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

IN RE:	)	
	)	**UNITED STATES' MEMORANDUM IN**
CAMP LEJEUNE WATER LITIGATION	)	**OPPOSITION TO PLG'S MOTION FOR**
	)	**AN ORDER EXCLUDING CERTAIN**
This Document Relates To:	)	**OPINIONS OF ALEXANDROS**
ALL CASES	)	**SPILIOTOPOULOS, PH.D.**

INTRODUCTION

Dr. Alexandros Spiliotopoulos is a senior hydrogeologist and water modeling expert at S.S. Papadopulos & Associates, a well-known environmental consulting firm that has played an instrumental role in developing techniques for using computer models to evaluate groundwater contamination. The United States retained Dr. Spiliotopoulos to evaluate water models that were developed by the Agency for Toxic Substances and Disease Registry ("ATSDR") to support its epidemiological studies related to Marine Corps Base Camp Lejeune ("Camp Lejeune"). These models purportedly estimated mean monthly concentrations of contaminants in three water distribution systems at Camp Lejeune. As part of this effort, ATSDR simulated decades of historical groundwater qualities from the 1950s to 1980s based on a small number of samples taken after 1982. Based on his evaluation, Dr. Spiliotopoulos opines that ATSDR lacked sufficient data to reconstruct estimated monthly concentration levels at the level of detail presented in its analysis, and that ATSDR's water models are uncertain and biased-high.

Plaintiffs' Leadership Group ("PLG") asks this Court to exclude eight broad categories of opinions held by Dr. Spiliotopoulos in the Water Contamination Phase of this litigation. *See generally* Pls.' Mot., D.E. 376. PLG's arguments in support of excluding Dr. Spiliotopoulos's opinions are illogical and misleading. Further, PLG argues that Dr. Spiliotopoulos's opinions are unreliable, but PLG misapplies the standards that courts have used to determine admissibility under Federal Rule of Evidence 702. Therefore, PLG's Motion must be denied.

NATURE OF THE CASE

Plaintiffs have filed actions for personal injury and wrongful death related to exposure to contaminated water pursuant to the Camp Lejeune Justice Act of 2022, Pub. L. No. 117–168, § 804, 136 Stat. 1759, 1802–04 (2022).

STATEMENT OF FACTS

Dr. Spiliotopoulos is a Doctor of Civil and Environmental Engineering, with over twenty years of relevant experience in groundwater modeling and evaluating the fate and transport of contaminants in the environment. *See* Spiliotopoulos Rep., D.E. 377-3 at 10, 134–39. He has worked with various public and private sector clients to perform groundwater modeling and evaluate the fate and transport of contaminants, including at National Priorities List sites like the Hanford, Washington nuclear plant. *Id.* Dr. Spiliotopoulos is published and has presented at multiple conferences across the country. *Id*. Through their experts, PLG has advocated for the wholesale adoption of ATSDR's water modeling to determine the absolute concentrations of contaminants that individuals at Camp Lejeune were exposed to between 1953 and 1987.[1] In response to PLG's expert reports, Dr. Spiliotopoulos independently evaluated and offered opinions regarding the water modeling efforts carried out by ATSDR. *See generally id.*

Dr. Spiliotopoulos opines, *inter alia*, that (1) ATSDR lacked sufficient data to reconstruct historical concentrations of contaminants at the level of detail presented in its analyses; (2)

[1] The United States has filed a Motion in Limine to Exclude Plaintiffs' Phase I Expert Testimony in Support of Using ATSDR's Water Models to Determine Exposure Levels for Individual Plaintiffs. D.E. 367. In that motion, the United States argues that ATSDR's models were not intended to determine exposure levels for individuals. Accordingly, the models are not reliable under Rule 702 for determining individuals' exposure levels in this litigation. *See generally id.*

ATSDR's groundwater models were constructed using model inputs that were both incorrect and unrepresentative of the real-world conditions at Camp Lejeune; and (3) ATSDR's groundwater models produced biased-high estimates of monthly contaminant concentrations. *See id.* at 3–4. Dr. Spiliotopoulos's opinions are consistent with contemporary reviewers of ATSDR's water models, including those from the Department of the Navy ("Navy") and the National Research Council ("NRC").

PLG asks this Court for an Order to exclude eight broad categories of opinions from Dr. Spiliotopoulos:

(1) opinions on ATSDR's intent and purpose with respect to conducting its water modeling;

(2) opinions from a section of his report titled "Timeline and Scientific Discourse on ATSDR's Camp Lejeune Water Modeling";

(3) opinions on how ATSDR's modeling results can or should be used by epidemiologists, doctors, or public health professionals;

(4) opinions that ATSDR's modeling approaches were "cutting-edge" or still in the research stages;

(5) opinions regarding ATSDR's uncertainty and sensitivity analyses;

(6) opinions regarding the loss of contaminants from drinking water during the water treatment process;

(7) opinions on the timing of the release of perchloroethylene ("PCE") into the environment at Tarawa Terrace; and

(8) opinions on water quality data collected from water supply well HP-634.

Pls.' Mem., D.E. 377, at 1–2.

LEGAL STANDARD

Fed. R. Evid. 702 seeks to ensure that expert witness testimony evidence is reliable and relevant. *Daubert v. Merrell Dow Pharms., Inc.*, 509 U.S. 579, 589 (1993) [hereinafter *Daubert*]. The focus of the inquiry under Fed. R. Evid. 702 "must be solely on principles and methodology, not on the conclusions that they generate." *In re Lipitor (Atorvastatin Calcium) Mktg., Sales Pracs. & Prods. Liab. Litig. (No II) MDL 2502*, 892 F.3d 624, 631 (4th Cir. 2018) (quoting *Daubert*, 509 U.S. at 595). Moreover, "the court should not resolve contested factual issues at the admissibility stage." *Mountain Valley Pipeline, LLC v. 0.32 Acres of Land*, 127 F.4th 427, 435 (4th Cir. 2025).

ARGUMENT

PLG argues that Dr. Spiliotopoulos's opinions are not supported by sufficient facts or data, that he failed to apply a reliable methodology in rendering his opinions, and that his "opinions critiquing ATSDR's methodology fail all of the *Daubert* factors." Pls.' Mem., D.E. 377, at 8 (citing *Daubert v. Merrell Dow Pharms., Inc.*, 43 F.3d 1311, 1318–19 (9th Cir. 1995) [hereinafter *Daubert II*]). However, beyond these conclusory statements, PLG fails to demonstrate how any of Dr. Spiliotopoulos's opinions are unreliable under Fed. R. Evid. 702 and *Daubert*. PLG also repeatedly misstates the record and identifies several areas of factual dispute between the Parties' Water Contamination Phase experts. PLG's argument merely reveals their disagreement with Dr. Spiliotopoulos's opinions that should be subject to traditional means of challenging expert opinions, including "[v]igorous cross-examination," and "presentation of contrary evidence." *Daubert*, 509 U.S. at 596. PLG has not made an appropriate admissibility challenge to Dr. Spiliotopoulos's opinions under the standards of Fed. R. Evid. 702. Therefore, PLG's Motion must be denied.

I. Dr. Spiliotopoulos Properly Considered the Contemporaneous Statements of ATSDR, its Employees, and Independent Evaluators When Offering Opinions on the Qualities of ATSDR's Modeling Work.

A. Dr. Spiliotopoulos Considered ATSDR's Contemporaneous Statements about the Intent and Purpose of Developing the Water Models in Forming His Opinions.

After Camp Lejeune was placed on the National Priorities List by the Environmental Protection Agency ("EPA"), ATSDR began conducting epidemiologic health studies on the effects of exposure to contaminated drinking water at Camp Lejeune. These studies sought to investigate the potential impacts of exposure to contaminated drinking water. However, as ATSDR stated in one of its water modeling reports, "[b]ecause limited measurements of contaminant and exposure data [were] available to support the epidemiological study, ATSDR [used] modeling techniques to reconstruct historical conditions of groundwater flow, contaminant fate and transport, and the distribution of drinking water contaminated with [volatile organic compounds] delivered to family housing areas." ATSDR, Chapter A: Summary of Findings, D.E. 370-3, at A1.

Dr. Spiliotopoulos considered this, and similar statements made contemporaneously by ATSDR regarding the purpose of the models, in forming and offering his opinions. Spiliotopoulos Rep., D.E. 377-3, at 23 (quoting ATSDR's stated purpose of the Hadnot Point water modeling effort). Considering the intent and purpose of a model is necessary as part of employing a reliable methodology. PLG's water modeling experts agree that when evaluating a model, it is important to consider the model's purpose. *See* Davis Dep. Tr., D.E. 357-3, at 69:11–70:3, 211:1–6; Konikow Dep. Tr., D.E. 357-9, at 129:1–130:19; *see also* **Exhibit 1**, Mustafa Aral, *Environmental Modeling and Health Risk Analysis (Acts/Risk)* 40 (2010) [hereinafter "Aral Book Excerpts"] ("All models are developed to answer a specific question about the system outcome. The use of models in a specific application cannot and should not go beyond the question posed during the model development stage.”).

According to Dr. Spiliotopoulos, evaluating model calibration (or “history matching”) is “important for evaluating a model’s fit for purpose.” Spiliotopoulos Rep., D.E. 377-3, at 10; *see also* Spiliotopoulos Dep. Tr., D.E. 377-2, at 153:12–25 (testifying that he included a statement about the water modeling being done for epidemiologic studies because it “support[s his] work in looking at whether the modeling work that was done provided good results to rely on and support such evaluations”). Contrary to PLG’s contention, Dr. Spiliotopoulos is not offering any opinion inferring the intent or purpose of ATSDR’s studies—rather, he is properly considering ATSDR’s own statements of its intent and purpose in support of his opinions.[2] PLG’s Motion seeking to exclude Dr. Spiliotopoulos’s discussion of ATSDR’s intent and purpose in creating the water models should therefore be denied.

B. Dr. Spiliotopoulos Considered and Relied on the Documents Summarized in Section 3.3 of his Report in Forming his Opinions.

In Section 3.3 of Dr. Spiliotopoulos’s report, he lays out a timeline of events and scientific discourse that he considered in rendering his opinions on the reliability of ATSDR’s water models. For example, Dr. Spiliotopoulos notes in the timeline that EPA placed Camp Lejeune on the National Priorities List, triggering a public health assessment by ATSDR, which ultimately led to the decision to create water models. Spiliotopoulos Rep., D.E. 377-3, at 16–17. He noted the occurrence of expert panels and other external reviews of the modeling by the

[2] In a footnote, PLG asserts that Dr. Spiliotopoulos’s citation to bench books on hydrologic modeling and deposition testimony “raises questions as to who wrote certain portions of [his] report.” Pls.’ Mem., D.E. 377, at 11. In response to PLG’s subpoena, the United States has produced almost two hundred fifty pages of detailed billing records for the period 2022 onward, which show Dr. Spiliotopoulos invoiced at least 180 hours for work on his report in that timeframe (and not including the hours of staff or assistants working under Dr. Spiliotopoulos). Moreover, when asked at deposition whether he wrote his report, Dr. Spiliotopoulos replied, “Yes, I did.” Spiliotopoulos Dep. Tr., D.E. 377-2, at 100:14–15.

Government Accountability Office, the Navy, and the NRC. *Id.* at 17–22. Dr. Spiliotopoulos returns to these assessments throughout the body of his report to inform and support his opinions. *See, e.g., id.* at 31–32, 36, 46, 68, 70, 78. Next, Dr. Spiliotopoulos notes the passing of a bill to provide medical benefits to those impacted by water contamination at Camp Lejeune, a policy decision informed by ATSDR's modeling efforts. *Id.* at 22. In support of his opinions, Dr. Spiliotopoulos also cited to the ATSDR's epidemiology studies which included analyses derived from ATSDR's water modeling. *Id.* at 23–24.

PLG argues that Section 3.3 of Dr. Spiliotopoulos's report, titled "Timeline and Scientific Discourse on ATSDR's Camp Lejeune Water Modeling" must be excluded because it constitutes a "summary of events, narration of select documents, and opinions on the intent, motive, or state-of-mind of third parties and are not proper topics of expert testimony." Pls.' Mem., D.E. 377, at 10. In support of this argument, PLG cites two cases: *City of Huntington v. AmerisourceBergen Drug Corp.*, No. CV 3:17-01362, 2021 WL 1436672 (S.D.W. Va. Apr. 15, 2021), and *In re Davol, Inc./C.R. Bard, Inc., Polypropylene Hernia Mesh Products Liability Litigation*, 546 F. Supp. 3d 666 (S.D. Ohio 2021). Both are inapposite.

In *City of Huntington*, the District Court for the Southern District of West Virginia excluded the testimony of a former Drug Enforcement Agency ("DEA") agent who offered an overview of the laws that governed the case and how DEA enforces those laws. 2021 WL 1436672, at *1–3. The court in *City of Huntington* held that the former DEA agent's testimony constituted an impermissible narrative because it was not necessary to support his opinions. *Id.* The court found that the former DEA agent's narrative was "the end in itself" because it was not provided in support of any separate opinions. *Id.* at *3. Similarly, in *In re Davol*, the District Court for the Southern District of Ohio excluded a portion of the testimony of a materials science expert that summarized corporate documents because the expert did not rely on those documents in forming his opinions. 546 F. Supp. 3d at 670–80.

These cases are distinguishable. Dr. Spiliotopoulos relied on the timeline in Section 3.3 of his report in forming and supporting his opinions. This section outlines the history and purpose of the ATSDR's model, and even PLG's experts agree that knowing the purpose of a model is essential for any modeling effort. *See, e.g.,* Konikow Dep. Tr., D.E. 357-9, at 129:15–23, 213:14–18; Davis Dep. Tr., D.E. 357-3, at 69:11–21, 211:1–6; *see also* Ex. 1, Aral Book Excerpts, at 40. Dr. Spiliotopoulos's assessment of the purpose of the model is informed by the context of its creation and the scientific discourse surrounding the model's development. Spiliotopoulos Dep. Tr., D.E. 377-2, at 97:25–98:7 (testifying that whether a model is properly calibrated "depends on the intended purpose of the model, and it also depends on what data are available to perform that calculation, and, therefore, how confident you are in the calibrated model that you have"). Unlike the experts in *City of Huntington* and *In re Davol*, Dr. Spiliotopoulos substantively relied on the documents summarized in Section 3.3 of his report in forming his opinions. PLG' Motion seeking to exclude this Section should therefore be denied.

C. Dr. Spiliotopoulos Has Not Disclaimed the Opinion That Certain of ATSDR's Modeling Approaches Were Cutting-Edge, but Rather Considered the Conclusions of the NRC in Forming His Opinions.

PLG next contends that Dr. Spiliotopoulos should be precluded from offering opinions regarding ATSDR's modeling approaches that "allegedly were 'cutting-edge' and/or still in the research stages" because he "disclaimed" them. Pls.' Mem., D.E. 377, at 12. In support of this contention, PLG cites the following portion of the deposition transcript:

> Q: No. You say that, "Some of the modeling approaches used by ATSDR were cutting edge, meaning that they used computer codes and modeling techniques that are still in the research stage." Which computer codes and modeling techniques are you referring to there?
> A. First of all, that's a quote; right.

> Q. Sure. In your opinion, which computer codes and modeling techniques of ATSDR were still in the research stage that they used for their modeling of Tarawa Terrace?
> MR. ANWAR: Object to form.
> THE WITNESS: I believe that's something for the NRC to articulate.
> BY MS. BAUGHMAN: Can you identify any today?
> A. That's not part of the opinions that I provide. So I don't have an opinion on that.

