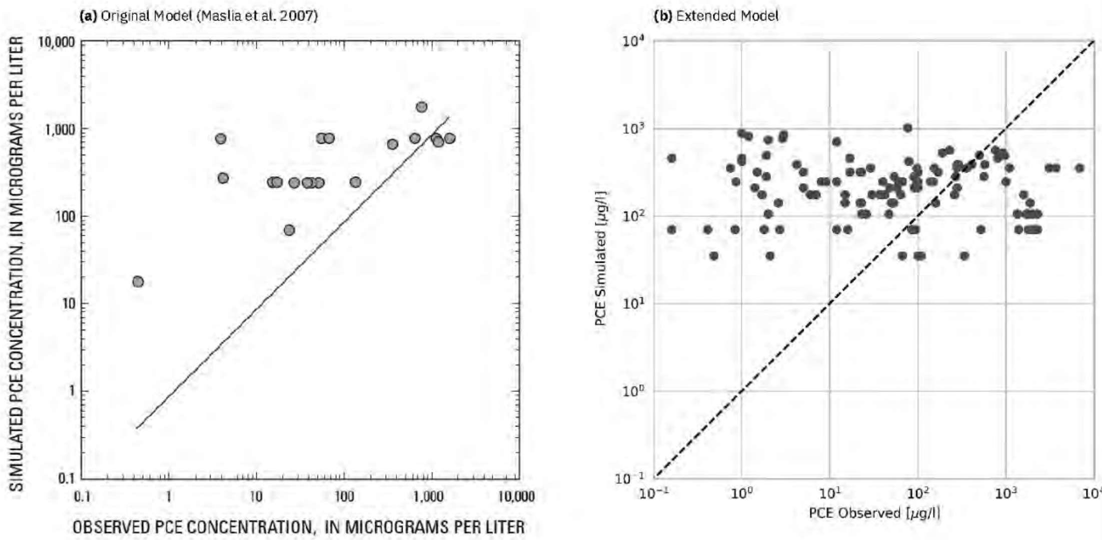
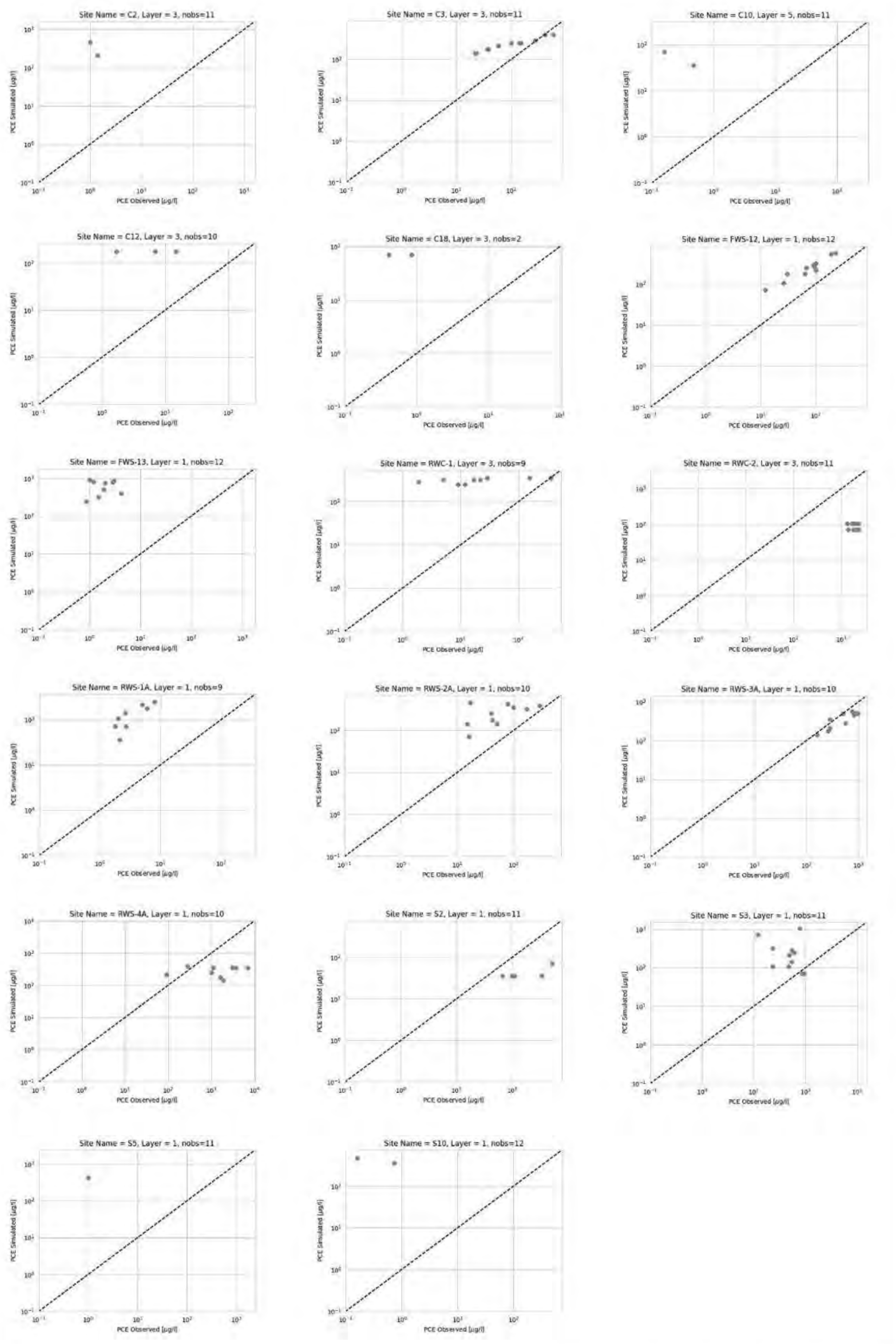
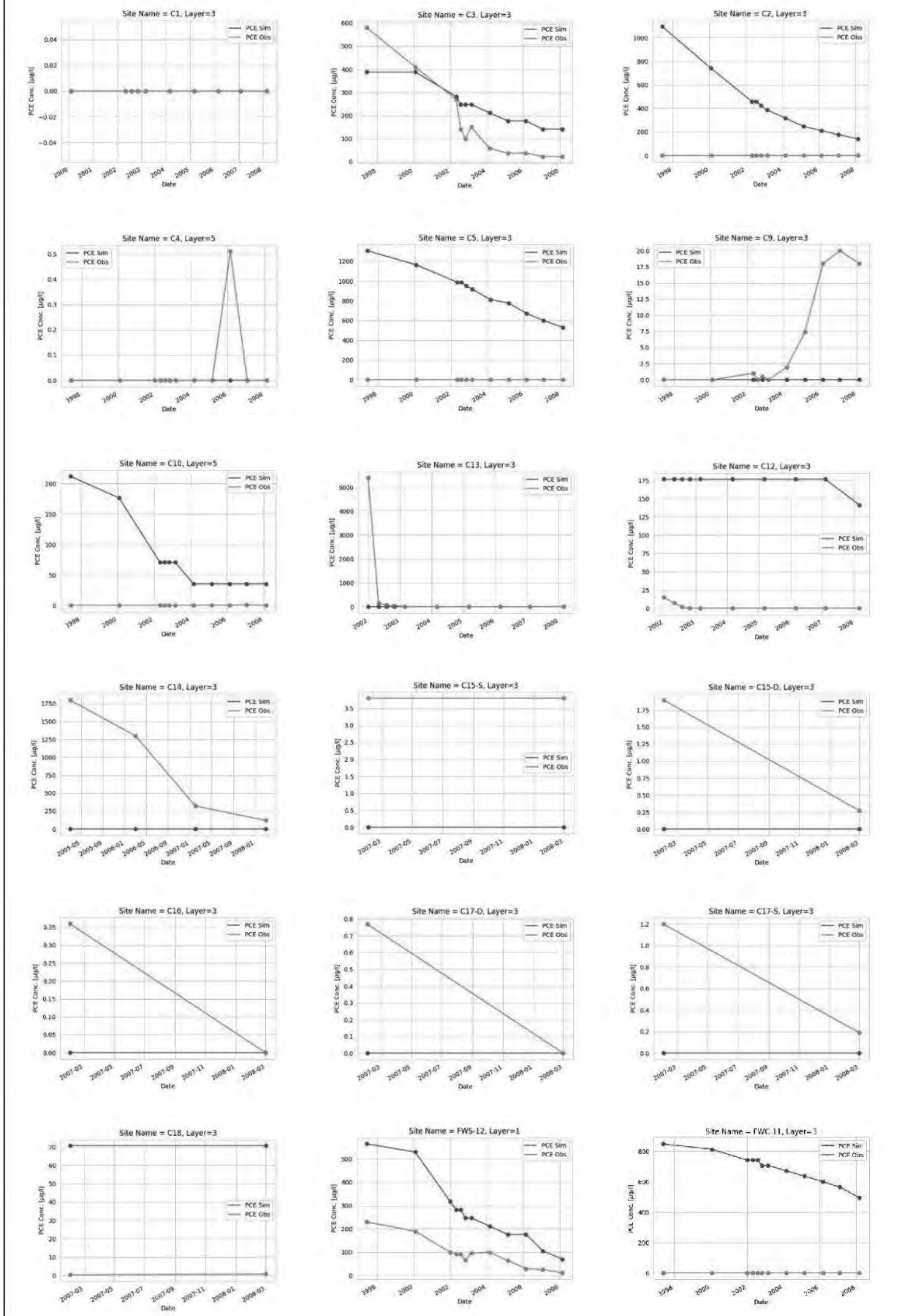


Figure 6.
Simulated vs. Observed PCE Concentrations from (a) Original Model and (b) Extended Model
Tarawa Terrace Flow and Transport Model Post-Audit



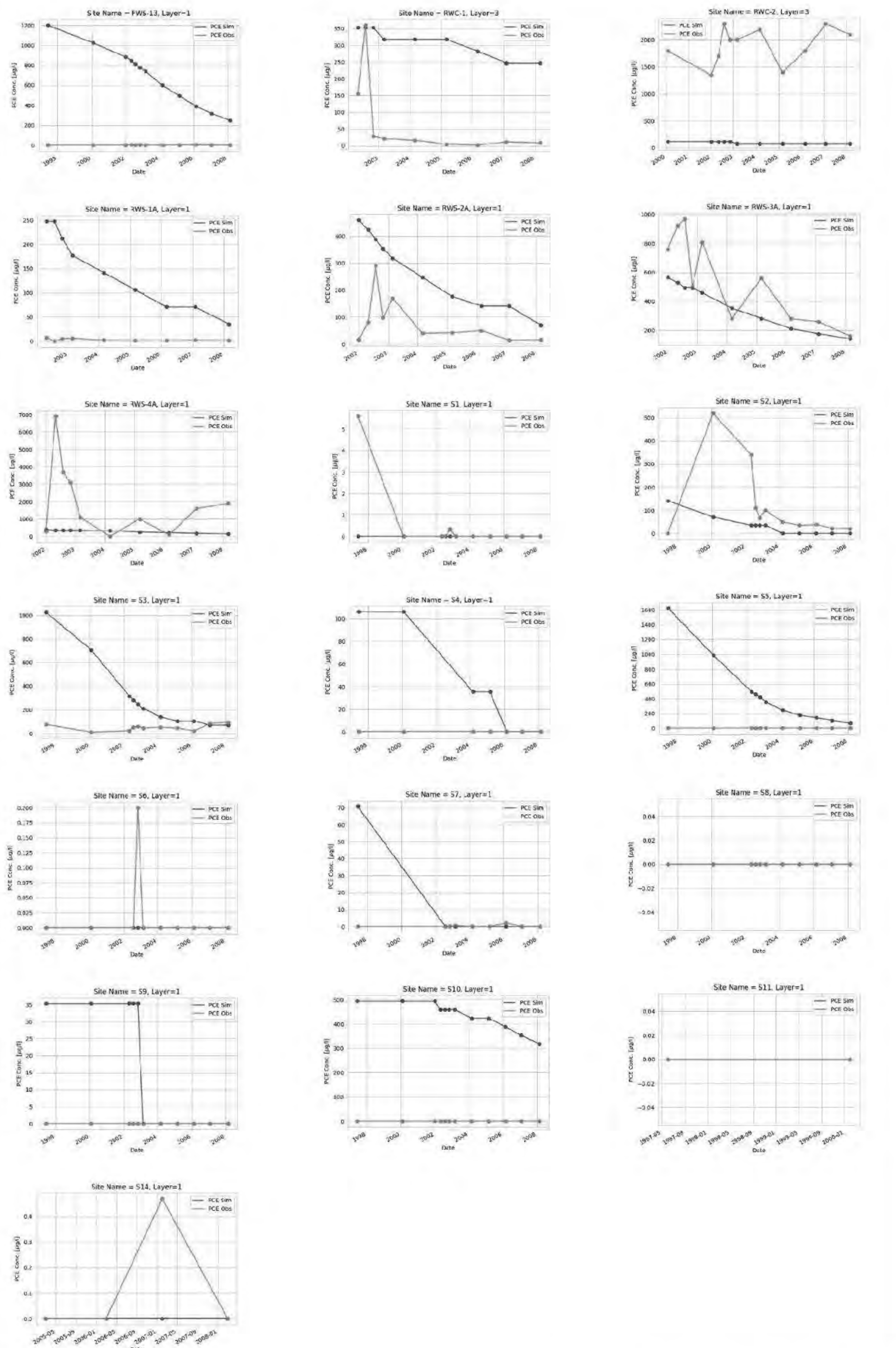
integral

Figure 7.
Simulated vs. Observed PCE Concentrations for Monitoring Well Locations
Tarawa Terrace Flow and Transport Model Post-Audit



integral

Figure 8a.
Time Series Plots of Simulated and Observed PCE Concentrations at Monitoring Well Locations
Tarawa Terrace Flow and Transport Model Post-Audit



integral

Figure 8b.
Time Series Plots of Simulated and Observed PCE Concentrations at Monitoring Well Locations
Tarawa Terrace Flow and Transport Model Post-Audit

