Environmental Modeling - Vol. I

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

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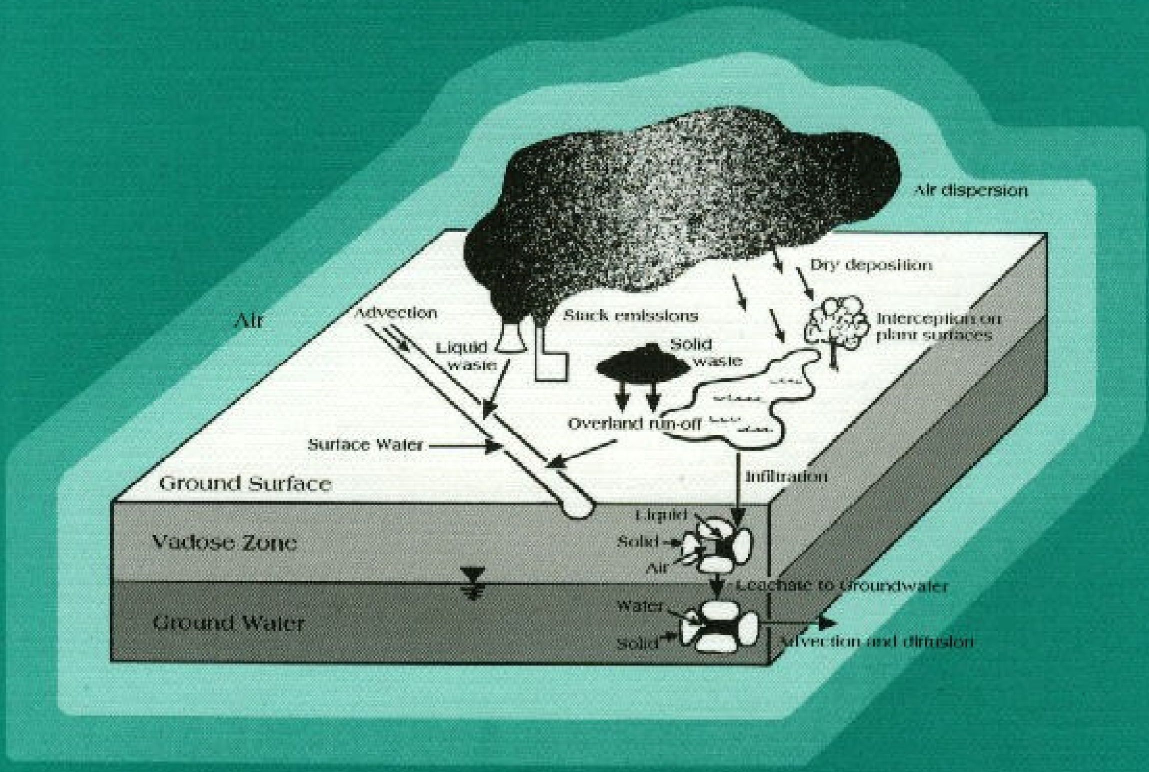

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P. Zannetti
Failure Analysis Associates., Inc.
149 Commonwealth Drive
P.O. Box 3015
Menlo Park, California 94025
USA

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Chapter 1

Introduction and overview

P. Zannetti

Failure Analysis Associates, Inc., 149 Commonwealth Drive, Menlo Park, California 94025, USA

Abstract

This chapter provides an introduction to the book series and an overview of the environmental modeling topics that are covered in this volume (Volume I).

Key words

Environmental Modeling, Environmental Monitoring, Pollution, Computer Sciences, Research and Development

1 Why environmental modeling?

The science of environmental modeling in the 90s is reminiscent of the science of chess simulation in the early 70s. Chess simulation then was treated in two different, opposing ways. On one side, among a large fraction of chess experts, computer simulation of chess was not taken seriously, and many experts were solemnly predicting that never would a computer be able to learn to play chess at a level similar to that played by any adult, let alone a grand master. On the other side, in the popular press, it was not unusual to read articles on the exceptional abilities of some computer chess program developed in some unknown university. As far as I am concerned, I must admit that, still in the late 70s, in spite of my awareness of the computer revolution, I would have never guessed that just a few years later a chess program running on a simple Macintosh would have humiliated my own limited chess skills.

