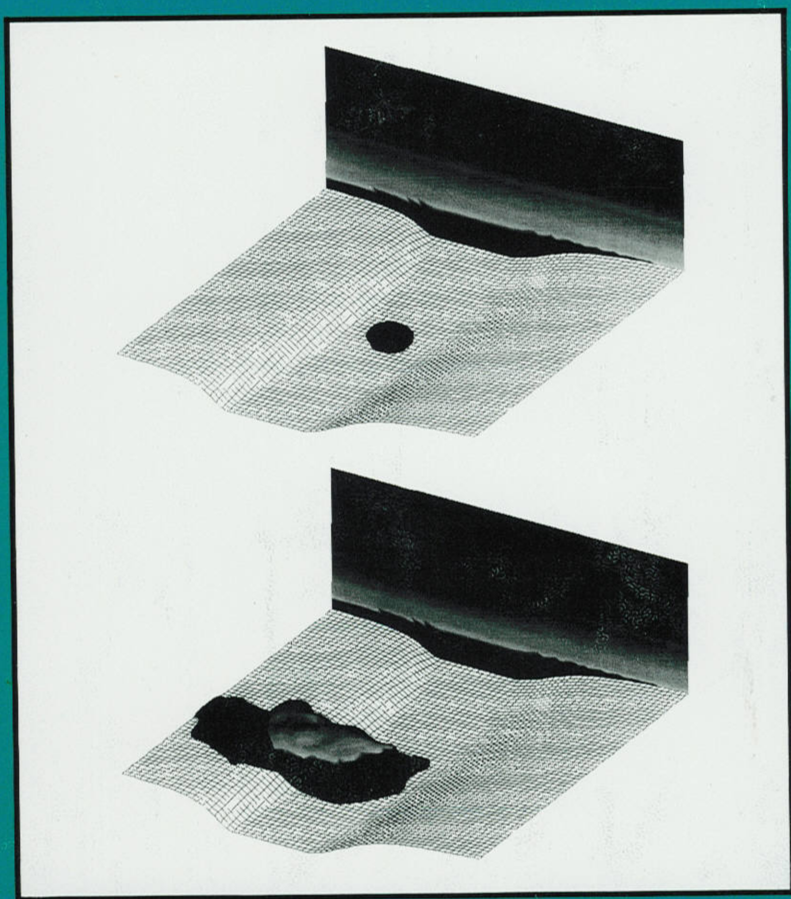
Air Pollution II Volume 1:

Computer Simulation

Editors: J.M. Baldasano, C.A. Brebbia, H. Power, P. Zannetti



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SPECIAL KEYNOTE ADDRESS

Computer modeling of air pollution; science, art or fiction?(*)

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ABSTRACT

This keynote address explores the issues related to air pollution modeling as an emerging scientific field often greeted with appreciation but sometimes with skepticism and mistrust. The article explores the complex relationship between the modeling community and the rest of the scientific world. Finally, a discussion is presented of future trends in air pollution modeling and, in particular, the expected development of Comprehensive Modeling Systems (CMS) by the end of the decade.

WHAT IS COMPUTER MODELING OF AIR POLLUTION?

Air pollution modeling (Zannetti, 1990) is an essential tool for most air pollution studies. 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 familiar with the first type of physical or laboratory models since we all have played with *toys*. What are toys? Well, most toys are a small-scale representation of real things, for example cars, cranes, people, appliances, rifles, and tanks. And these toy "models" possess some of the characteristics and physical properties of the original objects they try to imitate; for example, a toy boat floats 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

(*) This article is based, in part, on sections taken from two introductory chapters that the author wrote for a book series on Environmental Modeling, Vols. I and II, published by Computational Mechanics Publications in 1993 and 1994, respectively.

real car, can withstand impacts and rollovers that would seriously damage a real automobile.

Physical models in air pollution science are built to provide tools for experimentation. For example, 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 systems. 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 to use simulation results with care.

The second type of modeling approach is 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–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, that is 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 need 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 air pollution phenomena are concerned, the real world–the atmosphere–is three-dimensional, never at rest, and seldom homogeneous. Fortunately, in the last few decades, computers have come 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 air pollution scientists in particular.

