ENVIRONMENTAL MODELING
Vol. II

Computer Methods and Software for Simulating Environmental Pollution and its Adverse Effects

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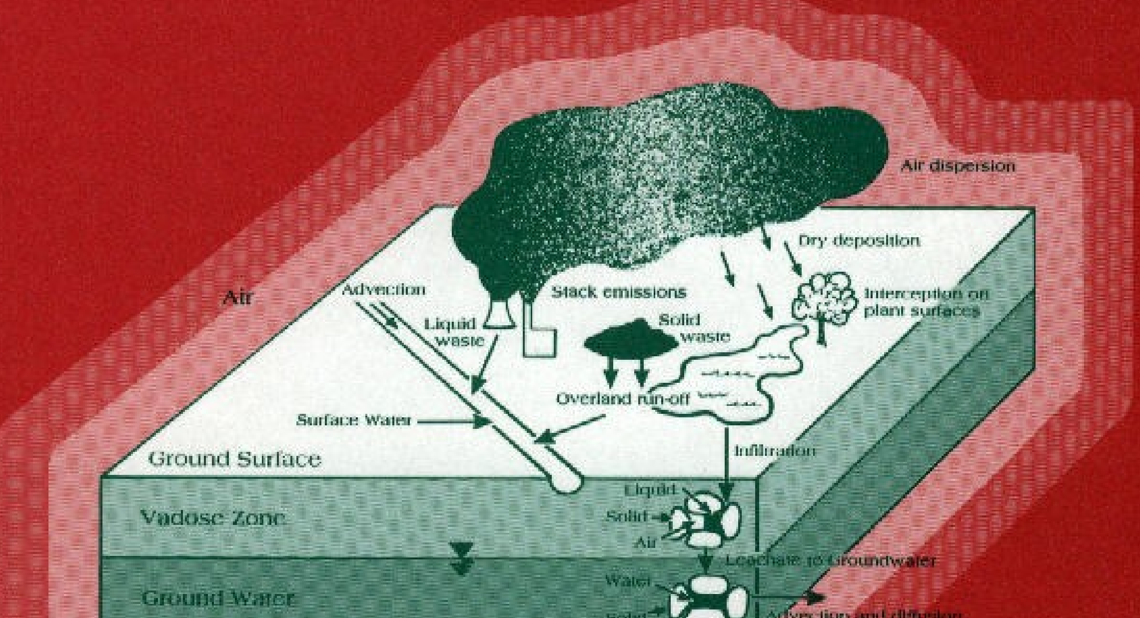

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Chapter 1

Introduction to Environmental Modeling

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Abstract

This chapter provides an introduction to the topic of Environmental Modeling and a guide to the contents of the first two volumes of the book series.

Key words

Environmental Modeling, Pollution, Computer Simulation, Numerical Modeling, Computer Sciences, Research and Development

1. A Definition of Environmental Modeling

Definitions are always difficult. They can be too general and therefore mean nothing. Or they can be too specific and, consequently, restricting and incomplete. It is useful and necessary, however, to try to give a working definition to the subject of this book series.

Let us start with "environment" and "environmental sciences." Can we define the topics that are encompassed by the adjective "environmental?" The risk of giving a too general definition is very high. I have been working for more than two decades on environmental research and I can hardly imagine any subject that is more multidisciplinary than the environment. Understanding environmental issues requires a good knowledge of their physical, chemical, and biological aspects for both small and large geographical scales. Pollution control requires good engineering practice. Environmental simulations require sophisticated mathematical and numerical techniques and the use of state-of-the-art computational facilities. Environmental adverse effects cover the damage to human health, ecological impacts, and aesthetic damage, such as visibility degradation and the deterioration of art work. Environmental planning requires accurate cost-benefit analyses and econometrical assessments. Environmental issues often require a good understanding of laws and regulations, since these laws affect industrial and urban development, influence the environmental business, and drive environmental litigation. Last but not least, environmental problems pose new philosophical questions by challenging industrial managers–often under community pressure–to do what is ethically right and not just what is legally acceptable. In summary, physics, chemistry, biology, engineering, computing, medicine, psychology, art, economy, law, and philosophy all play an intricate and interconnecting role in the study of the environment.

But let us try to be more specific. Obviously, environmental sciences are the scientific disciplines that cover the *environment* in which we live. They therefore could be seen as synonymous with "earth sciences" or "planetary sciences" and include traditional and well established scientific fields such as geology, oceanography, and meteorology. However, in my opinion the label "environmental" gives a precise, new connotation. After all, to the best of my knowledge, environmental studies have been labeled "environmental" starting only in the 1960s even though "earth sciences" have been around for a much longer time.

