Air Pollution

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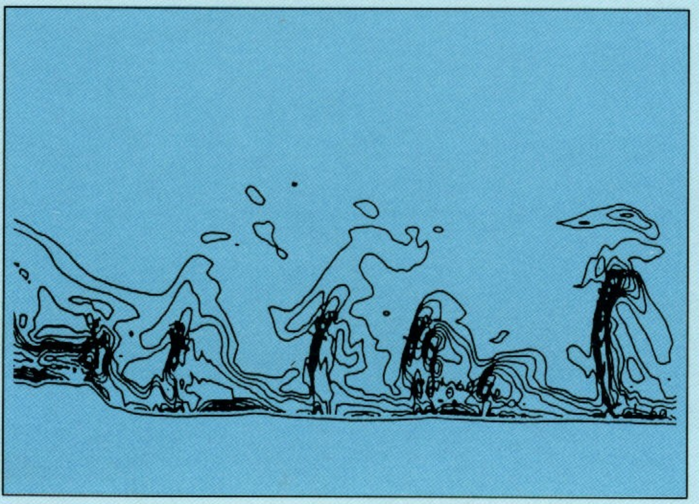

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Numerical simulation modeling of air pollution: an overview

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Abstract

This article presents an overview of mathematical and numerical methods used to simulate air pollution phenomena. Each method is discussed without introducing its mathematical notation. Advantages, disadvantages and limits of applicability of each technique are addressed.

1. INTRODUCTION

If air pollution is a "problem," mathematical modeling cannot claim to be the "solution" to this problem. Mathematical modeling, however, is an indispensable tool for several important air quality analyses. As a matter of fact, no strategy for emission reduction and control can be cost-effective without a previous serious application of mathematical modeling techniques.

Mathematical models are the only practical 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.

This article presents a review of current mathematical methods for air quality studies and is based on recent surveys (e.g., Zannetti, 1990; Finzi and Brusasca, 1991; Milford and Russell, 1992; etc.). These are the main modeling topics to be discussed:

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- *Meteorological models*, i.e., the simulation of those meteorological parameters, such as wind, intensity of turbulence, etc., that affect the dispersion of pollutants in the atmosphere
- *Plume-rise models*, i.e., the simulation of the initial dispersion phase of buoyant plumes, characterized by a rise of the plume above its emission level
- *Gaussian models*, i.e., those techniques in which atmospheric diffusion is approximated by assuming that the concentration field inside each plume maintains a Gaussian distribution horizontally and vertically
- *Eulerian models*, i.e., those numerical codes in which the computational domain is divided into cells and continuity equations are solved in each cell
- *Lagrangian models*, i.e., numerical techniques in which plumes are broken up into "elements" such as segments, puffs, or particles
- *Chemical modules*, which simulate the often nonlinear chemical and photochemical transformations of atmospheric pollutants
- *Deposition modules*, which simulate the dry and wet deposition phenomena in which a fraction of atmospheric pollution is deposited on the surface
- *Indoor air pollution models*, which simulate the accumulation of pollutants inside buildings and poorly ventilated areas
- *Receptor models*, i.e., techniques that, solely through the chemical analysis of air pollution measurements, are able to apportion the contribution of each source (or each group of sources) to the measured concentrations without the need for reconstructing the dispersion pattern of pollutants
- *Stochastic models*, i.e., statistical or semiempirical techniques to understand trends, periodicities, and interrelationships of air quality measurements and to forecast the evolution of pollution episodes
- *Interpolation methods and graphical techniques*, such as Kriging, pattern recognition, cluster analysis, and fractals
- *Optimization methods* to identify the optimal allocation of monitoring networks or to minimize either the adverse effects of pollution or the cost of controlling it
- *Statistical techniques* to evaluate the performance of dispersion models when their simulations are compared with actual pollution measurements
- *Modeling of adverse effects of pollution*, such as visibility impairment, climate changes, and stratospheric ozone depletion
- *Available computer packages*

These fifteen topics are covered in the next section.

2. MAIN MODELING TOPICS

2.1. Meteorological models

Meteorological models are developed for two purposes:

1. To understand local, regional, or global meteorological phenomena; and
2. To provide the meteorological input required by air pollution dispersion models.

