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ADVANCES IN ENVIRONMENTAL SCIENCE AND ENGINEERING

Edited by
James R. Pfafflin
Edward N. Ziegler

Volume 1
FUNDAMENTALS

PREFACE

Wolman† has pointed out that "It is undoubtedly true that the intellectual forces which created a better life for man, and likewise violated some of the environment, are the same forces to which one must look for correcting past and avoiding future deteriorations." The successful search for new fundamental knowledge and rapid technological advances are weapons in the arsenal of the environmental worker, on whom the world may so heavily depend. The environmental scientist and engineer, indeed all professionals and concerned citizens, are themselves dependent on the dissemination of new knowledge. The work presented here, and in succeeding years, is and will be but a small contribution to the overall international effort. We have endeavoured in the Advances series to bring together the recent contributions of respected scholars and practitioners and so make their work and views available to a wide multidisciplinary audience. The techniques of environmental science and engineering are of great significance in maintaining and enhancing the future quality of terrestrial life. They must be applied both to prepare for and to counteract the impact of industrially, domestically and naturally produced deleterious substances on the atmosphere, the bodies of water and the terrain.

Much of the philosophy and scope of the Advances is based on the editors' earlier *Encyclopedia of Environmental Science and Engineering*. However, as the challenges to our ecosystem change, so the procedures for analyzing and ameliorating the effect of both presently identified and emerging detrimental factors will require revision and there must be a concurrent expansion of our knowledge. It is thus logical that an Advance series should occupy a humble but finite space within our globe, hopefully with a long halflife before its ultimate passage to recyclable solid waste.

Progress in environmental science may be thought of as occurring on two frontiers: one of increasing depth within a confined subject area, which we shall call Fundamentals; and one that deals with the broader and more interactive subject matter, which for convenience we designate Resource Management.

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†Dr. Abel Wolman (1976), Introduction to *Encyclopedia of Environmental Science and Engineering*, edited by J. R. Pfafflin and E. N. Ziegler (Gordon and Breach, New York–London).

The former section will deal with subjects related to air, water and land including: analysis; physical and biological processes; pollutant control; theory and modeling; health effects; physiological ecology; and occupational health and safety. On the other hand, the Resource Management section will deal with legal aspects; impact statements; modeling; standards of safety (nuclear and alternative energy sources); transportation impact; urban environmental planning; environmental protection administration; and ecosystem concepts.

The Advisory Board and the authors, international in scope, have been drawn from distinguished scholars and practitioners representing a broad spectrum of disciplines and professional endeavors. One of the editors wishes to express appreciation for the constructive comments and advice of Mr. Bo R. Nilsson.

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CONTENTS

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METEOROLOGICAL ASPECTS OF REGIONAL-SCALE AIR-QUALITY MODELING

1.0 Introduction

The overall problem of constructing a general, predictive air-quality model is considered, with emphasis placed on the meteorological aspects of the modeling problem.

A scale analysis of the pollutant-conservation equation indicates that different physical processes are important on the urban, regional, and global scales of pollutant transport and diffusion. Thus different types of models, initial conditions and boundary conditions are appropriate for these distinct scales.

The physical and numerical aspects of predictive meteorological models on the regional scale are reviewed in detail. The major problems are associated with the measurement of the data required by numerical models, the analysis of these data, the specification of lateral boundary conditions on a limited-area domain, the modeling of the important physical processes, and the numerical solution of the finite-difference equations.

Next, some general classes of air-pollution transport and diffusion models are discussed. These range from simple box models to complicated and expensive three-dimensional models. The limitations and potentialities of each type of model are discussed.

Finally, an example of a simple combined meteorological–air-quality model is given. The meteorological model, which is a one-layer model of the planetary boundary layer, provides detailed meteorological data for use in a particle-in-cell transport and diffusion model. A hypothetical 12-h forecast of an SO_2 plume on the regional scale is given, to illustrate the model's potential use.