Spiliotopoulos Dep. Tr., D.E. 377-2, at 147:14–148:6.

Page 21 of Dr. Spiliotopoulos's report contains a quote from a study published by the NRC, which discusses the "cutting-edge" modeling approaches used by ATSDR in their Camp Lejeune modeling efforts. Spiliotopoulos Rep., D.E. 377-3, at 21. The NRC stated:

> Some of the modeling approaches used by ATSDR were "cutting-edge," meaning that they used computer codes and modeling techniques that are still in the research stage and have yet to be validated. Furthermore, the absence of measurement data for the first 30 years of the contamination period means the predictions, even if based on validated codes and models, cannot be evaluated for accuracy. The actual concentrations may have been higher or lower than the predictions, but that cannot be assessed.

National Research Council, *Contaminated Water Supplies at Camp Lejeune: Assessing Potential Health Effects* 4 (2009), D.E. 372-3. Moreover, PLG's own expert and the project manager for ATSDR's water modeling efforts, Morris Maslia, acknowledged that ATSDR's use of water models was "a novel application." June 30, 2010 Maslia Dep. Tr., D.E. 370-6, at 45:15–17. While Dr. Spiliotopoulos is not offering an independent opinion about cutting-edge techniques, he considered the NRC's evaluation and Mr. Maslia's testimony in forming his own opinions and evaluation. For example, Dr. Spiliotopoulos noted that "ATSDR used the Linear Control Model (LCM), an alternative methodology for reconstructing the historical concentrations of the [volatile organic compound] degradation by-products." Spiliotopoulos Rep., D.E. 377-3, at 82. PLG's expert, Dr. Aral, agrees. *See* Aral Rep., D.E. 359-2, at 15–20 (stating that the LCM was implemented by the use of TechControl, a sub-model developed by Dr. Aral's research laboratory for the Camp Lejeune modeling effort). Dr. Spiliotopoulos continued, "[a]pplication of [the

LCM] methodology relied on the same limited set of observed data, available after 1985. As illustrated in Figure 33, the historical reconstruction prior to 1985 cannot be verified, due to lack of observed data for the period." Spiliotopoulos Rep., D.E. 377-3, at 82.

Even though Dr. Spiliotopoulos never disputed the novelty of ATSDR's water model, but instead merely deferred to the NRC in that regard, any allegedly inconsistent testimony is not a basis for exclusion under Fed. R. Evid. 702. *See Sanchez v. Bos. Sci. Corp.*, No. 2:12-CV-05762, 2014 WL 4851989, at *21 (S.D.W. Va. Sept. 29, 2014) (finding that the existence of inconsistent opinions goes to the weight, and not admissibility, of an expert's testimony).

D. Without Offering Any Specific Opinions on the Appropriate Use of Models by Epidemiologists or Health Professionals, Dr. Spiliotopoulos Rightly Acknowledges that the Inaccuracy and Uncertainty of ATSDR's Water Models Could Impact Decisions about Health Effects.

PLG next asserts that Dr. Spiliotopoulos "has no experience or expertise that qualifies him to offer an opinion as to whether or how a health professional can or should use ATSDR's modeling results to assess individual exposures to contaminants or to conduct an epidemiological study." Pls.' Mem., D.E. 377, at 12. However, Dr. Spiliotopoulos has not offered any such opinions. PLG contends these opinions are expressed on page 25 of Dr. Spiliotopoulos's report. Pls.' Mem., D.E. 377, at 2. Rather than expressing any opinion on how a health professional can use ATSDR's modeling results, however, Dr. Spiliotopoulos merely quoted ATSDR's reports regarding their intended purpose. *See* Spiliotopoulos Rep., D.E. 377-3, at 25.

Dr. Spiliotopoulos does not opine whether or how a health professional should use ATSDR's modeling results. Instead, he opines that the accuracy of the contaminant concentrations these models simulated are highly uncertain and likely to be biased-high. Spiliotopoulos Rep., D.E. 377-3, at 33–55, 87–89. The accuracy of the contamination levels simulated by the model is unquestionably relevant to the purpose of determining exposure levels in individuals, and to the purpose of determining health effects associated with exposure—which is how PLG has proposed using ATSDR's water models. Dr. Spiliotopoulos recognized:

> [W]hen models are used for hindcasting or forecasting conditions that are directly translated to substantially more important decisions, such as health impacts, the implications of model uncertainty have to be viewed more critically. Camp Lejeune is a suitable case in point. ATSDR reconstructed historical conditions at Camp Lejeune to calculate how much contamination (i.e., dose) people at Camp Lejeune were exposed to, by implementing "*a unique application of -- of going backward in time,*" and "*reconstructing backwards in time for 30, 35 years at a monthly interval,*" using "*[n]ovel application*" of significant complexity.

Spiliotopoulos Rep., D.E. 377-3, at 28 (emphasis in original) (citations omitted). While Dr. Spiliotopoulos does not opine on the appropriate use of water models by health professionals, he does acknowledge that, from an engineering perspective, the accuracy of these models is insufficient to meet the stated purpose of determining how much contamination was historically present in drinking water. *Id.* This opinion is wholly within Dr. Spiliotopoulos's realm of expertise and PLG has not offered an appropriate basis under Rule 702 to exclude it.

II. Dr. Spiliotopoulos's Opinions about the Tarawa Terrace Model Sensitivity Analysis and Hadnot Point-Holcomb Boulevard Uncertainty Analysis Are Supported by Peer-Reviewed Literature and Based on the Same Standards That He Would Use in His Non-Litigation Practice.

PLG argues that the broad category of Dr. Spiliotopoulos's opinions related to ATSDR's sensitivity and uncertainty analyses must be excluded. Pls.' Mem., D.E. 377, at 2, 4–10. Sensitivity and uncertainty analyses are steps in the groundwater modeling workflow. In the words of PLG's expert, Dr. Konikow, "there's always uncertainty and certainly errors in every model, and what you try to do in standard practice is assess how serious those errors might be, how they might affect the results." Konikow Dep. Tr., D.E. 357-9, at 228:18–229:11; *see also* Ex. 1, Aral Book Excerpts, at 17 ("Because models are not a precise and complete depiction of the real system, they need to be presented and analyzed in a computational environmental which should include an analysis of uncertainty."). Groundwater modelers perform "sensitivity tests and uncertainty analysis to help assess what confidence [one] should have in the model because we recognize that the model is not the reality." Konikow Dep. Tr., D.E. 357-9, at 228:18–229:11. Dr. Spiliotopoulos opined, *inter alia*, that ATSDR's uncertainty and sensitivity analyses for Tarawa Terrace and Hadnot Point-Holcomb Boulevard were not supported by sufficient data, were incomplete, and did not account for site-specific conditions. *See* Spiliotopoulos Rep., D.E. 377-3, at 2–4. PLG's arguments against the admissibility of these opinions fail.

A. Dr. Spiliotopoulos Considered and Relied on Peer-Reviewed Literature and Other Reputable Authorities in Forming His Opinions.

PLG repeatedly misrepresents that Dr. Spiliotopoulos failed to cite to published literature to support his opinions. Pls.' Mem., D.E. 377, at 5–9. Even a cursory reading of Dr. Spiliotopoulos's report reveals that he repeatedly cites to published scientific literature in support of his opinions, and his report includes a reference list identifying published literature that he considered in forming his opinions. On the topic of uncertainty analysis, Dr. Spiliotopoulos cited numerous studies and books published by his peers in groundwater modeling. For example, Dr. Spiliotopoulos identified the "general rule for the calibrated model output (prediction)" from John Doherty, *Calibration and Uncertainty Analysis for Complex Environmental Models* 52 (2015), and explained that ATSDR's models failed to obey that rule:

> Recall the discussion in Section 3.1.5 about the general rule for the calibrated model output (prediction): "*[i]deally, the value of that prediction should lie somewhere near the centre of the uncertainty band of the prediction. In this way, the potential for predictive error is minimized*."[294] Inspection of Figure 36 indicates that the calibrated model fails to conform with this rule at two critical times: (a) in the early 1950s, when the model estimates the arrival of TCE at the pumping wells and, thus, the influent to the WTP, and (b) after 1972, when pumping well HP-651 was put in service.
>
> . . . .
>
> [294] Doherty (2015), p. 52

Spiliotopoulos Rep., D.E. 377-3, at 92 (emphasis in original); *see also id.* at 48 (referring to an earlier citation of Doherty (2015) in support of the proposition that ATSDR's uncertainty analysis demonstrates that the calibrated model is biased-high). Mr. R. Jeffrey Davis, an expert for the Plaintiffs, testified that the Doherty text cited here by Dr. Spiliotopoulos is reliable. Davis Dep. Tr., D.E. 357-3, at 306:25–307:8. Dr. Spiliotopoulos modified model inputs and re-ran portions of ATSDR's models to test for compliance with this rule based on the use of site-specific, rather than generic, data. Spiliotopoulos Rep., D.E. 377-3, at 48–54, 81–82.

In his introductory discussion of aspects of groundwater model development, which includes model calibration, sensitivity analysis, and uncertainty analysis, Dr. Spiliotopoulos also cites to, *inter alia*, Anderson et al. (2015), Zheng & Bennet (2002), Reilly and Harbaugh (2004), and Harter et al. (2018). Spiliotopoulos Rep., D.E. 377-3, at 8–11.

In Section 4 of his report, Dr. Spiliotopoulos further cites to published literature sources. By way of example, Dr. Spiliotopoulos cited a 2002 study by Meyer and Orr (2002) in support of the proposition that uncertainty ranges can be skewed upward when site-specific data are ignored in favor of generic datasets. *Id.* at 28. Similarly, Dr. Spiliotopoulos quotes peer reviewed studies from Sepulveda et al. (2015) and Clement (2011) to support his opinion that ATSDR's Tarawa Terrace model did not consider the "observed system behavior," meaning measured or observed data taken from the Tarawa Terrace water supply wells and water treatment plant. *Id.* at 45–46.

When questioned at deposition, Dr. Spiliotopoulos confirmed the numerous sources he relied on in forming his opinions:

> Q. Can you cite any discussion in the literature, textbooks, standards that supports your criticism of how ATSDR did its uncertainty analysis for Tarawa Terrace?
> MR. ANWAR: Object to form.
> THE WITNESS: I have cited references with respect to how the uncertainty analysis is supposed to be conducted, but it includes various aspects of it. I'm not sure you want me to --

BY MS. BAUGHMAN: I want to know about this range issue. . . .

Spiliotopoulos Dep. Tr., D.E. 377-2, at 305:19–306:5. When the attorney for PLG pressed Dr. Spiliotopoulos on the justification for his opinions, he elaborated:

> Q: Are you relying on your professional judgment?
> A: And I'm referencing literature sources where a discussion is made about how the --
> Q: Show me where the literature in your -- specifically where you're criticizing the uncertainty analysis in your report, what's the literature source for that?
> A: I'm sorry. Which part of the criticism that I provided?
> Q: Where you're criticizing uncertainty analysis, what's your literature source for that?
> A: I believe -- let me just go and check. One aspect is, for example, the value of that predictions should --
> Q: What -- I'm sorry?
> A: Page 92.
> Q: Tell me what I want is the citation to a textbook or a standard in your field or a published document. Is that what you're telling me [you] cited to?
> A: Yes, [footnote] 294, yes.
> Q: What page?
> A: 92.
> Q: So Doherty --
> A: That's one that I can --
> Q: Is this about the uncertainty analysis?
> A: Yes.
> Q: The page 52. Anything else?
> A: And [footnote] 35, that's section 3[.]1[.]5.
> Q: What page?
> A: Page 8.
> Q: What source are you relying on here?
> A: Hill and Tiedeman talking about precision accuracy of the model outputs when we're looking at uncertainty analysis.
> Q: What about the sections of your report where you discuss your criticisms of the uncertainty analysis, did you cite any literature or textbook there in support of your analysis or your opinions?
> A: I'm not sure I had to.
> Q: Did you? Yes or no.
> A: I don't think I did specific for some --
> Q: Let's move on because I don't have much time left.

Spiliotopoulos Dep. Tr., D.E. 377-2, at 313:5–314:25.

In short, PLG's conclusory allegation that Dr. Spiliotopoulos "cite[d] no peer reviewed literature or other authorities in support of his critiques of ATSDR's methodology" is contradicted by both Dr. Spiliotopoulos's report and the testimony PLG elicited from him at deposition. Pls.' Mem., D.E. 377, at 5.

Even if Dr. Spiliotopoulos had cited no published literature in support of his opinions—which is not the case—his opinions would still be admissible under *Daubert*. This Court has held that, in the absence of "specific industry standard[s]," experts are permitted to "base their opinions on a comparison with their experience." *Bouygues Telecom, S.A. v. Tekelec*, No. 4:05-CV-78-FL, 2007 WL 9718141, at *9 (E.D.N.C. Feb. 12, 2007); *see also McCullock v. H.B. Fuller Co.*, 61 F.3d 1038, 1044 (2d Cir. 1995) ("Disputes as to . . . lack of textual authority for [an] opinion, go to the weight, not the admissibility, of [the] testimony."). Indeed, PLG's own experts agree with Dr. Spiliotopoulos that contaminant fate and transport modeling require the subjective judgment of the modeler. *See, e.g.,* Konikow Dep. Tr., D.E. 357-9, at 289:6–17 (agreeing that calibration targets are subjective and that assessing whether a model is calibrated is "partly subjective."); Davis Dep. Tr., D.E. 357-3, at 132:7–25 (testifying that the amount of data needed to accurately perform water modeling is "completely subjective."); Konikow Groundwater Modeling Chapter, D.E. 370-2, at 14 ("However, even with regression modeling, the hydrologic experience and judgment of the modeler continues to be a major factor in calibrating a model both accurately and efficiently.").

Contrary to PLG's unsupported assertions, Dr. Spiliotopoulos identified peer reviewed literature and other reputable authorities that support his critiques of ATSDR's methodology in his report and in his deposition testimony. Moreover, PLG's own experts agree that water modeling requires some subjective analysis on the part of the modeler, for which textual authority does not exist. *See* Davis Dep. Tr., D.E. 357-3, at 132:10–25 (testifying that "there's not a definition written" for how much data is needed to accurately perform modeling); *see also*

ATSDR Response to DON Letter, D.E. 357-7, at 10 ("Note, however, that published or accepted groundwater-flow or contaminant fate and transport model calibration standards are currently not established.") (emphasis in original). Finally, lack of textual authority in support of expert opinions is more properly raised on cross-examination, not under a motion to exclude pursuant to Fed. R. Evid. 702. *McCullock*, 61 F.3d at 1044. Accordingly, to the extent PLG's Motion is based on arguments related to Dr. Spiliotopoulos's cited authorities, it should be denied.

B. Dr. Spiliotopoulos's Opinions About the Adequacy of the ATSDR's Uncertainty Analysis of the Tarawa Terrace and Hadnot Point Models are Entirely Consistent with Each Other, as Demonstrated by His Report and Deposition Testimony.

PLG next claims that Dr. Spiliotopoulos's opinions are contradictory. *See* Pls.' Mem., D.E. 377, at 5, 6–7. In support of this claim, PLG argues that Dr. Spiliotopoulos contradicts himself by alternatively "endorsing" and critiquing ATSDR's selection of parameter ranges for its model calibration. Pls.' Mem., D.E. 377, at 6 (quoting Spiliotopoulos Rep., D.E. 377-3, at 87).

PLG is conflating two separate opinions that are wholly distinct and do not contradict one another. One involved the Tarawa Terrace model and the other involved the Hadnot Point model; both critiqued ATSDR's failure to match site-specific conditions. At deposition, Dr. Spiliotopoulos stated that his report referred to the parameter ranges that ATSDR itself, not Dr. Spiliotopoulos, indicated were reasonable for Tarawa Terrace. Spiliotopoulos Dep. Tr., D.E. 377-2, at 311:13–312:1.