Numerical meteorological models can be divided into two groups:

1. Diagnostic models, i.e., models that interpolate and extrapolate available meteorological measurements and contain no time-tendency terms; and
2. Prognostic models, i.e., models with full time-dependent equations.

Diagnostic models are simpler but include little physics in their calculations. They are often used to calculate mass-consistent wind flow over complex terrain. Prognostic models are used to forecast the evolution of the atmospheric system through the space-time integration of equations for conservation of mass, heat motion, water, and, if necessary, other substances such as gases and aerosols. Most prognostic models are hydrostatic. Complex terrain simulation and small-grid applications, however, require the use of more complex nonhydrostatic models.

Any three-dimensional air pollution simulation requires good data input from a meteorological model.

2.2 Plume-rise models

In most cases, pollutants injected into ambient air possess a higher temperature than the surrounding air. Most industrial pollutants, moreover, are emitted from smokestacks or chimneys and therefore possess an initial vertical momentum. Both factors (thermal buoyancy and vertical momentum) contribute to increasing the average height of the plume above that of the smokestack. Plume-rise models calculate the vertical displacement and general behavior of the plume in this initial dispersion phase.

Both semiempirical and advanced plume-rise formulations are available. Special cases of plume rise include the interaction of plumes from multiple sources, the partial penetration by the buoyant plume of an elevated inversion, and the plume rise from stacks equipped with scrubbers.

2.3 Gaussian models

The Gaussian plume model is the most common air pollution model. It is based on the assumption that the plume concentration, at each downwind distance, has independent Gaussian distributions both in the horizontal and in the vertical. Almost all the models recommended by the U.S. Environmental Protection Agency (EPA) are Gaussian.

Gaussian models have been modified to incorporate special dispersion cases, such as plumes in the wakes of buildings, dispersion over water, coastal dispersion, and plumes in complex terrain. A simplified version of the Gaussian model (the Gaussian climatological model) can be used to calculate long-term averages such as annual concentration impacts.

The most refined use of the Gaussian model consists in splitting the plume into a series of elements. These elements are then independently treated as Gaussian segments or puffs. In this way the Gaussian model, which in its basic formulation is a steady-state equation, can be used to simulate non-homogeneous, time-dependent diffusion scenarios.

2.4 Eulerian models

The Eulerian approach is based on the equation for conservation of mass of a single pollutant species. This equation can be solved analytically under special, simplifying assumptions. By superimposing a grid, however, the equation can be solved using numerical methods such as the finite-difference method.

Advanced Eulerian models include second-order closure models and large-eddy simulation models. The latter are especially useful for simulating convective conditions since they calculate the large-scale turbulent motions by directly solving a set of modified Navier-Stokes equations.

2.5 Lagrangian models

Lagrangian models describe fluid elements that follow the instantaneous flow. They include all models in which plumes are broken up into elements such as segments, puffs, or particles.

Particle modeling is the most recent and powerful computational tool for the numerical discretization of a dynamic system. Particle models use a certain number of computational (fictitious) particles to simulate the dynamics of a selected physical parameter. Particle motion can be produced by both deterministic velocities and, more interestingly, by semirandom pseudovelocities generated using Monte Carlo techniques.

In air pollution applications that use Lagrangian particle methods, the emitted pollutants are simulated by a set of computational particles that are moved by pseudovelocities at each time step. These velocities are computed to take into account the transport caused by the average wind, the turbulent terms due to wind fluctuations, and, if necessary, atmospheric molecular diffusion (which is often negligible).

One of the major advantages of particle models versus Eulerian grid models is their ability to correctly simulate the transport terms without adding artificial numerical diffusion.

2.6 Chemical modules

Atmospheric chemistry deals essentially with four major issues: photochemical smog, aerosol chemistry, acidic deposition, and air toxics. Several air pollution models include modules for the calculation of chemical reactions. These modules can include a simple, first-order reaction (e.g., a transformation of sulfur dioxide into sulfates) or perform complex multispecies chemical and photochemical reactions.