As industrialized urban areas continue to grow, air-pollution problems extend farther and farther away from the localized pollution sources, becoming regional, national and even global in extent. The scientific, political, economic and pathological aspects of these larger-scale pollution problems become enormously complex. Unlike the local problem, in which the people who do the polluting suffer by diminished local air quality, on the regional and larger scales it is people far downwind who must pay the price.

Besides the obvious economic, biological and aesthetic penalties associated with increased regional pollution, it is possible that the earth's climate may be vulnerable to increasing emissions of various gases and particulates. The documented (SMIC, 1971) increase in CO_2 over the last 20 years and the associated modifications to the global radiation balance is one example. Another possible change in climate that is currently receiving much attention is the emission of freon at the ground and its subsequent diffusion upward to the stratosphere, where the chlorine atoms formed by its photodissociation threaten the ozone layer (Basuk, 1975). On the smaller scale, there is increasing concern that the use of cooling towers associated with giant energy parks may significantly affect the temperature, cloud cover and precipitation for tens of kilometers around the site (Hanna and Gifford, 1975). There is already considerable evidence that warm-season rainfall is increased by as much as 30% within 50 km of major urban areas (Huff and Changnon, 1973; Semonin and Changnon, 1974). Harnack and Landsberg (1975) have found cases where the urban thermal effect was the likely triggering mechanism for shower development over Washington, D.C.

The significance of such possible changes to the weather and climate, as well as the known association between decreasing air quality and increasing morbidity and mortality (e.g., Landsberg, 1969), demands quantitative studies of the fate of pollutants after they leave their source. Quantitative studies, in turn, require models, since we wish to be able to predict the future air quality from a given set of initial conditions or the consequences of a given pollution-control strategy in advance. Simply monitoring a given pollutant or atmospheric condition, while a necessary part of a pollution-control program, is insufficient to make predictions hours, days or years in advance.

The general term "air-quality model" may be used to describe a large number of models of varying types and complexities. Even a qualitative assessment of the meteorological conditions and their probable effect on the transport and diffusion of a pollutant represents the use of a simple air-quality model—an imprecise conceptual model built in the mind of the forecaster by previous experience. On the other end of the complexity scale, we may stagger our imaginations with the idea of an enormous mathematical, physical and chemical model which predicts all scales of atmospheric motion that affect the transport and diffusion of a contaminant, as well as the chemical reactions that modify each species. Such a complete model is well beyond our present scientific and computational skills. Clearly there must be models in between the two extremes that can provide acceptably accurate quantitative answers at a reasonable cost.

The purpose of this paper is to consider the overall air-quality prediction problem on a regional scale† and to summarize the potential uses and limitations of various types of mathematical models that are either in operational use now or are currently under development. Because the problem is very large, only a brief look at each of the components of air-quality modeling is possible. In fact, many of the individual components are so complex that they deserve a separate, more detailed review.

After briefly enumerating some of the potential uses for accurate air-quality models, we discuss the general problem of forecasting the concentration of a contaminant Q at a given point. This forecast involves two major components, a meteorological model and a pollutant transport and diffusion model. The problems of developing a realistic, predictive meteorological model are considered first. Then the modeling of the transport and diffusion of a contaminant by the wind field is discussed. A specific example of the combination of a time-dependent meteorological model and a transport and diffusion model to produce an air-quality model is then presented. This example is based on one aspect of the mesoscale modeling work being carried out at the Pennsylvania State University.

1.1 Potential Uses for Predictive Air-Quality Models‡

Before discussing the various types of air-quality models, it is useful to speculate on the potential uses of a truly predictive air-quality model—one which starts with an observed state of the atmosphere, and together with the proper boundary conditions (including known emission rates) accurately predicts the behavior of the pollutant in space and time. The question is not whether a perfect forecast of this type is possible; we know that the answer to that question is no. The question is: how close, and at what cost, can we approach this ideal?