The unique connotation that the label "environment" adds is the role of anthropogenic factors and manmade pollution. For example, oceanographic research aiming at a better understanding of ocean currents can be seen as a study in the field of oceanography; but if the same study aims, as a principal goal, at the understanding of transport and fate of oil spills of anthropogenic origin, the study is better characterized as environmental. Therefore, I would like to propose the following definition:

> *Environmental sciences are defined as the sciences that cover, as their principal subject, anthropogenic pollution: its generation, its transport and fate in different environmental media (air, water, soil, groundwater, and biota), and its adverse effects.*

We could use a more general characterization, if you prefer, and define environmental sciences as those concerned with pollution, population control, and resource conservation. But I would resist the temptation of "contaminating" environmental sciences with the inclusion of controversial and ideological topics that better belong to the political and economic sciences and to the agendas of modern-day environmentalism.

Now what about modeling? Let us first clarify that "modeling" may indicate two very different things: 1) small-scale physical or laboratory modeling, and 2) mathematical or numerical modeling. We are all very familiar with the first type of models since we all have played with *toys*. What are toys? Well, most toys are a small-scale representation of real things (e.g. cars, cranes, people, appliances, rifles, and tanks). And these toy "models" do possess some of the characteristics and physical properties of the original objects they try to imitate; for example, a toy boat does float on water and a toy crane is capable of lifting weights. A child discovers very soon, however, that the models are different from the real things. Even when the shapes and the colors of the models are very realistic, their structural behavior and response to external stimulation are different. For example, a toy car, even when built as an accurate small-scale representation of a real car, can withstand impacts and rollovers that would seriously damage a real automobile.

Physical models in environmental sciences are built to provide a tool for experimentation. For example, a physical model of a complex lagoon can simulate the expected behavior of the internal water currents if modifications are made to the lagoon structure. Similarly, a smog-chamber experiment in controlled laboratory conditions can lead to the identification and quantification of complex chemical reactions among atmospheric pollutants. Physical models are needed to understand some of the characteristics of a system that would be impossible to study otherwise. Moreover, physical models allow us to perform experimentation on small-scale replicas of large structures and entities, where the cost of experimenting directly on the real objects would be unaffordable.

Of course, physical models cannot replicate all the properties of the real system. For example, the laws that rule the transport of mass in the environment possess nonlinear terms (for example, viscosity). Therefore, any small-scale representation, no matter how sophisticated and detailed, will provide results that cannot perfectly replicate the real world. The scientific challenge is to understand, quantify, and minimize the inaccuracies of the physical models and use their simulation results with care.

This book series on environmental modeling does not exclude the topic of physical modeling. However, all the chapters so far deal with the second type of modeling approach: mathematical and numerical modeling. Historically, like many other sciences that originated from military needs, the science of mathematical modeling probably started with ballistic computations in the sixteenth century. The goal was to understand the trajectories of cannonballs and improve accuracy in hitting enemy targets. Under a set of simplifying conditions, equations were found that describe the trajectory of the cannonball. These equations were solved to provide an *analytical solution*, i.e. a *formula* that gives the point of impact as a function of the initial velocity and the shooting angle. These equations constituted a "mathematical model" of reality, i.e., the representation of physical properties solely with mathematical tools, pen, and paper.

In the last two centuries, scientists have been very successful in discovering new equations that describe reality. Differential calculus, in particular, has been the key mathematical tool in this endeavor. Equations representing reality became more and more complex and included fewer and fewer simplifying factors. Of course, finding new equations was only part of the problem. To be used for practical applications, equations needed to be solved. However, the more complex the equations representing reality, the more difficult it was to find analytical solutions. Scientists were capable of solving complex equations only in extremely simplified conditions, under steady-state, homogeneous assumptions, and in one or at most two dimensions.

Unfortunately, as far as environmental phenomena are concerned, the real world is three-dimensional, never at rest, and seldom homogeneous. However, in the last few decades, computers came to the rescue. The ability of electronic computers to perform hundreds, thousands, and today millions of operations per second has made it possible to solve the equations *numerically*. A numerical solution is not a general solution, such as an analytical solution. A numerical solution can only describe a specific set of conditions. However, we can solve any set of equations numerically, no matter how complex. This is the source of the success of numerical simulations and the use of computers in science. Computers have become indispensable tools to scientists in general and environmental scientists in particular. More precisely, computer techniques are more than just tools. Computer analysis is a method, an attitude, a research direction, a science in itself (the "third branch" of science), and, more importantly, an extension of the scientist's thinking power.