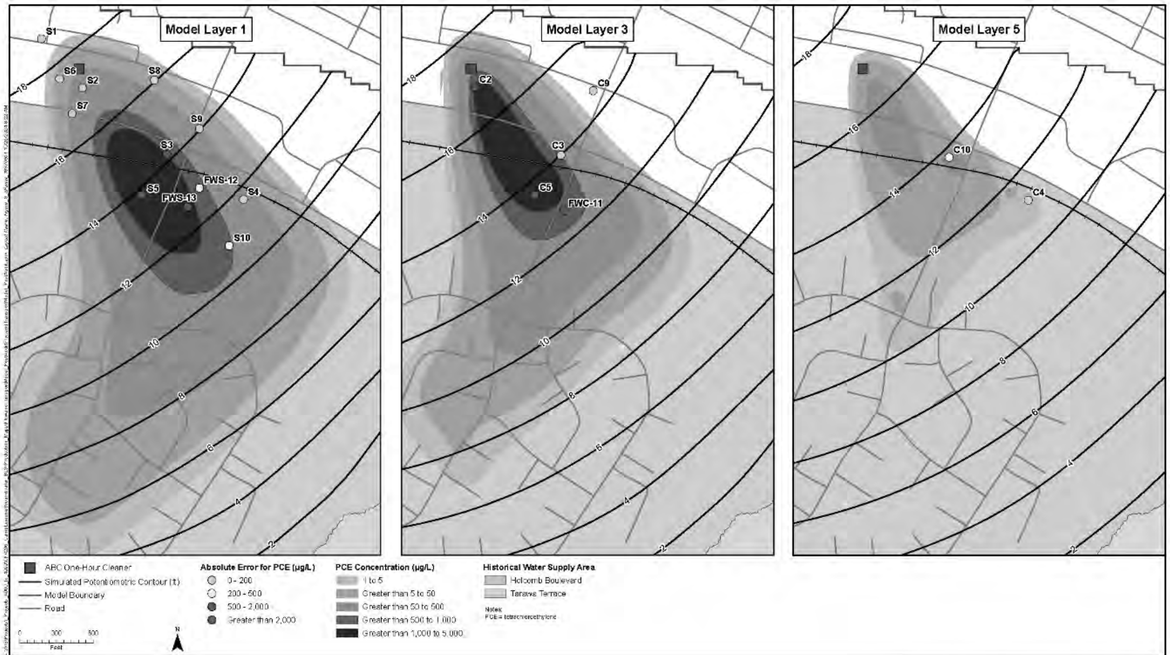


Figure 9.
Simulated PCE Concentration for Three Model Layers
Compared to Measured Values, June 1997
Tarawa Terrace Flow and Transport Model Post-Audit

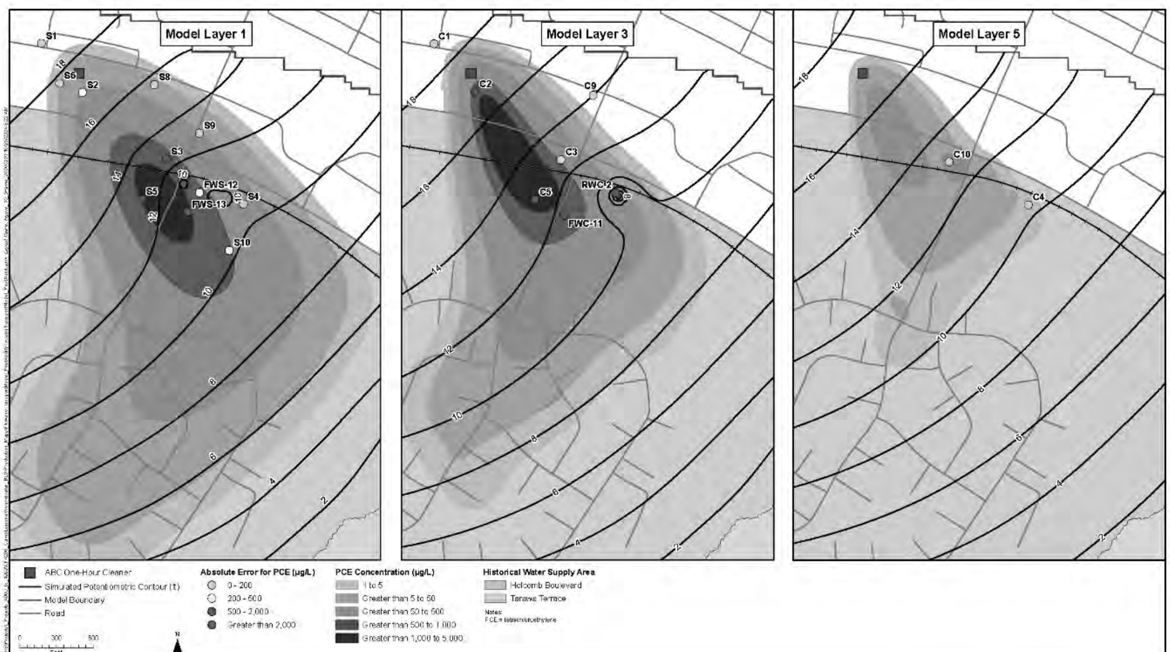


Figure 10.
Simulated PCE Concentration for Three Model Layers
Compared to Measured Values, February 2000
Tarawa Terrace Flow and Transport Model Post-Audit

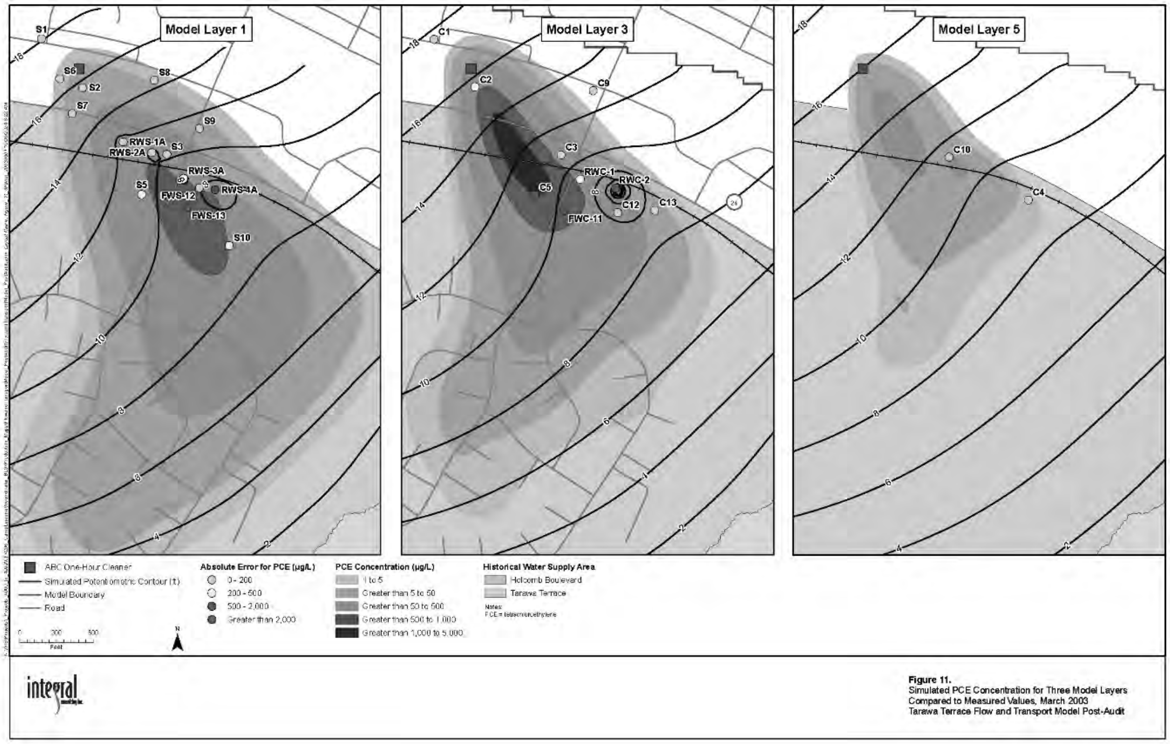


Figure 11.
Simulated PCE Concentration for Three Model Layers
Compared to Measured Values, March 2003
Tarawa Terrace Flow and Transport Model Post-Audit

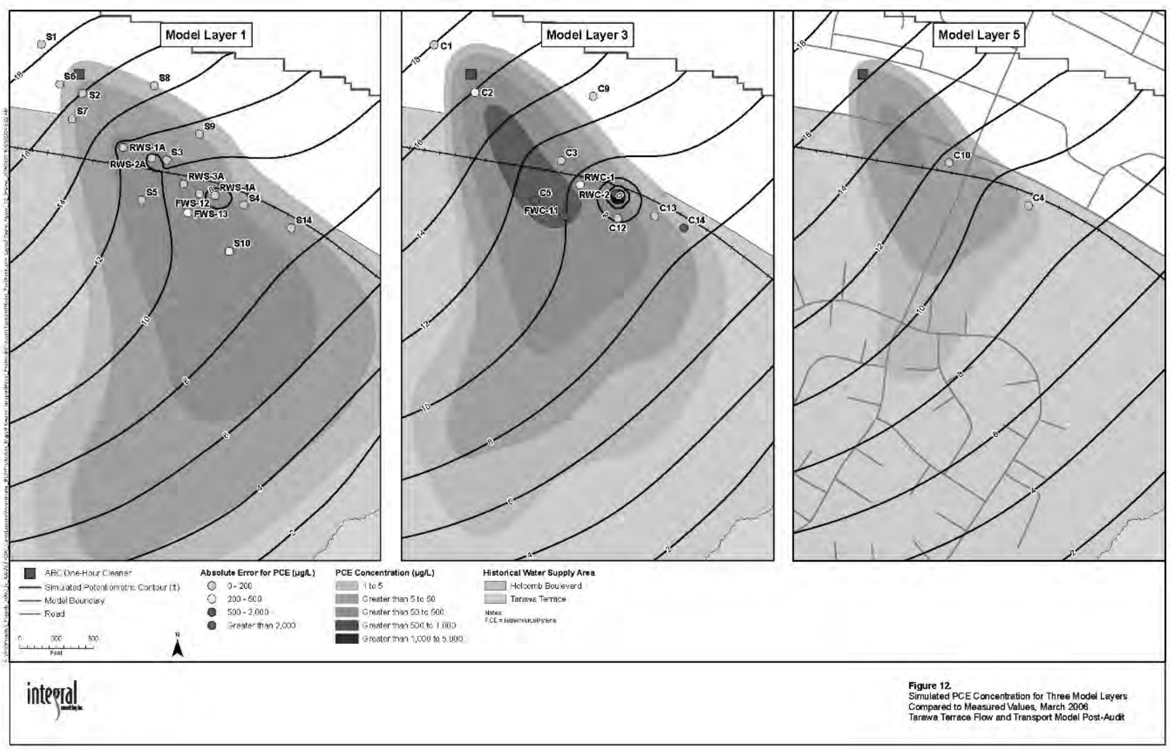


Figure 12.
Simulated PCE Concentration for Three Model Layers
Compared to Measured Values, March 2006
Tarawa Terrace Flow and Transport Model Post-Audit

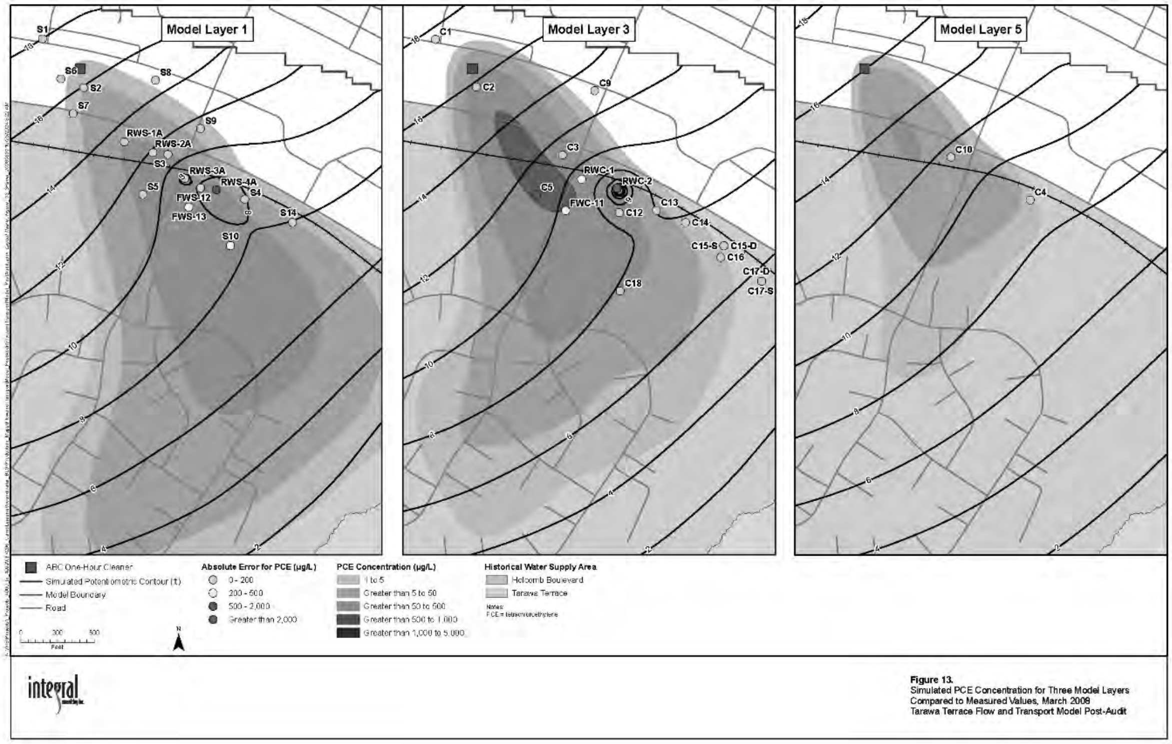
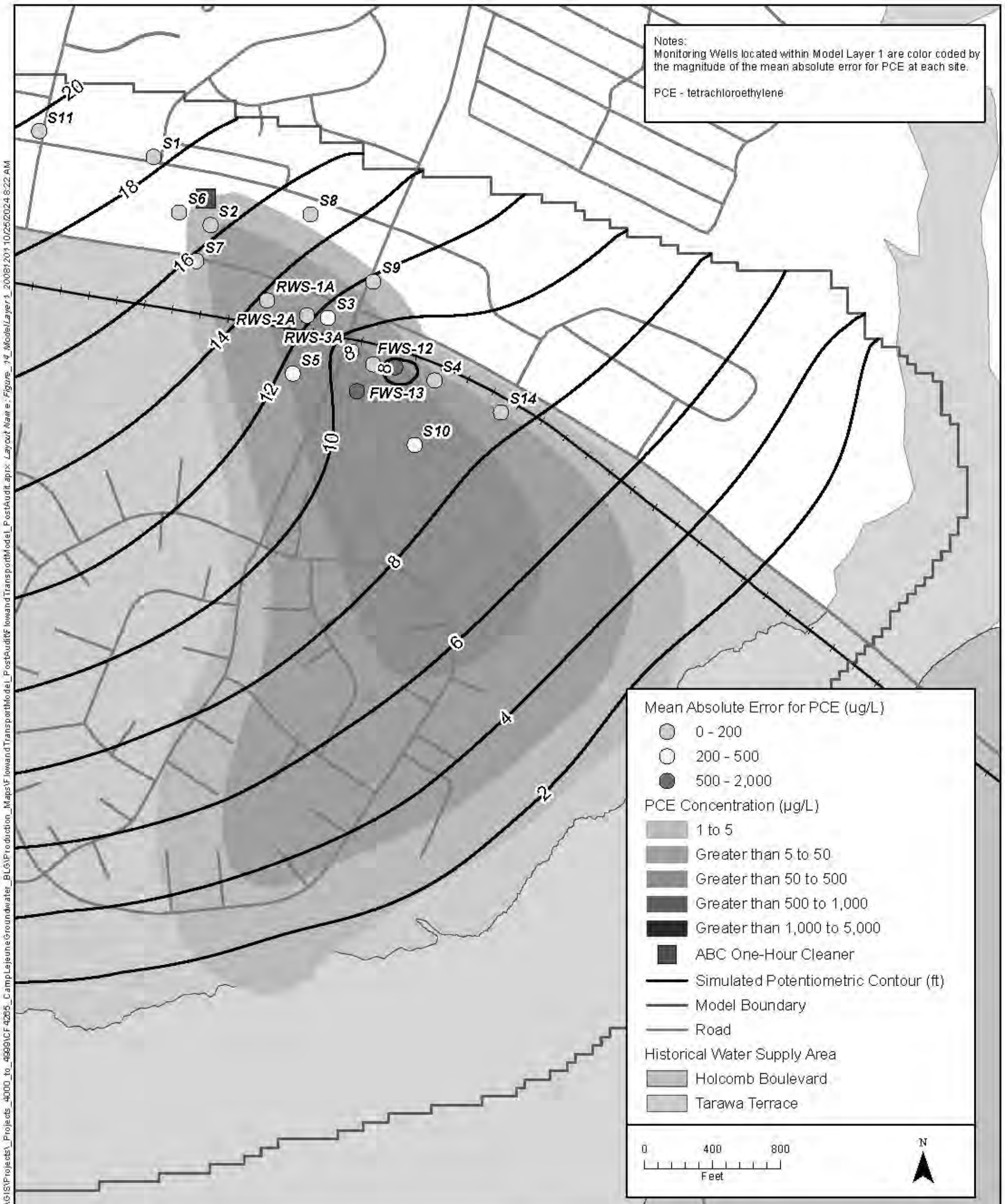