Environmental modeling sometimes still encounters skeptical reactions in a fraction of the scientific community and too optimistic descriptions in part of the media. The latter attitude is easy to understand, since popular articles are often designed to attract the attention of the inexperienced reader by overstating (and, less often, understating) the ability of the scientists. The former attitude is more complex and deserves more discussion.

Environmental modeling–the ability of numerically simulating environmental phenomena–is still an evolving science. Models have expanded, decade after decade, in complexity and size. The *scale* of the problem, in particular, has expanded enormously. For example, in air quality modeling we deal today with global issues such as the depletion of stratospheric ozone and the effects of the global increase of greenhouse gases, while in the 60s and 70s most studies dealt with short-range (i.e., up to 10 km) impact of industrial and urban sources.

Environmental models are becoming today a *numerical laboratory*, that is, a setting in which scientists can test hypotheses, develop experiments, and assess scenarios. Complex environmental models today, especially when linked to powerful 3D visualization techniques, are not just a tool to provide a numerical solution of a predefined set of equations. In fact, numerical modeling is becoming a new branch of science, not just a solution method to assist scientific researchers.

In pollution studies, in particular, the role of simulation modeling is unique. Certainly, if environmental pollution is a 'problem,' mathematical modeling cannot claim to be the 'solution' to this problem. Mathematical modeling is, however, an indispensable tool for several important environmental analyses. As a matter of fact, no strategy for pollution reduction and control can be cost-effective without a previous rigorous application of both simulation modeling and optimization techniques.

Mathematical models are the only practical and objective tool that can answer our 'what if' questions. Contrary to the common belief that environmental *point measurements* are the 'real world,' it should be firmly stated that only a well-tested and well-calibrated simulation *model* can be a good representation of a *three-dimensional* real world, its dynamics and its responses to possible future perturbations.

In spite of all the considerations above, we–as environmental modelers–must continue to face some criticism, both fair and unfair, from segments of the scientific community. Unfortunately some scientists–especially experimental scientists–still view computers with diffidence. With the advance of a new generation of scientists, this phenomenon will certainly disappear, but it will take some time. Also, the majority of the funds for environmental research are still oriented toward experimental studies. Therefore, we–as modelers–are in a competition for the allocation of resources. This may explain why we continue to hear scientific opinions about models that emphasize their limitations (that is, what the models *cannot* do) instead of their strengths (what the model *can* do).

Ideally, there should be no competition between experimentalists and modelers, since both cover different needs in science. Unfortunately, however, too often data are collected without good coordination with the scientists that will eventually have to use them. Therefore, too often data remain unutilized on paper or computer media. On the other side, modelers sometimes tend to isolate themselves inside an 'ivory tower' and lack a deep practical understanding of the real world.

One of the problems we face is the fact that collected data are too often seen by the experimentalist as a final result, while we–environmental modelers–know that collecting data is just the beginning of the process of understanding the complex realities of the physical world.

Environmental modeling should be seen as an objective frame laid over subjective interpretations. From this perspective, Dr. Tiziano Tirabassi wrote an interesting and humorous piece in which he addressed the basic misunderstanding that still persists between mathematical modelers and the rest of the world. The column was written in Italian and published as a chapter of the book *Viaggi con Afrodite* (Traveling with Aphrodite) by Sandro Boccini, Editoriale Centro Studi Vanoni, Terni, Italy, 1987. A translation of excerpts from this chapter is provided below.