For the Tarawa Terrace model, Dr. Spiliotopoulos opined that ATSDR's selection of parameter ranges for calibrated values "did not consider appropriate parameter values based on site-specific data." Spiliotopoulos Rep., D.E. 377-3, at 52–53. This opinion was based on Dr. Spiliotopoulos re-running the model using modified parameter values within the range of site-specific data, then comparing those results to ATSDR's. *Id.* at 53.

For the Hadnot Point-Holcomb Boulevard sensitivity analysis, Dr. Spiliotopoulos opined that ATSDR selected extreme parameter values that are both outside the range of values used for the Tarawa Terrace analysis, and not representative of site conditions. *Id.* at 88–89. Bearing in mind that ATSDR was modeling the same aquifer at Hadnot Point and Tarawa Terrace, it is clear these opinions do not contradict one another. Dr. Spiliotopoulos's opinions are entirely consistent and appropriate, and should not be excluded.

C. Dr. Spiliotopoulos Applied the Same Standards Used in His Non-Litigation Work to Reach His Opinions in this Case.

PLG next asserts that Dr. Spiliotopoulos has failed to apply the same standards he uses in his non-litigation work to his opinions in this case. Pls.' Mem., D.E. 377, at 5, 7–8. Despite their earlier critique of Dr. Spiliotopoulos's qualifications, PLG acknowledges within this argument that he previously served as the "lead modeler" for a high-profile groundwater flow and contaminant transport model for a decommissioned nuclear production complex. *Id.* at 7. PLG states that Dr. Spiliotopoulos "criticized the uncertainty analysis for Hadnot Point as being limited to the effects of historical pumping variability," and argues that the uncertainty analysis he performed for the Hanford nuclear site was "at least as limited." *Id.* at 8. PLG also notes that "there is no indication that the parameter range used for Hanford met the not-too-narrow and not-too-wide standard applied by Dr. Spiliotopoulos here." *Id.*

Despite their argument to the contrary, PLG demonstrated through deposition questioning that Dr. Spiliotopoulos is applying exactly the same standards to ATSDR's work that he applied to his non-litigation work at the Hanford site. Dr. Spiliotopoulos testified that "it was impossible to do" history matching for contaminant concentrations at the Hanford site "because we had very limited data." Spiliotopoulos Dep. Tr., D.E. 377-2, at 87:3–10. At the Hanford site, Dr. Spiliotopoulos performed an uncertainty analysis on the only parameter for which they had enough data; this was followed by a period of data collection and iterative model refinement. *See id.* at 84:11–88:10. PLG's argument ignores the critical difference between what Dr. Spiliotopoulos was doing at Hanford, which was *forecasting future* contaminant levels based on existing and evolving data, and what ATSDR was trying to do for Camp Lejeune, which was *hindcasting historic* concentration levels with limited data. At Hanford, Dr. Spiliotopoulos necessarily did not yet have the contaminant concentrations that PLG argues that he should have used to perform an uncertainty analysis there.

PLG's argument obfuscates the fact that, for the Hanford site, Dr. Spiliotopoulos's limited uncertainty analysis was the first step in a decade-long, multistep process of designing a contaminant remediation scheme and continually refining the model as more data were collected. *See id.* at 95:20–96:3. Dr. Spiliotopoulos's criticism of ATSDR's uncertainty analysis is based on the fact that, for Hadnot Point, the uncertainty analysis on historical pumping variability was the only systematic uncertainty analysis performed. *See* Spiliotopoulos Rep., D.E. 377-3, at 92. Because of the historical nature of ATSDR's work, there was no opportunity to collect more data to refine the models. *Id.* PLG's critique conflates these two very different processes to misrepresent Dr. Spiliotopoulos's opinions.

Moreover, PLG's assertion that "there is no indication that the parameter range used for Hanford met the not-too-narrow and not-too-wide standard applied by Dr. Spiliotopoulos here" is misleading. Pls.' Mem., D.E. 377, at 8. Dr. Spiliotopoulos testified at deposition that the range of hydraulic conductivity parameter values used to calibrate the Hanford model was based on the available data at the time. Spiliotopoulos Dep. Tr., D.E. 377-2, at 90:3–10. Moreover, Dr. Spiliotopoulos made clear that the purpose of his modeling work at the Hanford site was to predict future characteristics of the contaminant plume in the aquifer in support of groundwater remediation efforts. *Id.* at 78:14–17. Because of the predictive nature of this work, Dr. Spiliotopoulos did not know the potential range of hydraulic conductivities and thus could not have applied any "not too-narrow and not-too-wide" standard to evaluate them. However, as additional data became available over time, the potential range of hydraulic conductivities and other model parameters were further evaluated. This is obviously distinguishable from ATSDR's Camp Lejeune modeling, which employed "historical reconstruction" to look back in time rather than to forecast future conditions. PLG's Motion regarding the standards Dr. Spiliotopoulos applied should therefore be denied.

D. Dr. Spiliotopoulos's Opinions on ATSDR's Uncertainty and Sensitivity Analyses are Based on a Reliable Methodology.

PLG next asserts that Dr. Spiliotopoulos's opinions on the uncertainty and sensitivity analyses conducted by PLG are unreliable because "all of the work Dr. Spiliotopoulos has done to form his opinions in this case was done for or in anticipation of litigation." Pls.' Mem., D.E. 377, at 8 (citing *Daubert II*, 43 F.3d at 1317). PLG cites an isolated statement from the Ninth Circuit's decision in *Daubert II*, but they fail to acknowledge the ensuing paragraphs, which make clear that "preexisting or independent research" is not the standard for admission, but only one part of determining whether any expert is employing a reliable methodology. 43 F.3d at 1317–18 ("If the proffered expert testimony is not based on independent research, the party proffering it must come forward with other objective, verifiable evidence that the testimony is based on 'scientifically valid principles.'").

It is true that all of the work Dr. Spiliotopoulos has done on the topic of groundwater modeling Camp Lejeune has been in the context of litigation, but it is based on methods that he has frequently used outside the context of litigation. It is not necessary that each expert have non-litigation experience on a particular site for their opinions to be admitted; otherwise most of the expert opinions offered in this case would be excludable, including those of PLG's own Water Contamination Phase experts, Mr. Davis, Dr. Jones, and Dr. Sabatini. As shown by his prior work on the Hanford project, Dr. Spiliotopoulos is employing the same methods here that formed the basis of his past research and non-litigation experience. That Dr. Spiliotopoulos is employing standard non-litigation methodologies in his critique of ATSDR's water models is also demonstrated by the fact that his opinions are consistent with those of other reviewers of ATSDR's water models, including the Navy, the NRC, and Dr. Prabhakar Clement's published critiques in the journal *Groundwater*. *See, e.g.,* June 19, 2008, Navy Letter to ATSDR, D.E. 370-5; 2009 NRC Rep., D.E. 372-3, at 50 ("Without historical geochemical data, the uncertainty associated with many of the input parameters (such as the biodegradation parameters) could be very high."); T. Prabhakar Clement, *Complexities in Hindcasting Models—When Should We Say Enough Is Enough?*, 49 Groundwater 620 (2010), D.E. 372-4, at 6 ("One of the important concerns that limit the use of bioreactive transport models at chlorinated solvent sites is the lack of problem-specific information on input parameters.").

Furthermore, Dr. Spiliotopoulos's testimony in this case is based on the totality of his experience as a civil and environmental engineer and his research on groundwater modeling. *See, e.g.,* Spiliotopoulos Rep., D.E. 377-3, at 1 ("To conduct my evaluation and render my expert opinions, I relied on my education, research, and professional experience."); Spiliotopoulos Dep. Tr., D.E. 377-2, at 244:10–17 (testifying that his opinion that there were insufficient data to conduct a reliable model calibration and uncertainty analysis was based on his professional judgment and experience). Dr. Spiliotopoulos employed reliable methodology in forming his opinions, and therefore, PLG's Motion should be denied.

III. Dr. Spiliotopoulos Properly Considered and Relied on Information Provided by Other Experts in in Informing His Own Opinions.

PLG next argues that Dr. Spiliotopoulos's opinions on two subjects are "neither helpful nor admissible" because they are "parroted opinions of other experts." Pls.' Mem., D.E. 377, at 13. PLG seeks to prevent Dr. Spiliotopoulos from testifying as to losses of volatile organic compounds in water during the water treatment process, and the earliest time at which PCE began entering the environment. *Id.* at 13–14. PLG alleges that Dr. Spiliotopoulos simply relied on the opinions of other experts in this litigation, without offering "additional findings." *Id.* However, Dr. Spiliotopoulos does not parrot the opinions of other experts as his own; rather, he relies on facts or data supplied by other experts. Given that an expert in Dr. Spiliotopoulos's field would reasonably rely on these types of facts and data in forming his opinions, this is permitted under Fed. R. Evid. 703.

A. Dr. Spiliotopoulos Relied on the Fact that Contaminant Losses Would Occur During Water Treatment, and Incorporated that Fact into His Own Opinions.

Contrary to PLG's assertion, Dr. Spiliotopoulos has not offered an opinion quantifying the losses of volatile organic compounds during the water treatment process. *See generally* Spiliotopoulos Rep., D.E. 377-3. Dr. Spiliotopoulos testified:

> Q: . . . Have you, yourself, performed any calculations regarding alleged volatilization losses at the water treatment plant?
> A: No, I have not, my calculations [e]nd at the treatment plant.
> Q: So are you relying on the calculations and the opinions of Dr. Hennet regarding the quantification of any alleged VOC losses at the water treatment plants?
> A: Yes, I do.

Spiliotopoulos Dep. Tr., D.E. 377-2, at 192:23–193:10. As his deposition testimony and report make clear, Dr. Spiliotopoulos is relying on Dr. Hennet's calculations for the general proposition that VOC losses occurred during treatment and incorporating that proposition into his own opinions.[3]

For example, Dr. Spiliotopoulos opines that ATSDR's reference to "finished water" or "groundwater that has undergone treatment" in its studies is more appropriately described as "concentrations in the influent to the treatment plant." Spiliotopoulos Rep., D.E. 377-3, at 30–31. That is because ATSDR "ignored contaminant losses that would occur during treatment." *Id.* at 30. Based on this understanding, Dr. Spiliotopoulos opined that "treatment of the influent to the treatment plant resulted in evaporative and other losses, reducing contaminant concentrations in the 'finished' water." *Id.* at 68–69. In support of this opinion, Dr. Spiliotopoulos relied both on Dr. Hennet's calculations, as he testified at deposition, and on his reading of ATSDR's report, as evidenced by the citation which follows this proposition. *See id.* at 30. For this reason, PLG's Motion should be denied.

B. Dr. Spiliotopoulos Relied on a Historian to Determine a Historical Fact, then Incorporated that into His Own Opinions.

Also contrary to PLG's assertion, Dr. Spiliotopoulos did not offer the opinion that the PCE source release date at ABC One-Hour Cleaners was incorrect without "additional corroboration, validation, or explanation." Pls.' Mem., D.E. 377, at 13 n.3. As Dr. Spiliotopoulos testified at deposition, he relied on the report of the United States' expert historian, Dr. Brigham, to support the proposition that the off-base dry cleaner began operating in June of 1954. Spiliotopoulos Dep. Tr., D.E. 377-2, at 223:2–18. Dr. Spiliotopoulos also testified that he reviewed for himself the documents Dr. Brigham cited. *Id.* Dr. Spiliotopoulos properly relied on a historian to search and interpret the historical record. *See vonRosenberg v. Lawrence*, 413 F.

[3] Despite PLG's challenge to this opinion, PLG's expert, Dr. Sabatini, also opines that contaminant losses would occur during water treatment. *See* Sabatini Rebuttal Rep., D.E. 374-5, at 13–14 (opining that the percentage loss of VOCs of interest during water treatment was "less than 6 to 12%").

Supp. 3d 437, 450 (D.S.C. 2019) (collecting cases) (finding that historians generally possess the specialized knowledge to identify, review, and synthesize voluminous historical texts).

Dr. Spiliotopoulos then incorporated this expert's information into his own opinions by explaining how the earlier contamination start date impacted ATSDR's water models. For example, Dr. Spiliotopoulos wrote that "the impact of this discrepancy in release start dates is that the PCE plume reached the water supply wells sooner in ATSDR's model." Spiliotopoulos Rep., D.E. 377-3, at 36. Moreover, to demonstrate the impact on model outputs of changing the PCE release start date and other suggested corrections, Dr. Spiliotopoulos ran a modified version of ATSDR's simulation. *Id.* at 39–41. This analysis compared the results of ATSDR's original model with Dr. Spiliotopoulos's corrections, based, in part, on a later contamination start date. *Id.* This is clearly the type of information that an expert like Dr. Spiliotopoulos reasonably relies upon. Fed. R. Evid. 703.

In support of the proposition that Dr. Spiliotopoulos's opinions on contaminant losses during water treatment and the contamination start date should be excluded, PLG cites to *In re Davol*, 546 F.Supp.3d at 676, and *Funderburk v. S.C. Elec. & Gas Co.*, 395 F. Supp. 3d 695, 721–22 (D.S.C. 2019). Pls.' Mem., D.E. 377, at 13-14. In *In re Davol*, the Southern District of Ohio acknowledged that experts may "base an opinion on another expert witness for a point of expert knowledge not personally possessed," but may not "simply parrot another expert's opinion." 546 F.Supp.3d at 676 (internal quotations omitted). The court, in fact, declined to exclude the opinions of an expert, even though the expert did not independently validate the findings of another expert before relying on them. *Id.* at 675–76. This is because the expert in *In re Davol* also made "many of his own findings, which [were] well-supported by scientific literature and his own testing and experience." *Id.* at 676.

As with the expert in *In re Davol*, Dr. Spiliotopoulos is taking data points supplied by experts in different fields into consideration in forming his ultimate opinions. *Id.* at 675–76. Dr. Spiliotopoulos is then incorporating that data into his own opinions, offering context or performing new analysis using that information.

In *Funderbunk*, the District of South Carolina excluded as unreliable the opinion of an expert based only on his review of another expert's report. 395 F. Supp. 3d at 721–22. Unlike the expert in *Funderbunk*, Dr. Spiliotopoulos has not simply repeated opinions that another expert is prepared to provide. *Id.* Rather, Dr. Spiliotopoulos reviewed the documents that support the information provided by other experts in addition to their reports. He then utilized that data to inform his own opinions. Accordingly, Dr. Spiliotopoulos's opinions related to contaminant losses during treatment and the PCE release start date should not be excluded.

IV. Dr. Spiliotopoulos's Opinion on Well HP-634 is Reliable, and PLG's Attack on This Opinion is Based on their Disagreement with His Ultimate Conclusion, Not His Methodology.