One of the most useful applications of a predictive air-quality model would be the prediction of the concentration of a particular pollutant at a receptor in order to provide a rational basis for an air-pollution control strategy. Models for this purpose could be used in real time during air-pollution episodes to regulate industrial and domestic uses of energy or on a long-term basis to study the consequences of proposed changes in pollutant emissions. Such a prediction on the regional scale demands an accurate

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†See also the article by Meyers *et al.* in this volume.

‡Fortak (1974) provides an excellent comprehensive discussion of the applications of air-quality modeling.

accounting of contributions from possibly many sources upwind of the receptor. With the knowledge of the relative contribution from each source, the efficacy of a proposed control measure can be evaluated. An example of the use of an air-quality model to test particular emission-control strategies for the New York City region is given by Slater (1974).

A second application of air-quality models is in land-use planning. As major new polluting sites are proposed, it may be possible to take advantage of local meteorological conditions to minimize the effect of emissions on the local population. Models may be used to determine which location of major transportation systems, fossil-fuel and nuclear power parks or industries will least affect the environment. In some cases, models may indicate that the proposed construction should not proceed at all in the region, because the cost to the local air quality or climate would be too great. Obviously, the models whose results determine the fate of such million- or billion-dollar projects must be accurate. It is also obvious that when considering changes to the micro- and mesoscale climate—such as the possibility of dramatically increasing the frequency of winter fogs and summer thunderstorms by the construction of a major cooling-tower complex (e.g., Hanna and Gifford, 1975)—the models must be sufficiently general to handle the complicated feedback between the pollution and the atmosphere. It is in such problems associated with land-use planning and the preparation of environmental-impact statements that the most complicated air-quality models will probably be most useful.

A third use of air-quality models is the real-time forecasting of air quality. Real-time forecasting of air quality can be useful to people planning outdoor activities and domestic chores even during relatively noncritical situations, as well as during critical air-pollution episodes when health warnings might become necessary. The benefits of accurate real-time forecasting in determining the impact of controls such as a switch to cleaner fuels or a curtailment of industrial activities have been discussed above.

Finally, a fourth potential use of air-quality models is the evaluation of a particular control strategy. In this role, the model may be utilized to determine whether the pollution problem has improved because of the controls or because of changing meteorological conditions.

An air-quality model that also includes time-dependent meteorological parameters can be a very useful research tool for the determination of minimum meteorological conditions in a given location such that concentrations do not exceed a prescribed standard. Thus, many model experiments under varying large-scale meteorological conditions may determine the local conditions necessary for a 3-h average to exceed the standard for a given emission rate. For example, in a coastal city it might be found that the necessary conditions for a standard to be exceeded were as follows:

a) a large-scale geostrophic wind speed of less than 5 m/s;
b) a lapse rate near the ground of less than 3°C/km; and
c) a surface heat flux of less than 0.2 cal $\cdot$ cm^{-2} $\cdot$ min^{-1}.

Forecasting in real-time would be greatly aided at a very low cost by statistical statements of this kind.

In a related example of the utility of a combined meteorological–air-quality model, we consider the possibility of generating local climatological statistics in data-poor regions as a function of known large-scale climatological parameters, as measured by standard observing systems. In a related use, we might imagine "filling in" observations between stations through the use of models. Such local meteorological statistics could then be used in simple air-quality models, such as the Gaussian model. Statistics such as those included in a stability wind rose (joint probability distribution of wind directions, speeds and stability class), or those which describe the mean afternoon mixing depth and mean depth of the nocturnal inversion, could be generated by the model and used to provide estimations of annual average concentrations. The input would be derived from each possible large-scale condition; the output would be a probability distribution of the expected air quality.