2. Models and Modelers versus the Rest of the World

As a modeler, my interactions with the rest of the world have been complex and sometimes frustrating. In most cases, I have received gratifying and competent appreciation of modeling work and a fair understanding of what models can do. But in other cases things have been complicated. Often, in certain circles, I have found it difficult to explain what computer modeling is. This is because computer illiteracy in certain segments of the population, including medium-high management levels, is still not uncommon today in spite of the clear progress made in the last decade by the personal-computer revolution.

In many cases, I faced a profound skepticism for the capabilities of environmental models. How many times I heard, even from scientists, the simplistic statement that "models do not work," or the other famous statement claiming that models are just "garbage in, garbage out!" In some cases, I have experienced profound diffidence toward the modelers themselves. They were seen as desk scientists working in isolation, living in a special world detached from the "real world," playing with computer toys, and unable to connect and interact with the rest of the environmental community, especially with the people who go into the field and understand what pollution really is from practical, direct experience.

Of course, any criticism has some fraction of truth. Nevertheless, I have never believed (and never will believe) that walking with boots on a polluted landfill or visiting a monitoring station can improve my ability to simulate groundwater pollution or perform a statistical analysis of the collected data. However, a few months ago, to better explore this issue, I mailed a questionnaire to a few dozen scientists. I selected these individuals because of their general environmental expertise. They are well-established environmental experts who are not modelers but know about environmental modeling and interact with computer modelers. The questionnaire asked the following three questions:

1) *What is your current opinion of environmental models? Has your opinion changed in the last 2-3 years? Which role do you see for environmental modeling in the future?*

2) *How do you characterize your interactions and communications with environmental modelers? Can you specify the positive and negative aspects of your current and past working relationship with modelers?*

3) *In your opinion, is there competition, contrast, or misunderstanding between computer modelers and other environmental professionals? If so, what are the roots of the problem and what can be done to improve communication and collaboration?*

I received few answers, but all were from very qualified people. A summary of the answers is presented below.

1) Most people who responded indicated that their opinions about models have risen. ("My opinion of current atmospheric models has improved in the last 2-3 years; so have the models.") They generally have a good opinion of models ("Models are more useful than ever"), especially after the arrival of low-cost, high-performance workstations that allow easier application of the most advanced models. Some people pointed out that models are sometimes grossly misused but clarified that this is not the fault of the modeler who developed the code. Some people criticized the "PC mentality," described as insistence on using personal computers instead of more powerful workstations. Almost anyone expected models to improve in their ability to represent reality and become more user-friendly. ("We will eventually come out of the present dark ages into a time when modeling is a proper tool that can be trusted to give believable answers.") Some people suggested that models should refuse to run when the input parameters are not appropriate and should optimize themselves given a few data points. (This particular feature is called "data assimilation" and is discussed at lengths in Chapter 9 of this volume).

2) The responses characterized the relationship with modelers as relatively good, but with some problems. The major criticism is that some modelers seem to believe more in their modeling simulations than in the actual measurements. Moreover, it was claimed that some modelers "seem to have rigged the input data" to obtain the results they wanted. Another criticism is that modelers "sometimes create model parameters that cannot be measured for calibration/validation." Regarding the last statement, I must add that it is apparently true that some model parameters are difficult or impossible to measure directly. Indirect measurements, however, are always possible. Also, I want to clarify that the identification of parameters that cannot be measured is the consequence of the application of the scientific method and not a trick invented by the modelers to escape accountability.

3) Some responses are conciliatory ("I do not believe there should be a competition"), but others are more realistic: "When resources for research are finite and dwindling, there is always competition, not only between modelers and experimentalists, but between local modelers and global modelers, and between atmospheric physicists and atmospheric chemists". Some people expressed strong criticism of the U.S. Environmental Protection Agency (EPA) for not providing better and more credible models: "They [the EPA] presently have a definite 'NIH' [not invented here] bias in what they recognize, and are using models known to be defective in reaching very expensive conclusions". One person identified the EPA as "the biggest problem by far, at least in the U.S.," because of the agency's "entrenched attitude" of not promoting more advanced modeling techniques: "Models which were 'approved' [by the EPA] more than a decade ago are still mandated in spite of their manifest inadequacies. Outdated models continue to be applied, at government insistence, to situations were accuracy is being sacrified in the name of 'consistency' or 'conservatism'."