Finally, PLG seeks to exclude Dr. Spiliotopoulos's opinion that ATSDR misinterpreted a water quality sample taken from well HP-634 on January 16, 1984. Pls.' Mem., D.E. 377, at 14. PLG argues that Dr. Spiliotopoulos's analysis of this issue is "not based on sufficient facts or data, nor is it the product of reliable principles and methods" because Dr. Spiliotopoulos relied on: (1) Dr. Hennet's analysis of the issue, (2) the fact that HP-634 is upgradient from contamination sources, and (3) other samples taken at that well around the same time. *Id.*

PLG does not explain how or why Dr. Spiliotopoulos's reliance on these three sources is insufficient or unreliable. Rather, they argue that Dr. Spiliotopoulos ultimately reached the wrong conclusion from those sources. *See generally id.* at 14–16. In support of this, PLG cites their own expert rebuttal report five times. *Id.*

For example, PLG asserts that Dr. Spiliotopoulos offered an opinion on the water quality sample "without the identification of a reliable methodology, performance of any calculations or measurements, or citation to authority . . . ." *Id.* at 15. In support of this argument, PLG cites the rebuttal report of their own expert, Dr. Konikow, who does not identify any employed methodology, perform any calculations or measurements, or cite to any authority in reaching the opposite conclusion. *See* Konikow Rep., D.E. 377-6, at 21–23. Rather, both experts rely on general principles of hydrogeology to reach differing conclusions from the same data. *See id.*

This is plainly a dispute between the Parties' experts on the interpretation of the same sampling data, not a dispute over the reliability of Dr. Spiliotopoulos's testimony. PLG asks this Court to exclude Dr. Spiliotopoulos's testimony not because it is irrelevant or unreliable, but because PLG's experts disagree with it. This is not a proper basis for the exclusion of testimony under Fed. R. Evid. 702. *Bresler v. Wilmington Tr. Co.*, 855 F.3d 178, 195 (4th Cir. 2017); *see also Funderburk*, 395 F. Supp. 3d at 721 (finding that a party's *Daubert* challenge improperly focused on the way in which an expert interpreted data, not the methodology underlying the opinion).

In *Bresler*, the defendant challenged the plaintiffs' expert accountant on the basis that his calculations were erroneous and used an improper discount rate. 855 F.3d at 195–96. The Fourth Circuit affirmed the trial court's refusal to exclude the testimony, holding that, "[t]o determine whether an opinion of an expert witness satisfies *Daubert* scrutiny, courts may not evaluate the expert witness' conclusion itself, but only the opinion's underlying methodology." *Id.* at 195. The Fourth Circuit further stated that "questions regarding the factual underpinnings of the expert witness' opinion affect the weight and credibility of the witness' assessment, not its admissibility." *Id.* (cleaned up). As in *Bresler*, PLG is challenging Dr. Spiliotopoulos's interpretation of the sampling data because the result is unfavorable to them. This argument is inapposite under the Fed. R. Evid. 702 analysis, and PLG's Motion should therefore be denied.

CONCLUSION

For the foregoing reasons, the United States requests that the Court deny PLG's Motion for an Order Excluding Certain Opinions of Alexandros Spiliotopoulos, Ph.D.

[Signature page to follow.]

Dated: June 4, 2025

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CERTIFICATE OF SERVICE

I hereby certify that on June 4, 2025 I electronically filed the foregoing using the Court's Case Management/Electronic Case Files system, which will send notice to all counsel of record.

/s/ Giovanni Antonucci
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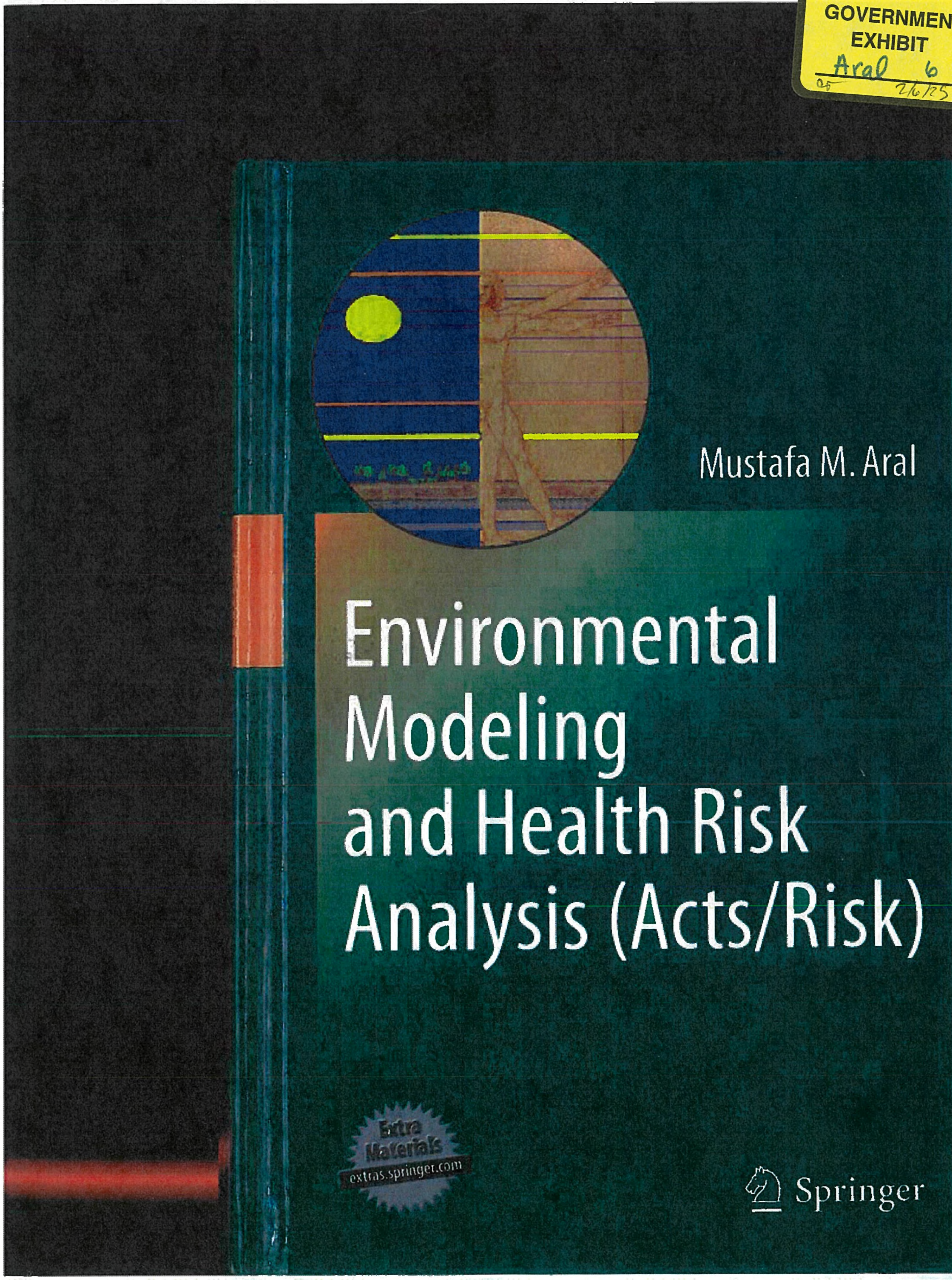
EXHIBIT 1

GOVERNMENT EXHIBIT
Aral 6
2/6/25



$$\sum \text{Mass flux in} - \sum \text{Mass flux out} \pm \sum (\text{sources/sinks}) = 0 \qquad (1.3)$$

Most of the models that are used in contaminant transformation and transport simulations, which are based on the conservation of mass principle, can be studied as deterministic models. That is, these models will yield one expected outcome at a spatial point and time, based on a given set of initial and boundary conditions and a set of parameters used in defining the process. In this approach one assumes that there is no uncertainty in conceptualization, data, model structure or the scale selected. It is well established in the literature that there are numerous uncertainties in each phase of the modeling effort, which may lead to the predictive uncertainty. To address uncertainty issues, models may also be used in a probabilistic sense, yielding not only the expected outcome, but also the variance of that expected outcome. In the probabilistic analysis of the models reviewed in this book, the Monte Carlo approach will be adopted to address uncertainty issues. There are also more recent approaches that can be categorized as non-probabilistic analysis or possibilistic analysis. The possibilistic approach has demonstrated that it can be employed in addressing uncertainty in environmental or health risk modeling where the uncertainty is heuristic. The possibilistic approaches include the Fuzzy systems approach (Kosko 1997; Kentel and Aral 2004; Kentel and Aral 2005), will not be covered in this book but the reader is referred to the above references since this type of analysis is important health risk analysis.

1.2 Environmental Modeling Concepts

A review of the modeling field indicates that several environmental models with varied degrees of complexity and different simulation objectives are available in the literature. One problem with most of these models is that it is often very difficult to implement them. These difficulties are due in part to the inaccessibility of the computer codes used in the solution, and in part to the problem-oriented design employed in the development of these models and codes. Thus some of these models are either never used or used by few users who have access to their computational platforms.

Models and model building is at the core of environmental management studies and significant time and effort must be spent to make proper decisions to appropriately represent the system being modeled. Several authors have discussed extensively the importance of models and model building in their books on scientific methods (Rosenbluth and Wiener 1945; Bloschl and Sivapalan 1995; Schnoor 1996). The following statement can be considered to be a consensus:

> No substantial part of the universe is so simple that it can be grasped and controlled without abstraction. Abstraction consists in replacing the part of the universe under consideration by a model of similar but simpler structure. Models . . . are thus a central necessity of scientific procedures.

$\sum$ (sources/sinks) = 0 (1.3)

...transformation and transport ...of mass principle, can be studied ...yield one expected outcome at a ...and boundary conditions and a ...approach one assumes that ...model structure or the scale ...are numerous uncertainties ...to the predictive uncertainty. ...used in a probabilistic sense, ...variance of that expected ...reviewed in this book, the ...uncertainty issues. There are also ...non-probabilistic analysis or ...demonstrated that it can be ...health risk modeling where ...include the Fuzzy systems ...and Aral 2005), will not be ...references since this type

...mental models with ...are available in ...often very difficult ...accessibility of the ...-oriented design ...some of these ...access to their

...gement studies ...to appropri- ...discussed exten- ...on scientific ...1995; Schnoor

...without ...deration ...sity of

Thus, a scientific model can be defined as an abstraction of some real system, an abstraction that can be used for prediction and management purposes. The purpose of a scientific model is to enable the analyst to determine how one or more changes in various aspects of the modeled system may affect other aspects of the system or the system as a whole. Because models are not a precise and complete depiction of the real system, they need to be presented and analyzed in a computational environment which should include an analysis of uncertainty. Uncertainty analysis may take the form of sensitivity analysis, or for more complicated applications, statistical uncertainty analysis may be utilized. We should also emphasize the difference between two commonly used terms in modeling "uncertainty" and "variability." As expected they refer to two distinct concepts:

Uncertainty is a measure of the knowledge of the magnitude of a parameter. Uncertainty can be reduced by research, i.e., the parameter value can be refined through further experimentation or further data collection.

Variability is a measure of the heterogeneity of a parameter or the inherent variability in a chemical property. Variance cannot be reduced by further research, but a model can be developed such that it would mimic the variability of the parameter used in the model.

There are many advantages to the use of mathematical models. According to (Fishman 1996), these advantages are:

i. Enable investigators to organize their theoretical beliefs and observations about a system and to deduce the logical implications of this organization;
ii. Lead to improved system understanding;
iii. Bring into perspective the need for detail and relevance;
iv. Expedite the analysis;
v. Provide a framework for testing the desirability of system modifications;
vi. Allow for easier manipulation than the system itself permits;
vii. Permit control over more sources of variation than direct study of a system would allow; and,
viii. Analysis is generally less costly than observing the system.

On the other hand, there are at least three reservations one should always bear in mind while constructing and using a model (Rubinstein 1981). First, there is no guarantee that the time and effort devoted to modeling will return useful results and satisfactory benefits. Occasional failures are expected to occur because of limited resources allocated to modeling. More often, however, failure results when the investigator relies too much on the method and not enough on ingenuity in constructing the model. The proper balance between the two is the key to success in modeling. The second reservation concerns the tendency of the investigator to treat his or her mathematical description of the problem as the best representation of the reality. One should be open minded in understanding the limitations of the proposed model. The third reservation concerns the use of the model outside the predictive range of the model developed. When working with a model, care must be given to ensure that the analysis remains within the valid representation range of the model. These are important concepts of concern when working with models.

It is well known that model design, almost by definition, is a pragmatic process. The simulation objectives determine the basic form, usability, and generality of the model proposed. Further, an investigation of the various environmental models, approved by U.S. Nuclear Regulatory Commission Regulatory Guide (Till and Meyer 1983), which focuses on their usability and applicability in predicting the transport of effluents in a surface water environment following an accidental spill, clearly indicates the necessity of the availability of user-friendly and well documented computer models. In this book, a review of the most common environmental models used in environmental health risk assessment studies is provided for the groundwater, air and surface water pathways, along with a user-friendly software interface to implement them and to facilitate their use.

Environmental transformation and transport models are built for the following purposes: (i) to evaluate the transformation and transport of contaminants in the environment by quantifying physical, chemical and biological processes that affect migration; (ii) to evaluate dynamic point-of-contact concentration levels that may have occurred in the past, are occurring presently or will occur in the future; and, (iii) to evaluate the outcome of different scenarios under various loading or management action alternatives. Since determination of exposure concentrations to toxicants constitutes the first step in health risk assessment, and direct field measurements may not be always available environmental modeling is becoming more and more of a permanent part of environmental health risk assessment studies.

Among the models that are available for environmental modeling, the first category of models may be identified as empirical models. In these models the description of cause-and-effect relationships is based on observational data sets with minimum analytic understanding of how the system works based on the relationships developed through the analysis of the data. These models are tied to empirical constants obtained from field or experimental data which may become the source of considerable uncertainty in applications.

The other category of models may be identified as mechanistic models. When we express the cause-and-effect relationships for a certain process or a system in terms of mathematical equations (differential or algebraic), the resulting models are identified as mechanistic (deterministic). Mechanistic models, in principle, reflect our understanding of how the system works, and they are based on certain accounting principles such as conservation of mass, energy or momentum. The complexity of these models depends on the level of detail for a process in a specific model or the dimensionality of the model developed.

Model accuracy and reliability are two of the more important aspects of modeling, which should not be overlooked. If a model is to be accepted as a reliable predictive tool, the numerical error bounds generated in computation should be within acceptable limits, and the model should be calibrated regionally or locally using available data. Proceeding in this direction, much of the recent work done in environmental quality modeling has been oriented towards improving models and incorporating better numerical solution techniques, the accuracy of which by far surpasses the availability and accuracy of the field parameter data that have to be used with such models. Scarcity of the field data, especially in air, groundwater and

definition, is a pragmatic process.
usability, and generality of the
various environmental models,
Regulatory Guide (Till and
applicability in predicting the
following an accidental spill,
user-friendly and well docu-
of the most common environmen-
studies is provided for the
with a user-friendly software

models are built for the following
transport of contaminants in the
biological processes that affect
concentration levels that
or will occur in the future;
under various loading or
of exposure concentrations to
and direct field mea-
modeling is becoming more
risk assessment studies.
modeling, the first
In these models the des-
observational data sets with
based on the relation-
models are tied to empirical
may become the source of

models. When we
or a system in terms
resulting models are
in principle, reflect
based on certain account-
The complexity
specific model or the

aspects of model-
accepted as a reliable
computation should be
regionally or locally
work done in
models and
which by far
that have to be
groundwater and

surface water quality modeling, is well known to researchers and engineers working in this field. Currently there is some disagreement among researchers as to whether higher priority should be placed on still further developments in model sophistication or on parameter prediction to improve accuracy.