1.2 Generalized Air-Quality Models

The general goal of an air-quality model is to forecast the concentration of a contaminant, Q (in dimensions of mass per volume), over space and time, given the initial conditions on the atmospheric structure and on the distribution of Q, and given the boundary conditions. For limited domains, the boundary conditions generally consist of the meteorological and concentration values on the upwind side of the domain (lateral boundary conditions); the conditions at the surface including surface heat, moisture and momentum fluxes; the emission rates in space and time over the domain; and appropriate upper boundary conditions. Mathematically, we wish to solve the equation for the time rate of change of $Q(x, y, z, t)$

$$\frac{\partial Q}{\partial t} = -\mathbf{V}_{\mathrm{H}} \cdot \nabla Q - w\frac{\partial Q}{\partial z} - Q\nabla \cdot \mathbf{V} - \nabla_{\mathrm{H}} \cdot \overline{\mathbf{V}'_{\mathrm{H}} Q'} - \frac{\partial \overline{w'Q'}}{\partial z} + \text{sources} + \text{sinks}, \tag{1.1}$$

given $Q(x, y, z, t_0)$, the time-dependent mean† horizontal and vertical veloc-

†Here the mean refers to averages over appropriate space and time scales. In a grid-point numerical model, for example, the spatial average is the average over a single mesh volume; the time average is over one time step.

ities ($\mathbf{V}_H$ and w), the horizontal and vertical eddy fluxes represented by $\nabla_H \cdot \overline{\mathbf{V}'_H Q'}$ and $\partial \overline{w'Q'}/\partial z$, and the volume sources (emission rates) and sinks (e.g., deposition, rainout, reactions).

It is obvious from Eq. (1.1) that the mean wind and the turbulent fluxes play a major role in determining the behavior of the concentrations. The truly predictive model will consist of forecast equations for these meteorological variables as well as the prediction of Q itself. For example, Pandolfo and Jacobs (1973) describe experimental forecasts of CO over the Los Angeles area utilizing a combined meteorological–pollutant model. However, solutions of Eq. (1.1) alone for specified wind distributions may be of some use in strategy planning, for example. in answering "what if" questions such as, "What would the local concentration be if the wind behaved in a certain way?" Real-time forecasting of particular pollution episodes, however, requires a predictive model for the meteorology as well as the pollutant.

Because it is possible and sometimes useful to utilize fairly sophisticated models to predict air quality without simultaneously predicting the meteorology (for example, by solving Eq. (1.1) for specified or observed wind distributions) it is convenient to break the general air-quality model into two major components: the meteorological model and the pollutant model (Figure 1). The meteorological model, which may range in complexity from simple empirical models to vast, sophisticated computer-oriented models, provides the meteorological variables that affect the transport, diffusion, and reaction of a pollutant, Q. These variables are then utilized in the pollutant model to forecast the advection and diffusion of Q. If Q is passive—that is, its behavior does not appreciably affect the meteorology—the meteorological and pollutant models may be run in series. The meteorological model is run first; the appropriate data are stored and then used in the subsequent pollutant model. In the more difficult situation in which the pollutant affects the weather, both models must be run simultaneously. Fortunately, for many air-pollution problems, the pollutant does not significantly affect the dynamics and thermodynamics on the regional scale. However, an important exception, occurs in the stratosphere, where several pollutants threaten the ozone layer.

The meteorological and pollutant components of the general air-quality model are discussed in Sections 2 and 3 respectively. At this point we discuss the special requirements for air-quality models that arise on different scales of motion and for different meteorological conditions. This analysis demonstrates that different types of air-quality models are required for different conditions. Thus in building air-quality models, it is very useful for the modeler to know the specific requirements for the model, including the horizontal scale of interest, the length of the forecast, the pollutant to be modeled, the available input data and the computation resources available. That is, the particular problem must be defined as precisely as possible.

