Environmental Modeling - Vol. 3

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

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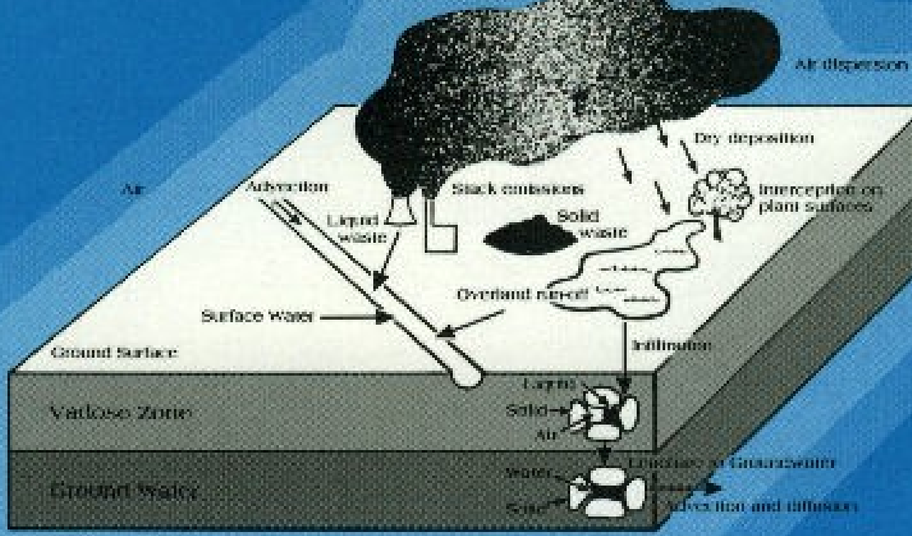

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Chapter 1

Environmental modeling: today and tomorrow

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Abstract

This chapter provides an introduction to the topic of Environmental Modeling, a discussion on current and future trends, and a guide to the contents of the first three volumes of the book series.

Keywords

Environmental Modeling, Pollution, Computer Simulation, Numerical Modeling, Computer Sciences, Research and Development, Multimedia Modeling, Comprehensive Modeling Systems, Virtual Reality

1. Environmental Modeling Today

In the previous volume's Introduction, a definition of environmental sciences was presented. This definition, which seems to be acceptable to most of scientists I interacted with, is reproduced below.

> *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.*

In Volume 2, I discussed and analyzed the fact that part of the scientific community is sometimes skeptical about the use of environmental models, i.e., computer simulation techniques that reproduce and forecast environmental phenomena. To understand and clarify this issue, the results of an opinion survey were presented, in which a selected number of scientists responded to three questions soliciting constructive criticism. These scientists were well-established environmental experts who were not modelers but knew about environmental modeling and interacted with computer modelers. Their answers were interesting and provocative.

For Volume 3, I decided to submit the same questionnaire (slightly reworded) to environmental modelers, i.e., scientists who develop new environmental models or apply existing models to simulate environmental phenomena.

The questionnaire asked the following three questions:

1. *As an environmental modeler, what is your current opinion about environmental models? Has your opinion changed in the last few years? Which role do you see for environmental modeling in the future?*

2. *How do you characterize your interactions and communications with other environmental professionals (i.e., nonmodelers)? Can you specify the positive and negative aspects of your current and past working relationship with them?*

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 communications and collaborations?*

Several answers were received from very qualified people. A summary of the answers is presented below.

1) The answers, as expected, show confidence in environmental modeling and their increasing role and importance in the near future. Models are defined as "a tool for better understanding of what is going on in the real world" and "the only way to predict the future". It is pointed out that "the quality of environmental models has improved in the last 5-10 years" and that "the most important purpose of environmental models is to predict the impact of human activities". It is mentioned, however, the fact that models may "give right answers for the wrong reasons" and require accurate "calibration and validation". A scientist suggests two major roles for models in the future: 1) complicated scientific models to be used for environmental protection and restoration; and 2) fast, efficient, and simple models for decision makers and authorities. Some scientists also mention the fact that environmental models should include in the future social aspects and policy-oriented applications.

   These answers are not much different from those provided by the nonmodelers and discussed in Volume 2, even though modelers are certainly more optimistic about the present and future role of computer models.