A very simplistic model may use a very crude definition of a physical process, with few parameters to define the process. A very complex model may use a very detailed definition of a physical process, with a significant increase in parameters that is used to define the process. Naturally, improved sophistication of models is associated with an increase in the number of model parameters. Since it is likely that many of the additional parameters included in the model would be defined only in qualitative terms or with lesser accuracy, a relatively more sophisticated model can be less reliable than a simpler version. On the other hand, some systems and some physical phenomena are so complex in nature that there is often little reason to believe that good simulations are possible with simplified representations. In such cases, the need for more detailed and realistic models should be clear. A simple and crude example can be found in the case of effluent transport models for a river system. Given our current understanding and knowledge of turbulence characteristics, secondary currents, roughness concepts and sediment transport characteristics of natural rivers, it may be overly ambitious to develop a three-dimensional effluent transport model for a river network system just because it is possible numerically. Going to the other extreme, if in order to simplify such a model, that is, in order to reduce the model's dependence on complex field parameters, if one ignores the diffusive transport terms while keeping the convective transport terms in the analysis, the reliability of the model becomes questionable, at least for certain problem types such as accidental spills of pollutants or daily cyclic variation of spills, as is the case in sewage output. Thus, it is not necessarily true that models become more accurate as more complex definitions are used to define the model's processes. Inaccuracies may also result from the increase in the number of parameters associated with the detailed definition of a process or system. As observed in many applications, the likelihood of accurately defining these parameters is very low, resulting in an inherent loss of accuracy for complex models. On the other hand simplifying models has pitfalls as indicated in the example above. Thus, in developing models, the optimum solution is between these two extremes. In an attempt to achieve this balanced goal, an effort is made in this book to introduce the reader to one-, two- and three-dimensional screening level models and analytical solutions to these models, which, in most cases, provide sufficient detail for understanding the bounds of the problem at hand at a screening level.

Evaluation of advection and dispersion of effluents in natural or manmade environments is a complex phenomenon, especially if an effort is made to cover all aspects of their evaluation. In an industrialized society, a great variety of pollutants may get mixed into groundwater, surface waters or air. Dissolved matters such as chemicals, radioactive materials and salt, solid matters such as sediments, and temperature gradients introduced by power plants can be cited as a few of the sources of environmental pollution. Different models are needed to describe the transport characteristics of different pollutants. Thus, in environmental mod building, the decision or selection of the contaminant type is the first step whic needs to be addressed. A conservative chemical behaves differently than a non conservative chemical. The stage of effluent transport is another variable th needs to be considered, since mathematical models describing initial mixin zones are considerably different than mathematical models that are used to evaluat conditions for well mixed zones. In building an environmental model, the thir variable to consider is the choice of model dimensions. Given the present knowledg in numerical and analytical methods, it is usually tempting to develop a three dimensional model, with the assumption that the parameters needed in implementing such a model are readily available. Thus, determination of the dimensionality o physical and kinematic parameters is the third complexity encountered in modeling transformation and transport of pollutants in natural or manmade environments Within this set of available choices and options the best approach to modeling is very difficult to identify. That is why modeling is considered to be both a science and art in the current literature.

In the course of time, a number of deterministic, empirical or stochastic models have been proposed to predict mass transport in multipathway environments such as air, groundwater and surface water. Contaminant transformation and transport models, as they are treated in this book, fall under the category of mechanistic models. These models are generic models which may be used in the analysis of a wide range of conditions and site specific applications. Mechanistic models may also be used in a statistical sense, in which case one or more of the parameters will be defined in terms of probability density functions. This approach would yield the outcome in terms of statistical (probability) distributions. This mode of analysis, i.e. Monte Carlo analysis, will be used extensively in this book. Stochastic models seek to identify the probability of the occurrence of a given outcome based on probabilistic variations that are introduced to the model. They may be used to identify the variability in output based on variability in input parameters or variability of the boundary conditions of the problem analyzed.

The environmental modeling field has its own terminology and associated definitions. A review of the important terms used in this field is given in Appendix 2. In addition to the definitions of the terminology given in Appendix 2, the acronyms and abbreviations given in Appendix 1 are commonly used in the environmental modeling literature. It is important for the reader to familiarize themselves with their definitions.

1.3 Environmental Toxicology

Chemicals on earth are plenty and diverse. In addition to their presence, the chemical industry worldwide manufactures and markets thousands of new synthetic chemicals each year. Thus, it is safe to say that we are constantly being exposed to natural or synthetic chemicals in our ambient environment. The task of of accidental radioactivity releases to power plant. Nuclear Regulatory Com-

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Chapter 2
Principles of Environmental Modeling

Everything should be made as simple as possible, but not simpler.
Albert Einstein

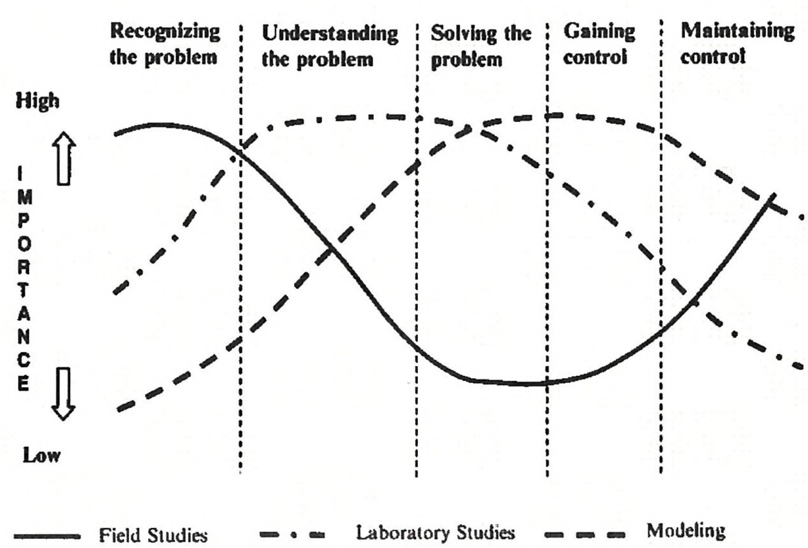
We have three primary scientific tools at our disposal to evaluate transformation and transport processes in the environment or to find solutions to environmental pollution problems and make decisions based on these solutions. These are, in no particular order: (i) direct field observations; (ii) laboratory scale tests and physical modeling studies; and, (iii) mathematical modeling. We recognize that transformation and transport processes that may occur in the environment and the accurate characterization of these processes both in the physical and also the mathematical domain are extremely complex. Thus, each of these tools has its appropriate place and mutually supporting role, as well as advantages and disadvantages of its use in understanding and solving environmental pollution problems.

It is well established in the literature that field observations tend to be costly but necessary. They are commonly used after the primary symptoms of the problems emerge at a contamination site. In this sense, they are extremely useful in characterizing the extent of the environmental problem, identifying its bounds or in evaluating whether the proposed remedial strategies are contributing to the solution of the environmental problem at a specific site. Laboratory studies, on the other hand, may be only useful in understanding the basic principles governing the problem at a micro or molecular scale. Findings and knowledge gained at this scale may experience significant problems in up-scaling the results to the field-scale analysis. Nevertheless, laboratory studies are extremely useful for both solving problems and for understanding micro scale issues at various stages of environmental pollution investigations and remediation.

In this book, among other topics, we will focus our attention on the use of mathematical modeling techniques in evaluating environmental transformation and transport processes. Thus it is important that we discuss problems we may encounter during model building and application, and the expectations we may have from a modeling study in an environmental application. First we should agree that mathematical models cannot help us in the problem recognition stage of an environmental pollution problem. However, they are very useful tools in the "gaining control" and "finding solutions" stages of our problem solution spectrum. They are cost effective and can be easily set up to test "what if" scenarios associated with a remedial application or a contamination problem. This cannot be easily studied with the other two scientific tools. The downside is the approximate nature of these tools which should always be kept in mind when their outcome is utilized. The level of contribution of each of these three tools to an analysis throughout the environmental problem solving spectrum is shown in Fig. 2.1.

Mathematical models are an abstraction of the environmental system and they are based on our understanding of the physical principles that govern the system. Since models are always going to be an abstraction of a system or a physical process, their outcome should always go through a careful and detailed interpretation stage before the results obtained from a model are determined to be representative of the behavior of the process or the system modeled (Fig. 2.2).

The purpose of mathematical model building and modeling is to simulate the behavior of the environmental system being modeled. Models are built to represent the system behavior in a controlled and cost effective computational environment. In this sense, modeling has become a common building block of most scientific applications. Using this tool we may observe, analyze, synthesize and rationalize the behavior of these systems under controlled conditions, and also we may evaluate the performance of the proposed solutions to an environmental problem. A common feature of all models is that they are all based on the "concept" of



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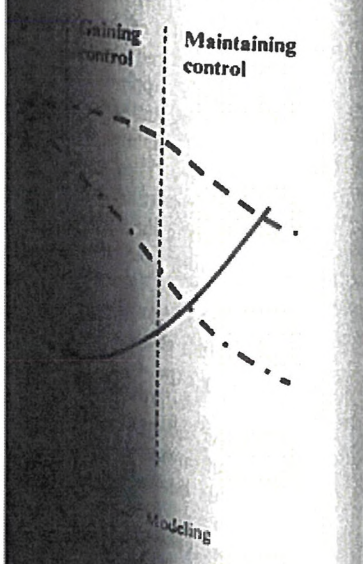

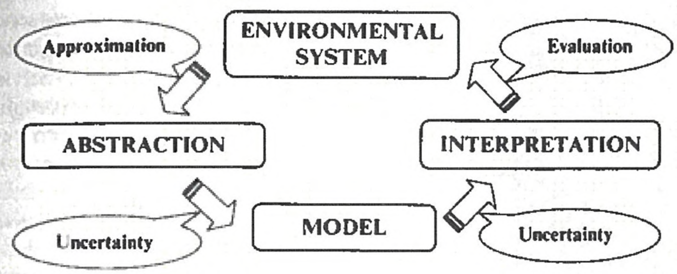

Fig. 2.2 Principles of modeling philosophy

simplification of the environmental system they are built to represent. This simplification may be achieved either through reducing the dimensionality of the system, elimination of less important processes that govern or affect the system, or through the introduction of simplified definitions for the parameters and variables that are used to describe the system. All of these or a selected subset of these simplifications are always observed in models built to represent an environmental process or an environmental system. Before we describe and make use of the models that are included in this text and also in the ACTS and RISK computational platforms, it is important that we review the modeling terminology from this perspective since it is necessary and extremely important for the reader to understand the limitations of models and modeling procedures in general. Otherwise, models or modeling may end up becoming a dangerous tool if their output is interpreted as the absolute truth without regard to the inherent simplifications and limitations they may have, or used as if they represent the environmental system under all circumstances. As a rule of thumb, modeling should always be considered to be a cost effective, efficient but approximate substitute for observing the modeled system behavior in its natural environment. Since observation of a process cannot always be achieved in a timely and cost effective manner, the models are here to stay among our scientific arsenal of tools as an important and alternative method.

The three evaluation tools identified above also differ from one another in the instruments that they may use to perform the analysis. In this sense, field study tools and laboratory tools are more closely related. Both of these methods may use electronic instrumentation to record and measure macro scale or micro scale processes. To provide a systematic procedure, these instruments may be linked to a computer or the observations can be done manually. On the other hand, computers are an essential component of all mathematical modeling studies. The language used in this analysis is primarily the language of mathematics. The interpretation of mathematics in the computer is done through coded systems, which nowadays can take the form of object or class oriented computer programming languages. As a simple definition one can say that a computer program written in any language to solve a mathematical problem is an orderly collection of coded instructions to the as software. The ACTS and RISK computational platforms, in this sense, can b identified as software that can be used in the modeling of multimedia environmenta transformation and transport problems and health risk analysis.

Finally, the analysis tools described above should always be used in coordinatio with one another. Field studies should support the laboratory studies or vice versa and mathematical modeling should support both of these efforts and vice versa. Th advantages of any one tool should be exploited to the utmost for the benefit o finding a satisfactory solution to the problem. The outcome of each tool should b checked and verified with the outcome of the other tool. In this sense, these tool should be viewed as complementing, rather than competing scientific methods.

2.1 Modeling Principles

Principal steps involved in modeling and the uncertainty and approximation introduced at each step are summarized in Fig. 2.2 in their simplest form. As a preliminary definition, one can say that to model is to abstract from the natural system a description which addresses a question we have posed for the system. All models are developed to answer a specific question about the system outcome. The use of models in a specific application cannot and should not go beyond the question posed during the model development stage. This is an inherent approximation and limitation that is involved in all models. After this stage several other uncertainties are introduced in model coding and analysis. Some of these uncertainties are associated with mathematical representations used in modeling and others are related to the choice of model parameter characterization during implementation. When the model is used in the simulation phase it may produce a significant amount of output. The evaluation of this output is identified as the interpretation stage. Thus the overarching goal of mathematical modeling is first to come up with an abstract representation of an environmental system and to characterize this abstraction in a mathematically consistent manner such that it yields easy to use and understandable representations of the outcome, and second to use the outcome to interpret the behavior of the modeled system within the bounds of the model. Within this sequence, approximations and uncertainties are introduced to the analysis at each stage as shown in Fig. 2.2.

A common aspect of all mathematical models is that there is an input and an output component. Outputs are tied to inputs in some mathematical sense which describes the behavior of the abstracted physical problem. Since all models are approximate representations of a natural system, they are commonly designed to accept only a subset of all possible inputs an environmental system may have. Consequently models can only generate a subset of outputs that is expected from an environmental system. In other words we can never see the complete output or picture of the modeled system. To the extend that the inputs are limited the outputs will be limited as well.

When completed, models are used in simulation. Simulations are done to provide the data necessary in decision making or in evaluating the behavior of nal platforms, in this sense, can be deling of multimedia environmental th risk analysis.

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the system that is modeled. Decision making is based on simulation results and simulations themselves should not be interpreted as decision making. Human interaction or other heuristic mathematical models are always necessary in decision making which will be based on the outputs obtained from a model. Simulation results generated by models only provide us with the pieces of the puzzle that will help us make the appropriate decision. Evaluating the behavior of the modeled system should also be interpreted the same way. Simulation output only gives us the pieces of the puzzle needed to evaluate the system behavior.

Developing abstracted conceptual systems and a computational code for the conceptual systems is the scientific part of the modeling effort which may introduce scientific uncertainties (Lemons 1996). Simulation can be identified as the labor intensive part. Interpretation of the outcome and decision making can be considered to be the artistic part of the overall modeling effort (Fig. 2.2).

Fallout in modeling is the tendency to model in too much detail rather than modeling a finite manageable abstraction. The key to avoid this pitfall is to model around a question that needs to be answered rather than shooting for a universal representation. A simple model can always be fine tuned (calibrated) to overcome the approximations introduced through simplification. As a rule of thumb the following are key elements of a successful modeling effort:

i. Understand the problem and clearly state the question that needs to be addressed.
ii. Evaluate existing models first, do not re-invent the wheel.
iii. Create a conceptual model that is logical and represents the conceptual model in consistent mathematical terms.
iv. In developing the model involve the user or think like a user.
v. Simplify the conceptual model, its mathematical interpretation and its user interface. This may lead to a trial and error process. Don't be shy of remodeling.
vi. When complete make sure that the model satisfies the objective and mission of the effort (see item 1).
vii. Design the simulations such that they provide answers to the question posed. Do not expect answers beyond the questions posed.
viii. Always remember that the purpose of modeling is the knowledge gained from a model and not the models themselves.

2.2 Model Building and Model Types

In model building the starting point should always be the identification of the goals of the modeling study. In this context, the following alternative goals can be cited:

i. The modeling study is going to be a scientific study in which different hypotheses regarding the governing principles of the study will be tested, dominant processes of the problem will be identified, bounds of the parameter ranges that define these processes will be quantified.

ii. The modeling study will be used to characterize a study area, i.e. to determine the site specific parameters that are associated with the processes included in the model.

iii. The model will be based on well established basic principles and will be used as a predictor either to reconstruct a past event or simulate the future behavior of an environmental process at a site.

iv. The model will be used as an imbedded predictor (slave application) within a master application and will be used repeatedly to supply data to the master application. Simulators used in optimization models or statistical applications (Monte Carlo analysis) fall into this category and may include the goals identified in item 3.

v. The model will be used to support engineered decisions that will be made at a site and the purpose of modeling is the evaluation of the performance of these decisions.