Figure 13.
Simulated PCE Concentration for Three Model Layers
Compared to Measured Values, March 2009
Tarawa Terrace Flow and Transport Model Post-Audit



integral consulting inc.

Figure 14.
Simulated PCE Plume for December 2008 for Model Layer 1
Tarawa Terrace Flow and Transport Model Post-Audit

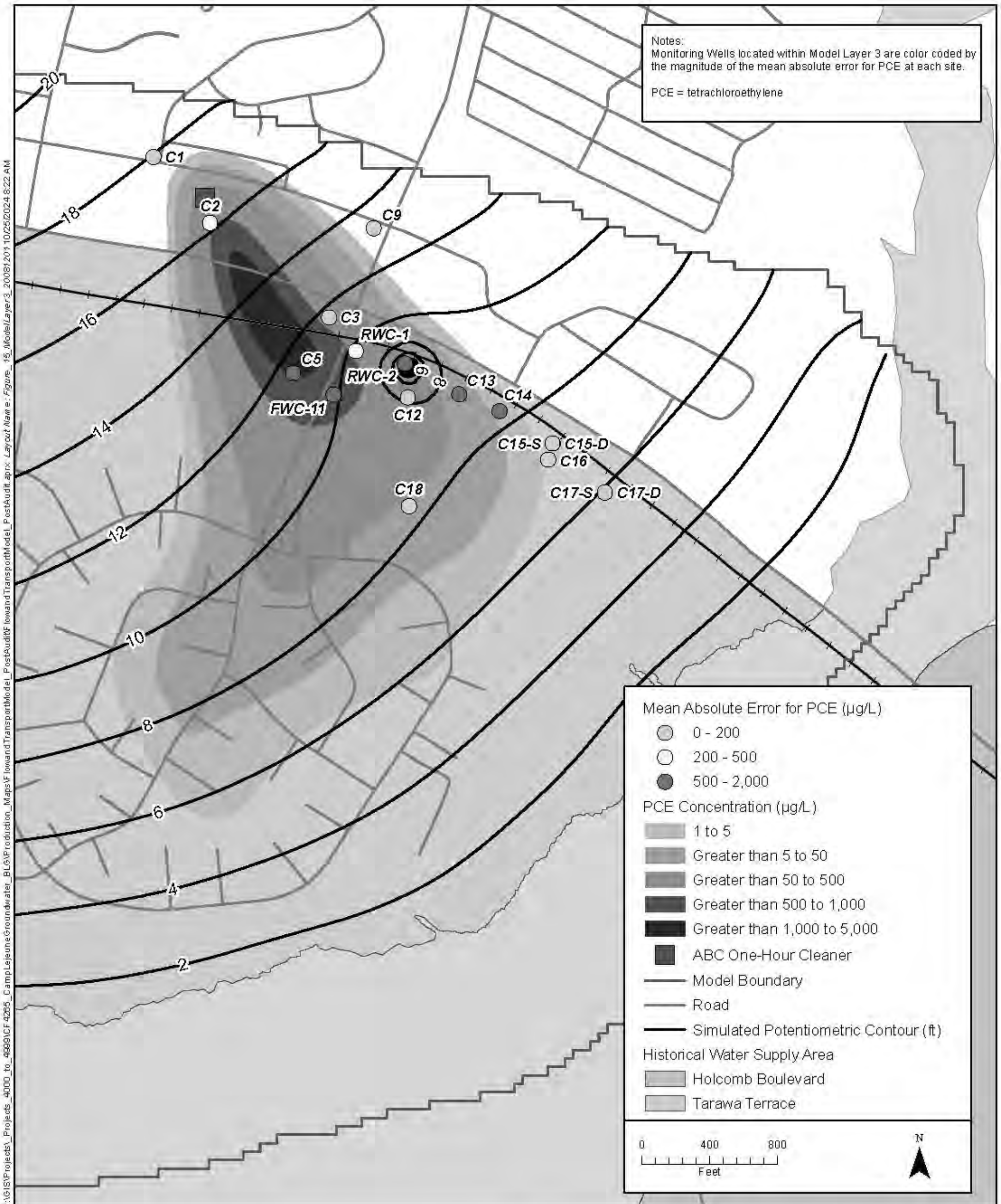


Figure 15.
Simulated PCE Plume for December 2008 for Model Layer 3
Tarawa Terrace Flow and Transport Model Post-Audit

integral consulting inc.

Figure 16.
Simulated PCE Plume for December 2008 for Model Layer 5
Tarawa Terrace Flow and Transport Model Post-Audit

Tables

Table 1. Annual Rainfall and Effective Recharge Rates

	Rainfall (in./yr)				Effective Recharge	
Year	Wilmington Airport	Wilmington 7N	New River MCAF	Average Rainfall	(in./yr)	(ft/day)
1995	65.1	64.4	48.6	59.3	13.94	0.00318
1996	64.4	52.7	75	64	15.04	0.00343
1997	49.6	51	53.6	51.4	12.07	0.00276
1998	64.2	77.2	70.1	70.5	16.55	0.00378
1999	72.1	82.1	63.2	72.5	17.02	0.00389
2000	53.8	59.2	50.4	54.5	12.79	0.00292
2001	38	57.4	43.5	46.3	10.87	0.00248
2002	49.3	56.9	49.4	51.9	12.18	0.00278
2003	63.6	72.8	50.5	62.3	14.64	0.00334
2004	50.7	71.7	51.7	58.1	13.63	0.00311
2005	69.3	68.4	59.2	65.6	15.41	0.00352
2006	63.8	62.7	62.5	63	14.8	0.00338
2007	33.4	37.3	60.4	43.7	10.26	0.00234
2008	60.8	48.4	56.4	55.2	12.96	0.00296
2009	59.7	59.4	53.6	57.6	13.53	0.00309

Notes:

Data publicly available at: https://www.weather.gov/wrh/Climate?wfo=ilm

Annual rainfall data were available for three locations proximal to the Tarawa Terrace: Wilmington Airport, Wilmington 7N, and New River MCAF.

Table 2. Pumping Rates for Remediation Wells Operating 1995 to 2008

Well	Northing	Easting	Model Layer	Pumping Rate (gpm)							
				11/1/1999	11/6/2001	3/7/2004	12/16/2004	3/31/2005	3/6/2006	2/20/2007	3/11/2008
RWS-1A	364445.7	2491125	1	5.5	18	20.8	12.1	20	20	0	0
RWS-2A	364351.5	2491359	1	3.8	18	3.5	2.34	28	24	0	0
RWS-3A	364146.8	2491620	1	29.2	24	18	1.07	15	30	30	30
RWS-4A	364053.7	2491878	1	13.3	24	24	22.5	28	25	30	25
RWC-2	364067.5	2491842	3	28.2	40	40	32.1	40	42	40	40

Notes:
Northing and easting values are given in NAD 1983 HARN North Carolina State Plane FIPS 3200 (US Feet)
gpm = gallons per minute

Table 3. Monitoring Wells Included in Extended Simulation

Monitoring Well	Northing	Easting	Model Layer	Well Completion Date	Borehole Depth (ft)	Finished Well Depth (ft)	Well Type
C1	365285.0	2490460.1	3	4/4/1992	104	100	Monitoring Well
C2	364895.7	2490794.3	3	4/8/1992	87	84.5	Monitoring Well
C3	364338.9	2491496.9	3	4/9/1992	90.5	89.4	Monitoring Well
C4	363971.9	2492116.1	5	4/3/1992	200	130	Monitoring Well
C5	364012.1	2491285.3	3	4/7/1992	92.5	90.5	Monitoring Well
C9	364864.6	2491760.5	3	9/10/1993	76.5	76	Monitoring Well
C10	364321.6	2491468.6	5	9/28/1993	80	0	Monitoring Well
C12	363867.4	2491961.7	3	11/6/2001	84	70	Monitoring Well
C13	363886.1	2492264.8	3	11/6/2001	83	76	Monitoring Well
C14	363787.1	2492503.0	3	5/12/2005	87	84.9	Monitoring Well
C15-D	363596.3	2492817.1	3	2/9/2007	110	110	Monitoring Well
C15-S	363596.3	2492816.1	3	2/9/2007	110	89	Monitoring Well
C16	363501.3	2492790.7	3	2/13/2007	95	94	Monitoring Well
C17-D	363306.6	2493125.4	3	2/13/2007	117	95	Monitoring Well
C17-S	363306.6	2493124.4	3	2/13/2007	117	85	Monitoring Well
C18	363226.0	2491968.6	3	2/15/2007	87	84	Monitoring Well
FWC-11	363884.0	2491523.5	3	--	89	88.6	--
FWS-12	364070.4	2491748.5	1	--	40	39.6	Monitoring Well
FWS-13	363912.7	2491653.1	1	--	38.5	38.2	Monitoring Well
RWC-1	364140.6	2491654.6	3	1/3-4/1998	91.5	--	Recovery Well
RWC-2	364067.5	2491944.6	3	1/5-6/1998	90	--	Recovery Well
RWS-1A	364445.7	2491125.4	1	--	55.5	55.5	Recovery Well
RWS-2A	364357.4	2491359.9	1	--	56	48.5	Recovery Well
RWS-3A	364146.8	2491620.4	1	--	60	55	Recovery Well
RWS-4A	364053.7	2491877.8	1	--	58.2	53	Recovery Well
S1	365289.2	2490457.3	1	3/22/1992	28	25.5	Monitor Well
S2	364889.0	2490792.7	1	3/26/1992	39.7	39.7	Monitor Well
S3	364343.6	2491482.1	1	4/2/1992	39.5	39.5	Monitor Well
S4	363976.4	2492109.4	1	4/3/1992	34	34	Monitor Well
S5	364016.2	2491275.9	1	4/1/1992	28	28	Monitor Well
S6	364962.4	2490607.3	1	3/26/1992	40.5	40.5	Monitor Well
S7	364677.4	2490707.9	1	4/5/1992	30.3	30.3	Monitor Well
S8	364951.7	2491380.5	1	4/4/1992	28	28	Monitor Well
S9	364555.9	2491748.8	1	3/21/1992	40	28.3	Monitor Well
S10	363597.3	2491992.8	1	3/20/1992	40	35	Monitor Well
S11	365440.7	2489784.3	1	9/11/1993	31	--	Monitor Well
S14	363788.1	2492499.8	1	5/10/2005	87	29	Monitor Well

Notes:

Northing and easting values are given in NAD 1983 HARN North Carolina State Plane FIPS 3200 (US Feet).

-- = information not available

[a] Estimated value

Table 4. Observed PCE Concentrations at Monitoring Wells, 1995 to 2008

Monitoring Well	Model Layer	PCE Concentration (µg/L)											
		6/1/1997	2/1/2000	1/1/2002	5/1/2002	8/1/2002	11/1/2002	3/1/2003	3/1/2004	3/1/2005	3/1/2006	2/1/2007	3/1/2008
C1	3	–	<DL	–	<DL	<DL	<DL	<DL	<DL	<DL	<DL	<DL	<DL
C2	3	<DL	<DL	–	1	<DL	<DL	<DL	<DL	<DL	1.4	<DL	<DL
C3	3	580	410	–	270	140	100	150	58	37	38	23	22
C4	5	<DL	<DL	<DL	<DL	<DL	<DL	<DL	<DL	<DL	0.51	<DL	<DL
C5	3	<DL	<DL	–	<DL	<DL	<DL	<DL	<DL	<DL	<DL	<DL	<DL
C9	3	<DL	<DL	–	1	<DL	0.48	<DL	1.9	7.4	18	20	18
C10	5	<DL	<DL	–	<DL	<DL	0.16	<DL	<DL	<DL	<DL	0.48	<DL
C12	3	–	–	15	7	1.7	<DL	<DL	<DL	<DL	<DL	<DL	<DL
C13	3	–	–	5,400	140	68	44	6	3	2.8	2.5	2.7	7.8
C14	3	–	–	–	–	–	–	–	–	1,800	1,300	320	120
C15-D	3	–	–	–	–	–	–	–	–	–	–	1.9	0.27
C15-S	3	–	–	–	–	–	–	–	–	–	–	3.8	3.8
C16	3	–	–	–	–	–	–	–	–	–	–	0.36	<DL
C17-D	3	–	–	–	–	–	–	–	–	–	–	0.77	<DL
C17-S	3	–	–	–	–	–	–	–	–	–	–	1.2	0.19
C18	3	–	–	–	–	–	–	–	–	–	–	0.41	0.84
FWC-11	3	<DL	<DL	<DL	<DL	<DL	<DL	<DL	<DL	<DL	<DL	<DL	<DL
FWS-12	1	230	190	100	92	90	67	96	100	64	30	26	12
FWS-13	1	<DL	<DL	1	3	1.2	2.9	2	<DL	1.9	4.2	1.5	0.86
RWC-1	3	–	–	–	155	360	29	22	17	5	1.9	12	9.1
RWC-2	3	–	1,800	1,350	1,700	2,300	2,000	2,000	2,200	1,400	1,800	2,300	2,100
RWS-1A	1	–	–		8	<DL	5	6	2.6	2	1.8	2.7	2.1
RWS-2A	1	–	–	17	79	290	98	170	40	42	50	15	16
RWS-3A	1	–	–	760	920	970	500	810	280	560	280	260	160
RWS-4A	1	–	–	280	6,900	3,700	3,100	1,100	<DL	1,000	92	1,600	1,900
S1	1	5.6	<DL	–	<DL	<DL	0.32	<DL	<DL	<DL	<DL	<DL	<DL
S2	1	0	520	–	340	110	67	100	50	35	38	22	20
S3	1	77	12	–	23	54	60	48	53	47	23	85	94
S4	1	<DL	<DL	–	–	–	–	–	<DL	<DL	<DL	<DL	<DL
S5	1	<DL	<DL	–	<DL	<DL	1	<DL	<DL	<DL	<DL	<DL	<DL
S6	1	<DL	<DL	–	–	<DL	0.2	<DL	<DL	<DL	<DL	<DL	<DL
S7	1	<DL	–	–	–	<DL	<DL	0.5	<DL	<DL	1.9	<DL	<DL
S8	1	<DL	<DL	–	<DL	<DL	<DL	<DL	<DL	<DL	<DL	<DL	<DL
S9	1	<DL	<DL	–	<DL	<DL	<DL	<DL	<DL	<DL	<DL	<DL	<DL