In conclusion, computer modeling of air pollution is today the ability to numerically simulate air pollution phenomena. In other words, computers have become a numerical laboratory in which air pollution phenomena are reproduced, examined, and controlled through numerical experiments. We call this process computer modeling of air pollution–the ability to use computers to solve the basic equations that describe the dynamics of meteorological and air pollution phenomena and, ultimately, the adverse effects of pollution.

WHY DO WE NEED TO MODEL?

Computer modeling of air pollution 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, 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 the impact of industrial and urban sources at short-range (that is, impact confined to a few kilometers).

Air pollution 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, especially when linked to powerful 3D visualization techniques, are not just tools to provide a numerical solution of a predefined set of equations. In fact, numerical modeling is becoming a new branch of science and not just a solution method to assist scientific researchers.

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

Air pollution 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 conclusion, air pollution modeling should be seen as an objective frame laid over subjective interpretations.

MODELERS AND NON-MODELERS

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 relatively high levels of management, 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 have faced a profound skepticism for the capabilities of environmental models. How many times I have 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 noticed profound diffidence toward the modelers themselves. They were seen as desk scientists working in isolation, living in an ivory tower–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. 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 who know about air pollution modeling and interact with computer modelers. The questionnaire had 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 everyone 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

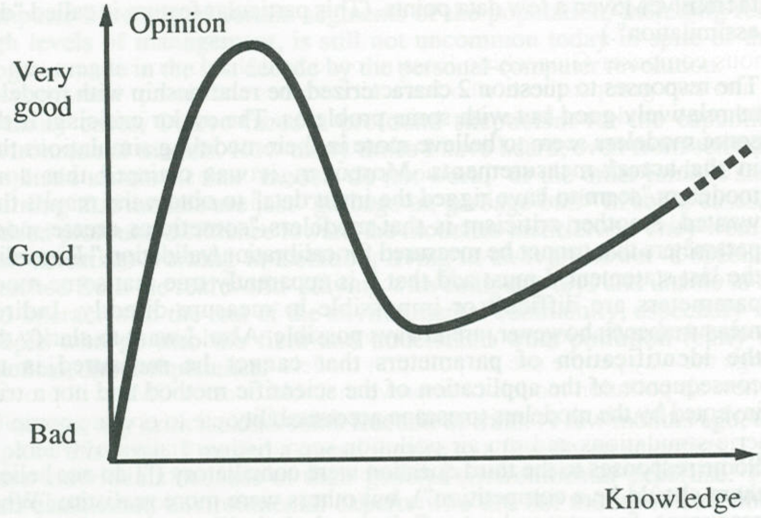
themselves given a few data points. (This particular feature is called "data assimilation".)

2) The responses to question 2 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 to the third question were conciliatory ("I do not believe there should be a competition"), but others were 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 where accuracy is being sacrified in the name of 'consistency' or 'conservatism'."

I encourage everyone to reflect seriously on these statements. I intend to collect more opinions on this topic and expand the analysis. Therefore, I would really appreciate it if many colleagues (modelers and nonmodelers) would share with me their comments and frank opinions on this matter.

I would like to conclude this section with a picture that depicts, in a semi-facetious manner, what I think is the prevalent opinion among environmental professionals about air pollution models. Opinion is plotted as a function of the professionals' knowledge of and experience about models. I do not profess that this curve applies to everybody. However, in my experience, it often works very well.



Environmental professionals with no knowledge about models tend to have a bad opinion of them. This still puzzles me because I cannot explain it in rational terms. With some initial knowledge, something very drastic happens: people thinks that models can do everything and are the solution to all our problems; models are God. With more knowledge and experience, skepticism sets in and people reassess their trust and expectations. With more knowledge, there is a steady growth and the return of some optimism about the capabilities of air pollution models. Does this curve make sense to you? Let me know.

IS ENVIRONMENTAL MODELING POSSIBLE?

Most scientists strongly believe in environmental modeling. A 1992 issue of *Science* magazine 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 fields from biology to high-energy physics a way to perform experiments that would be otherwise impossible." In particular, computer visualization of numerical simulations was depicted as an extension of the scientist's thinking power.

But there are scientists who disagree with this assessment. For example Oreskes et al. (1994) state that "verification and validation of numerical models of natural systems is impossible" and that "models can only be evaluated in relative terms, and their predictive value is always open to question." They conclude that "the primary value of models is heuristic."