2) Communications with other environmental professionals are described as "difficult"; "often with a barrier, especially between computer modelers and experimentalists";

characterized by a "different culture"; "not easy"; affected by experimentalists adopting a "distant attitude"; and "good" in spite of models "still intimidating many people". A few scientists observe the tendency by nonmodelers "to blindly trust model results or to abandon them all". Many complain that nonmodelers "just do not understand" models and their mathematical and numerical aspects. Some scientists, however, blame the modelers themselves for failing to educate and explain models' assumptions, limitations, and uncertainties. A few modelers, however, are satisfied with the constructive climate within their multi-disciplinary working groups.

These responses are quite different from those provided by the nonmodelers in Volume 2, who characterized the relationship with modelers as relatively good, but with some problems. Modelers do not hesitate to express some constructive (and sometimes destructive) criticism, such as: "for nonmodelers, the computer models are something like 'hocus-pocus' or 'black magic'". One scientist also complains that nonmodelers tend to use models "as a black box" without understanding the science underneath.

3) Answers are quite different here. Some modelers do not see competition or friction between the two communities, but the majority do. Almost everybody, however, mention the need for future cooperation and multi-disciplinary activities. Where friction is found, two reasons are often mentioned: the contrast for proper allocation of financial support and the different culture affecting the modeling community versus the other communities. However, one modeler observes that, at least in his country (located in Northern Europe), "there is not much competition between modelers and nonmodelers; however, there is competition among modelers".

These responses are somehow similar to those of nonmodelers in Volume 2. However, in general, nonmodelers complain louder about what they believe is often an inappropriate, preferred allocation of research funds toward monitoring and experimental activities. Modelers also imply, in their criticism, that other communities do not make a sufficient effort to properly understand simulation modeling and its important role in environmental sciences.

I encourage readers to reflect 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.

Perhaps we could try to draw some preliminary conclusions from the analysis of the opinions presented above. 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 today not uncommon, 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.

The fact of the matter is that environmental modeling, like most things on earth, can be perfectly done or can result in "garbage in, garbage out", with most applications, of course, lying in the middle of these two extremes. It is difficult to define how a modeling application can be perfectly done, but I have tried to make a list below of nine conditions for what we can call "excellence in modeling".

1. The computer code must be fully tested, both as a whole and in its individual modules.

2. The code should be used by other groups, besides the developers, to assure external peer-review and approval.

3. The code should be fully documented. All equations and assumptions should come from formulations and methods published in peer-reviewed publications.

4. The input data should be reliable and pertinent to the specific application. The spatial and temporal resolution of the input data should be consistent with the time and space scales of the phenomenon that one wants to simulate.

5. The code should apply the best available science, e.g., by using full three-dimensional (3D) representations and avoiding the use of steady-state solutions to simulate time-varying phenomena.

6. The code should be numerically correct (e.g., all iterative calculations should reach full convergence and results should not be affected by the size of the grid or the length of the integration time).

7. The code should be fully validated against reliable field data. This validation should include a careful evaluation of the physical significance of both model outputs and field measurements. For example, a comparison between model outputs on large spatial grids with point measurements can be phenomenologically incorrect.

8. Any calibration of the code should be done properly. Proper calibration means the tuning of some input parameters within their range of uncertainty in order to maximize the agreement between model outputs and field data. Calibration, however, is not proper when it ends up making the model work for the wrong reason! (This has happened, unfortunately in several occasions in the past. A well-known example is the application of photochemical models to simulate ozone concentrations in urban areas. In the past, reaction rates in these photochemical models were "tuned" to allow the models to agree with the available measurements of ozone in the region. Later, it was discovered that the main model inputs, i.e., the emissions of VOC and NO_x in the region, were incorrect. That means that these models could be tuned to provide "correct" ozone concentrations with highly incorrect emission values of the ozone precursors. Therefore, what people called "calibration" in that case was just forcing the models to work for the wrong reason. Any practical application of these models, for example to calculate the emission reductions in VOC and NO_x required to achieve a certain pre-defined reduction of ozone concentrations in the region, was clearly incorrect.)

9. The model application should be fully documented in a report presenting all assumptions and a description of all computer runs. The reader should be capable of rerunning the application on his computer and obtaining the same results in an independent manner.