I encourage readers to reflect seriously on this section and the statements above. I intend to collect more opinions on this topic and expand the analysis. Therefore, I would really appreciate it if many readers (modelers and nonmodelers) could send me their comments and frank opinions on this matter.

3. The Contents of *ENVIRONMENTAL MODELING,* Volume 2

Environmental Modeling, volume 2 is the second volume of an edited series of publications on computer methods for simulating environmental pollution and its adverse effects. It presents an organized collection of invited review papers covering environmental modeling topics. Each chapter was authored by a leading scientist in the field and was written to provide the reader with an organized and consistent approach to the field of mathematical and numerical simulation of environmental phenomena. In addition to the discussion of the mathematical, numerical, physical, chemical, biological and ecological aspects of environmental phenomena, *Environmental Modeling* provides a critical review of software available for environmental simulations.

This *Environmental Modeling* series represents an effort that is unique in its contents and especially in its long-term goals. Volumes I and II contain 17 technical chapters on different environmental subjects plus two introductory chapters. Subsequent volumes will expand the coverage of environmental topics by including new material and rearranging or rewriting previously published chapters. In other words, each new volume will change the structure of the entire publication series and provide the reader with an updated, expanded, and reorganized review. An introductory chapter in each new volume will assist the reader and guide the reading process through the different volumes.

In this volume (volume 2), Chapters 2 through 5 cover atmospheric topics at different scales, Chapter 6 deals with rainfall-runoff modeling and catchment hydrology, Chapters 7 and 8 discuss groundwater contamination issues, Chapter 9 covers variational data assimilation techniques, and Chapter 10 deals with expert-system support for environmental decisions. A brief description of each chapter is presented below.

Chapter 2 discusses atmospheric modeling at a short scale of 10-100 m. The chapter reviews **aerial spray drift modeling**, i.e. the assumptions, approaches, and techniques applied to the modeling of spray drift from aerial application of agricultural pesticides. In this review, the authors examine some of the traditional ways of modeling the trajectories of spray material that is released from aircraft, falls through the atmosphere, evaporates, and is deposited upon crops and the ground. It is important to note that aerial spray modeling has reached the point today where it is a tool running on personal computers and available to an application specialist seeking alternative spray strategies.

Chapter 3 discusses atmospheric modeling at the urban scale of 1-10 km. The chapter describes the development of a **metropolitan airshed pollution model** applied to the city of Perth, Australia. The simulation approach combines a numerical mesoscale meteorological model with a simple Langevin scheme to simulate the dispersion of pollutants emitted from both point and area sources. The method is applied to simulate the transport of automotive emissions in the city of Perth.

Chapter 4 discusses atmospheric modeling for mesoscale applications with a scale of 100-1000 km. The chapter focuses on **Lagrangian particle dispersion modeling** (or Monte-Carlo modeling) and describes two dispersion modeling systems: the Mesoscale Dispersion Modeling System (MDMS) and the Hybrid Particle Concentration Transport (HY-PAC) model. Two examples of applications of the Lagrangian particle dispersion model for complex terrain in the southwestern United States and eastern Europe demonstrate a design of computationally intensive air-quality studies with the aid of modern workstations.

Chapter 5 discusses atmospheric modeling at the long-range scale of 1000 km and more. The chapter presents an overview of state of the art in **long range dispersion models** of pollutants in the atmosphere. It includes the treatment of the most important mechanisms of pollutant removal from the atmosphere, such as dry and wet deposition and chemical reaction. The chapter also presents the results of a recent intercomparison study of long-range transport models applied to simulate the transport of the radioactive plume emitted during the Chernobyl accident on April 1986.

Chapter 6 discusses a new method of **rainfall-runoff modeling** and its applications in catchment hydrology. Rainfall-runoff models play a central role in catchment hydrology, assisting in a wide range of investigations such as assessment of the hydrological impacts of land use and possible climate changes, real-time flood forecasting and "design flood" estimation, assessment of the reliability of natural water resources, and investigations of river water quality. The chapter describes a new rainfall-runoff modeling method and presents several of its applications. A discussion is also included of the potential for information-transfer to ungauged catchments (regionalization) using statistical relationships linking Physical Catchment Descriptors (PCDs) and Dynamic Response Characteristics (DRCs) derived from Unit Hydrographs (UHs) parameters.