MISTER JOURDAIN AND THE MATHEMATICAL MODELS

by Tiziano Tirabassi

Mister Jourdain: . . . I am in love with a very refined woman and I would like you to help me to write a note to her that I will drop at her feet.
Philosophy Teacher: Very well.
Mister Jourdain: It should be a charming note.
Philosophy Teacher: Of course. Do you want to write in verse to her?
Mister Jourdain: No, I don't .
Philosophy Teacher: You want to write in prose, then.
Mister Jourdain: No, neither in prose nor in verse.
Philosophy Teacher: It must be one or the other.
Mister Jourdain: Why?
Philosophy Teacher: For the reason, sir, that one can express himself only in prose or in verse.
Mister Jourdain: That's all we have?
Philosophy Teacher: That is all. What is not in verse is in prose; and what is not in prose is in verse.
Mister Jourdain: But when we talk, what is that?
Philosophy Teacher: That is prose.
Mister Jourdain: You mean that, when I ask my servant, "Nicole, bring me my slippers," that is prose?
Philosophy Teacher: Yes, sir.
Mister Jourdain: I can't believe it. I have been talking in prose for more than 40 years and I did not know it . . . .

This dialogue, from a play by Moliere, always comes to my mind when I hear opinions about mathematical models from people that are not very familiar with them. The lack of familiarity, together with the difficulty of understanding the mathematical language, tends to generate two different, opposing reactions. On one side, some people accept the results of the models without hesitation and believe everything the model says. On the other side, other people express strong reservations on the model results and emphasize the superiority of experimental data over theoretical computer simulations.

The latter position does not account for the fact that theories and data are strongly linked. There are no data without theories and no theories without data. In fact every experimental data set has its own theory, since experimental data collection requires previous identification of the parameters to be measured and definition of measurement protocols and objectives.

Any interpretation of experimental data derives from a simple or complex theoretical model. Furthermore, a mathematical model is just an interpretation scheme of a phenomenon, based upon our theoretical knowledge. Therefore, a mathematical model is not different, from a qualitative point of view, from the mental models that we use, consciously or not, when we perform experimental studies and interpret the collected data.

It should be clear, by now, why the opinions of some of my colleagues remind me of the Moliere piece. We all operate naturally through models in the same way in which we speak in prose.

Let's make an example to clarify this concept. Let's discuss the Gaussian model, a simple mathematical formulation that describes the transport and diffusion of pollutants in the atmosphere. The Gaussian formula says that the concentration in any point downwind from a source is directly proportional to the source emission rate and inversely proportional to the wind speed. Moreover, the formula states that the polluting material is distributed horizontally and vertically in the shape of a Gaussian distribution and that the growing size of the plume is a function of both the distance from the source and the turbulent status of the atmosphere.

What is important to point out, however, is the fact that every model, no matter how complex, is a representation, in logical and mathematical terms, of a physical phenomenon. The mathematical representation is better than others mostly because it can be easily translated into a computer program. This allows calculations that would be otherwise impossible to perform by hand.

That is the analogy with the dialogue in the Moliere piece. I always smile when I think of the astonishment that some of my colleagues would experience if they realized–as Mr. Jourdain when he suddenly realized that he spoke in prose–that they have always used models in their evaluations of physical phenomena.

Often people do not like models for another reason. They see models, in their ultimate development, as *objective* tools for decision making. Therefore, models that provide the best solution or the best alternative decrease the *subjective* power of the decision makers and force them to choose strategies that are different from those that they would prefer to choose. In particular, politicians often do not like models. Why use a model to simulate pollution and optimize pollution control instead of following the traditional political process in which one favors friends and obstructs enemies?

We–as environmental modelers–must remain optimistic about the ability of our approach and the eventual success of our studies. In a decade or two this debate will be over and computer modeling will have a full, independent role in science[1]. It is

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[1] A recent issue of *Science* (Vol. 256, 3 April 1992) was dedicated to 'Computers in Science.' Computer simulation was identified as 'the third branch of science,' stating that 'computer simulation has opened a new eye on the world, giving scientists in the fields from biology to high-energy physics a way to perform experiments that would be otherwise impossible.' In particular, computer visualization of numerical simulations is depicted as an extension of the scientist's thinking power.

exciting to live and work in these years that represent a turning point.

2 Numerical modeling and the computer revolutions

A very interesting interpretation of human, industrial and computer evolution was provided by Dr. Enrico Clementi in his MOTECC 90 and MOTECC 91 volumes (published by ESCOM Science Publishers B.V., Leiden, the Netherlands). He notes that ages are often classified by their production tools: stone, bronze and iron ages. Therefore, today we must live in the *computer* age (not in the *nuclear* age as previously thought) and are surrounded by an *information* society. He also borrows the concepts related to the industrial revolution and applies them to computer evolution. The former revolution was characterized by human-sized assembly lines. We are in the process of entering the third industrial revolution where intelligent robots will be in charge and constitute intelligent robot-sized assembly lines.