The author of this paper belongs to the group that believes in environmental modeling. Certainly, there are intrinsic limitations in computer simulation and difficulties and uncertainties in simulating environmental processes (and, in particular, atmospheric processes). Nevertheless, we should be confident that in this decade environmental modeling will be fully established as a very reliable science, in spite of some current skepticism.

THE FUTURE: CMS

The famous composer Gioacchino Rossini once said that opera singers can be divided into two groups: those who have nice voices and do not know how to sing and those who do not have nice voices and do not know how to sing. In the same facetious manner, we could claim that there are two types of air pollution models available today: those that incorporate rigorous assumptions and are poorly documented and difficult to use and those that use overly simplified assumptions and are poorly documented and difficult to use. It is a matter of fact that air pollution modeling software was not developed for a large number of paying customers, such as users of other scientific software.

The expected future development of a Comprehensive Modeling System (CMS) will change the way people use air pollution models–and also the way scientists develop new air pollution models or improve their old ones. A CMS will provide a set of tools to allow both scientists and nontechnical people to operate complex atmospheric simulations and run air pollution scenarios virtually anywhere. A CMS will initially include a set of different simulation modules but, more importantly, will also provide a set of rules (that is, a simulation environment) for the incorporation of additional simulation modules.

What is a CMS?

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. Clicking (with a foot mouse) the button *Beginners click here* brings up a series of windows. Some of these windows contain detailed information sections and one contains an animated user's guide that describes the entire system. Clicking the button *Education* brings up a new series of windows and "chapters." These sections are connected to CD's, laserdisks and multimedia devices that provide, on the *Penta III* screen, interactive education tools on the subjects of atmospheric sciences, air pollution, laws/regulations, simulation modeling, 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, locking the execution of the simulations into 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 to access the master version of CMS (in remote computer storage) and to modify, add, or 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 meteorological fields, emission data, transport and diffusion, 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. A special *Real-time* button allows real-time simulation for emergency response to accidental releases, if proper connections are made to access meteorological and other data on-line. At any time the user can extract input/output data for his or her own purposes and move to different computational environments (such as new versions of *Mathematica*, *Spyglass*, *Systat*, etc.) on the *Penta III* screen.

Science fiction? Not really. Many groups (including IBM before its recent business crisis) have given a lot of thought to the development of environmental workstations or workbenches to offer some of these features. The concepts of a CMS were recently discussed by Hansen et al. (1994), who define CMS as "an advanced set of tools for air quality managers to use in making scientifically based decisions." CMS is presented as a tool to properly simulate phenomena such as tropospheric ozone, toxic airborne materials, visibility impairment, acid rain, and real or hypothetical emergencies. They consider the attributes of a CMS to be: regulatory approval, accessibility, versatility, reliability, self consistency, convenience, and efficiency.

A CMS can also be defined as a system 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 other endeavors. As such, a CMS should provide the following:

1. A platform for modeling pollutant emissions, atmospheric physics and chemistry, and impacts in as scientifically sound a fashion as is desired or possible.

2. A readily accessible interface, so that its use is a benefit, not a distraction.

3. A powerful set of graphical, visual, economic, and scientific analysis tools, including report preparation.

4. A method to make maximum use of the available computational resources, including CPU power, disk storage, communication, etc.

Air quality modeling has been listed as one of the grand challenges of computational science (Levin, 1989). CMS is the answer to this challenge.

<u>Current Developments</u>

Two major efforts are currently under development.

The US EPA has been developing, testing, and evaluating increasingly complex mathematical modeling systems. A recent document (Novak et al., 1994) provides a conceptual overview of Models-3, an air quality modeling system expected to serve as a user-friendly foundation and to provide air quality assessment and decision-support tools for direct use by regulatory analysts and scientists.

The Consortium for Advanced Modeling of Regional Air Quality (CAMRAQ) Steering Committee has drawn up a Technical Work Plan (Hanna, 1993) that summarizes research plans on CMS development for the next 10 years. Additional information on this ongoing effort is found in Hansen et al. (1994). Close collaboration has been established between the EPA and the CAMRAQ groups.

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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).

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