Table 4. Observed PCE Concentrations at Monitoring Wells, 1995 to 2008

Monitoring Well	Model Layer	PCE Concentration (µg/L)											
		6/1/1997	2/1/2000	1/1/2002	5/1/2002	8/1/2002	11/1/2002	3/1/2003	3/1/2004	3/1/2005	3/1/2006	2/1/2007	3/1/2008
S10	1	<DL	<DL	<DL	<DL	<DL	0.16	<DL	<DL	<DL	<DL	0.74	<DL
S11	1	<DL	<DL	--	--	--	--	--	--	--	--	--	--
S14	1	--	--	--	--	--	--	--	--	<DL	<DL	0.47	<DL

Notes:

-- = no sample collected

<DL = sample result reported below the detection limit

PCE = tetrachloroethene

Table 5. Observed and Simulated PCE Concentrations at Monitoring Well Locations

Date	Monitoring Well	PCE Observed Concentration (µg/L)	PCE Simulated Concentration (µg/L)	Error	Abs(Error)
2/1/2000	C1	<DL	<DL	0	0
5/1/2002		<DL	<DL	0	0
8/1/2002		<DL	<DL	0	0
11/1/2002		<DL	<DL	0	0
3/1/2003		<DL	<DL	0	0
3/1/2004		<DL	<DL	0	0
3/1/2005		<DL	<DL	0	0
3/1/2006		<DL	<DL	0	0
2/1/2007		<DL	<DL	0	0
3/1/2008		<DL	<DL	0	0
6/1/1997	C2	<DL	1095	1095	1095
2/1/2000		<DL	742	742	742
5/1/2002		1	459	458	458
8/1/2002		<DL	459	459	459
11/1/2002		<DL	424	424	424
3/1/2003		<DL	388	388	388
3/1/2004		<DL	318	318	318
3/1/2005		<DL	247	247	247
3/1/2006		1.4	212	210	210
2/1/2007		<DL	177	177	177
3/1/2008		<DL	141	141	141
6/1/1997	C3	580	388	-192	192
2/1/2000		410	388	-22	22
5/1/2002		270	283	13	13
8/1/2002		140	247	107	107
11/1/2002		100	247	147	147
3/1/2003		150	247	97	97
3/1/2004		58	212	154	154
3/1/2005		37	177	140	140
3/1/2006		38	177	139	139
2/1/2007		23	141	118	118
3/1/2008		22	141	119	119
6/1/1997	C4	<DL	<DL	0	0
2/1/2000		<DL	<DL	0	0
1/1/2002		<DL	<DL	0	0
5/1/2002		<DL	<DL	0	0
8/1/2002		<DL	<DL	0	0
11/1/2002		<DL	<DL	0	0
3/1/2003		<DL	<DL	0	0
3/1/2004		<DL	<DL	0	0
3/1/2005		<DL	<DL	0	0
3/1/2006		0.51	<DL	-1	1
2/1/2007		<DL	<DL	0	0
3/1/2008		<DL	<DL	0	0

Table 5. Observed and Simulated PCE Concentrations at Monitoring Well Locations

Date	Monitoring Well	PCE Observed Concentration (µg/L)	PCE Simulated Concentration (µg/L)	Error	Abs(Error)
6/1/1997	C5	<DL	1307	1307	1307
2/1/2000		<DL	1165	1165	1165
5/1/2002		<DL	989	989	989
8/1/2002		<DL	989	989	989
11/1/2002		<DL	953	953	953
3/1/2003		<DL	918	918	918
3/1/2004		<DL	812	812	812
3/1/2005		<DL	777	777	777
3/1/2006		<DL	671	671	671
2/1/2007		<DL	600	600	600
3/1/2008		<DL	530	530	530
6/1/1997	C9	<DL	<DL	0	0
2/1/2000		<DL	<DL	0	0
5/1/2002		1	<DL	-1	1
8/1/2002		<DL	<DL	0	0
11/1/2002		0.48	<DL	0	0
3/1/2003		<DL	<DL	0	0
3/1/2004		1.9	<DL	-2	2
3/1/2005		7.4	<DL	-7	7
3/1/2006		18	<DL	-18	18
2/1/2007		20	<DL	-20	20
3/1/2008		18	<DL	-18	18
6/1/1997	C10	<DL	212	212	212
2/1/2000		<DL	177	177	177
5/1/2002		<DL	71	71	71
8/1/2002		<DL	71	71	71
11/1/2002		0.16	71	70	70
3/1/2003		<DL	71	71	71
3/1/2004		<DL	35	35	35
3/1/2005		<DL	35	35	35
3/1/2006		<DL	35	35	35
2/1/2007		0.48	35	35	35
3/1/2008		<DL	35	35	35
1/1/2002	C12	15	177	162	162
5/1/2002		7	177	170	170
8/1/2002		1.7	177	175	175
11/1/2002		<DL	177	177	177
3/1/2003		<DL	177	177	177
3/1/2004		<DL	177	177	177
3/1/2005		<DL	177	177	177
3/1/2006		<DL	177	177	177
2/1/2007		<DL	177	177	177
3/1/2008		<DL	141	141	141

Table 5. Observed and Simulated PCE Concentrations at Monitoring Well Locations

Date	Monitoring Well	PCE Observed Concentration (µg/L)	PCE Simulated Concentration (µg/L)	Error	Abs(Error)
1/1/2002	C13	5400	<DL	-5400	5400
5/1/2002		140	<DL	-140	140
8/1/2002		68	<DL	-68	68
11/1/2002		44	<DL	-44	44
3/1/2003		6	<DL	-6	6
3/1/2004		3	<DL	-3	3
3/1/2005		2.8	<DL	-3	3
3/1/2006		2.5	<DL	-3	3
2/1/2007		2.7	<DL	-3	3
3/1/2008		7.8	<DL	-8	8
3/1/2005	C14	1800	<DL	-1800	1800
3/1/2006		1300	<DL	-1300	1300
2/1/2007		320	<DL	-320	320
3/1/2008		120	<DL	-120	120
2/1/2007	C15-D	1.9	<DL	-2	2
3/1/2008		0.27	<DL	0	0
2/1/2007	C15-S	3.8	<DL	-4	4
3/1/2008		3.8	<DL	-4	4
2/1/2007	C16	0.36	<DL	0	0
3/1/2008		<DL	<DL	0	0
2/1/2007	C17-D	0.77	<DL	-1	1
3/1/2008		<DL	<DL	0	0
2/1/2007	C17-S	1.2	<DL	-1	1
3/1/2008		0.19	<DL	0	0
2/1/2007	C18	0.41	71	70	70
3/1/2008		0.84	71	70	70
6/1/1997	FWC-11	<DL	848	848	848
2/1/2000		<DL	812	812	812
1/1/2002		<DL	742	742	742
5/1/2002		<DL	742	742	742
8/1/2002		<DL	742	742	742
11/1/2002		<DL	706	706	706
3/1/2003		<DL	706	706	706
3/1/2004		<DL	671	671	671
3/1/2005		<DL	636	636	636
3/1/2006		<DL	600	600	600
2/1/2007		<DL	565	565	565
3/1/2008		<DL	494	494	494

Table 5. Observed and Simulated PCE Concentrations at Monitoring Well Locations

Date	Monitoring Well	PCE Observed Concentration (µg/L)	PCE Simulated Concentration (µg/L)	Error	Abs(Error)
6/1/1997	FWS-12	230	565	335	335
2/1/2000		190	530	340	340
1/1/2002		100	318	218	218
5/1/2002		92	283	191	191
8/1/2002		90	283	193	193
11/1/2002		67	247	180	180
3/1/2003		96	247	151	151
3/1/2004		100	212	112	112
3/1/2005		64	177	113	113
3/1/2006		30	177	147	147
2/1/2007		26	106	80	80
3/1/2008		12	71	59	59
6/1/1997	FWS-13	<DL	1201	1201	1201
2/1/2000		<DL	1024	1024	1024
1/1/2002		1	883	882	882
5/1/2002		3	848	845	845
8/1/2002		1.2	812	811	811
11/1/2002		2.9	777	774	774
3/1/2003		2	742	740	740
3/1/2004		<DL	600	600	600
3/1/2005		1.9	494	493	493
3/1/2006		4.2	388	384	384
2/1/2007		1.5	318	316	316
3/1/2008		0.86	247	246	246
5/1/2002	RWC-1	155	353	198	198
8/1/2002		360	353	-7	7
11/1/2002		29	353	324	324
3/1/2003		22	318	296	296
3/1/2004		17	318	301	301
3/1/2005		5	318	313	313
3/1/2006		1.9	283	281	281
2/1/2007		12	247	235	235
3/1/2008		9.1	247	238	238
2/1/2000	RWC-2	1800	106	-1694	1694
1/1/2002		1350	106	-1244	1244
5/1/2002		1700	106	-1594	1594
8/1/2002		2300	106	-2194	2194
11/1/2002		2000	106	-1894	1894
3/1/2003		2000	71	-1929	1929
3/1/2004		2200	71	-2129	2129
3/1/2005		1400	71	-1329	1329
3/1/2006		1800	71	-1729	1729
2/1/2007		2300	71	-2229	2229
3/1/2008		2100	71	-2029	2029

Table 5. Observed and Simulated PCE Concentrations at Monitoring Well Locations

Date	Monitoring Well	PCE Observed Concentration (µg/L)	PCE Simulated Concentration (µg/L)	Error	Abs(Error)
5/1/2002	RWS-1A	8	247	239	239
8/1/2002		<DL	247	247	247
11/1/2002		5	212	207	207
3/1/2003		6	177	171	171
3/1/2004		2.6	141	139	139
3/1/2005		2	106	104	104
3/1/2006		1.8	71	69	69
2/1/2007		2.7	71	68	68
3/1/2008		2.1	35	33	33
5/1/2002	RWS-2A	79	424	345	345
1/1/2002		17	459	442	442
8/1/2002		290	388	98	98
11/1/2002		98	353	255	255
3/1/2003		170	318	148	148
3/1/2004		40	247	207	207
3/1/2005		42	177	135	135
3/1/2006		50	141	91	91
2/1/2007		15	141	126	126
3/1/2008		16	71	55	55
1/1/2002	RWS-3A	760	565	-195	195
5/1/2002		920	530	-390	390
8/1/2002		970	494	-476	476
11/1/2002		500	494	-6	6
3/1/2003		810	459	-351	351
3/1/2004		280	353	73	73
3/1/2005		560	283	-277	277
3/1/2006		280	212	-68	68
2/1/2007		260	177	-83	83
3/1/2008		160	141	-19	19
1/1/2002	RWS-4A	280	388	108	108
5/1/2002		6900	353	-6547	6547
8/1/2002		3700	353	-3347	3347
11/1/2002		3100	353	-2747	2747
3/1/2003		1100	353	-747	747
3/1/2004		<DL	318	318	318
3/1/2005		1000	247	-753	753
3/1/2006		92	212	120	120
2/1/2007		1600	177	-1423	1423
3/1/2008		1900	141	-1759	1759

Table 5. Observed and Simulated PCE Concentrations at Monitoring Well Locations

Date	Monitoring Well	PCE Observed Concentration (µg/L)	PCE Simulated Concentration (µg/L)	Error	Abs(Error)
6/1/1997	S1	5.6	<DL	-6	6
2/1/2000		<DL	<DL	0	0
5/1/2002		<DL	<DL	0	0
8/1/2002		<DL	<DL	0	0
11/1/2002		0.32	<DL	0	0
3/1/2003		<DL	<DL	0	0
3/1/2004		<DL	<DL	0	0
3/1/2005		<DL	<DL	0	0
3/1/2006		<DL	<DL	0	0
2/1/2007		<DL	<DL	0	0
3/1/2008		<DL	<DL	0	0
6/1/1997	S2	<DL	141	141	141
2/1/2000		520	71	-449	449
5/1/2002		340	35	-305	305
8/1/2002		110	35	-75	75
11/1/2002		67	35	-32	32
3/1/2003		100	35	-65	65
3/1/2004		50	<DL	-50	50
3/1/2005		35	<DL	-35	35
3/1/2006		38	<DL	-38	38
2/1/2007		22	<DL	-22	22
3/1/2008		20	<DL	-20	20
6/1/1997	S3	77	1024	947	947
2/1/2000		12	706	694	694
5/1/2002		23	318	295	295
8/1/2002		54	283	229	229
11/1/2002		60	247	187	187
3/1/2003		48	212	164	164
3/1/2004		53	141	88	88
3/1/2005		47	106	59	59
3/1/2006		23	106	83	83
2/1/2007		85	71	-14	14
3/1/2008		94	71	-23	23
6/1/1997	S4	<DL	106	106	106
2/1/2000		<DL	106	106	106
3/1/2004		<DL	35	35	35
3/1/2005		<DL	35	35	35
3/1/2006		<DL	<DL	0	0
2/1/2007		<DL	<DL	0	0
3/1/2008		<DL	<DL	0	0