Given the list of goals stated above, we should expect the following characteristics to be the dominant features of the model built. In case 1 the model should be considered to be modular. The construction and solution method of the model should allow for inclusion or exclusion of certain sub-processes to the model with relative ease. Complexity of the model is of no concern in these applications. The purpose is to include all possible and important sub-processes into the model. In case 2 the model will be used in the inverse modeling sense. In these applications, independent parameters of the model are treated as unknowns and dependent variables are treated as known variables and the solution process is based on the intrinsic relation between the independent and dependent variables. These models are not expected to include many independent parameters; otherwise, the solution becomes impossible. These models rely heavily on accurate field data on dependent variables. In case 3 the model will be used as a predictor. In this case the model should include all the dominant sub-processes of the problem studied, independent of the availability of accurate definitions of the parameters that are necessary to define these sub-processes. During simulation these parameters will be varied anyway, and the model output sensitivity with respect to these parameters will be documented. In case 4 the model should yield results efficiently with minimal computation time. For this to happen one may either resort to closed form solutions (analytical) or simplified models that may not include complex sub-processes which may exist in the overall system. In this case, as another simplification alternative, one may choose to represent complex processes in their simplest approximate forms. For example, in contaminant transformation and transport analysis one may either choose not to include chemical reactions, that is only simulate transport of a conservative chemical behavior, or represent this chemical reaction as a first order reaction for a single species application. These are all acceptable simplifications for a class of applications. For case 5 the model will be used to test the "what if" scenarios with respect to an environmental decision that

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will be made at a site. In this sense, the model should definitely include the best and most accurate definition of the sub-process that is being evaluated at the site. Secondary sub-processes that may not influence the main process may be given lesser importance in the construction of the model. In all of these cases the dimensionality of the model is determined based on the available data and the complexity desired by the model builder. Whatever the goal of the modeling study is, one always has to recognize that the tool at hand is an approximate representation of the process that is being modeled.

From the perspective of inclusion of some mathematical reasoning into the analysis of system behavior, as a general rule, the three procedures discussed above are available: (i) physical modeling (laboratory); (ii) empirical modeling (laboratory and field scale); and, (iii) computational modeling. In physical modeling the natural system being modeled is duplicated by a scaled model which is geometrically and dynamically similar to the large scale system. In this case the mathematical processes are used to arrive at similarity laws that are based on the similarity of the force ratios which govern the behavior of the natural system. Observations are conducted on the scaled model and the results are projected to the large scale system, again using the same similarity laws. Mathematical reasoning behind empirical models is based on induction supported by the data collected in field or laboratory studies. In a sense, the empirical approach represents our declaration that the system modeled is very complex, or not fully understood, and that the only alternative left for us is to represent the system by the use of a black box approach. In some cases, the empirical equations that are developed may even end up being dimensionally non-homogeneous, such as the case of the well known Manning's equation in open channel flow analysis. This is a further an indication that the natural process modeled is not well understood. Sometimes modelers get around the issue of dimensional non-homogeneity by attributing dimensions to the proportionality constants that are used in the empirical model. This of course may lead to a dimensionally homogeneous equation but does not resolve the issue of how well we understand the process that is modeled. Some of these models are so well established in the technical literature that we do not question their validity, such as the Manning's equation used in open channel flow analysis, which is sometimes inhibiting. In other cases statistical methods are used to verify the predictions made from these models.

Finally, computational models (mechanistic modeling) are based on deductive reasoning. Derivation of these models is tied to fundamental principles that govern the system. In these models, more often than not, it is impossible to include all sub-processes affecting the behavior of a complex system. Thus, as stated earlier, these models commonly include simplifying assumptions which should be accounted for when they are put to use. In this sense, although these models are generic models, i.e. can be used in any large or small scale modeling study, we use calibration methods to overcome this deficiency and adjust the model response to a site or an application to represent a specific behavior. A classification of mathematical models is given in Fig. 2.3.

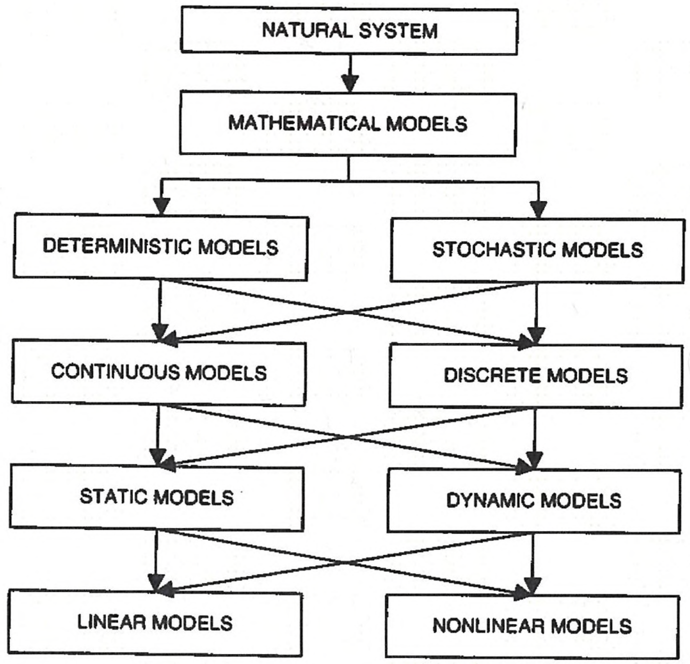
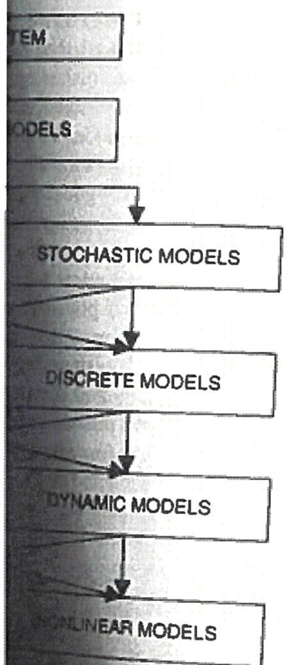


Fig. 2.3 Classification of mathematical models

The distinction in this classification is that deterministic models always produce the same output for a given input. On the other hand stochastic, a word of Greek origin which is synonymous with "randomness" and means "pertaining to chance," describes models in which a random set of inputs producing set of outputs that are interpreted statistically. Thus, stochastic is often used as the counterpart of the modeling exercise which is "deterministic," which means that random phenomena are not involved. Continuous models are based on the general mathematical property obeyed by mathematical objects and imply expressions in which all elements of the objects are within a neighborhood of nearby points. The continuity principle applies to dependent as well as independent variables of a mathematical model and implies smoothly varying properties, i.e. at least continuous first derivatives. Their counterpart is discrete models in which mathematical objects are not continuous and abrupt variation of parameters is expected. Static and dynamic refer to the dependence of the model on the independent variable "time". Static models are time independent and dynamic models are time dependent. Mathematical models that satisfy both the principles of additivity and homogeneity are considered to be linear models. These two rules, the additivity and homogeneity – taken together, lead to the possibility of the use of the principle of superposition. Nonlinear models are mathematical systems in which the behavior of the system is not expressible as



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a linear operation of its descriptors. Nonlinear models may exhibit behavior and results which are extremely hard (or impossible) to predict under current knowledge or technology.

Mathematical model building is a complex process. However, a systematic path to successful model building can be defined and this path should be followed to avoid common mistakes that may render the overall effort fruitless. Following the commonly accepted principles, a model building path is given in Fig. 2.4. The modeling framework, as identified in Fig. 2.4, includes standard checks and balances that should be used in model building, no matter what the purpose of the model may be. Remodeling is always an integral path of this process to improve on what is being built.

2.3 Model Calibration, Validation, Verification and Sensitivity Analysis

Since all models are simplifications of a complex system they need to be calibrated and verified before they are used in simulation. Validation and sensitivity analysis of models is also another concept that needs to be addressed and clarified. The literature on the definition and use of these concepts is abundant and sometimes confusing. Most of the confusion is associated with the concept of validation of models (Gentil and Blake 1981; Tsang 1991; Mayer and Butler 1993; Power 1993; Oreskes et al. 1994a, b; Rykiel 1996). For example validation is sometimes considered essential (Power 1993) and sometimes validation of models is considered impossible (Starfield and Bleloch 1986; Oreskes et al. 1994a, b), and some technicians of this field indicate that models can only be invalidated (Holling 1978; McCarl 1984). Due to this confusion and conflicting definitions it is appropriate to review the meaning of these terms as well as the interpretation of the very important terms "calibration" and "sensitivity analysis" from a mathematical modeling perspective.

Model Calibration: Models include parameters and constants that need to be associated with values. These parameters are used as input to the mathematical models to produce numerical output. Ideally, these parameters should have a good definition and a physical basis for the environmental system studied. Usually these parameters either are calculated using the mathematical representation of this physical basis, or they are measured in field or laboratory studies. More often than not, however, the values of these parameters are unknown or only known approximately. Thus a range of these parameters can be input to a model to yield the best outcome when compared to an observation made in a field or laboratory study. Thus, appropriate values of the parameters are needed in the model to achieve the appropriate output that is observed at a site. Calibration of a model can then be identified as the stage where we adjust the parameters of the mathematical model such that the model agreement is maximized with respect to the observation data we have on the modeled system. In this sense, model calibration is fine tuning the

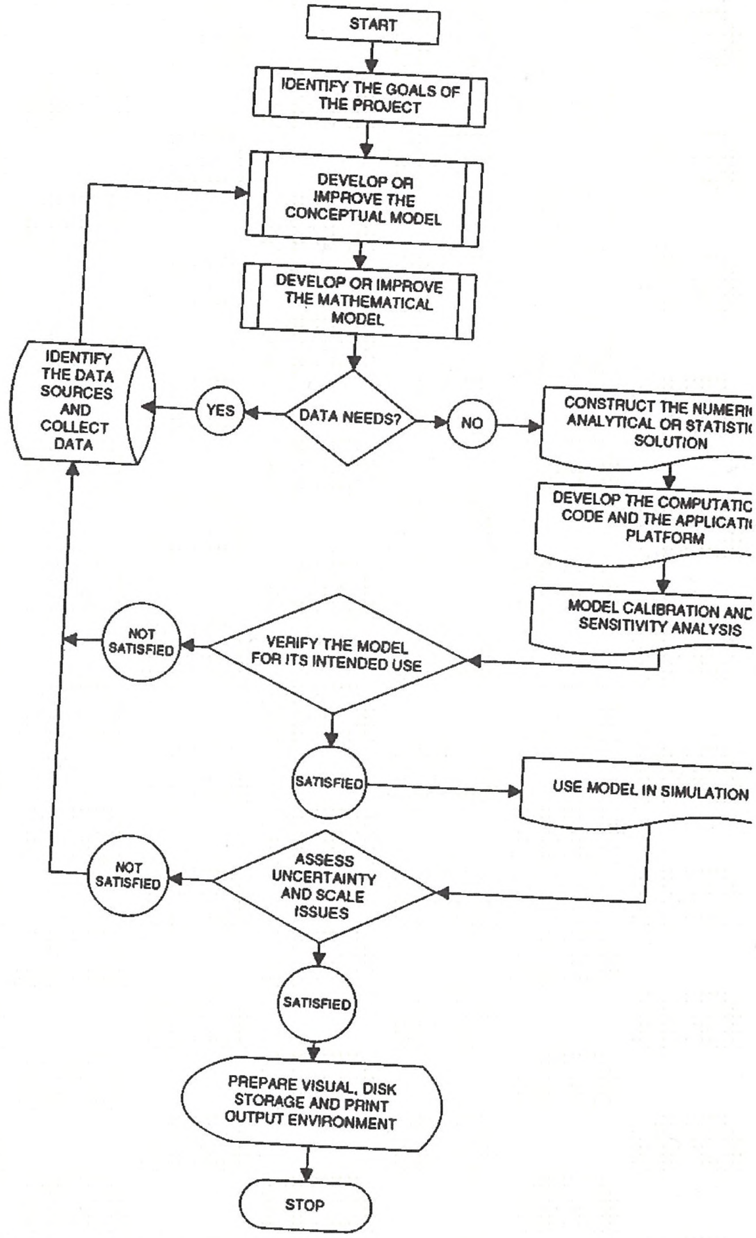
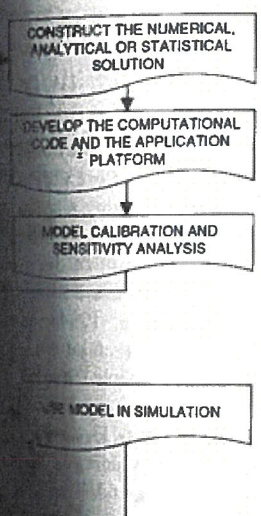


Fig. 2.4 Model building framework



model to a set of data on the natural system. Calibration of a model can be done manually, i.e. by trial and error adjustment of model parameters or it can be automated using stochastic procedures. Success in calibration, or lack of it, may yield information on how reasonable the modeler was in conceptualizing the natural system and mathematical representation of the conceptualized system. If a model fails to calibrate, it may mean that the conceptualization and mathematical representation stages need to be revisited. This also emphasizes the importance of remodeling in model development (Fig. 2.4). Calibration should not be interpreted as an inverse modeling technique which is used in parameter identification problems. Calibration procedure basically readies a model for its further use in simulation.

Model Verification: The confusion pointed out earlier may originate from the way we use the words 'verify' and 'validate'. In ordinary language, they are synonymous. From the perspective of modeling terminology these two words are used to describe two distinct concepts. Verification is a demonstration that the modeling formalism is correct. There are two types of verification avenues in modeling: (i) mechanical; and, (ii) logical. The former is associated with the debugging process of a computer program and in mathematical models, which shows that the mathematics and their numeric calculations are mechanically correct. A more important and difficult verification issue is the latter: showing that the program logic is correct. Some logical errors in a model may only appear under special circumstances that may not routinely occur in an application. Thus, these errors may not be recognized in routine applications of the model. Verification is thus a technical matter that identifies how faithfully and accurately ideas are translated into a computer code or mathematical formalisms (Law and Kelton 1991). In the case of large (complex) models, it is extremely difficult to verify that the model is entirely accurate and error free under all circumstances. Models are thus generally verified for the normal circumstances in which they are expected to be applied, and such verification is presumed inapplicable if the model is run outside this range. It is important to distinguish verification logic which relates to program operation from conceptual model logic which refers to the ecological logic used in structuring the model. Verification of models is needed in both aspects.

In summary, verification of a model is the stage at which we quantify the predictive capability of a mathematical model. This may be accomplished through a comparison of the output obtained from a model, which is based on input data, or with a set of observation data we have on a natural system which is based on the same input data. It is important to note that the observation data used in the calibration stage should be distinctly different from the data set used in the verification stage. That is, the data used for verification should be such that the calibration parameters should be fully independent of the verification data. The verified model can then be used for forecasting.

Model Validation: The absolute validity of a model can never be determined (NRC 1990). This statement is a strong reference to the impossibility of validation of a model. This reference to the impossibility of validation of models is somewhat relaxed in a statement in which Hoover and Perry state that: "The computer model is verified by showing that the computer program is a correct implementation of the logic of the model. Verifying the computer model is quite different from showing that the computer model is a valid representation of the real system and that verified model does not guarantee a valid model" (Hoover and Perry 1989), which implies that "validity" of a model is a possibility. To clear this confusion we need to expand on these definitions.