2. Environmental Modeling Tomorrow

This section presents a discussion on the expected future developments of environmental modeling. Three factors are discussed: 1) the increasing use of multimedia models; 2) the current design and development efforts toward the creation of comprehensive modeling systems; and 3) the possible incorporation of virtual reality techniques into environmental models.

2.1 Multimedia Modeling

Traditionally, environmental models were designed to cover the dynamics of pollution in one particular medium, e.g., the atmosphere or a body of water. Recently, multimedia models have become necessary (Seigneur, 1993), since pollutants such as pesticides can migrate and be detected in different media. Conceptually, a multimedia model is not necessarily more complex than a model designed for a specific medium. However, multimedia simulations require a more extensive set of input parameters (they must include, for example, intermedia transport terms such as atmospheric deposition, sedimentation, volatilization, and erosion).

2.2 Comprehensive Modeling Systems

In the early 1990s, a few project teams, typically formed by environmental and computer scientists, have explored the possibility of developing comprehensive modeling systems (CMS) for environmental sciences. In a nutshell, a CMS should include (Zannetti, 1993) three major functions:

1. Education. The Education section of a CMS should contain several modules designed for environmental education. These modules could typically cover six topics: the atmosphere, rivers and lakes, seas and oceans, soil and groundwater, human health, and environmental effects.

2. Simulation. The Simulation section of a CMS should contain modules that simulate environmental phenomena and adverse effects of pollution. Results could be visualized by still images or animation. The simulation modules could cover ten topics: air, watershed, soil and groundwater, surface water, multimedia, indoor pollution, noise, human health, environmental damage, and environmental engineering.

3. Management. The Management section of a CMS should contain several modules to assist the environmental manager and the environmental regulator. These modules could address eight topics: environmental information management, regulatory compliance, risk assessment, emergency response, pollution control, environmental remediation, litigation support, and literature search.

Much progress has been made recently toward the development of a CMS for air pollution (Hansen et al., 1994 and 1995; Zannetti et al., 1995; Dennis et al., 1995). These efforts are expected to be extended to other media in the near future. The air pollution CMS, as preliminary envisioned by its designers, should provide an infrastructure that helps its users to do their jobs better and faster, whether those jobs be regulatory and policy analysis, source impact assessment, understanding atmospheric chemistry and physics, or performing atmospheric research studies. As such, this CMS should provide the following:

- A platform for modeling pollutant emissions, atmospheric physics and chemistry, and the impact of pollution in as scientifically sound a fashion as is desired or possible.
- A readily accessible interface, so that its use is a benefit, not a distraction.
- A powerful set of analysis and decision-support tools, such as graphical, visual, economic, or scientific, including report preparation.
- A method to make maximum use of the available computational resources, including CPU power, disk storage, and communication systems.

The CMS is being designed in a way that facilitates its continuous evolution with science, computer capabilities, and user needs. This will require that it employ well-acknowledged standards (e.g., computer languages and data protocols).

Perhaps the best way to illustrate the CMS is to provide a realistic description of its future use, as is done below:

> Palo Alto, 7 April 1999. The user sits in front of an Apple-IBM *Penta III* computer screen. The screen shows a stylish *CMS* logo and several other buttons. By issuing a voice command to the system, or clicking (with a foot mouse) the button *Beginners click here*, a series of windows are displayed. These windows contain detailed information sections and an animated user's guide to describe the entire system. By clicking the button *Education* a new series of "windows" and "chapters" are available. These sections are connected to CDs, Laserdisks and multimedia devices and provide, on the *Penta III* screen, interactive education tools on the subjects of atmospheric sciences, air pollution, laws/regulations, simulation modeling, and databases. A special *Communication* button allows the user to communicate, via user-friendly interfaces, with library databases, meteorological/air quality databases, and other users.
>
> By clicking the *CMS Regulatory* button, the user accesses a subset of the CMS system in which only models and techniques that have received some regulatory approval are available. The use of these models is "locked," in the sense that they can only be used with computational options that are acceptable to the regulatory agencies. Regulations of different countries (USA, Canada, ECC, Japan, etc.) can be selected; therefore, locking the execution of the simulations under different regulatory constraints. By clicking the *CMS full set* button, the user accesses the entire simulation system. Through a password and a voice recognition check, a user-developer is allowed access to the master version of CMS (in remote computer storage) and modify/add/update modules and functions.