Chapter 7 discusses groundwater pollution modeling and focuses on **finite-element modeling of the transport of reactive contaminants in variably saturated soils**. The chapter presents the fundamental equation of nonlinear groundwater flow in variably saturated soils and develops a basic finite-element method for its solution under steady and transient conditions. The advantage of using finite-element techniques is that they provide high accuracy and can be used to simulate irregular three-dimensional domains with complex boundary conditions. The contaminant-transport model is expressed for both local equilibrium assumption (LEA) conditions (i.e. conditions in which contaminant sorption onto solid grains is simplified by assuming that chemical equilibrium is achieved instantaneously) and non-LEA conditions. The non-LEA model is solved by an integrodifferential approach involving a convolution integral, thus achieving a significant saving of computer storage and CPU time. The numerical models are successfully tested by comparing simulation results with solutions reported in the literature.

Chapter 8 discusses an important subtopic of groundwater pollution: the mechanisms and models for **aggressive-permeant interactions with soils**. This is a significant issue because aggressive permeants are capable of altering the hydraulic properties of the soils through which they flow. Consequently, they may alter the hydraulic conductivity of soil barriers used to contain them and escape into the environment. The chapter presents a comprehensive look at the subject of aggressive-permeant interactions with soils and discusses strategies for modeling the impact of aggressive permeants and for analyzing their preferential flow pathways. In addition, algorithms are presented for testing alternative aggressive-permeant interaction and for extracting the required model coefficients from typical permeameter observations.

Chapter 9 discusses theory and application of **variational data assimilation**. The objective of variational four-dimensional data assimilation is to find the solution to a numerical forecast that will best fit a series of observational fields distributed over some space and time interval. The basis of variational data assimilation is to use all the available information in order to produce the best possible initial state in a least-square norm optimal sense. Available information includes observations that are distributed more or less regularly in both time and space and vary greatly in their nature and accuracy, along with a numerical prediction model that describes physical conservation laws. This chapter presents the main aspects underlying a rigorous derivation of variational data assimilation, with special emphasis on meteorological applications.

Finally, chapter 10 discusses **expert-system support for environmental decisions**. Expert systems differ from traditional mathematical models in their ability to handle qualitative information that is very common in environmental decision problems. This chapter revises the architecture and the most important features of expert systems and shows how they can support environmental decision-makers. Two available environmental expert systems–OASIS and PigE–are described. Moreover, five roles for expert systems in environmental applications are identified: 1) to help in selecting appropriate models, 2) to help in calibrating the chosen models, 3) to predict adverse environmental effects, 4) to help users in understanding model outputs, and 5) to generalize model structures.

4. A Guide to the Reader of *ENVIRONMENTAL MODELING*, Volumes 1 and 2

This section provides some guidance to the reader of both volumes.

For a **general introduction to pollution modeling** in different environmental media, read Chapter 5 of volume 1. This chapter addresses multimedia modeling, i.e. the transport and fate of chemicals in the atmosphere, surface water, soil (including groundwater), and biota. The physico-chemical processes that govern the transport and fate of chemicals in each of these media are described, and the basic equations that represent these processes are discussed. The chapter includes a section on available software. Note that the topics in this chapter have recently been expanded into a series of technical articles in the quarterly journal *Environmental Software*, currently published by Elsevier. Additional useful information can also be found in Chapter 1 of each volume.

For the reader interested in **atmospheric modeling**, we suggest the following sequence of reading:

> Chapter 2 of volume 1 gives an introduction to atmospheric models and in particular the dynamics of atmospheric pollution. Different components and scales of the phenomenon are discussed: indoor air pollution; local-scale, urban, and regional scale pollution; and global air pollution. Different frameworks for air-quality modeling are presented, and several modeling applications are discussed. The chapter includes a section on available software.
>
> For a comprehensive description of air pollution modeling topics, the reader can also examine the textbook by Zannetti (1990).
>
> Chapters 2,3,4, and 5 of volume 2 provide expanded discussions of atmospheric modeling issues at different scales–from the local scale to the continental one. They cover, respectively, aerial spray drift modeling, the development of a metropolitan airshed pollution model, Lagrangian particle dispersion modeling, and long-range dispersion models. See the previous section for a brief outline of these four chapters.