Several reaction schemes have been proposed for simulating the dynamics of interacting chemical species. These schemes have been implemented into both Lagrangian and Eulerian photochemical models. In Eulerian photochemical models, a three-dimensional grid is superimposed to cover the entire computational domain, and all chemical reactions are simulated in each cell at each time step. In the Lagrangian photochemical models a single cell (or a column of cells or a wall of cells) is advected according to the main wind in a way that allows the injection of the emissions encountered along the cell trajectory. For the simulation of atmospheric chemistry, Lagrangian formulations are faster. However, they provide concentration outputs only along trajectories and, therefore, their outputs are difficult to compare with concentration measurements at fixed locations.

2.7 Deposition modules

Deposition phenomena are the way in which the atmosphere cleans itself. The process is efficient, as only a few gases (most notably carbon dioxide) show signs of global increase, in spite of the large and increasing worldwide emission of pollutants. There are two types of deposition mechanisms: dry deposition, i.e., uptake at the earth's surface, and wet deposition, i.e., absorption into droplets followed by droplet precipitation or impact on the earth's surface.

Several air pollution models include simple or complex modules for the calculation of atmospheric deposition. Simple methods decrease the concentration of pollutants using an exponential decay term, with a time constant that is a function of the type of pollutant, meteorological parameters, and type of deposition surface.

2.8 Indoor air pollution models

It is evident that the air people breathe inside buildings (at home or at work) and while traveling (by car, bus, subway, airplane, etc.) is quite different from the air outdoors. Outdoor pollutants can infiltrate into buildings. The real problem with indoor air quality, however, is the indoor emission of pollutants and their accumulation due to poor ventilation and air exchange.

Since a large majority of the population in the industrialized world spends most of its time indoors, it is clear that indoor air quality has a major effect on public health. Studies on health effects of air pollutants should be seriously challenged when they fail to account for this important factor.

Major indoor air pollution problems include radon, asbestos fibers, formaldehyde, other volatile organic compounds, biological pollutants, pesticides, and environmental tobacco smoke (ETS)(*). Indoor air quality modeling generally simulates indoor pollution dynamics by representing a building by a set of interconnected chambers, where pollutants are well mixed in each chamber.

2.9 Receptor models

Receptor models are the dream of the air pollution experimentalist - a dream that till now has been only partially fulfilled. Dispersion models compute the contribution of a source to a receptor as the product of the emission rate multiplied by a dispersion factor. In contrast, receptor models start with observed concentrations of ambient aerosols at a receptor and seek to apportion the observed concentrations among several source types (such as industry, transportation, or soil), based on the known chemical composition (the chemical fractions) of source and receptor materials.

Receptor models are based on mass-balance equations and are intrinsically statistical in the sense that they do not include a deterministic relationship between emissions and concentrations. However, mixed dispersion-receptor modeling methodologies have been developed and are very promising.

2.10 Stochastic models

Stochastic models are based on statistical or semiempirical techniques to analyze trends, periodicities, and interrelationships of air quality and atmospheric measurements and to forecast the evolution of pollution episodes. Several techniques are used to achieve this goal, e.g., frequency distribution analysis, time series analysis using Box-Jenkins and other models, spectral analysis, etc.

Stochastic models are intrinsically limited because they do not establish cause-effect relationships. However, statistical models are very useful in situations such as real-time short-term forecasting, where the information available from measured trends in concentration is generally more relevant (for immediate forecasting purposes) than that obtained from deterministic analyses.

2.11 Interpolation methods and graphic techniques

Several techniques, which can be labeled as interpolation methods and graphic techniques, have been used with success to analyze atmospheric data and air pollution measurements. They are Kriging, pattern recognition, cluster analysis, and fractals.

Kriging is an interpolation technique that presents three major advantages over other standard methods: its interpolations are made with weights that do not depend upon data values; it provides an estimate of the interpolation error; and it is an exact interpolation since the interpolation at any observation point is the observation itself.

(*) The author finds it extremely ironic to attend "air pollution" or "environmental" conferences in Europe and the Third World where smokers, while talking about protecting the environment, expose colleagues and friends to the highly toxic fumes generated by their bad social habit. It is very unfortunate that North America is still the only region in the world where some respect is shown for nonsmokers' rights.