A typical CMS session consists of a CMS-guided computer simulation and "report" preparation. The user defines the computational domain, the simulation period, and other user-specified options. CMS assists the user in performing a sequence of simulations and choices to calculate emission data, meteorological fields, transport and diffusion scenarios, chemical reactions, dry and wet deposition, and some adverse effects of air pollution, such as visibility impairment. Any step can be fully visualized by superimposing input/output data on geographical information using a GIS and full 3D views (in a fly-through fashion). A special *Real-time* button allows real-time simulation for emergency response of accidental releases, if proper connections are made to access meteorological and other data on-line. At any time the user can select input/output data and ask CMS to perform special calculations and analyses in different computational environments (such as new versions of *Mathematica*, *Spyglass*, *Systat*, etc.) on the *Penta III* screen.

What is described above illustrates the first and, by far, the most important goal of the CMS – to let the computer do the work. In the crudest sense, this means more complex and more sophisticated computations, but this is only the tip of the iceberg. Far more important is using the computer to compile, cross-reference, and comprehend intentions. The goal of the CMS is as much a manifesto as a plan; it is meant to be revolutionary, not incremental.

2.3 Virtual Reality

In the world of information sciences, two trends seem particularly relevant in the mid-1990s. The first trend is the increasing power of PCs (IBM-compatible and Macintosh-type machines). Internal PC clocks can now run at more than 100 MHz; thus, providing very substantial computer power.

Many scientists have invested their time and resources heavily in Unix workstations in the last few years. This investment was certainly a smart move at the beginning of the decade, when it became clear that mainframe computers and supercomputers were not cost-effective in comparison with the new generation of Unix-based microcomputers. A similar phenomenon is occurring now – scientists are discovering the increased power of the new generation of personal computers running under new, powerful operating systems such as IBM OS/2, Microsoft Win95/NT, and Apple OS. These new hardware/software platforms, and especially Microsoft NT, are expected to substantially erode the market for Unix workstations by providing high speed, advanced features, user-friendliness, and inexpensive software for scientific calculations and simulations.

The second trend is virtual reality (VR). VR may appear frivolous in nature because of its close relation to interactive games and, therefore, its "arcade" connotation. But VR techniques appear to be the most interesting trend in computer software today.

VR has been defined as

> ". . . a computer-synthesized, three-dimensional environment in which a plurality of human participants, appropriately interfaced, may engage and manipulate simulated physical elements in the environment and, in some forms, may engage and interact with representations of other humans, past, present or fictional, or with invented creatures" (Nugent, 1991, quoted in Larijani, 1994)

and

> "... an interactive computer system so fast and intuitive that *the computer disappears from the mind of the user,* leaving the computer-generated environment as the reality" (Goldfarb, 1991, quoted in Larijani, 1994).

According to Goerbe (1992),

> "... virtual reality enables users to immerse themselves in computer-generated environments that include three-dimensionality through sound, sight, and touch."

Larijani (1994) simply describes VR as

> "... a cartoon world you can get into."

VR techniques cover two basic applications: 1) those in which the user puts on appropriate gadgets and enters an artificial world in which he or she manipulates objects in an interactive manner; and 2) those in which the user observes and moves virtual humans operating in a virtual world.

VR techniques differ from multimedia tools, where the reader should note that in this section the term "multimedia" has a different connotation. "Multimedia" here indicates the expansion of our communication capabilities and the inclusion of sounds, images, animations, and video. VR techniques employ multimedia tools and expand upon them, allowing an interaction between the user and "objects" in a virtual world. Examples of VR applications are some of the most sophisticated video games and some training techniques used by the military (for example, jet fighter simulations).

VR techniques are expanding rapidly. According to Martin (1994), the marketing firm Forst & Sullivan reported that the VR market is expected to exceed $1 billion in 1997, following a growth rate in which the market almost tripled from 1991 to 1993 (from $49.7 million to $130 million).

I expect VR techniques to become, within 10 years (and perhaps even 5), the *preferred* way in which the user (any user) interacts with a computer (any computer). To understand why, one must look at the history of the computer user interface. There we find a logical evolution: from primitive techniques such as punched cards and dumb terminals to today's microcomputer software, developed using object-oriented techniques and available to users through GUIs (graphical user interfaces). The next step is, clearly, the use of 3D icons and, almost inevitably, the total immersion of the user in a 3D world – a VR world.