Table 5. Observed and Simulated PCE Concentrations at Monitoring Well Locations

Date	Monitoring Well	PCE Observed Concentration (µg/L)	PCE Simulated Concentration (µg/L)	Error	Abs(Error)
6/1/1997	S5	<DL	1624	1624	1624
2/1/2000		<DL	989	989	989
5/1/2002		<DL	494	494	494
8/1/2002		<DL	459	459	459
11/1/2002		1	424	423	423
3/1/2003		<DL	353	353	353
3/1/2004		<DL	247	247	247
3/1/2005		<DL	177	177	177
3/1/2006		<DL	141	141	141
2/1/2007		<DL	106	106	106
3/1/2008		<DL	71	71	71
6/1/1997	S6	<DL	<DL	0	0
2/1/2000		<DL	<DL	0	0
8/1/2002		<DL	<DL	0	0
11/1/2002		0.2	<DL	0	0
3/1/2003		<DL	<DL	0	0
3/1/2004		<DL	<DL	0	0
3/1/2005		<DL	<DL	0	0
3/1/2006		<DL	<DL	0	0
2/1/2007		<DL	<DL	0	0
3/1/2008		<DL	<DL	0	0
6/1/1997	S7	<DL	71	71	71
8/1/2002		<DL	<DL	0	0
11/1/2002		<DL	<DL	0	0
3/1/2003		0.5	<DL	-1	1
3/1/2004		<DL	<DL	0	0
3/1/2005		<DL	<DL	0	0
3/1/2006		1.9	<DL	-2	2
2/1/2007		<DL	<DL	0	0
3/1/2008		<DL	<DL	0	0
6/1/1997	S8	<DL	<DL	0	0
2/1/2000		<DL	<DL	0	0
5/1/2002		<DL	<DL	0	0
8/1/2002		<DL	<DL	0	0
11/1/2002		<DL	<DL	0	0
3/1/2003		<DL	<DL	0	0
3/1/2004		<DL	<DL	0	0
3/1/2005		<DL	<DL	0	0
3/1/2006		<DL	<DL	0	0
2/1/2007		<DL	<DL	0	0
3/1/2008		<DL	<DL	0	0

Table 5. Observed and Simulated PCE Concentrations at Monitoring Well Locations

Date	Monitoring Well	PCE Observed Concentration (µg/L)	PCE Simulated Concentration (µg/L)	Error	Abs(Error)
6/1/1997	S9	<DL	35	35	35
2/1/2000		<DL	35	35	35
5/1/2002		<DL	35	35	35
8/1/2002		<DL	35	35	35
11/1/2002		<DL	35	35	35
3/1/2003		<DL	<DL	0	0
3/1/2004		<DL	<DL	0	0
3/1/2005		<DL	<DL	0	0
3/1/2006		<DL	<DL	0	0
2/1/2007		<DL	<DL	0	0
3/1/2008		<DL	<DL	0	0
6/1/1997	S10	<DL	494	494	494
2/1/2000		<DL	494	494	494
1/1/2002		<DL	494	494	494
5/1/2002		<DL	459	459	459
8/1/2002		<DL	459	459	459
11/1/2002		0.16	459	459	459
3/1/2003		<DL	459	459	459
3/1/2004		<DL	424	424	424
3/1/2005		<DL	424	424	424
3/1/2006		<DL	388	388	388
2/1/2007		0.74	353	352	352
3/1/2008		<DL	318	318	318
6/1/1997	S11	<DL	<DL	0	0
2/1/2000		<DL	<DL	0	0
3/1/2005	S14	<DL	<DL	0	0
3/1/2006		<DL	<DL	0	0
2/1/2007		0.47	<DL	0	0
3/1/2008		<DL	<DL	0	0

Notes:

<DL = sample result reported below the detection limit

PCE = tetrachloroethene

Table 6. Mean Error and Mean Absolute Error for Monitoring Wells

Monitoring Well	Model Layer	Mean Error	Mean Absolute Error	Mean Absolute Error Category
C1	3	0	0	0-200
C2	3	423.6	423.6	200-500
C3	3	74.6	113.3	0-200
C4	5	0	0	0-200
C5	3	882.9	882.9	500-2,000
C9	3	-6.1	6.1	0-200
C10	5	77	77	0-200
C12	3	170.7	170.7	0-200
C13	3	-567.7	567.7	500-2,000
C14	3	-885	885	500-2,000
C15-D	3	-1.1	1.1	0-200
C15-S	3	-3.8	3.8	0-200
C16	3	-0.2	0.2	0-200
C17-D	3	-0.4	0.4	0-200
C17-S	3	-0.7	0.7	0-200
C18	3	70	70	0-200
FWC-11	3	688.6	688.6	500-2,000
FWS-12	1	176.4	176.4	0-200
FWS-13	1	693	693	500-2,000
RWC-1	3	242.1	243.6	200-500
RWC-2	3	-1817.9	1817.9	500-2,000
RWS-1A	1	141.8	141.8	0-200
RWS-2A	1	190.2	190.2	0-200
RWS-3A	1	-179.2	193.8	0-200
RWS-4A	1	-1677.6	1786.9	500-2,000
S1	1	-0.5	0.5	0-200
S2	1	-86.3	111.9	0-200
S3	1	246.2	253.1	200-500
S4	1	40.4	40.4	0-200
S5	1	462.2	462.2	200-500
S6	1	0	0	0-200
S7	1	7.6	8.1	0-200
S8	1	0	0	0-200
S9	1	16.1	16.1	0-200
S10	1	435.5	435.5	200-500
S11	1	0	0	0-200
S14	1	-0.1	0.1	0-200

Notes:

Northing and easting values are given in NAD 1983 HARN North Carolina State Plane FIPS 3200 (US Feet).

Exhibit 1

Resume for R. Jeffrey Davis

Education & Credentials

M.S., Civil & Environmental Engineering, Brigham Young University, Provo, Utah, 1998

B.S., Civil & Environmental Engineering, Brigham Young University, Provo, Utah, 1993

Professional Engineer, Utah (License No. 189690-2202), Texas (License No. 125406), Florida (License No. 74838), Colorado (License No. 0051575), Alabama (License No. PE52096), Idaho (License No. P-21839), Oregon (License No. 104270PE)

Certified Groundwater Professional, NGWA (2023)

Continuing Education

Certificate of Specialization in Leadership and Management, Harvard Business School Online (2023)

MSHA certified (2020)

First Aid and CPR certified (2020)

Professional Affiliations

National Ground Water Association

Utah Groundwater Association

Groundwater Resources Association of California

R. Jeffrey Davis, P.E., CGWP

Principal, Water Resources

(385) 955-5184

Salt Lake City, UT

jdavis@integral-corp.com

Mr. Jeff Davis is a licensed civil and environmental engineer, hydrogeologist, and certified groundwater professional with almost 30 years of global experience working on every continent except Antarctica. He currently serves on the Board of Directors for the National Ground Water Association. Mr. Davis has supported numerous litigation cases involving groundwater impacts and has experience as an expert witness. He has spent much of his career solving complicated water problems involving mining, oil and gas, and water resources. These projects include the clean water supply side as well as the remediation of contaminated sites. The contaminated sites include coal combustion residual (CCR) landfills and other waste impoundments, mining remediation sites, and industrial cleanup sites—both RCRA and CERCLA sites. In working with per- and polyfluoroalkyl substance (PFAS) compounds, MTBE, chlorinated solvents, hydrocarbons, nitrates, and road salt, he has developed and used numerous groundwater models for the mining, energy, chemical, and agricultural industries. Other projects have involved environmental impact statements, environmental assessments, water management, groundwater–surface water contamination, dewatering, and water supply and treatment. He has extensive knowledge of groundwater flow-and-transport principles and has taught numerous workshops and classes in the U.S. and around the world. His current focus is on water and groundwater sustainability and drought resiliency. Mr. Davis has extensive experience in the design and implementation of aquifer storage and recovery (ASR) projects across the country.

Relevant Experience

WATER MANAGEMENT

ASR Feasibility, Utah County, Utah — Served as principal investigator for a feasibility study for an ASR project. During the spring runoff of 2023, the team measured the runoff in several rivers, creeks, and ditches, and constructed a new infiltration basin, all in an effort to advance aquifer storage projects within the county.

ASR Feasibility, Utah County, Utah — Served as principal for a feasibility study for an ASR project. Former agricultural water rights were converted for industrial use and the effluent was being considered for aquifer replenishment. Both infiltration and direct injection of the treated water were considered as part of the feasibility study.

Provo ASR, Provo, Utah — Served as the project manager and engineer of record for the current Provo ASR project. Five sites (three infiltration and two direct injection) are currently permitted

integral

for pilot studies that have been ongoing since 2020. Final engineering design and permitting have been completed for all five sites.

Water Reuse and Aquifer Sustainability, Eagle Mountain, Utah — Served as the client manager and engineer of record for the current Eagle Mountain City, Utah, water-reuse planning and aquifer sustainability project. Water rights for Eagle Mountain were evaluated along with the groundwater system to understand aquifer sustainability for the city, which is expecting tremendous future growth, including large industrial water demands.

ASR Evaluation, Weber County, Utah — Served as the project manager and engineer of record for the current evaluation of the Weber Basin Water Conservancy District, Utah, ASR project. This project has been actively operating for more than 10 years. Hired to evaluate the storage capacity of the program and obtain greater recovery volumes from the system, working with the Utah Division of Water Rights.

Drainage Reuse Initiative, Harris County, Texas — Served as part of a team for the development of the Drainage Reuse Initiative for Harris County Flood Control District in Harris County, Texas. The project investigated the feasibility of alternative methods of flood mitigation by conveying stormwater to the subsurface, including natural infiltration to groundwater, enhanced infiltration or injection into aquifers, and mechanical injection to deep aquifers.

Roseville ASR, Roseville, California — Served as one of the groundwater leads for the development of an ASR program for the city of Roseville, California. Initial efforts involved developing a regional- scale conceptualization for the major portion of the Central Valley area. Developed a subsequent regional multilayer groundwater model, followed by a number of local-scale transport models to simulate pilot tests and understand the ASR process.

COAL COMBUSTION FACILITIES

Coal Combustion Residual Waste and Disposal, Bonanza, Utah — Served as the engineer of record for a coal power plant. Oversaw all efforts related to the monitoring and compliance of the facility's CCR waste and disposal. This included semiannual reporting, development of alternative source demonstrations, and annual groundwater monitoring reports.

Hexavalent Chromium Investigation, United States — Served as the principal investigator for a study to understand and evaluate the proposed EPA changes to hexavalent chromium (Cr(VI)) as it would apply to the monitoring and management of CCR landfill facilities. The work included examining potential regulatory levels from a human health perspective.

Alternate Water Sources Investigation, United States — Served as the principal investigator for a study to understand and evaluate differences at CCR facilities between upgradient and downgradient sources, and locate potential evidence of alternate sources using isotopes and microbial fingerprinting. After development of a sampling and analysis plan, advanced statistical and multivariate methods were used to document analyses that show potential for distinguishing source water from alternate sources.

OIL AND GAS WASTE MANAGEMENT

Oil and Gas Waste Facility, De Beque, Colorado — Served as the principal engineer for the permitting and operating of an 800-acre oil-and-gas waste-disposal facility southeast of De Beque, Colorado. Involved in several aspects of the permitting process, including the hydrogeological study and groundwater investigations; stormwater design; pond liner design and construction; closure certification; and submittal of the revised engineering design and operation plan.

Remedial Investigation, Billings, Montana — Served as the groundwater lead for the Yale Oil of South Dakota Facility in Billings, Montana. The Superfund site facility is in the remedial investigation phase; the risk-assessment work plan has been submitted to the Montana Department of Environmental Quality, and the client is waiting for comments before proceeding with the risk assessment.

EPA Study, Washington, DC — Served as participant and technical reviewer for EPA's "Study of Hydraulic Fracturing for Oil and Gas and Its Potential Impact on Drinking Water Resources." Participated in technical roundtables and technical workshops and completed a peer review of the EPA's five retrospective case studies.

Fate and Transport Modeling, Texas — Served as groundwater lead for fate-and-transport modeling and analysis of chloride contamination in southern Texas near the Gulf of Mexico. As part of the site mitigation phase, modeling was used to determine the potential migration of the chloride through the shallow aquifer system and nearby receptors.

Lockwood Solvent Groundwater Plume Site, Billings, Montana — Served as one of the groundwater leads performing groundwater modeling for the Lockwood Solvent Groundwater Plume site, an EPA Superfund site in Billings, Montana. The site spans 580 acres, and much of the groundwater there is contaminated with volatile organic compounds, including tetrachloroethene, trichloroethene, cis-1,2- dichloroethene, and vinyl chloride.

PLANNING AND PERMITTING

Beverage Can Manufacturing and Filling, Salt Lake City, Utah — Served as principal investigator for wastewater, stormwater, and Utah Pollutant Discharge Elimination System permitting, monitoring, and compliance for an aluminum can manufacturing and filling facility. Worked closely with the client, its operations team, and state and municipal regulators to regularly monitor and report all discharges from the facility.

Ely Energy Center EIS, White Pine County, Nevada — Served as principal lead for the development of a regional groundwater model for Steptoe Valley in White Pine County, Nevada. The investigation and model were part of the EIS for construction of the Ely Energy Center.

Haile Gold Mine EIS, Kershaw, South Carolina — Served as groundwater lead as the third-party contractor developing an EIS for the proposed Haile Gold Mine near Kershaw, South Carolina. The EIS analyzed the potential direct, indirect, and cumulative environmental effects of the proposed project and its alternatives. Work included project-team coordination for geology, groundwater, and surface water resources areas; review of applicant-supplied information; agency coordination; and public involvement.

Four Corners Power Plant EIS, Farmington, New Mexico — Served as groundwater lead as the third- party contractor in developing an EIS for the Four Corners Power Plant and Navajo coal mine in Farmington, New Mexico. The EIS analyzed the potential direct, indirect, and cumulative environmental effects of the proposed project and its alternatives. The groundwater portion included analyzing field investigations, pump tests, conceptual and numerical modeling of the project and surrounding area, and remediation and reclamation activities.

Iron Ore Operations Cumulative Impact Assessment, Pilbara, Western Australia — Served as one of the groundwater leads for a cumulative impact assessment for a proposed expansion of iron ore operations in the Pilbara in Western Australia. Work included identifying the methodology and developing the conceptual models to perform the assessment. The groundwater modeling included both quantitative and qualitative approaches.

LITIGATION SUPPORT

Expert Witness for PFAS Litigation, Martin County, Florida — Served as the groundwater expert witness for a litigation case in Martin County. The multidistrict litigation bellwether case involved PFAS contamination of groundwater affecting public drinking water. Opinions were given regarding PFAS sourcing, and fate and transport in groundwater, and regarding public water supply planning.

Water Resources Litigation, Grand County, Colorado — Served as principal investigator for a litigation case involving flooding damages caused by a canal breach. Surface water modeling was used to determine amount and extent of erosion and sedimentation from the flooding.

Water Resources Litigation, Northwest Minnesota — Served as principal investigator and expert witness for a litigation case involving agricultural water rights and pumping near tribal lands. Developed a conceptual model to understand the hydrogeological conditions and constructed a groundwater model to determine possible impacts due to the agriculture activities.