The term model uncertainty which is linked to model validation is used to represent lack of confidence that the mathematical model is a "correct" formulation of the problem solved. Model uncertainty exists if the model produces an incorrect result even if we input the exact values for all of the model parameters. The best method for assessing model uncertainties is through model validation (Hoffman and Hammonds 1994), a process in which the model predictions are compared to numerous independent data sets obtained. Thus, as is the case with verification, validation is better understood as a process that results in an explicit statement about the behavior of a model. A common definition of validation can be the demonstration that a model, within its domain of applicability, possesses satisfactory accuracy consistent with the intended application of the model (Sargent 1984; Curry et al. 1989). This demonstration indicates that the model is acceptable for use. But that does not imply that it represents the absolute truth for the system modeled, nor even that it is the best model available. For operational validation, this demonstration involves a comparison of simulated data with data obtained by observation and measurement of the real system. Such a test cannot demonstrate the logical validity of the model's scientific content (Oreskes et al. 1994b). Validation only demonstrates that a model meets some specified performance standard under specified conditions. It is often overlooked that the "specified conditions" include all implicit and explicit assumptions about the real system the model represents as well as the environmental context it covers. That is, that a model is declared validated only within a specific context, is an integral part of the certification. If the context changes, the model must be re-validated; however, that does not invalidate the model for the context in which it was originally validated (Rykiel 1996). Validation is a "yes" or "no" proposition in the sense that a model does or does not meet the specified validation criteria. These criteria may include requirements for statistical properties (goodness-of-fit) of the data generated by the model, and thus are not necessarily deterministic. Ambiguous situations may develop when the model meets some but not all of the criteria. The criteria may need to be prioritized, and the model may be validated with respect to these priorities. Because modeling is an iterative process, validation criteria may evolve along with the model. This is more typically the case with scientific research models than with engineering models. From a technical perspective, a valid model is the one whose scientific or conceptual content is acceptable for its purpose.

Sensitivity Analysis: Sensitivity analysis, on the other hand, can be considered to be a component of simulation through which the modeler evaluates the response of the model to changes in input parameters or boundary conditions of the model.

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el validation is used to ; a "correct" formulation lel produces an incorrect lel parameters. The best lel validation (Hoffman lictions are compared to e case with verification, in an explicit statement f validation can be the ility, possesses satisfac- ne model (Sargent 1984; model is acceptable for ute truth for the system erational validation, this with data obtained by test cannot demonstrate ces et al. 1994b). Valida- d performance standard e "specified conditions" real system the model That is, that a model is gral part of the certifica- ; however, that does not inally validated (Rykiel se that a model does or ria may include require- generated by the model, tions may develop when criteria may need to be these priorities. Because evolve along with the arch models than with del is the one whose

d can be considered aluates the response ditions of the model.

Sensitivity of model response to the input data and parameters of the model and the model output obtained is critical and must be quantified both during calibration and verification stages. Through this process, discrepancies between the model output and observation must be minimized to the extent that is possible by identifying and minimizing sources of error. These error sources include measurement errors, conceptual error in model development and approximation errors that may exist in mathematical representations. The goal of sensitivity analysis is to estimate the rate of change in the output of a model with respect to changes in model inputs or parameters. This knowledge is important for:

i. Evaluating the applicability range of the model developed;
ii. Determining parameters for which it is important to have more accurate values; and,
iii. Understanding the behavior of the system being modeled at critical points of solution – possibly at singular points.

The choice of the method of sensitivity analysis depends on:

i. The sensitivity measure employed;
ii. The desired accuracy in the estimates of the sensitivity measure; and
iii. The computational cost involved in calculating the error.

Consider a contaminant transport model in which several parameters P_i characterize the contaminant concentration C as a continuous function in a linear mathematical function, $C = f(P_1, P_2, P_3, \ldots, P_n)$ from which some reference value of C can be calculated, $C_o = f(P_1^o, P_2^o, P_3^o, \ldots, P_n^o)$. For this case some of the more common sensitivity measures S_{ij}, which can be used, are:

$$
\begin{aligned}
&\text{Local gradient measure:} && S_{ij} = \frac{\partial C_i}{\partial P_j^i} \\
&\text{Normalized gradient measure:} && S_{ij} = \frac{\partial C_i}{\partial P_j^i}\frac{P_j^i}{C_i} \\
&\text{Normalized variance measure:} && S_{ij} = \frac{\partial C_i}{\partial P_j^i}\frac{std\{P_j\}}{std\{C_i\}} \\
&\text{Expected value measure:} && S_{ij} = C_i[\mathrm{E}(P_i)] \\
&\text{Extreme value measure:} && S_{ij} = \left\{\max C_i\left(P_j^i\right), \min C_i\left(P_j^i\right)\right\} \\
&\text{Normalized response measure:} && S_{ij} = \left(C_o - C_i\left(P_j^i\right)\right) / C_i(P) \\
&\text{Average response measure:} && S_{ij} = \sum_j C_i\left(P_j^i\right) / \sum_j P_j^i
\end{aligned}
\tag{2.1}
$$

where E is the expected value measure and the expected value of P_i is the mean value of parameters P_i.

Based on the choice of the sensitivity measure and the variation in the mc parameters, methods of sensitivity analysis can be broadly classified into one of following categories:

i. Variation in parameters or model formulation: In this approach, the mode run for a set of sample points (different combinations of parameters concern) or with straightforward changes in model structure (e.g., model resolution). Sensitivity measures that are appropriate for this type analysis include the response from arbitrary parameter variation, normaliz response and extreme value measure. Of these measures, the extreme valu are often of critical importance in environmental applications.
ii. Sensitivity analysis over the solution domain: In this case the sensitivi involves the study of the system behavior over the entire range of paramet variation, often taking the uncertainty in the parameter estimates into accour
iii. Local sensitivity analysis: In this case the model sensitivity to input ar parameter variation in the vicinity of a sample point(s) is evaluated. Th sensitivity is often characterized through gradient measures.

The discussion of the terms calibration, verification, validation and sensitivit analysis given above outlines the basic principles involved in any modeling an model development effort. There are numerous models that are available in th scientific literature which may be used to analyze a multitude of physical processes These models are sometimes identified as off-the-shelf models from which the user may download a code and implement it in a specific application that is of interest tc the user. Here, it is important to note that the user must be fully aware of the limitations and the application range of the model used for the intended purpose. Ir certain cases some of these models have become so common in the literature that we no longer truly check the application rage of the model downloaded and we do not verify if the model truly fits the physical problem being modeled. In certain cases there are model applications in which the physical system modeled is restricted just to fit the system into a readily available off-the-shelf model. This practice can be characterized as fitting a physical system to a model rather than fitting a model to a physical system. This approach in modeling should be avoided at all times, at all cost. One should never try to define a physical system based on the limitations of the model that may be readily available. One should always remember the hierarchical steps involved in modeling. The description of the physical system always comes first, while the development of the model to describe the system follows behind.

2.4 Model Scales, Error and Uncertainty

The term "scale" refers to the characteristic spatial or temporal dimensions at which entities, patterns, and processes can be observed and characterized to capture the important features of an environmental process. Borrowing from cartography and the variation in the model broadly classified into one of the

n: In this approach, the model is combinations of parameters of in model structure (e.g., in are appropriate for this type of parameter variation, normalized e measures, the extreme values ental applications.

n: In this case the sensitivity er the entire range of parameter rameter estimates into account. model sensitivity to input and point(s) is evaluated. This measures.

validation and sensitivity volved in any modeling and that are available in the de of physical processes. models from which the users lication that is of interest to be fully aware of the he intended purpose. In in the literature that downloaded and we do modeled. In certain system modeled is shelf model. This a model rather than should be avoided system based on the always remem- of the physical to describe the

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concepts, as environmental modelers we define scale as having two components: grain and extent. The former corresponds to the smallest spatial and temporal sampling units used to gather a series of observations or perform a computation. Extent is the total area or time frame over which observations or computations related to a particular grain are made (O'Neill and King 1998). For example, this may be defined for an observation of a hydrologic process, or it may be defined for a modeled environment (Klemes 1983; Bloschl and Sivapalan 1995; Singh 1995). All environmental processes, large-scale or small-scale, have their own characteristic scales of reference, which are necessary to capture details of the processes modeled or observed. Independent of the size of the model used, all environmental models, as covered in this book, are based on some mathematical representation of a physical process which is scale dependent (Gupta et al. 1986). When analysts use large-scale models to predict small-scale events, or when small-scale models are used to predict large-scale events, problems may arise (Fig. 2.1).

From groundwater flow and contaminant transport models to flow and transport in river channel networks to overland flow in a watershed or air shed models, the environmental processes occur over a wide range of scales and may span about ten orders of magnitude in space and time. When we attempt to model an integrated system the first question one should ask is: "if it is necessary to link all components of the environmental cycle into one system model?" The answer to that question should not be based on whether these components are separable or not. In a global sense they are not. However, the answer to that question should be based on whether one wants to separate them or not depending on the goals of the project and the importance of the contribution of the sub-processes to the understanding and evaluation of that goal. For example, if one is not interested in observing or reflecting the effect of one subcomponent on the other, then one can easily isolate an environmental process and analyze that subcomponent alone. For example, there are numerous groundwater flow and contaminant transport models which are extensively used in the literature just to study groundwater systems (McDonald and Harbaugh 1988; Aral 1990a, b). In their analysis, groundwater would receive input from surface water, but the reverse influence cannot be considered. On the other hand, if the simulation of multipathway interaction of an environmental process is the goal, than an integrated systems modeling approach is a must, and therein one encounters the difficulties of integration over scales (Gunduz and Aral 2005).

The transfer of data or information across scales, or linking sub-process models through a unified scale, is referred to in the literature as "scaling." Up-scaling consists of taking information from smaller scales to derive processes at larger scales, while downscaling consists of decomposing information at one scale into its constituents at smaller scales (Jarvis 1995). In the context of absolute space and time, scaling primarily involves a change in the geometric and temporal structure of the data and their corresponding attributes. In using the term "absolute scale" here we are referring to the definitions used in an Eulerian coordinate system in which distances between points in time and space are well defined geometric and differential entities. Thus, linking sub-process parameters within the well defined rules can be considered to be objective and to be independent of one's viewpoint or frame of reference in solving a problem. From a relative perspective, scaling becomes a more complex task than it would be in an absolute framework. In a relative scale framework one focuses on the sub-environmental processes and defines space and time as a measure of the relationship between these sub-processes. In a way one can interpret this definition as a Lagrangian frame of reference.

The relative scales concept represents the transcending concepts that link processes at different levels of space and time. It entails a change in scale that identifies major factors operational on a given scale of observation, their congruency with those on lower and higher scales, and the constraints and feedbacks on those factors (Caldwell et al. 1993). With this definition, one can observe that two processes that occur in close proximity by the definition of an absolute scale may be very distant from one another in terms of a relative scale sense. An example could be the case of the two hydrologic processes, overland flow and saturated groundwater flow, that normally are separated by an unsaturated zone. These two hydrologic processes could be close to each other in an absolute sense, but in terms of their interaction with one another, they could be very distant in a relative space and time frame of reference, due to limiting transfer rates that may exist in the unsaturated zone. In such cases, when scaling is considered the relative frame of reference should take precedence.

As expressed by Jarvis (1995), what makes scaling a real challenge is the nonlinearity between processes and variables scaled, and the heterogeneity in the properties that determine the rates of processes in a relative frame of reference. Therefore, it is important to realize that scaling requires an understanding of the complex hierarchical organization of the geographic and temporal worlds in which different patterns and processes are linked to specific scales of observation, and in which transitions across scales are based on geographically and temporarily meaningful rules (Marceau 1999).

Scaling and its effects on environmental modeling are commonly linked to the heterogeneity of the system modeled. However, this link should also include the refinement necessary to resolve the mathematical nonlinearities incorporated into an environmental process. Scale differences necessary to resolve nonlinearities, such as the nonlinearities introduced by the dependence of the higher order chemical reaction terms on rate constants as opposed to the easily solved differential equation that accompanies the first order reaction rates can be given as an example. Thus nonlinearity and heterogeneity are the two important factors that need to be considered in scaling. The greater the degree of heterogeneity and nonlinearity, the smaller the scale one would have to use to represent such variability or resolve such nonlinearity.

The other component of scaling effect arises in the interpretation of field data. Integrated environmental models use a variety of parameters to represent the characteristics of an application domain. However, data on large scale domain parameters are often limited. The task is then to transform this spatially limited data to a scale which can be used as an input in large scale applications. The question to answer here is what scale one should use to represent this data without losing accuracy during the extrapolation process. As the spatial scale of the model increases from a small area to a large area, the extrapolation of limited spatial data

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... cending concepts that link pro- ... s a change in scale that identifies ... rvation, their congruency with ... and feedbacks on those factors ... observe that two processes that ... olute scale may be very distant ... An example could be the case of ... turated groundwater flow, that ... These two hydrologic processes ... in terms of their interaction ... space and time frame of ... in the unsaturated zone. In ... frame of reference should take

... real challenge is the non- ... and the heterogeneity in the ... relative frame of reference. ... an understanding of the ... temporal worlds in which ... of observation, and in ... and temporarily mean-

... commonly linked to the ... should also include the ... incorporated into an ... nonlinearities, such as ... order chemical reac- ... differential equation that ... ple. Thus nonline- ... to be considered in ... the smaller the ... such nonlinearity. ... ation of field data. ... to represent the ... scale domain ... atially limited ... lications. The ... data without ... of the model ... spatial data

to a large scale system would introduce errors in the analysis from the start, which should be avoided.

An optimum scale of an integrated model should then reflect the "functional scale" (Aral and Gunduz 2003), that provides a compromise between the resolution of nonlinearities of the mathematical model, availability and extrapolation of data and the heterogeneity of the system. Thus, in environmental modeling, in order to resolve scale and scaling problems, one should first attempt to answer the following fundamental questions:

i. What is the appropriate scale of study for a particular hydrologic sub-process in the study?
ii. How close these sub-processes are in a relative frame of reference?
iii. How can one accurately transfer the necessary information from one process scale to another for closure?

When answering these questions we end up with a so called compromised scale which we identify as the functional scale (Aral and Gunduz 2003).

Scales of Sub-processes: Different scales of space and time govern the flow and transport phenomena in the environmental cycle. For an integrated environmental model these scales vary by several orders of magnitude in terms of the idealization of the solution domain, the computational step size and the simulation extent that is necessary to capture the important aspects of the process modeled as well as the proper scales that are necessary to interpret the input data.

One important aspect of integrating various sub-processes is the selection of the method applied to solve the equations that define the system. In this regard, coupling via iterative solution and coupling via simultaneous solution are the most advanced levels of solving the sub-processes in an integrated fashion. In iterative solutions, each sub-process model is solved separately and integrated sequentially by using the contributions from the other sub-processes. When each sub-model is solved, the common parameters linking these systems are checked for convergence (i.e., deviation from the previous solution). If the solutions of these common parameters are not sufficiently close, the solution procedure is repeated until the differences between subsequent solutions are below a pre-determined convergence criteria. This iterative coupling approach is slow, especially when more than two sub-processes are linked together. On the other hand this approach would be less restrictive from the perspective of scaling concerns since each sub-process can be analyzed within its own scale.