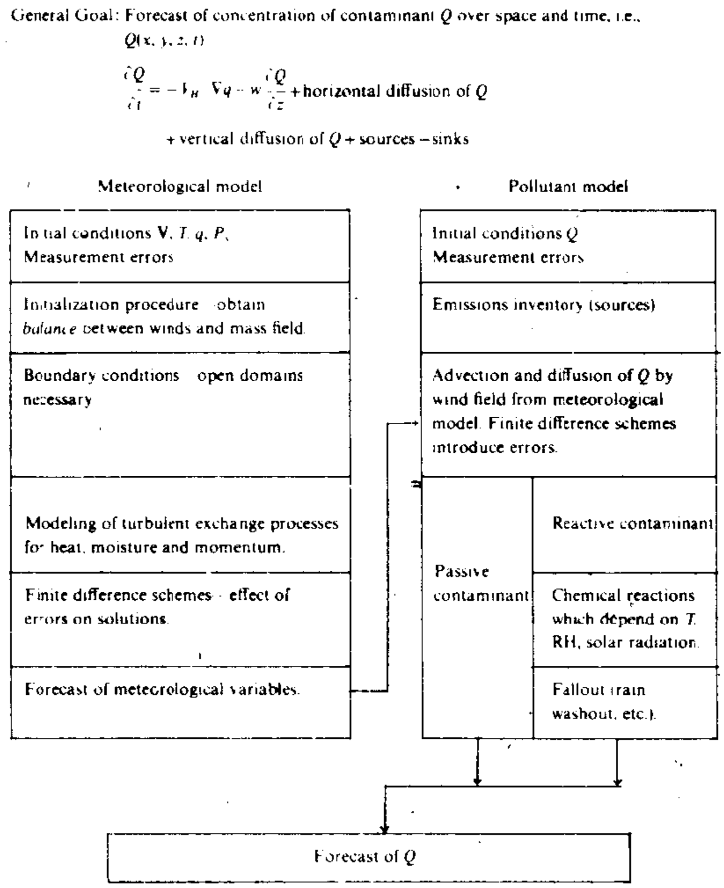

Figure 1 Schematic view of the components of a general air-quality model.

1.3 Scale Analysis of the Pollutant-conservation Equation

Some of the fundamental differences between air-quality predictions on the regional (400×400 km), urban (5×5 km) and single-plume scales may be seen from a scale analysis of Eq. (1.1). Grønskei (1974) has made a similar calculation. This analysis for the regional and urban scales assumes that the variation of the pollutant concentration is of the same scale throughout the domain and that the characteristic scale of variation is comparable to the size of the domain itself—in other words, that the typical distance from a relative maximum in concentration to a relative minimum is of the same order of magnitude as the domain size. Thus this analysis does not apply to the problem of tracing an individual plume on the regional scale. This problem, which should be approached by a trajectory-diffusion model, is discussed in Section 4.

Without loss of generality we may assume that the average v-component of the horizontal wind is zero and combine the sources and sinks of Q into a single term, S. We then define the nondimensional variables

$$
\begin{aligned}
Q' &= Q/\hat{Q};\\
u' &= u/\hat{u};\\
w' &= w/\hat{w};\\
x' &= x/L_x;\\
y' &= y/L_y;\\
z' &= z/L_z;\\
t' &= t/T,
\end{aligned}
\tag{1.2}
$$

where $\hat{u}$ and $\hat{w}$ are the magnitudes of the typical mean horizontal and vertical velocity components; $\hat{Q}$ is the amplitude of the variation in pollution concentration over the domain; L_x and L_y are the typical horizontal scales associated with the spatial variation of Q; L_z is the vertical scale of variation; and T is the time scale of the variation of Q. We also assume for order-of-magnitude purposes that the horizontal and vertical turbulent fluxes can be represented by gradient-transport or K theory, and that the term including the three-dimensional divergence is small compared to the advection terms. With these definitions and assumptions, Eq. (1.1) may be written as