Groundwater Litigation, Ventura County, California — Served as the groundwater expert for a litigation case in Ventura County. The case includes the development of a basin-wide groundwater- surface water model, not only for purposes of litigation but also for compliance with Sustainable Groundwater Management Act requirements. The groundwater basin in question is currently listed as a priority basin by the State of California.

Pipeline Spill Litigation, Williston, North Dakota — Provided litigation services for groundwater and surface water contamination from a pipeline spill in North Dakota. A large spill of produced water (brine) impacted surface streams as well as the shallow aquifer system. Work included groundwater modeling, field investigations, and remedial strategies.

Road Salt Contamination Litigation, Vandalia, Ohio — Performed fate-and-transport modeling and analysis of sodium chloride contamination of an aquifer in Vandalia, Ohio. Stored road salt caused limited contamination of a shallow aquifer that supplied drinking water to nearby residential homes. The groundwater model included the local domestic pumping wells, which helped determine the possible extent of chloride impacts. Largely due to the conceptual site model and transport modeling results, litigation was settled out of court to the satisfaction of the client.

GROUNDWATER MODELING

Subsidence Monitoring/Modeling, Fort Bend and Harris Counties, Texas — Served as the groundwater lead and engineer on several groundwater development projects in Fort Bend and Harris counties. Groundwater withdrawals are strictly curtailed due to historical subsidence. The Subsidence Districts have installed GPS Port-A-Measure (PAM) units and used InSAR mapping. Using this data plus the output from the models PRESS and MODFLOW-SUB to measure subsidence impacts.

Groundwater Model Development, New Jersey — Led a team of hydrogeologists to construct a groundwater flow and fate and transport model of perfluorononanoic acid and other contaminants. The model will be used to design a pump and treat system and possible aquifer replenishment with the treated groundwater.

Hydrogeological Services, Montgomery County, Texas — Provided modeling and hydrogeological consulting services for the Lone Star Ground-water Conservation District's (Montgomery County, Texas) update of its desired future conditions and groundwater management plans. Also provided litigation services for the district.

Groundwater Model Development, Havana, Florida — Provided consulting services for Northwest Florida Water Management District as it updated its regional groundwater model—an integrated groundwater-surface water model that provides regulatory control of the groundwater withdrawals and manages saltwater intrusion in the Floridan aquifer due to pumping.

Crop Production Services, Various Locations, U.S. — Served as the groundwater lead to provide modeling and hydrogeological consulting services for a number of crop production services legacy sites. The groundwater at the sites was contaminated with nitrates from long-term fertilizer use. Groundwater modeling was used to determine the fate and transport of the nitrates and to develop a remedial strategy for cleanup.

Legacy Way Tunnel Design, Brisbane, Australia — Provided senior oversight and technical review for all hydrogeologic assessments related to the Legacy Way tunnel design project, a 4.6 km underground tunnel in northern Brisbane, Australia. Work included evaluating field tests, preparing geotechnical and environmental reports, and modeling the entire project area.

Mercury Fate and Transport, Cincinnati, Ohio — Served as the groundwater lead for performing fate and-transport modeling and analysis of a mercury spill at a municipal landfill in Cincinnati, Ohio. As part of the project management phase, modeling was used to determine the potential migration of mercury through the landfill to the leachate collection system. Modeling efforts examined both the spatial distribution and the temporal component of the mercury transport.

Due Diligence Environmental Review, Pascagoula, Mississippi — Served as the environmental lead for performing an environmental assessment at a chemical plant in Pascagoula, Mississippi, as part of a due diligence effort. A number of groundwater and surface water contamination issues due to spills, leaks, and storage of hazardous materials were addressed. The location of the plant on the Gulf of Mexico makes possible environmental impacts from operation of the chemical plant a sensitive issue.

MINING

Bingham Canyon Mine Closure Planning, Copperton, Utah — Completed an independent third-party audit for a closure-plan pit-lake study for Bingham Canyon Mine. Reviewed the consultant scope of work for the pit-lake study and discussed the study, methodology, and pathway to completion with consultant staff. An independent audit report was compiled and submitted to the client.

Hooker Prairie Mine, Bartow, Florida — Served as the model expert to develop a contaminant and water budget and management model for the Hookers Prairie Mine in Florida using the GoldSim modeling software. The purpose of the model was to evaluate the probabilities of the mine meeting its current and future nutrient NPDES loading limits for certain contaminants. The project also included an evaluation of current monitoring data within the mine operations and at discharge locations, and the development of a complete monitoring plan integrated into a GIS as part of the model calibration and validation.

Bridger Coal Mine Investigation, Rock Springs, Wyoming — Served on a technical team to reevaluate groundwater conditions, and treatment and discharge alternatives at the Bridger coal mine in southwest Wyoming. Previous studies' predicted maximum flows into the mine had been exceeded. Reassessed the situation and provided solutions.

EMERGENCY RESPONSE

Emergency Response to Battery Fire, Confidential Location — Served as the principal in charge leading a team of multidisciplinary scientists, engineers, toxicologists, and risk assessors for an environmental emergency response at a large-scale battery power storage unit at a solar farm. A thermal incident where several cargo container boxes caught fire and burned required immediate action to assess the environmental and human health impacts.

ECOLOGICAL RESTORATION

Ecological Restoration, Northeast Idaho — Serves as the principal in charge leading a team of scientists, engineers, and ecologists for an ecological restoration effort in northeast Idaho. The project has involved restoring flow to a creek and working with a number of state and federal agencies to develop and implement a conceptual restoration plan and a mitigation and monitoring plan. The project will also include obtaining the necessary permits and overseeing the restoration in an area of critical habitat.

PROJECT MANAGEMENT

GMS Software Development, Utah — Served as chief engineer for the original development of the software Groundwater Modeling System (GMS) at the Environmental Modeling Research Laboratory at Brigham Young University. A sophisticated graphical environment for groundwater model pre- and post-processing, 3-dimensional site characterization, and geostatistics, GMS is the official groundwater application of the U.S. Department of Defense and is also used by the U.S. Department of Energy, EPA, and thousands of users across the world.

NATURAL RESOURCE DAMAGE ASSESSMENT

Natural Resources Damage Assessment, Southeastern Idaho — Served as the groundwater expert determining groundwater damages in southeastern Idaho due to decades of phosphate mining. Led a team of hydrogeologists evaluating the impacts of selenium and other contaminants and changes in natural groundwater flows across the entire region. The damage assessment included a number of mining areas as well as the facilities where the phosphate material was processed.

Presentations / Posters

Davis, R.J. 2023. Challenges limiting managed aquifer recharge (MAR) adoption in the West. National Ground Water Association Groundwater Summit. December 5–7. Las Vegas, NV.

Davis, R.J. 2023. Water, AI, and us: What does the future hold for solving Utah's water challenges. Hint: It can't be solved without you and me. Salt Lake County Watershed Symposium. November 15–16. Salt Lake City, UT.

Davis, R.J. 2023. Building climate resilience through sustainable remediation in the western region. Groundwater Resources Association of California Western Groundwater Congress. September 12–14. Burbank, CA.

Davis, R.J. 2023. Water in Utah: Navigating the present and shaping the future. American Groundwater Trust. August 14–15. Provo, Utah.

Davis, R.J. 2023. More managed aquifer recharge and saving the Great Salt Lake—A balancing act. Idaho Water Users Association. June 12–13. Sun Valley, ID.

Davis, R.J. 2023. More managed aquifer recharge: Deliberate resiliency to combat droughts and climate change in the West. Association for Environmental Health of Soils. March 20–23. San Diego, CA.

Davis, R.J. 2023. Resilient and sustainable remediation. ESG|Climate Resilient & Sustainable Remediation Symposium. Groundwater Resources Association of California Western Groundwater Congress. February 6–7. San Diego, CA.

Davis, R.J. 2022. More managed aquifer recharge: Solutions to combat droughts and climate change in the West. National Ground Water Association Groundwater Summit. December 6–8. Las Vegas, NV.

Davis, R.J. 2022. Saving our aquifers: Climate change and managed aquifer recharge. Salt Lake County Watershed Symposium. November 16–17. Salt Lake City, UT.

Davis, R.J. 2022. More managed aquifer recharge—A solution to combat droughts and climate change in the West. Groundwater Resources Association of California Western Groundwater Congress. September 21–23. Sacramento, CA.

Davis, R.J. 2022. Saving our aquifers—Climate change, sustainability, and managed aquifer recharge. International Water Holdings. August 24–25. Salt Lake City, UT.

Davis, R.J. 2022. More managed aquifer recharge (MMAR) a solution to combat droughts and climate change in the West. Groundwater Protection Council Annual Forum. June 21–23. Salt Lake City, UT.

Davis, R.J. 2022. Aquifer storage and recovery—Hydrogeologic considerations. American Water Resources Association. May 17. Salt Lake City, UT.

Davis, R.J. 2022. Utah hydrology—What you do and don't know about Utah hydrogeology. National Ground Water Association. May 4, 2022. Virtual.

Davis, R.J. and B. Lemon. 2022. Provo, Utah: From planning to pilot to a final aquifer storage and recovery (ASR) program. Utah Water Users Workshop. March 21–23. St. George, UT.

Davis, R.J. 2021. Provo, Utah, from planning to pilot to a final managed aquifer recharge (MAR) program. National Ground Water Association Groundwater Summit. December 7–8. Virtual.

Davis, R.J. 2021. Provo City aquifer storage and recovery project. Ground Water Protection Council Annual Forum, September 27–29. Virtual.

Davis, R.J. 2021. Provo, Utah, from planning to pilot to a final managed aquifer recharge (MAR) program. American Public Works Association Utah Section Annual Conference. September 21–22. Sandy, UT.

Davis, R.J. 2021. Provo City aquifer storage and recovery project. Utah Water Users Workshop. May 17–19. St. George, UT.

Davis, R.J. 2021. Provo, Utah: From planning to pilot to a final managed aquifer recharge (MAR) program. ASR for Texas, Virtual Webinar. May 4–5.

Davis, R.J. 2021. Provo aquifer storage and recovery—From planning to pilot. American Water Works Association Virtual Summit on Sustainable Water, PFAS, Waterborne Pathogens. February 10–11.

Davis, R.J. 2020. Update on Provo's aquifer storage and recovery program. American Water Works Association Virtual Intermountain Section Annual Conference. October 21–23. Sun Valley, ID.

Davis, R.J. 2020. Are you prepared for the new federal permit process for CCR facilities? Second Annual Coal Ash and Combustion Residual Management Webinar, October 7–8. Virtual.

Invited Participant, Expert Panels, and Workshops

Bulk Water Innovation Partnership (BWIP): More managed aquifer recharge: Deliberate resiliency to combat droughts and climate change in the West. December 6, 2023. Virtual.

Rocky Mountain Association of Environmental Professionals (RMAEP): Great Salt Lake of Utah: watershed, legislative, and community issues surrounding it. September 20, 2023.

Salt Lake Chamber: Utah Water Outlook. April 13, 2022.

EDCUtah Webinar: Water: Constraints and Opportunities for Development in Utah panel. June 11, 2021.

ULI Utah: Trends Conference—Water: Constraints and Opportunities for Development in Utah panel. October 27, 2021.

Exhibit 2

Resume for Norman L. Jones

Norman L. Jones, Ph.D.
Professor
Department of Civil & Construction Engineering
Brigham Young University

Education

Ph.D.	Civil Engineering, University of Texas at Austin, 1990
M.S.	Civil Engineering, University of Texas at Austin, 1988
B.S.	Civil Engineering, Brigham Young University, 1986

Academic Experience

Department Chair, Civil & Construction Engineering, Brigham Young University (BYU), 2018-2024
Professor, Civil & Construction Engineering, BYU, 2002–present
Associate Professor, Civil & Environmental Engineering, BYU, 1997–2002
Assistant Professor, Civil & Environmental Engineering, BYU, 1991–1996

Current Membership in Professional Organizations

American Society of Civil Engineers (ASCE)
American Water Resources Association (AWRA)
National Ground Water Association (NGWA)
American Geophysical Union (AGU)

Professional Committees

AWRA 2014 GIS in Water Resources Technical Program Chair
NGWA Groundwater Modeling Interest Group Committee
American Society of Civil Engineers
EWRI Groundwater Management Committee
EWRI Emerging Technologies Committee
International Editorial Board for the Journal of HydroInformatics
Editor of AQU Amundi Journal
Great Salt Lake Basin Integrated Plan - Groundwater Technical Advisory Team
Tethys Geoscience Foundation - Board Member

Selected Honors and Awards

2001 Walter L. Huber Civil Engineering Research Prize
2002 College of Engineering & Technology Special Commendation Award
2003 Brigham Young University Technology Transfer Award
2007 Utah Engineering Educator of the Year – ACEC
2012 Brigham Young University Karl G. Maeser Research and Creative Arts Award
2016 AWRA Educator of the Year – Utah Section
2021 NGWA John Hem Award for Science and Engineering
2023 Brigham Young University Sponsored Research Award

University Courses Taught

CE En 101 - Introduction to Civil and Environmental Engineering
CE En 201 - Infrastructure
CE En 270 – Computer Methods in Civil Engineering
CE En 341 – Elementary Soil Mechanics
CE En 540 – Geo-Environmental Engineering
CE EN 544 - Seepage and Slope Stability Analysis
CCE 547 – Ground Water Modeling

CE En 641 – Advanced Soil Mechanics

Software

Led the development of the Groundwater Modeling System (GMS) software. GMS is a state-of-the-art three-dimensional environment for ground water model construction and visualization. It includes tools for site characterization including geostatistics and solid modeling of soil stratigraphy. GMS is the most comprehensive and sophisticated groundwater modeling software available and is used by over 10,000 organizations in over 100 countries. Currently managed and distributed by Aquaveo, LLC, a company I co-founded in 2007.