In the simultaneous solution approach, all sub-process models are solved together using a common idealization scale and a common time step. In this approach all sub-model solution matrices are grouped in a single matrix structure and solved at once. Hence, this method requires the use of the smallest idealizations and smallest time step of all sub-models, which may be impractical for the coupling processes requiring idealization and time steps from the two extremes. For example linking the two processes such of saturated groundwater flow and transport and the unsaturated groundwater flow and transport falls into category. Attempting to solve such a system simultaneously results in small idealization scales and time steps and creates incompatibility between systems. For example, unsaturated flow requires small time steps in the order of seconds to describe the vertical movement of moisture in the unsaturated domain whereas the groundwater flow can be run with time steps in the order of days. If a simultaneous solution technique is used to couple these two systems, then the entire system would need to be run with the time step of the unsaturated zone. This condition is computationally costly and inefficient for the groundwater flow and contaminant transport simulations. On the other hand, this approach is more accurate than the iterative method since it does not involve improvement of the solution by iterating on the common parameters of the two sub-models (Gunduz and Aral 2003a, b, c, d). Thus the wide array of time scales required to simulate efficiently the flow and transport processes in the environment is the most important problem of environmental modeling. The incompatibility of the sub-process time scales makes the overall coupling of the system difficult and sometimes impractical.

Suggested Solutions to Scaling Problems in Integrated Environmental Modeling: In large scale environmental modeling, the scale issues and up-scaling or down-scaling difficulties outlined above must be resolved if we are to develop an integrated representation of these processes. Technicians in the field of modeling believe that these problems can be resolved through some compromises. In order to develop an order of importance list of compromises that can be considered, the modeler has to introduce concepts such as:

i. Order of importance;
ii. Domain of importance;
iii. Functional scales; and,
iv. Hybrid modeling concepts.

In an integrated modeling effort, the order of importance ranking of different sub-processes can be achieved by the analysis of the data associated with the environment under study. For example in an environment where the groundwater table is high and the unsaturated flow zone thickness is very small, it may not be a significant loss of accuracy if the unsaturated zone is not modeled as a distributed model but instead is represented in terms of lump parameter models. Similar order of importance analysis evaluation can be made for overland flow as well as for the contaminant transport modeling. In arid regions or for rainfall events which are not significant, the contribution of this component may also be represented in terms of lumped parameter models rather than distributed parameter models. However, in all cases the groundwater flow zone and the river channel flow zone will play an important role in the overall watershed hydrology and should be included in the analysis in terms of distributed models for improved accuracy of representation of these sub-processes in the integrated environmental model.

The domain of importance concept arises from the analysis of the type of the problem solved. For example, if the concern is the transport of a certain contaminant source in the watershed, and if this source is not located in the unsaturated zone, then modeling the hydrologic processes in the unsaturated zone in detail with the use of distributed models may not be necessary. Similarly, if it is known that the

...ple, unsaturated flow requires ...be the vertical movement of ...roundwater flow can be run ...us solution technique is used ...would need to be run with the ...is computationally costly and ...transport simulations. On the ...rative method since it does ...on the common parameters ...d). Thus the wide array of ...and transport processes in ...ironmental modeling. The ...s the overall coupling of

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...ranking of different ...associated with the ...re the groundwater ...all, it may not be a ...ed as a distributed ...dels. Similar order ...as well as for the ...ts which are not ...nted in terms of ... However, in all ...ne will play an ...included in the ...resentation of

...type of the ...ain contami- ...unsaturated ...detail with ...wn that the

flux of water between the unsaturated and the saturated zones is negligible, there is no need to complicate the analysis by including the unsaturated zone. On the contrary, there may not be any need to model the saturated groundwater flow when the top few meters of the soil column are of concern to the modeler and the groundwater table is at a much deeper elevation. Such simplifying judgments are a direct consequence of the available data for the domain modeled and are essential components of engineering evaluations to be made in a modeling study.

The functional scales concept is associated with the limitations of the integrated domain scales. If all sub-processes are important in an integrated environmental modeling effort and the use of distributed models is the goal, then one has to analyze the final time and space scales that are necessary to combine these models in an integrated system. At that point one may clearly see that this is not possible given the computational difficulties or long computation times required to solve the system. In such cases a compromise, as described earlier, is again the only solution.

Data availability is another limiting aspect of the integrated large scale environmental modeling studies. More often than not, field data is not available to justify the use of a distributed model at a large scale. This may be observed at a sub-process scale, in which case there is no reason to force a distributed model application for that sub-process as well. Otherwise, unforeseen errors will be introduced to the modeling effort. The availability of the alternative models, which range from simplified to more detailed system representations, or from small scale to large scale models, aids in evaluating the applicability of the low resolution models. If the results of the low resolution models (either in detail or in scale complexity) agree closely with those of the high resolution models, then the low resolution models are preferable, since they typically require lower computational resources and lesser input data.

Given the limitations on computational resources, computational methods and data limitations, the outcome of the integrated modeling compromises, as discussed above, is clearly to direct the modeler towards the use of hybrid models in integrated environmental modeling. In these models, lumped parameter models are used along with distributed parameter models to develop an integrated system.

Uncertainty and Error: The discussion above leads to uncertainty and error associated with environmental models and modeling (Figs. 2.2 and 2.5). Uncertainty in transformation and transport models arises in the following two stages of modeling: (i) model conceptualization or model building; and, (ii) model application. As mentioned above, model building uncertainty arises under several conditions, including the following:

i. When alternative sets of scientific or technical assumptions for developing a model exist (model structure);
ii. When models are simplified for purposes of tractability (model detail – inclusion or exclusion of sub-processes); and,

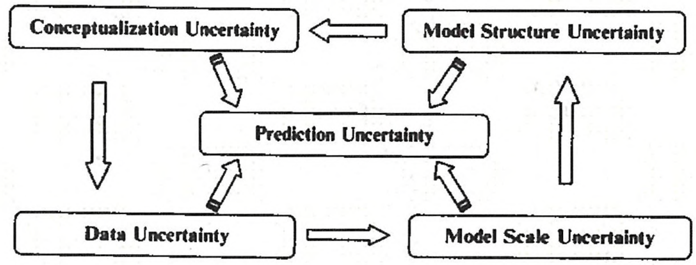


Fig. 2.5 Uncertainty sources in modeling

iii. When a coarse discretization and of data is used to reduce the computation demands of the model (model resolution – scale issues and statistical uncertainty).

The uncertainties and errors in simulation may arise from uncertainty in model inputs or parameters (i.e., parametric or data uncertainty). When a model application involves both model and data uncertainties, it is important to identify the relative magnitudes of the uncertainties associated with data and model formulation. Such a comparison is useful for focusing resources where they are most appropriate (e.g., data gaps versus model refinement).

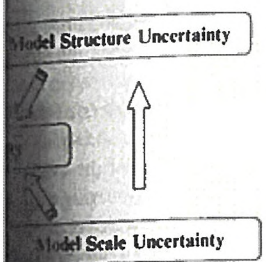
Uncertainties in model parameter estimates may stem from a variety of sources. Even though many parameters could be measured or calculated up to some degree of precision, there are often significant uncertainties associated with their estimates. Some uncertainties and errors can be identified as:

i. Random errors in analytic devices used in field and laboratory measurements;
ii. Systematic biases that occur due to imprecise calibration;
iii. Extrapolation of data from one scale to another; and,
iv. Inaccuracy in the assumptions used to infer the actual quantity of interest from observations of a "surrogate" parameter or estimation of parameters based on mildly representative samples.

Uncertainty analysis should not be confused with sensitivity analysis. In uncertainty analysis one attempts to describe the entire set of possible outcomes of a model together with their associated probabilities of occurrence. In sensitivity analysis one determines the relative change in model output given changes in model input values.

Model errors can be evaluated by analyzing the variation in dependent variables in the model based on the variation of the independent variables of the model, i.e. the parameters of the model. Taylor series analysis is commonly used in this analysis. Since Taylor series will be used in several different contexts in this book it is appropriate to introduce a review of this topic.

A Taylor series is the sum of functions composed of continually increasing derivatives. For a dependent variable such as contaminant concentration $C(P)$,



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...lly increasing ...ration $C(P)$,

which depends on only one independent parameter P, the value of the function $C(P)$ at points near P_o can be approximated by the following Taylor series,

$$C(P_o + \Delta P) = C(P_o) + \frac{\Delta P}{1!}\left(\frac{dC}{dP}\right)\Big|_{P_o} + \frac{(\Delta P)^2}{2!}\left(\frac{d^2C}{dP^2}\right)\Big|_{P_o} + \frac{(\Delta P)^3}{3!}\left(\frac{d^3C}{dP^3}\right)\Big|_{P_o} + \cdots + \frac{(\Delta P)^n}{n!}\left(\frac{d^nC}{dP^n}\right)\Big|_{P_o} + R_{n+1} \tag{2.2}$$

in which P_o is some reference value of the parameter P, ΔP is the increment in the parameter P and $(P_o + \Delta P)$ identifies the point where the concentration C is to be evaluated $C(P_o + \Delta P)$ and R_{n+1} represents the remainder terms of a Taylor series expansion. In Eq. (2.2) the derivatives of $C(P)$ are evaluated at P_o. Using the definition above a first order approximation can be defined by keeping the terms of the Taylor series up to and including the first derivative as follows,

$$C(P_o + \Delta P) \approx C(P_o) + \Delta P\left(\frac{dC}{dP}\right)\Big|_{P_o} \tag{2.3}$$

Similarly, the second and third order approximations to Taylor series are given by

$$C(P_o + \Delta P) \approx C(P_o) + \Delta P\left(\frac{dC}{dP}\right)\Big|_{P_o} + \frac{(\Delta P)^2}{2!}\left(\frac{d^2C}{dP^2}\right)\Big|_{P_o} \tag{2.4}$$

and

$$C(P_o + \Delta P) \approx C(P_o) + \Delta P\left(\frac{dC}{dP}\right)\Big|_{P_o} + \frac{(\Delta P)^2}{2!}\left(\frac{d^2C}{dP^2}\right)\Big|_{P_o} + \frac{(\Delta P)^3}{3!}\left(\frac{d^3C}{dP^3}\right)\Big|_{P_o} \tag{2.5}$$

respectively. The accuracy of a Taylor series approximation improves as the order of the Taylor series increasesas shown in Eqs. (2.3) through (2.5). In these equations an approximate relationship is implied since the remainder terms of the Taylor series are omitted. Referring back to Eq. (2.3), we can associate the point P_o with the mean value of the parameter distribution P. Accordingly, the Eq. (2.3) will represent the value of C(a space is needed here such as) C around the mean value of P. We can now write an equation for the variance of the concentration C, using the definition of variance of $C(P)$ about the mean P_o, $S^2(C(P_o))$.

$$S^2(C(P)) = S^2(P)\left(\frac{dC}{dP}\right)^2\Big|_{P_o} \tag{2.6}$$

where $S(P)$ is the sample standard deviation, and $S^2(P)$ is the sample variance around the mean P_o. Eq. (2.6) implies that the variance in the dependent variable (uncertainty) is a function of the variance (uncertainty) in the parameter P, the sensitivity of the dependent variable to the changes in the parameter P around its mean, $\left(\frac{dC}{dP}\right)^2\Big|_{P_o}$ and the variance in the parameters $S^2(P)$.

For a multivariate relationship, $C(P^i)$, $i = 1,2,3,\ldots,n$ the first order Taylor series expansion, Eq. (2.3), can be written as,

$$C\left(P_o^1 + \Delta P^1, P_o^2 + \Delta P^2, P_o^3 + \Delta P^3, \ldots, P_o^n + \Delta P^n\right) \approx C\left(P_o^1, P_o^2, P_o^3, \ldots, P_o^n\right) + \sum_{i=1}^{n} \Delta P^i \left(\frac{\partial C}{\partial P^i}\right)\Bigg|_{P_o^i} \quad (2.7)$$

which yields the variance relation,

$$S^2\left(C\left(P_o^1, \ldots, P_o^n\right)\right) \approx \sum_{i=1}^{n} S^2\left(P_o^i\right)\left(\frac{\partial C}{\partial P_o^i}\right)^2 + 2\sum_{j=1}^{n-1}\sum_{i=j+1}^{n}\left(\frac{\partial C}{\partial P_o^i}\right)\left(\frac{\partial C}{\partial P_o^j}\right) S\left(P_o^i\right) S\left(P_o^j\right) \Phi\left(P_o^i, P_o^j\right) \quad (2.8)$$

where P_o^i is the mean of the ith parameter, $S\left(P_o^i\right)$ and $S^2\left(P_o^i\right)$ are the standard deviation and the variance of the ith parameter around its mean respectively, $S^2\left(C\left(P_o^i\right)\right)$ is the variance of $C(P^i)$ around the means P_o^i, $\Phi\left(P_o^i, P_o^j\right)$ is the correlation coefficient in a linear least squares regression between the parameters P^i and P^j (Crow et al. 1960; Reckhow and Chapra 1983; Bogen and Spear 1987; Ayyub and McCuen 1997; Conover 1999).

Monte Carlo analysis is another method used to evaluate parameter sensitivity to solution. Since this approach is used extensively in the ACTS and RISK software we will review this topic in more detail in Chapter 7.

2.5 Methods of Solution

Some mathematical models are relatively simple and their solution can be achieved using analytical methods, sometimes referred to as a closed form solution. Numerical calculation based on an analytical solution can be exact or approximate. Its accuracy depends on the complexity of the analytical solution. More complex models may require numerical solution which are all inherently approximate solutions to the problem. Both solutions will require computer based calculations to relate the model inputs to model outputs.

As indicated above statistical models and statistical calculations are also a necessary component of a modeling exercise. If not explicitly used in the modeling

$S^2(P)$ is the sample variance
ance in the dependent variable
ainty) in the parameter P, the
in the parameter P around its
(P).
$3, ..., n$ the first order Taylor

$$..., P_o^n + \Delta P^n)$$

$$\left(\frac{\partial C}{\partial P^i}\right)\Bigg|_{P_o^i} \qquad (2.7)$$

$$S(P_o^i)S(P_o^j)\Phi(P_o^i, P_o^j) \qquad (2.8)$$

and $S^2(P_o^i)$ are the standard
around its mean respectively,
$\Phi(P_o^i, P_o^j)$ is the correla-
the parameters P^i and P^j
Spear 1987; Ayyub and

parameter sensitivity to
ACTS and RISK software

can be achieved
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approximate solu-
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itself, statistical methods will become an important component in the sensitivity, calibration and verification phases of the modeling exercise.

In the case of the ACTS and RISK software analytical solutions will commonly be employed, since the models included in these software platforms are considered as screening models and in that sense are simpler representations of the modeled system. To perform sensitivity analysis the ACTS and RISK software also includes a Monte Carlo module in all models where the models can be run in a stochastic mode.

2.6 Modeling Terminology

The modeling field is quite a diverse field of science. It is important for the professionals working in the environmental health field to familiarize themselves with various concepts and methods employed in this field to be able to understand the outcomes and limitations of environmental modeling and use them in environmental health analysis appropriately. For this purpose a review of the following references are recommended, (Gentil and Blake 1981; USEPA 1984; Starfield and Bleloch 1986; Hoover and Perry 1989; Law and Kelton 1991; Tsang 1991; Mayer and Butler 1993; Oreskes et al. 1994b; Lemons 1996; Schnoor 1996; Abdel-Magid et al. 1997; Saltelli et al. 2000; Anderson and Bates 2001; Nirmalakhandan 2002; Aral and Gunduz 2003). The acronyms used in this field are given in Appendix A of this book. The list of terms and their definitions given in Appendix B are also included in this book to familiarize the reader with the terminology used in the environmental modeling field as a starting point.

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