2 THE TOOL - MATHEMATICAL MODELING

Air quality modeling is an essential tool for most air pollution studies. Models can be divided into

- physical models -- small scale, laboratory representations of the phenomena (e.g., wind tunnel, water tank)
- mathematical models -- a set of analytical/numerical algorithms that describe the physical and chemical aspects of the problem

Physical models (Puttock, 1979; Willis and Deardorff, 1981; Mitsumoto and Ueda, 1983; Alessio et al., 1983) have shown interesting results, illuminating mechanisms and providing validation data to developers of mathematical models. Physical models will not be discussed further in this book on mathematical models.

2.1 DETERMINISTIC VERSUS STATISTICAL MODELS

Mathematical models can be

- deterministic models, based on fundamental mathematical descriptions of atmospheric processes, in which effects (i.e., air pollution) are generated by causes (i.e., emissions)
- statistical models, based upon semiempirical statistical relations among available data and measurements

An example of a deterministic model is a diffusion model, in which the output (the concentration field) is computed from mathematical manipulations of specified inputs (emission rates and atmospheric parameters such as dispersion rates). An example of a statistical model is given by the forecast, in a certain region, of the concentration levels in the next few hours, as a statistical function of (1) the currently available measurements and (2) the past correlation between these measurements and the concentration trends.(*)

Deterministic models are the most important ones for practical applications since, if properly calibrated and used, they provide an unambiguous, deterministic 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 developments. In other words, only a deterministic model can provide an unambiguous assessment of the fraction of responsibility of each pollutant source to each receptor area, thus allowing the definition and implementation of appropriate emission control strategies.

2.2 WHY AIR QUALITY MODELING?

Air quality models are a unique tool for (Seinfeld, 1975)

- establishing emission control legislation; i.e., determining the maximum allowable emission rates that will meet fixed air quality standards
- evaluating proposed emission control techniques and strategies; i.e., evaluating the impacts of future control
- selecting locations of future sources of pollutants, in order to minimize their environmental impacts
- planning the control of air pollution episodes; i.e., defining immediate intervention strategies, (i.e., warning systems and real-time short-term emission reduction strategies) to avoid severe air pollution episodes in a certain region
- assessing responsibility for existing air pollution levels; i.e., evaluating present source-receptor relationships

Figure 2-1 illustrates the elements of a comprehensive air pollution control strategy in a certain region.

It is important to clarify what air quality modeling is and what it is not. Air quality modeling is an indispensable tool for all the above analyses. It is,

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(*) The above distinction is not strict. Some diffusion models, for example, are based on statistical diffusion theories and the performance of a statistical model is always improved when some deterministic information is included in its structure. Mixed deterministic-statistical methods are also available (see Chapter 12).