External Research Grants

1. Automated Mesh Generation For the TABS-2 System, $19,000, 2/90 - 11/90, U.S. Army Engineer Waterways Experiment Station
2. A Geometry Pre-Processor for HEC-1 Employing Triangulated Irregular Networks, $20,048, 3/91 - 10/91, U.S. Army Engineer Waterways Experiment Station
3. Real-Time Visualization for the TABS-2 Modelling System, $14,123, 4/91 - 8/91, U.S. Army Engineer Waterways Experiment Station
4. An Investigation of X-Windows Interface Tools, $49,556, 1/92 - 8/92, U.S. Army Engineer Waterways Experiment Station
5. Descriptive Geometry and Solid Rendering, $24,000, 1/92 - 10/92, U.S. Army Engineer Waterways Experiment Station
6. An Investigation of Automated Pre-processing Schemes for TIN-Based Drainage Analysis, $34,750, 4/92-10/92, U.S. Army Engineer Waterways Experiment Station
7. A Comprehensive Graphical User Environment for Groundwater Flow and Transport Modeling, $246,526, 6/93-9/94, U.S. Army Engineer Waterways Experiment Station
8. An Integrated Surface Flow Modeling System, $131,848, 1/94-1/95, U.S. Army Engineer Waterways Experiment Station
9. Productivity and Management Tools for Groundwater Flow and Transport Modeling, $207,404, 5/94-4/95, U.S. Army Engineer Waterways Experiment Station
10. Enhanced Tools for Quality Control in Automated Groundwater Transport Modeling, $246,553, 1/95-12/95, U.S. Army Engineer Waterways Experiment Station
11. Visualization for Two-Dimensional Surface Runoff Modeling, $98,221, 1/95-10/95, U.S. Army Engineer Waterways Experiment Station
12. Visualization Tools for Two-Dimensional Finite Element Hydrologic Modeling, $93,933, 11/95-10/96, U.S. Army Engineer Waterways Experiment Station
13. A Graphical Environment for Multi-Dimensional Surface Water Modeling, $49,789, 3/96-9/96, U.S. Army Engineer Waterways Experiment Station
14. A Conceptual Modeling Approach to Pre-processing of Groundwater Models, $475,743, 11/95-11/97, U.S. Army Engineer Waterways Experiment Station
15. Hydrosystems Modeling, $2,458,083, 5/97-4/02, U.S. Army Engineer Waterways Experiment Station
16. Second Generation Hydroinformatics Research, $4,958,127. U.S. Army Engineer Research and Development Center.
17. Flux Calculations and 3D Visualization for the SCAPS Piezocone and GeoViz System, $34,931, U.S. Navy.
18. Development of modeling methods and tools for predicting coupled reactive transport processes in porous media under multiple scales. $949,000. US Dept. of Energy. 1/07-12/09.
19. CI-WATER: Cyberinfrastructure to Advance High Performance Water Resource Modeling, $3,435,873. National Science Foundation - EPSCoR. 9/11-8/14.

20. Comprehensive Streamflow Prediction and Visualization to Support Integrated Water Managment, $599,823. NASA SERVIR, 8/16-8/19.
21. Daniel P. Ames, E. James Nelson, Norman L. Jones, An AmeriGEOSS Cloud-based Platform for Rapid Deployment of GEOGLOWS Water and Food Security Decision Support Apps, $540,658, NASA GEO, 1/2018-12/2020
22. Geospatial Information Tools That Use Machine-Learning to Enable Sustainable Groundwater Management in West Africa, $657,232. NASA SERVIR, 11/19-11/22.
23. Advancing the NASA GEOGloWS Toolbox for Regional Water Resources Management and Decision Support. $1.2M. NASA GEOGLOWS. 2022-2025. Dan Ames, Jim Nelson, Gus Williams, Norm Jones.
24. CIROH: National Cyberinfrastructure Framework for Engaging the Hydrologic Community (NCF). $1,822,418. National Oceanographic and Atmospheric Administration. 2022-2025. Dan Ames, Jim Nelson, Gus Williams, Norm Jones.
25. CIROH: Advancing Science to Better Characterize Drought and Groundwater-Driven Low-Flow Conditions in NOAA and USGS National-Scale Models. $801,221. 2023-2025. Norm Jones, Gus Williams, T. Prabhakar Clement, Donna Rizzo.
26. Improved Hydrologic Prediction Services for Resilience with GEOGLOWS, $1,889,627, National Oceanic and Atmospheric Administration (NOAA), 4/1/2024-3/31/2027. Norm Jones, Jim Nelson, Andrew South.

Summary: PI or Co-PI on 26 projects totaling $22,026,639.

Peer-Reviewed Publications in the Past 10 Years

1. Jones, N., Nelson, J., Swain, N., Christensen, S., Tarboton, D. Dash, P. Tethys: A Software Framework for Web-Based Modeling and Decision Support Applications. In: Ames, D.P., Quinn, N.W.T., Rizzoli, A.E. (Eds.), Proceedings of the 7th International Congress on Environmental Modelling and Software, June 15-19, San Diego, California, USA. ISBN: 978-88-9035-744-2
2. Jones, N., Griffiths, T., Lemon, A., Kudlas, S. Automated Well Permitting in Virginia's Coastal Plain Using SEAWAT and GIS Geoprocessing Tools. In: Ames, D.P., Quinn, N.W.T., Rizzoli, A.E. (Eds.), Proceedings of the 7th International Congress on Environmental Modelling and Software, June 15-19, San Diego, California, USA. ISBN: 978-88-9035-744-2
3. Y. Fan, S. Richard, R. S. Bristol, S. E. Peters, S. E. Ingebritsen, N. Moosdorf, A. Packman, T. Gleeson, I. Zaslavsky, S. Peckham, L. Murdoch, M. Fienen, M. Cardiff, D. Tarboton, N. Jones, R. Hooper, J. Arrigo, D. Gochis, J. Olson and D. Wolock (2014), DigitalCrust – a 4D data system of material properties for transforming research on crustal fluid flow, *GeoFluids*, Article first published online: 7 OCT 2014 | DOI: 10.1111/gfl.12114.
4. Swain, N.R., K. Latu, S.D. Christensen, N.L. Jones, E.J. Nelson, D.P. Ames, G.P. Williams (2015). "A review of open source software solutions for developing water resources web applications." Environmental Modeling & Software 67: 108-117.
5. Jones, David, Norm Jones, James Greer, and Jim Nelson, "*A cloud-based MODFLOW service for aquifer management decision support*," Computers and GeoSciences, Vol. 78, pp. 81-87, 2015.
6. Dolder, H., Jones, N., and Nelson, E. (2015). "Simple Method for Using Precomputed Hydrologic Models in Flood Forecasting with Uniform Rainfall and Soil Moisture Pattern." *J. Hydrol. Eng.*,10.1061/(ASCE)HE.1943-5584.0001232 , 04015039.
7. Fatichi, S., Vivoni, E.R., Ogden, F.L., Ivanov, V.Y., Mirus, B., Gochis, D., Downer, C.W., Camporese, M., Davidson, J.H., Ebel, B., Jones, N., Kim, J., Mascaro, G., Niswonger, R., Restrepo, P., Rigon, R., Shen, C., Sulis, M., and Tarboton, D. (2016). *An Overview of Challenges, Current Applications and Future Trends of Distributed Process-based Models in Hydrology.*

3

Journal of Hydrology. Vol 537, 45-60. DOI:10.1016/j.jhydrol.2016.03.026

8. Snow, Alan D., Scott D. Christensen, Nathan R. Swain, E. James Nelson, Daniel P. Ames, Norman L. Jones, Deng Ding, Nawajish S. Noman, Cédric H. David, Florian Pappenberger, and Ervin Zsoter, 2016. *A High-Resolution National-Scale Hydrologic Forecast System from a Global Ensemble Land Surface Model.* Journal of the American Water Resources Association (JAWRA) 52(4):950–964, DOI: 10.1111/1752-
9. Perez, J. Fidel, Nathan R. Swain, Herman G. Dolder, Scott D. Christensen, Alan D. Snow, E. James Nelson, and Norman L. Jones, 2016. *From Global to Local: Providing Actionable Flood Forecast Information in a Cloud-Based Computing Environment.* Journal of the American Water Resources Association (JAWRA) 52(4):965–978. DOI: 10.1111/1752-1688.12392
10. Swain, N. R., S. D. Christensen, A. D. Snow, H. Dolder, G. Espinoza-Dávalos, E. Goharian, N. L. Jones, E. J. Nelson, D. P. Ames and S. J. Burian (2016). "A new open source platform for lowering the barrier for environmental web app development." Environmental Modelling & Software 85: 11-26.
11. Souffront Alcantara, Michael A.; Crawley, Shawn; Stealey, Michael J.; Nelson, E. James; Ames, Daniel P.; and Jones, Norm L. (2017) "Open Water Data Solutions for Accessing the National Water Model," Open Water Journal: Vol. 4 : Iss. 1 , Article 3.
12. Souffront Alcantara, Michael, C Kesler, M Stealey, J Nelson, D Ames, N Jones, 2017. Cyberinfrastructure and Web Apps for Managing and Disseminating the National Water Model, *Journal of the American Water Resources Association, JAWRA Journal of the American Water Resources Association* 54, no. 4 (2018): 859-871.
13. Christensen, Scott D., Nathan R. Swain, Norman L. Jones, E. James Nelson, Alan D. Snow, and Herman G. Dolder. "A Comprehensive Python Toolkit for Accessing High-Throughput Computing to Support Large Hydrologic Modeling Tasks." *JAWRA Journal of the American Water Resources Association* 53, no. 2 (2017): 333-343.
14. Nelson, E. J., Pulla, S. T., Matin, M. A., Shakya, K., Jones, N., Ames, D. P., Ellenberg, W.L., Markert, K.N., Hales, R. (2019). Enabling Stakeholder Decision-Making With Earth Observation and Modeling Data Using Tethys Platform. *Frontiers in Environmental Science, 7.* https://doi.org/10.3389/fenvs.2019.00148
15. Purdy, A. J., David, C. H., Sikder, M. S., Reager, J. T., Chandanpurkar, H. A., Jones, N. L., & Matin, M. A. (2019). An Open-Source Tool to Facilitate the Processing of GRACE Observations and GLDAS Outputs: An Evaluation in Bangladesh. *Frontiers in Environmental Science,* 7. https://doi.org/10.3389/fenvs.2019.00155
16. Souffront Alcantara, M. A., Nelson, E. J., Shakya, K., Edwards, C., Roberts, W., Krewson, C., Ames, D. P., Jones, N. L., Gutierrez, A. (2019). Hydrologic Modeling as a Service (HMaaS): A New Approach to Address Hydroinformatic Challenges in Developing Countries. *Frontiers in Environmental Science*, 7. https://doi.org/10.3389/fenvs.2019.00158
17. Evans, S.; Williams, G.P.; Jones, N.L.; Ames, D.P.; Nelson, E.J. Exploiting Earth Observation Data to Impute Groundwater Level Measurements with an Extreme Learning Machine. *Remote Sens.* 2020, *12*, 2044. https://doi.org/10.3390/rs12122044
18. Evans, S.W.; Jones, N.L.; Williams, G.P.; Ames, D.P.; Nelson, E.J. (2020). Groundwater Level Mapping Tool: An open source web application for assessing groundwater sustainability. *Environmental Modeling and Software*, Vol 131, September 2020. https://doi.org/10.1016/j.envsoft.2020.104782
19. Nelson, S. T., Robinson, S., Rey, K., Brown, L., Jones, N., Dawrs, S. N., et al. (2021). Exposure Pathways of Nontuberculous Mycobacteria Through Soil, Streams, and Groundwater, Hawai'i, USA. *GeoHealth*, 5, e2020GH000350. https://doi.org/10.1029/2020GH000350
20. Sanchez Lozano J, Romero Bustamante G, Hales R, Nelson EJ, Williams GP, Ames DP, Jones NL. A Streamflow Bias Correction and Performance Evaluation Web Application for GEOGloWS ECMWF Streamflow Services. *Hydrology*. 2021;

8(2):71. https://doi.org/10.3390/hydrology8020071
21. Dolder, Danisa; Williams, Gustavious P.; Miller, A. W.; Nelson, Everett J.; Jones, Norman L.; Ames, Daniel P. 2021. "Introducing an Open-Source Regional Water Quality Data Viewer Tool to Support Research Data Access" *Hydrology* 8, no. 2: 91. https://doi.org/10.3390/hydrology8020091
22. Bustamante, G.R.; Nelson, E.J.; Ames, D.P.; Williams, G.P.; Jones, N.L.; Boldrini, E.; Chernov, I.; Sanchez Lozano, J.L. Water Data Explorer: An Open-Source Web Application and Python Library for Water Resources Data Discovery. *Water* 2021, *13*, 1850. https://doi.org/10.3390/w13131850
23. Hales, R.C.C.; Nelson, E.J.J.; Williams, G.P.P.; Jones, N.; Ames, D.P.P.; Jones, J.E.E. The Grids Python Tool for Querying Spatiotemporal Multidimensional Water Data. *Water* 2021, *13*, 2066. https://doi.org/10.3390/w13152066
24. Khattar, R., Hales, R., Ames, D. P., Nelson, E. J., Jones, N., & Williams, G. (2021). Tethys App Store: Simplifying deployment of web applications for the international GEOGloWS initiative. *Environmental Modelling & Software*, 105227. https://doi.org/10.1016/j.envsoft.2021.105227
25. McStraw, T.C., Pulla, S.T., Jones, N.L., Williams, G.P., David, C.H., Nelson, J.E., and Ames, D.P.. 2021. "An Open-Source Web Application for Regional Analysis of GRACE Groundwater Data and Engaging Stakeholders in Groundwater Management." *Journal of the American Water Resources Association* 1– 15. https://doi.org/10.1111/1752-1688.12968.
26. Barbosa, S.A.; Pulla, S.T.; Williams, G.P.; Jones, N.L.; Mamane, B.; Sanchez, J.L. Evaluating Groundwater Storage Change and Recharge Using GRACE Data: A Case Study of Aquifers in Niger, West Africa. *Remote Sens.* 2022, *14*, 1532. https://doi.org/10.3390/rs14071532
27. Nishimura, R.; Jones, N.L.; Williams, G.P.; Ames, D.P.; Mamane, B.; Begou, J. Methods for Characterizing Groundwater Resources with Sparse In Situ Data. *Hydrology* 2022, *9*, 134. https://doi.org/10.3390/hydrology9080134
28. Ramirez, S. G., Hales, R. C., Williams, G. P., & Jones, N. L. (2022). Extending SC-PDSI-PM with neural network regression using GLDAS data and Permutation Feature Importance. *Environmental Modelling & Software*, 105475. https://doi.org/10.1016/j.envsoft.2022.105475
29. Hales, R. C., Nelson, E. J., Souffront, M., Gutierrez, A. L., Prudhomme, C., Kopp, S., Ames, D. P., Williams, G. P., & Jones, N. L. (2022) Advancing global hydrologic modeling with the GEOGloWS ECMWF streamflow service. *Journal of Flood Risk Management*, e12859. https://doi.org/10.1111/jfr3.12859
30. Ramirez, S.G.; Williams, G.P.; Jones, N.L. (2022) Groundwater Level Data Imputation Using Machine Learning and Remote Earth Observations Using Inductive Bias. *Remote Sens.* 2022, *14*, 5509. https://doi.org/10.3390/rs14215509
31. Jones, J.E.; Hales, R.C.; Larco, K.; Nelson, E.J.; Ames, D.P.; Jones, N.L.; Iza, M. (2023) Building and Validating Multidimensional Datasets in Hydrology for Data and Mapping Web Service Compliance. Water 2023, 15, 411. https://doi.org/10.3390/w15030411
32. Ramirez, S.G.; Williams, G.P.; Jones, N.L.; Ames, D.P.; Radebaugh, J. (2023) Improving Groundwater Imputation through Iterative Refinement Using Spatial and Temporal Correlations from In Situ Data with Machine Learning. Water 2023, 15, 1236. https://doi.org/10.3390/w15061236
33. Jones, N.L. and Mayo, A.L. (2023), Urban Thirst and Rural Water – The Saga of the Southern Nevada Groundwater Development Project. Groundwater. https://doi.org/10.1111/gwat.13364
34. Barbosa, S.A.; Jones, N.L.; Williams, G.P.; Mamane, B.; Begou, J.; Nelson, E.J.; Ames, D.P. (2023) Exploiting Earth Observations to Enable Groundwater Modeling in the Data-Sparse Region of Goulbi Maradi, Niger. *Remote Sens.* 2023, *15*,

5199. https://doi.org/10.3390/rs15215199
35. Sanchez Lozano, J. L., Rojas Lesmes, D. J., Romero Bustamante, E. G., Hales, R. C., Nelson, E. J., Williams, G. P., Ames, D. P., Jones, N. L., Gutierrez, A. L., & Cardona Almeida, C. (2025). Historical simulation performance evaluation and monthly flow duration curve quantile-mapping (MFDC-QM) of the GEOGLOWS ECMWF streamflow hydrologic model. *Environmental Modelling & Software*, *183*, 106235. https://doi.org/10.1016/j.envsoft.2024.106235

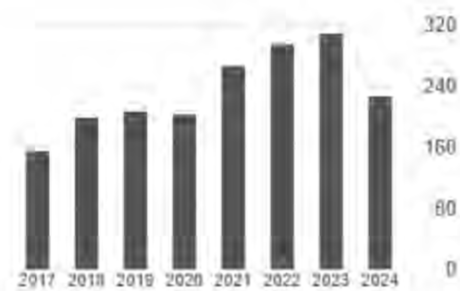
Summary: 88 total peer-reviewed publications.