Pattern recognition techniques categorize sets of observations graphically and perform forecasting. These methods have been applied in atmospheric studies for air pollution control, characterization of local sources, and automatic computation of mixing heights from LIDAR measurements.

Cluster analysis covers a variety of techniques that can be used to find out which objects in a set are similar.

Finally, fractals are useful for qualitative reproduction of natural phenomena, such as turbulent motion, and for image compression techniques. Their most interesting application is probably in conjunction with chaos theories.

2.12 Optimization methods

Air quality studies often call for optimization. It is unfortunate that so many important decisions (and so many mistakes) in air pollution and environmental problems are made by "decision-makers" and not by optimization models. For example, strategies for reduction of emissions should always be optimized in order to achieve the most effective reductions within allowable budgets.

The most common application of optimization methods occurs in the design of monitoring networks, where nonlinear programming techniques are used to determine the optimum number and location of stations to monitor the quality of ambient air.

2.13 Statistical evaluation techniques

The performance of both Lagrangian and Eulerian dispersion models can be estimated by comparing their predictions against field measurements. This comparison is performed using both qualitative data analysis techniques and quantitative statistical methods.

In performing a statistical evaluation of an air pollution model against field data, two caveats should be kept in mind. First of all, "garbage in, garbage out": even the most accurate model will not work with poor emission and meteorological data. More important, however, is the common belief that environmental measurements are the "real world" and that models are good only when they replicate measurements well. Environmental measurements are not the real world! In fact, their spatial and temporal resolution is generally poor. Only a well-tested and well-calibrated simulation model can be a good representation of the real world, its dynamics, and its responses to perturbations.

Unfortunately, all over the world huge efforts and investments are being made to collect data that too often remain unused. Frequently these monitoring activities are not well coordinated with numerical modelers nor followed up with appropriate investments in computer analyses, interpretation, and modeling studies that are the logical and indispensable continuation of the initial project.

2.14 Modeling of adverse effects of pollution

Often the real goal of an air pollution study is not only to evaluate the concentration field of atmospheric pollutants but also to quantify the pollutants' adverse effects. Adverse effects can be divided into

1. Short-term and long-term ecological damage to human health, animals, and plants
2. Damage to human "welfare," such as visibility impairment, odors, and weather changes
3. Economic damages to material, structures, real estate values, and artistic heritage
4. Global effects, such as greenhouse phenomena and stratospheric ozone depletion

Two major topics have been addressed by visibility modeling techniques:

1. Plume visibility, models of which simulate the visual effect of a single plume
2. Regional haze, models of which address visibility impairment (mainly a reduction in visual range) caused by large air masses containing high concentrations of fine particles such as sulfates

Global problems are simulated by global circulation models (GCM), i.e., complex Eulerian techniques that simulate atmospheric dynamics at the global scale.

2.15 Available computer packages

Many computer programs have been developed for meteorological and air quality simulations. Some of them, generally the simplest, are well documented and relatively easy to use. Most of them, however, require users with good technical skills and, often, the supervision of the developers of the codes. Available codes are discussed in Chapter 14 of Zannetti (1990). Roth et al. (1988) offer a comprehensive compendium of air quality models in their Appendix B, Part 2, and Appendix C.

Many air pollution models have been developed by or for the U.S. EPA, which has periodically provided guidelines and recommendations. Many non-EPA models can also be used, especially for studies that do not involve regulatory aspects and, therefore, need not be performed with "approved" software.

Models are also available for evaluating accidental emissions (Hanna and Drivas, 1987) and for local planning and assistance in emergency response (U.S. EPA, 1989).

3. CONCLUSIONS

An overview of air pollution modeling has been presented. Air quality modeling is an essential tool for most air pollution studies. Modeling is indispensable in at least three cases:

1. When measurements are not available or sufficient
2. For assessing the degree of responsibility of different polluting sources
3. To make pollution forecasts and evaluate "what if" scenarios

Both deterministic and stochastic-statistical techniques have been discussed. Deterministic models are the most important ones for practical application since, if properly calibrated and used, they provide an unambiguous, objective, source-receptor relationship. Such a relationship is the goal of any study aiming either at improving ambient air quality or preserving the existing concentration levels from future urban and industrial development.

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