Similar concepts apply to computers. Clementi identifies seven computer generations: the first (1946-55) characterized by static memory and vacuum tubes; the second (1955-65) with transistor logic and magnetized core memory; the third (1965-75) with integrated circuits and magnetic disks; the fourth (1975-90) characterized by vector processing and parallelism, mostly with only a few processors.

The fifth generation (1990-2000) has just started and is characterized by knowledge-processing computers, not just data and information processing. The sixth generation (1991-2000) is evolving at the same time and possesses massive parallelism, distributed computing and user-friendly systems. We can also try to outline the features of the seventh generation (1998-2010), which will probably be based on neural networks ideas and possess signal recognition capabilities (e.g., for the human voice) and full use of artificial intelligence concepts and user-friendly tools.

All the above considerations naturally apply to 'mainframe' or multiuser computers. The evolution of personal computers and workstations has been so fast in the last few years that it is hard to assess where it will go and how it will interfere with mainframe computing. It is a fact, however, that a huge number of applications have moved and will continue to move from mainframe computers to cheaper, but very powerful, desktop and laptop machines.

So, where do we stand today? Well, for industrialized activities we are moving towards intelligent robot-sized production lines, while for computers we are in a strange situation. We are at the end of the fourth generation, moving toward the sixth, and later, the fifth and seventh generations.

One of the most interesting parts of Clementi's analysis is his interpretation of how the three industrial revolutions are imitated by the development of computer solution approaches and simulation software.

The first stage is computer software that automates manual computation. This stage in simulation modeling can be called 'computerization of a simulation' and imitates what hundreds or thousands of humans could do by hand. It corresponds to the human-sized assembly lines in industry.

The second stage is 'global simulation,' i.e., modeling not as an independent, isolated activity but within a supporting simulation environment. We can find today partial realizations of this second stage in the space industry, where large and well-organized libraries of programs are used as a key tool for manufacturing activities and not just as a service. This stage in simulation modeling corresponds to robot-sized assembly lines in industry.

The third stage adds artificial intelligence to the simulation environment and therefore is capable of automatic detection and correction of errors. This stage of simulation modeling can be referred to as 'cognizant simulation' and corresponds to intelligent robot-sized assembly lines in industry.

But how does this discussion apply to environmental modeling and software? Well, we must admit that we are still in the first stage, even though many efforts are being performed to at least design the second stage. For example, several consulting and computer manufacturing groups are working today toward the design of a prototype 'environmental workstation'–an interactive, user-friendly computer system to provide all the tools that are needed to manage environmental projects, simulate environmental phenomena and visualize the results. The following section presents some of the concepts the author proposes for the development of a 'total approach' to environmental modeling and software.[2]

3 The total approach to envrionmental modeling and software

This section summarizes the features that an ideal computer package should possess in order to provide a general user with all the necessary tools to perform environmental analyses, simulations, assessments and evaluations, including report preparation and visualization of results. A prototype of this total approach – called FES, FaAA Environmental Software – has been developed by the author and is briefly described below.

FES provides a conceptual platform for a total approach to environmental modeling and software. It is designed to run on a PC 386 or 486 machine under ToolBook/Microsoft Windows/DOS. The prototype is user-friendly and mouse-driven.

FES initiates by displaying a 'cover page' containing several buttons. By clicking on these buttons, beginners' information, overview and other information are displayed. By clicking on the START button, the program moves to the main window and a working session begins.

The main window is characterized by three 'chapters' and six buttons. The buttons are always active at any time during the session. The chapters deal with

1. Education
2. Simulation
3. Management

The Education chapter contains several modules designed for environmental education. In its final configuration, the modules in this chapter are designed to cover

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[2] A prototype of this total approach (called FES, FaAA Environmental Software) has been developed by the author. A demonstration diskette is available to readers upon request. This demonstration can run on a PC 386 or 486 under Microsoft Windows/DOS.

six topics: the atmosphere, rivers and lakes, seas and oceans, soil and groundwater, human health, and environmental effects.