Clearly, the environmental modeling community will be affected, at least indirectly, by this trend. Certainly, the use and the development of environmental models will be influenced by the increasing availability of VR-based productivity tools. But the real question is how this trend will *directly* affect environmental scientists (Zannetti, 1995).

As discussed in the previous section (2.2), an important trend in environmental modeling today is the ongoing development effort directed toward "comprehensive" systems. These new air quality modeling systems are expected to be scientifically advanced, comprehensive (e.g., covering local, regional, and continental scales), easy to access and use, self-consistent, and computationally efficient. For example, a comprehensive modeling system (CMS), such as that described by Hansen et al. (1995), is expected to change the way people use air pollution models by allowing both scientists and non-technical people to operate complex atmospheric simulations and run air pollution scenarios almost anywhere.

I would argue that the ultimate step in the development of environmental models – and probably the only step that can assure full user-friendliness and accessibility to non-technical people – is the incorporation of VR techniques. After all, what is "environmental modeling?" Environmental modeling can be seen as an organized and interactive series of computational modules that transform one set of databases (emissions, human activities, meteorology, geography, etc.) into another set (concentrations, depositions, health damage, etc.) The more comprehensive environmental modeling systems become, the more users will be able to apply simulation techniques as black boxes, i.e., without necessarily understanding the details of the computations. Users, therefore, will be able to focus on exploring the relationships among the databases (inputs and outputs) and experimenting with changes without worrying about the computational details.

In less than 10 years, the use of environmental models may very well become a simple and entertaining VR exploration into databases. It may look like a video game, but it will incorporate the best science. Manipulations of input databases (e.g., emissions) will automatically generate related changes in output databases (e.g., concentrations). Inverse calculations (e.g., the emission controls required to achieve pre-defined concentration standards) could be simply triggered by imposing a constraint on an object in the output database. It is not science fiction to envision a user wearing a VR device such as a helmet, entering a virtual database, walking through objects and their functional relationships, and performing direct and inverse simulations, analyses, and optimizations by simple manual operations on 3D objects. It will be like walking through a gigantic spreadsheet in which a single cell may contain the same number of calculations as one of today's air pollution models (e.g., 10^5 to 10^6 lines of FORTRAN code).

Clearly, at this point one can hardly guess to what extent VR will figure in future environmental modeling studies. To forecast the evolution of computer systems and user needs is problematical, and one may easily be fooled by fashionable trends with no future. However, let me conclude this section with two pieces of advice to the reader. First, this is probably not the best time to make a big Unix investment – wait at least 6 months if you can. Second, next time your kids go to the arcade and start playing with helmets and other gadgets, join them; you may develop very useful skills for the computer work that is awaiting you just a few years ahead.

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

Environmental Modeling, Volume 3 is the third 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. The first three volumes contain 30 technical chapters on different environmental subjects plus a introductory chapter for each volume. 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 and guide the reader through the different volumes.

In this volume (Volume 3), Chapters 2 through 7 cover atmospheric topics at different scales; Chapters 8 and 9 deal with rainfall-runoff modeling and catchment hydrology; Chapter 10 discusses a peculiar issue in groundwater hydrology (seawater intrusion) while Chapter 11 introduces and revises the electrical resistivity method in groundwater studies. Chapter 12 presents a case study in ecological modeling, while Chapter 13 discusses and quantifies the total damage of air and water pollution. Finally, Chapter 14 discusses computer techniques and software for scientific visualization. A brief description of each chapter is presented below.

Chapter 2 discusses atmospheric modeling at a **short scale** of 10-100 m. The chapter discusses topics in **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 chapter, the authors discuss, in particular, the ongoing refinement and application of the USDA Forest Service aerial spray drift model FSCBG (Forest Service Cramer-Barry-Grim). The model intends to help applicators in achieving safe, efficient, and economical application of pesticides and herbicides.