$$
\frac{1}{T}\left(\frac{\partial Q'}{\partial t'}\right) = -\frac{\hat{u}}{L_x}\left(u'\frac{\partial Q'}{\partial x'}\right) - \frac{\hat{w}}{L_z}\left(w'\frac{\partial Q'}{\partial z'}\right) + \frac{K_H}{L_x^2}\left(\frac{\partial^2 Q'}{\partial x'^2}\right) + \frac{K_H}{L_y^2}\left(\frac{\partial^2 Q'}{\partial y'^2}\right) + \frac{K_z}{L_z^2}\left(\frac{\partial^2 Q'}{\partial z'^2}\right) + \frac{S}{\hat{Q}},
\tag{1.3}
$$

where K_H and K_z are the horizontal and vertical diffusivities, respectively. By the definition of the scaling parameters, all terms in parentheses are nondimensional and of order of magnitude one. Therefore, the relative importance of the horizontal and vertical advection, horizontal and vertical diffusion, and source/sink terms are given by the coefficients of the nondimensional terms. Furthermore, the time scales of each process are given by the inverse of the coefficients. Therefore, given certain space scales of variation and particular meteorological conditions, the importance of each process can be ascertained and the overall time scale of the pollution fluctuation at a given point can be estimated.

We analyze Eq. (1.3) for three space scales and six meteorological conditions. The three space scales are the regional, urban and single-plume scales, summarized in Table I. For the regional and urban scales, a uniform square-grid array of dimensions 40×40 was assumed to cover the domain. This array size, together with the size of the domain (given by L_x and L_y), determine the mesh size, Δs. For these horizontal scales, the vertical scale L_z is assumed to be equal to the mixing depth, H. The horizontal diffusion coefficient K_H is the parameter that is most arbitrary and difficult to determine. Here, we

TABLE I
Scales of air-quality models

	L_x	L_y	L_z	Δs	K_H
Regional	400 km	400 km	H	10 km	$10^4\ m^2 \cdot s^{-1}$
Urban	5 km	5 km	H	125 m	$125\ m^2 \cdot s^{-1}$
Plume	1000 m	100 m	100 m	—	K_z

relate K_H to a perturbation horizontal velocity V' (arbitrarily set equal to $1\ m \cdot s^{-1}$), and a mixing length which is taken to be the grid size of the model

$$K_H = V' \Delta s. \tag{1.4}$$

For the single-plume scale, the horizontal dimension L_x along the direction of the flow is greater than the scale across the flow, and the vertical scale is usually smaller than the mixing depth (Gifford, 1973, p. 8). Furthermore, on this small scale the order of magnitude of the horizontal diffusivity is taken equal to the magnitude of the vertical diffusivity K_z, which will be related to the meteorological parameters.

The six meteorological categories utilized in this analysis are listed in Table II. Moderate wind conditions are represented by $\hat{u}$ equal to $4\ m \cdot s^{-1}$ and $\hat{w}$ equal to $1\ cm \cdot s^{-1}$. The height of the mixed layer is 1 km except for the stable categories when it is reduced to 200 m.

The magnitude of the vertical diffusivity K_z is assumed to be equal to the vertical eddy coefficients for momentum. In the surface layer, under neutral conditions, K_z is given by

$$K_z = k u_* z, \tag{1.5}$$

where k is Kármáns constant (~ 0.4) and u_* is the friction velocity

$$u_*^2 = \tau / \rho; \tag{1.6}$$

TABLE II
Meteorology classes used in scale analysis

	Approximate Pasquill (1961) stability class	$\hat{u}$ ($m \cdot s^{-1}$)	$\hat{w}$ ($cm \cdot s^{-1}$)	H (m)	K_z ($m^2 \cdot s^{-1}$)
(a) Typical: moderate wind wind, neutral stability	D	4	1	1000	25
(b) Moderate wind, convective	B	4	1	1000	250
(c) Light wind, convective	A	1	0.25	1000	250
(d) Light wind, stable	F	1	0.25	200	1
(e) Calm, convective	A	0	0	1000	250
(f) Calm, stable	—	0	0	200	1