For the reader interested in **surface hydrology and water pollution**, we suggest the following sequence of reading:

> Chapter 6 of volume 2 discusses a new method of rainfall-runoff modeling and its applications in catchment hydrology. See the previous section for a brief outline.
>
> Chapter 3 of volume 1 describes the application of mathematical modeling to the marine environment. In particular, the main characteristics of a general time-dependent three-dimensional model of the marine environment are presented, and the possibility of extracting smaller submodels from the general model is examined. Also, case studies with applications to the northwest European continental shelf and to the northern Bering Sea are described.
>
> Chapter 4 of volume 1 covers the modeling of the water quality of rivers and lakes. Strategies of model-building, governing equations, and case studies are presented. The case studies cover the Hungarian Danube, Lake Balaton, Lake Kuortaneenjarvi, and Lake Tuusulanjarvi. The chapter ends with a discussion of decision-support

systems, i.e. structures in which models are not used in an independent fashion but are part of a larger set of user-friendly interface tools.

For the reader interested in **groundwater hydrology and water pollution**, we suggest the following sequence of reading:

For a comprehensive description of groundwater modeling topics the reader can examine the textbook by Anderson and Woessner (1992).

Chapter 7 of volume 2 discusses groundwater pollution modeling and focuses on finite element modeling of the transport of reactive contaminants in variably saturated soils.

Chapter 8 of volume 2 discusses an important subtopic of groundwater pollution: the mechanisms and models for aggressive-permeant interactions with soils. See the previous section for a brief outline of these two chapters.

For a discussion of **ecological modeling**, read Chapter 6 of volume 1. This chapter presents a survey of some important features in mathematical ecology, with a special emphasis on the structural properties and behavior of ecosystems rather than just numerical aspects. Adverse conditions may induce structural perturbations in normal environmental processes, and the approach outlined in this chapter can be used to assess their extent and how they propagate throughout the entire ecosystem. The chapter includes a section on available software.

For a discussion of **environmental noise modeling**, read Chapter 7 of volume 1. This chapter covers the prediction of noise propagation from industrial plants, transportation noise models (for traffic, rail, and air transportation), modeling applications, a discussion on the accuracy of the predictions, and the modeling of long-term noise impact. The chapter includes a section on available software.

For a discussion of **environmental information management**, read Chapter 8 of volume 1. Since environmental regulations are imposing increased record keeping and reporting requirements, automating environmental information is becoming an important issue. This chapter provides a review of the different kinds of software available commercially, including on-line systems, databases, information services, data management systems, decision-support aids, expert systems, and training packages.

For a discussion of theory and application of **variational data assimilation**, read Chapter 9 of volume 2. See the previous section for a brief outline of this chapter.

For a discussion of **expert systems**, read Chapter 10 of volume 2. See the previous section for a brief outline of this chapter. Additional information on the use of expert systems for water-quality studies can also be found at the end of Chapter 4 of volume 1.

Finally, for a discussion of the **future of environmental modeling**, read Chapter 9 of volume 1. It presents a stimulating discussion on the growing role of environmental modeling. Nine facets of the evolution of environmental modeling over the next decade are examined from the perspective of a computer scientist: capability (performance, new science, and challenges), uniformity (databases, nomenclature, and interfaces), and accessibility (lower cost, user-friendliness, and networking). Additional useful information can also be found in Chapter 1 of each volume.

5. Conclusion

In conclusion, I want to thank all the authors of the 17 technical chapters in volumes 1 and 2 for their valuable efforts under challenging conditions and strict deadlines.

Hopefully, the *Environmental Modeling* series will not be just black ink on white paper. In fact, we plan to include "computerized" chapters(*) and user-friendly software in the series soon. By examining computerized chapters provided on disk, the readers will be able to access information in which text, data, equations, numerical solutions, and graphics are fully interconnected. The readers will then be able to work with all the material provided in the chapters and, with just a few keystrokes, adjust equations, modify data, and recalculate and replot the results under modified assumptions. Also, the inclusion of user-friendly versions of environmental models as part of the chapter material will allow readers to run environmental simulations to verify their understanding of modeling theories and numerical implementations.

Finally, I thank the readers for their support and I encourage the environmental scientific community to provide input, suggestions, contributions, and constructive criticism.

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Disclaimer

The opinions presented herein are those of the author alone and should not be interpreted as necessarily those of Failure Analysis Associates, Inc. (FaAA).

(*) Computerized chapters can be made today using special programs, such as *Mathcad, Maple V,* or *Mathematica*. The most striking feature of these software packages is their ability to create, on personal computers, interactive documents that mix text, animated graphics, and sound with active formulae. Using these packages, an author can write an article or a book in which the reader can modify and solve, analytically or numerically, a set of equations. These solutions generate figures, sound, animation. A simple change of a parameter or a variable in the text causes new solutions, new figures, new animation. In this way, the book or the article becomes a learning and testing environment for the reader.