Chapter 3 discusses atmospheric modeling at the **intermediate scale** of 1-10 km. The chapter describes the evaluation of a new version of the AVACTA II model on **flat and complex terrain**. AVACTA II is a Gaussian segment-puff code that simulates air pollution dispersion. It maintains the basic Gaussian formula, but allows the simulation of nonstationary and nonhomogeneous conditions by treating plumes as a sequence of independent segments or puffs. The chapter describes the recent improvements made in the code and the encouraging evaluations performed using field and laboratory data.

Chapter 4 discusses atmospheric modeling for **mesoscale** applications, defined as the transport and diffusion of air pollutants over horizontal distances **between 2 and 2,000 km** with time periods ranging from 1 to 48 hours. The authors emphasize the need for accurate representation of multiscale atmospheric flow in mesoscale models and present a survey of current techniques to improve meteorology in dispersion models. The second part of the chapter is dedicated to the description of the Operational Multi-scale Environment model with Grid Adaptivity (OMEGA). This model development was conceived out of a need to advance the state-of-the-art in numerical weather prediction in order to improve the real-time prediction capability of the transport and diffusion of atmospheric pollutants. One of the unique characteristics of OMEGA is its use of unstructured and adaptive mesh numerical techniques.

Chapter 5 presents a **case study of regional atmospheric modeling** in the southwestern United States. The authors performed numerical simulations for the entire year of 1992 by linking a prognostic mesoscale model (the CSU Regional Atmospheric Modeling System, RAMS) together with a Lagrangian particle dispersion (LPD) model. The prime area of interest is the Colorado Plateau, including the Grand Canyon National Park. By comparing model outputs with tracer experiments, the authors reach interesting conclusions and make the important statement that models without sufficient resolution to adequately represent mesoscale motions will overestimate the impact from distant sources and, at the same time, underestimate the impact from local sources.

Chapter 6 discusses **soil moisture** and its role in **mesoscale meteorological modeling**. The author points out that meteorological models are highly sensitive to the initial soil moisture profile – a parameter that, however, is simply "guessed" in current modeling applications because no reliable soil moisture profile technology is available for routine measurements. This seems to translate into major forecasting errors for local wind and thunderstorm predictions. A new, *in situ*, measurement technology is also discussed (time domain reflectometry, TDR). This technology seems to provide a promising tool for the application of meteorological prognostic models with greater confidence and accuracy.

Chapter 7 presents a literature review of mathematical models for simulating **volcanic emissions** and gas and aerosol dispersion at both **mesoscale and global scale**. Both physical and chemical phenomena are discussed. The authors also present a few case studies, focusing mostly on CO_2 emissions.

Chapter 8 discusses the use of a stochastic integral equation to approximate **rainfall-runoff modeling**. The problem of predicting watershed runoff (i.e., flood flows) from rainfall data is of key importance to society. The state-of-the-art in rainfall-runoff modeling is to use computers to solve the various deterministic equations describing the related phenomena. 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. These models, however, often possess a high degree of uncertainty because of the lack of success in estimating runoff from rainfall data. This chapter presents an application of probabilistic thinking, instead of deterministic simulation.

Chapter 9 presents a **Decision Support System (DSS)** for **catchment management**. The DSS is designed to help catchment managers understand the future impact of current and proposed land management policies. Moreover, the DSS includes a Model Management System (MMS) to help design and evaluate catchment models.

Chapter 10 discusses a peculiar case of **groundwater** pollution: **seawater intrusion**. The chapter describes the physical aspects of the problem and its global extent. It also reviews various models that have been developed to simulate seawater intrusion in coastal aquifers. A range of case histories are also presented.

Chapter 11 introduces and reviews the **electric resistivity method**. This method, like other **geophysical methods**, allows us to make deductions about a subsurface structure from surface measurements. Most geophysical problems are of the *inverse* type; i.e., they allow us to deduce a "source" from an observed "response" to that source. In recent years, the resistivity method has undergone a resurgence of interest due to advances in data acquisition technology, better mathematical algorithms, and more interactive modeling software. The chapter concludes with a review of two commercial inversion software packages: the first (RINVERT for Windows) for one-dimensional models of the earth and the second (RES2DINV) for 2D models.

Chapter 12 presents a **case study** in **ecological modeling**. The study region is the Lagoon of Venice, Italy. The full conceptual model focuses on physiological descriptions of macroalgae (*Ulva rigida*) dynamics in response to the most important external factors. Attempts are made to clarify the feedback mechanism between algae and dissolved oxygen. The simulations were performed using software for automatic programming and modeling SIMSAB (simulation modeling system for aquatic bodies).