Books

Strassberg, G., Jones, N., Maidment, D. (2011). Arc Hydro Groundwater: GIS for Hydrology. ESRI Press, Redlands, California, 250 pp.

Google Scholar Metrics

	All	Since 2019
Citations	3287	1507
h-index	27	19
i10-index	51	30



Complete CV: https://www.et.byu.edu/~njones/vita/

Appendix P — Reliance Materials

1. The literature, publications, and documents identified in the References section of this report (Section 8).

2. The documents, information and data identified in Appendix A2 ("Information sources used to extract model-specific data for historical reconstruction analyses, U.S. Marine Corps Base Camp Lejeune, North Carolina") to Maslia et al., Analyses and Historical Reconstruction of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water Within the Service Areas of the Hadnot Point and Holcomb Boulevard Water Treatment Plants and Vicinities, U.S. Marine Corps Base Camp Lejeune, North Carolina—Chapter A: Summary and Findings, ATSDR 2013, and included with this report in **Appendix E**.

3. Maslia, M.L. et al. 2007. "Analyses of Groundwater Flow, Contaminant Fate, and Transport, and Distribution of Drinking Water at Tarawa Terrace and Vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina: Historical Reconstruction and Present-Day Conditions - Chapter A: Summary of Findings." ATSDR, July 2007.

4. Faye, R.E. et al. 2007. "Analyses of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water at Tarawa Terrace and Vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina: Historical Reconstruction and Present Day Conditions - Chapter B: Geohydrologic Framework of the Castle Hayne Aquifer System." ATSDR, September 2007.

5. Faye, R.E. et al. 2007. "Analyses of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water at Tarawa Terrace and Vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina: Historical Reconstruction and Present Day Conditions - Chapter C: Simulation of Groundwater Flow." ATSDR, November 2007.

6. Lawrence, S.J. et al. 2007. "Analyses of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water at Tarawa Terrace and Vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina: Historical Reconstruction and Present Day Conditions - Chapter D: Properties and Degredation Pathways of Common Organic Compounds in Groundwater." ATSDR, September 2007.

7. Faye, R.E. and Green, J.W. 2007. "Analyses of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water at Tarawa Terrace and Vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina: Historical Reconstruction and Present Day Conditions - Chapter E: Occurrence of Contaminants in Groundwater." ATSDR, December 2007.

8. Faye, R.E. et al. 2008. "Analyses of Groundwater Flow, Contaminant Fate, and Transport, and Distribution of Drinking Water at Tarawa Terrace and Vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina: Historical Reconstruction and Present-Day Conditions - Chapter F: Simulation of the Fate and Transport of Tetrachloroethylene (PCE)." ATSDR, February 2008.

9. Jang, W. et al. 2008. "Analyses of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water at Tarawa Terrace and Vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina: Historical Reconstruction and Present Day Conditions - Chapter

G: Simulation of Three-Dimensional Multispecies, Multiphase Mass Transport of Tetrachloroethylene (PCE) and Associated Degredation By-Products." ATSDR, April 2008.

10. Jang, W. and Aral, M.M.. 2008. "Analyses of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water at Tarawa Terrace and Vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina: Historical Reconstruction and Present Day Conditions - Chapter H: Effect of Groundwater Pumping Schedule Variation on Arrival of Tetrachloroethylene (PCE) at Water-Supply Wells and the Water Treatment Plant." ATSDR, February 2008.

11. Maslia, M.L. et al. 2009(a). "Analyses of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water at Tarawa Terrace and Vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina: Historical Reconstruction and Present-Day Conditions - Chapter I: Parameter Sensitivity, Uncertainty, and Variability Associated with Model Simulations of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water." ATSDR, February 2009.

12. Maslia, M.L. et al. 2013. "Analyses and Historical Reconstruction of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water Within the Service Areas of the Hadnot Point and Holcomb Boulevard Water Treatment Plants and Vicinities, U.S. Marine Corps Base Camp Lejeune, North Carolina - Chapter A: Summary and Findings." ATSDR, March 2013.

13. Sautner, J.B. et al. 2013. "Analyses and Historical Reconstruction of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water Within the Service Areas of the Hadnot Point and Holcomb Boulevard Water Treatment Plants and Vicinities, U.S. Marine Corps Base Camp Lejeune, North Carolina - Chapter A–Supplement 1 - Descriptions and Characterizations of Data Pertinent to Water-Supply Well Capacities, Histories, and Operations." ATSDR, March 2013.

14. Telci, I.T. et al. 2013. "Analyses and Historical Reconstruction of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water Within the Service Areas of the Hadnot Point and Holcomb Boulevard Water Treatment Plants and Vicinities, U.S. Marine Corps Base Camp Lejeune, North Carolina - Chapter A–Supplement 2 - Development and Application of a Methodology to Characterize Present-Day and Historical Water-Supply Well Operations." ATSDR, March 2013.

15. Faye, R.E. et al. 2013. "Analyses and Historical Reconstruction of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water Within the Service Areas of the Hadnot Point and Holcomb Boulevard Water Treatment Plants and Vicinities, U.S. Marine Corps Base Camp Lejeune, North Carolina - Chapter A–Supplement 3 - Descriptions and Characterizations of Data Pertinent to Water-Level Data and Groundwater Flow for the Brewster Boulevard and Castle Hayne Aquifer Systems and the Tarawa Terrace Aquifer." ATSDR, March 2013.

16. Suarez-Soto, et al. 2013. "Analyses and Historical Reconstruction of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water Within the Service

Areas of the Hadnot Point and Holcomb Boulevard Water Treatment Plants and Vicinities, U.S. Marine Corps Base Camp Lejeune, North Carolina - Chapter A–Supplement 4 - Simulation of Three-Dimensional Groundwater Flow." ATSDR, March 2013.

17. Guan, J. et al. 2013. "Analyses and Historical Reconstruction of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water Within the Service Areas of the Hadnot Point and Holcomb Boulevard Water Treatment Plants and Vicinities, U.S. Marine Corps Base Camp Lejeune, North Carolina - Chapter A–Supplement 5 - Theory, Development, and Application of Linear Control Model Methodology to Reconstruct Historical Contaminant Concentrations at Selected Water-Supply Wells." ATSDR, March 2013.

18. Jones, L.E. et al. 2013. "Analyses and Historical Reconstruction of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water Within the Service Areas of the Hadnot Point and Holcomb Boulevard Water Treatment Plants and Vicinities, U.S. Marine Corps Base Camp Lejeune, North Carolina - Chapter A–Supplement 6 Characterization and Simulation of Fate and Transport of Selected Volatile Organic Compounds in the Vicinities of the Hadnot Point Industrial Area and Landfill." ATSDR, March 2013.

19. Jang, W. et al. 2013. "Analyses and Historical Reconstruction of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water Within the Service Areas of the Hadnot Point and Holcomb Boulevard Water Treatment Plants and Vicinities, U.S. Marine Corps Base Camp Lejeune, North Carolina - Chapter A–Supplement 7 - Source Characterization and Simulation of the Migration of Light Nonaqueous Phase Liquids (LNAPLs) in the Vicinity of the Hadnot Point Industrial Area." ATSDR, March 2013.

20. Sautner, J.B. et al. 2013. "Analyses and Historical Reconstruction of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water Within the Service Areas of the Hadnot Point and Holcomb Boulevard Water Treatment Plants and Vicinities, U.S. Marine Corps Base Camp Lejeune, North Carolina - Chapter A–Supplement 8 - Field Tests, Data Analyses, and Simulation of the Distribution of Drinking Water with Emphasis on Intermittent Transfers of Drinking Water Between the Hadnot Point and Holcomb Boulevard Water-Distribution Systems." ATSDR, March 2013.

21. Faye, R.E. et al. 2012. "Analyses and Historical Reconstruction of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water Within the Service Areas of the Hadnot Point and Holcomb Boulevard Water Treatment Plants and Vicinities, U.S. Marine Corps Base Camp Lejeune, North Carolina - Chapter B: Geohydrologic Framework of the Brewster Boulevard and Castle Hayne Aquifer Systems and the Tarawa Terrace Aquifer." ATSDR, January 2012.

22. Faye, R.E. et al. 2010. "Analyses and Historical Reconstruction of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water Within the Service Areas of the Hadnot Point and Holcomb Boulevard Water Treatment Plants and Vicinities, U.S. Marine Corps Base Camp Lejeune, North Carolina - Chapter C: Occurrence of Selected

Contaminants in Groundwater at Installation Restoration Program Sites." ATSDR, October 2010.

23. Faye, R.E. et al. 2012. "Analyses and Historical Reconstruction of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water Within the Service Areas of the Hadnot Point and Holcomb Boulevard Water Treatment Plants and Vicinities, U.S. Marine Corps Base Camp Lejeune, North Carolina - Chapter D: Occurrence of Selected Contaminants in Groundwater at Above-Ground and Underground Storage Tank Sites." ATSDR, December 2012.

24. Maslia, M.L. (Editor). 2005. "Expert Peer Review Panel Evaluating ATSDR's Water-Modeling Activities in Support of the Current Study of Childhood Birth Defects and Cancer at U.S Marine Corps Base Camp Lejeune, North Carolina." ATSDR, Meeting March 28-29, 2005, published October 2005.

25. Maslia, M.L. (Editor). 2009. "Expert Panel Assessing ATSDR's Methods and Analyses for Historical Reconstruction of Groundwater Resources and Distribution of Drinking Water at Hadnot Point, Holcomb Boulevard, and Vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina." ATSDR, April 29-30, 2009, published December 2009.

26. March 28, 2005 Expert Peer Review Panel Meeting Transcript, available at https://www.atsdr.cdc.gov/sites/lejeune/panel_report_groundwater.html

27. March 29. 2005 Expert Peer Review Panel Meeting Transcript, available at https://www.atsdr.cdc.gov/sites/lejeune/panel_report_groundwater.html

28. April 29, 2009 Expert Peer Review Panel Meeting Transcript, available at https://www.atsdr.cdc.gov/sites/lejeune/expertpanels.html

29. April 30, 2009 Expert Peer Review Panel Meeting Transcript, available at https://www.atsdr.cdc.gov/sites/lejeune/expertpanels.html

30. February 8, 2012 Deposition of Elizabeth Ann Betz

31. June 30, 2010 Deposition of Morris Maslia

32. May 28, 2024 Deposition of General Anthony Zinni; Zinni Deposition Exhibits 1-8

33. August 5, 2024 Deposition of Kim Henderson; Henderson Deposition Exhibits 1-18

34. August 6, 2024 Deposition of Dan Waddill; Waddill Deposition Exhibits 1-20

35. August 14, 2024 Deposition of Jason Barry Sautner; Sautner Deposition Exhibits 1-10

36. August 15, 2024 Deposition of Rene Suarez-Soto; Suarez-Soto Deposition Exhibits 1-5

37. August 22, 2024 Deposition of Dr. Chris Rennix; Rennix Deposition Exhibits 1-6

38. September 26, 2024 Deposition of Morris Maslia; Maslia Deposition Exhibits 1-22

39. ATSDR Camp Lejeune Project File: CLJA_ATSDRWM01-0000000001-CLJA_ATSDRWM01-0000189563; CLJA_WATERMODELING-0000000001-CLJA_WATERMODELING-0000209307; CLJA_WATERMODELING_01-0000000001-CLJA_WATERMODELING_01-0000854197; ATSDR_WATERMODELING_01-0000854198-ATSDR_WATERMODELING_01-0000936235; CLJA_WATERMODELING_01-0000936236-CLJA_WATERMODELING_01-0001118025; CLJA_WATERMODELING_04-0000000001-CLJA_WATERMODELING_04-0000117996; CLJA_WATERMODELING_05-0000000001-CLJA_WATERMODELING_05-0001394405; ATSDR_WATERMODELING_05-0001394406-ATSDR_WATERMODELING_05-0001394413; CLJA_WATERMODELING_07-0000000001-CLJA_WATERMODELING_07-0002316354; CLJA_WATERMODELING_08-0000000001-CLJA_WATERMODELING_08-0000193508; CLJA_WATERMODELING_09-0000000001-CLJA_WATERMODELING_09-0000547124; ATSDR_WATERMODELING_09-0000547125-ATSDR_WATERMODELING_09-0000568329; CLJA_WATERMODELIING_09-0000568330-CLJA_WATERMODELIING_09-0000615612; CLJA_WATERMODELING_09-0000615613-CLJA_WATERMODELING_09-0000745917

40. 00897_PLG_0000067113-00897_PLG_0000067132

41. 00897_PLG_0000339484-00897_PLG_0000339588

42. 00897_PLG_0000063393-00897_PLG_0000063594

43. 00897_PLG_0000065633-00897_PLG_0000065659

44. CLJA_ATSDR_BOVE-0000006959-CLJA_ATSDR_BOVE-0000006960

45. September 25, 2024 Tarawa Terrace Flow and Transport Model Post-Audit by N.L. jones and R.J. Davis, Integral Consulting, Inc.

46. The forthcoming depositions of Frank Bove, Susan Martel, and Scott Williams, including any accompanying deposition exhibits