The Simulation chapter contains modules that simulate environmental phenomena and adverse effects of pollution. Results can be visualized by still images or animation. In its final configuration, the simulation modules in this chapter are expected to cover ten topics: air, watershed, soil and groundwater, surface water, multimedia, indoor pollution, noise, human health, environmental damage, and environmental engineering.

The Management chapter contains several modules to assist the environmental manager and the environmental regulator. In its final configuration, the modules in this chapter are expected to address eight topics: environmental information management, regulatory compliance, risk assessment, emergency response, pollution control, environmental remediation, litigation support, literature search.

All modules may include direct access to databases, laser disk and other multimedia devices. The buttons allow, at any moment, the initiation of other procedures and the generation of new windows as follows:

1. HELP button. To get on-line help.
2. INFO button. To get information such as references, acronyms, etc.
3. VISUAL button. To visualize data and simulation results with visualization software.
4. DATABASE button. To access on-line databases.
5. COMM button. To establish communications with other computers, e-mail or external devices, such as the laser disk.
6. GIS button. To superimpose data and simulation results over a geographical information system.

FES is not intended at this stage to be a commercial computer package. It is instead a conceptual platform that can be used to generate a customized product for any group dealing with environmental problems and interested in using advanced, computerized techniques.

FES is highly modular in design. For simple educational needs, selected educational modules may run with a basic configuration (PC 386 only). For advanced applications and handling of large databases, FES can be designed in a full configuration mode, with built-in connections with other computers, external databases, laser disk, etc. One interesting feature is that laser disk images can be projected directly on a window in the PC screen.

A demonstration diskette of FES is available to readers upon request. This demonstration can run on a PC 386 or 486 under Microsoft Windows/DOS.

4 A guide to *Environmental Modeling* - Volume I

Environmental Modeling - Volume I is the first 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 available software for environmental simulations.

This *Environmental Modeling* series represents an effort that is unique in its contents and especially in its long term goals. Volume I–which contains eight chapters on different environmental subjects plus this introductory chapter–deals both with major environmental topics, such as air pollution, and with some special issues, such as noise pollution. The following 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, Chapter 2 discusses **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, 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.

Chapter 3 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 sub-models 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 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 stretch, Lake Balaton, Lake Kuortaneenjarvi and Lake Tuusulanjarvi. The chapter ends with a discussion on 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 5 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 one of these media are described, and the basic equations that represent these processes are discussed. The chapter includes a section on available software.

Chapter 6 discusses **ecological modeling**. A survey of some important features in mathematical ecology is presented, with a special emphasis on the structural properties and behavior of ecosystems, rather than just numerical aspects. In fact, 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.

Chapter 7 addresses **environmental noise modeling.** It 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.

Chapter 8 deals with **environmental information management.** 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.

Finally, Chapter 9 discusses **the future of environmental modeling.** 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).

5 Conclusions

I would like to conclude this introductory chapter by encouraging the environmental scientific community to provide input, suggestions, contributions and constructive criticism. I would really appreciate help, encouragement and support, especially from the readers of our *Environmental Software* journal (currently published by Elsevier)–a publication that since its inception in 1986 has been dedicated to providing information on research activities, model development and software use to environmental scientists, engineers and decision makers. This *Environmental Modeling* series continues along the same path.

Hopefully, the *Environmental Modeling* series will not be just black ink on white paper. In fact, we plan to expand our editorial goals to include soon in the series 'computerized' chapters[3] 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 readers will then be able to actively interact with all the material provided in the chapters and, with just a few keystrokes, to adjust equations, modify data, recalculate and

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[3] Computerized chapters can be made today using special programs, such as *Mathematica*. The most striking feature of *Mathematica* is its ability to create interacting documents that mix text, animated graphics and sound with active formulae. In other words, using *Mathematica* the author can write an article or a book that is 'alive,' i.e., a text in which parameters are used to solve, analytically or numerically, a set of equations. These solutions trigger the generation of figures, sound, animation. Everything is connected and interactive. 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.

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.

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