Chapter 13 discusses the **impact analysis**, i.e., the quantification of the adverse impact of air and water pollution. This analysis is performed using the impact pathway methodology which traces the fate of each pollutant, from the source to the receptor, using dose-response functions to evaluate the damage. Formally, this can be represented by an equation for the incremental damage of a particular type (e.g., health effects) due to an incremental quantity of a pollutant emitted by a specific source. The method is applied to simulate the impacts from power plants in Europe and quantify the environmental costs of energy use.

Chapter 14 reviews the use of software **visualization** tools and their role in environmental modeling. Visualization used to be a "post-processing" activity during which scientists elaborated the results of their calculations to provide graphic summaries and presentation material. Today, visualization is (and has to be) an "on-line" process to help the scientist at each step of the research study and provide a method for exploration, verification, debugging, and interpretation. This chapter explains what scientific visualization is, how it is used, and discusses its future in environmental modeling. Moreover, the chapter provides a useful review and discussion of available visualization software toolkits on different computer platforms (e.g., Unix workstations and PCs).

4. A Guide to the Reader of *ENVIRONMENTAL MODELING*, Volumes 1 through 3

This section provides some guidance to the reader of all three 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 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 and Chapters 2, 3, 4, 5, 6, and 7 of Volume 3 provide expanded discussions of atmospheric modeling issues at different scales – from the local scale to the continental one. They cover: aerial spray drift modeling (Chapter 2 of Volume 2 and Chapter 2 of Volume 3), the development of a metropolitan airshed pollution model (Chapter 3 of Volume 2), segmented-puff techniques (Chapter 3 of Volume 3), Lagrangian particle dispersion modeling (Chapter 4 of Volume 2), mesoscale meteorological modeling (Chapters 4, 5, and 6 of Volume 3) and long-range dispersion models (Chapter 5 of Volume 2 and Chapter 7 of Volume 3; the latter with emphasis on volcanic emissions). See the previous section for a brief outline of the six chapters in Volume 3.

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.

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 3D 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.

Chapter 8 of Volume 3 discusses the use of a stochastic integral equation to approximate rainfall-runoff modeling response. See the previous section for a brief outline.

Chapter 9 of Volume 3 presents a decision support system for catchment management. See the previous section for a brief outline.

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.

Chapter 10 of Volume 3 discusses the issue of seawater intrusion in coastal aquifers. See the previous section for a brief outline of chapter.

Chapter 11 of Volume 3 discusses the electrical resistivity method and its use in groundwater studies. See the previous section for a brief outline of this chapter.

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. Also, Chapter 12 of Volume 3 presents a case study in ecological modeling (see the previous section for a brief outline of this chapter).

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 ofVolume 2. See the previous section for a brief outline of this chapter.

For a discussion of **expert systems**, read Chapter 10 of Volume 2. 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. Also, Chapter 9 of Volume 3 discusses a decision support system for catchment management (see the previous section for a brief outline of this chapter).

For a discussion on **impact analysis**, i.e., the calculation of the adverse effects of pollution, read Chapter 13 of Volume 3. See the previous section for a brief outline of this chapter.

For a discussion on **visualization**, read Chapter 14 of Volume 3, which also includes a software review. See the previous section for a brief outline of this chapter.

Finally, for a discussion of the **future of environmental modeling**, read Chapter 9 of Volume 1. It presents a 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 information can also be found in Chapter 1 of each volume and, in particular, in Section 2 of Chapter 1 of Volume 3.

5. Conclusion

In conclusion, I want to thank all the authors of the 30 technical chapters in Volumes 1 through 3 for their valuable efforts under challenging conditions and strict deadlines.

Hopefully, the *Environmental Modeling* series will not be just black ink on white paper. A parallel effort is under development for the production of "computerized" chapters * and user-friendly software. 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 reader 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.

For more information on available computerized chapters (e.g., an electronic book has already been produced on the topic of Air Pollution Modeling – Gaussian Models), the reader should contact the author by fax (415) 688-7269 or e-mail (paolo@cup.portal.com).

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* 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.

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

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).

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