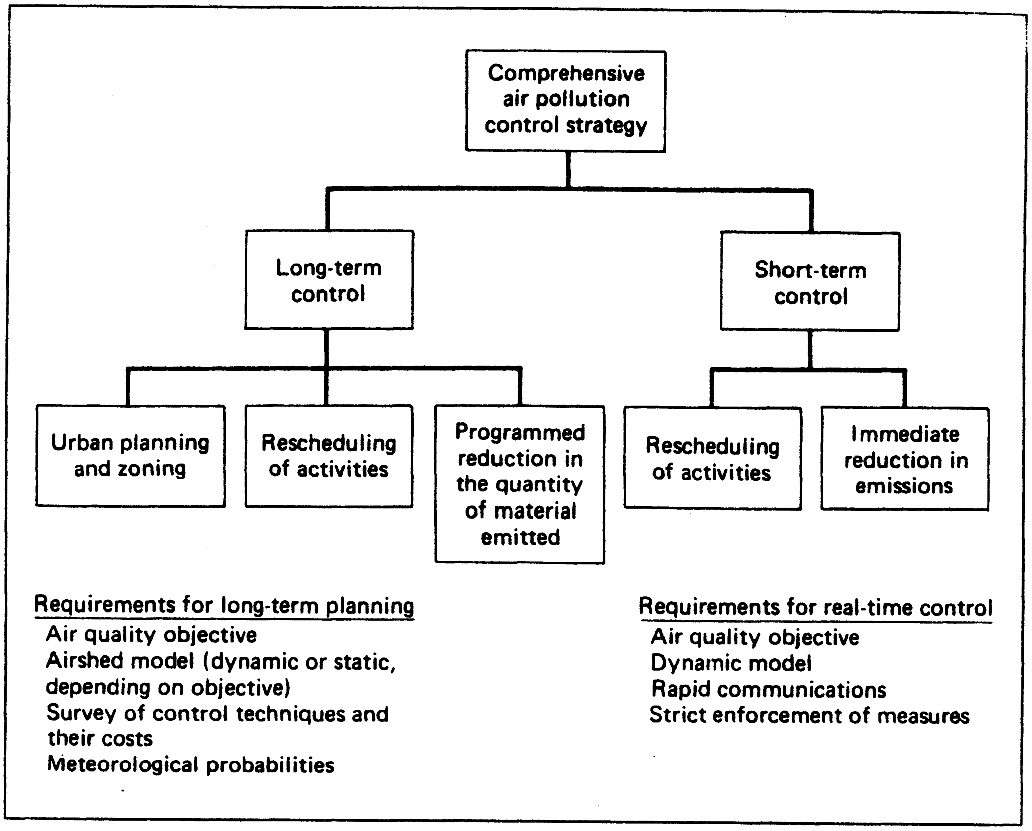

Figure 2-1. *Elements of a comprehensive air pollution control strategy for a region (from Seinfeld, 1975). [Reprinted with permission from McGraw-Hill.]*

however, only a tool. Modeling, like monitoring, is *not* the solution of the air pollution problem, even though each is sometimes presented as such. Monitoring and modeling studies constitute only a relatively inexpensive activity whose results, in the best case, provide useful information for possible future implementations of much more expensive emission reduction and control strategies.

It is also important to clarify the real role of modeling versus monitoring efforts. It is not unusual to hear qualified scientists making statements such as "Why do we need to model that? Let's measure it; that's all we need," "Models do not work," etc. These statements imply unscientific thinking. Science involves the development of theories (or "models") based on (1) the empirical interpretation of experimental data, (2) the generalization of experimental relationships, or (3) pure speculative thinking subsequently confirmed by experimental results. The advancement of science is not the consequence of monitoring activities, even though the collection of good, reliable experimental data is often (but not always) a necessary (but not sufficient) condition to it.

The above concepts, which are well-established in most scientific circles, are sometimes alien to the environmental community, where, for example, it is commonly believed that environmental measurements are the "real world." They are not! Monitoring data are indispensable for inferring theories or parameters and calibrating or validating computer simulation packages. Their spatial and temporal resolution, however, is generally insufficient to qualify them as the real world. 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 investments and efforts are made to collect data that too often remain unused on paper or computer tapes. Too often these monitoring activities are not well coordinated with numerical modelers or not followed by appropriate investment in computer analyses, interpretations and modeling studies that are the logical and indispensable continuation of the initial project.

2.3 MODELING TOPICS

Simulation modeling techniques can be applied to all aspects of the air pollution problem; i.e., (1) to evaluating emission rates, (2) to describing phenomena that take place in the atmosphere, and (3) to quantifying adverse pollutant effects (damage computation) in a certain region. In this book, only the second modeling category will be extensively covered. This will include mathematical models for simulating

- atmospheric transport
- turbulent atmospheric diffusion
- atmospheric chemical and photochemical reactions
- ground deposition

Even with the above limitation, the problem remains formidable. A correct representation of these phenomena and their multimedia (i.e., air-water-land) interactions requires several sets of equations, as illustrated schematically in Figure 2-2. The situation is actually even more complex, because Figure 2-2 does not contain the chemical processes explicitly. Drake (1979) has discussed a complete set of governing equations. Businger (in Nieuwstadt and van Dop, 1982) has given another important survey of equations and concepts in

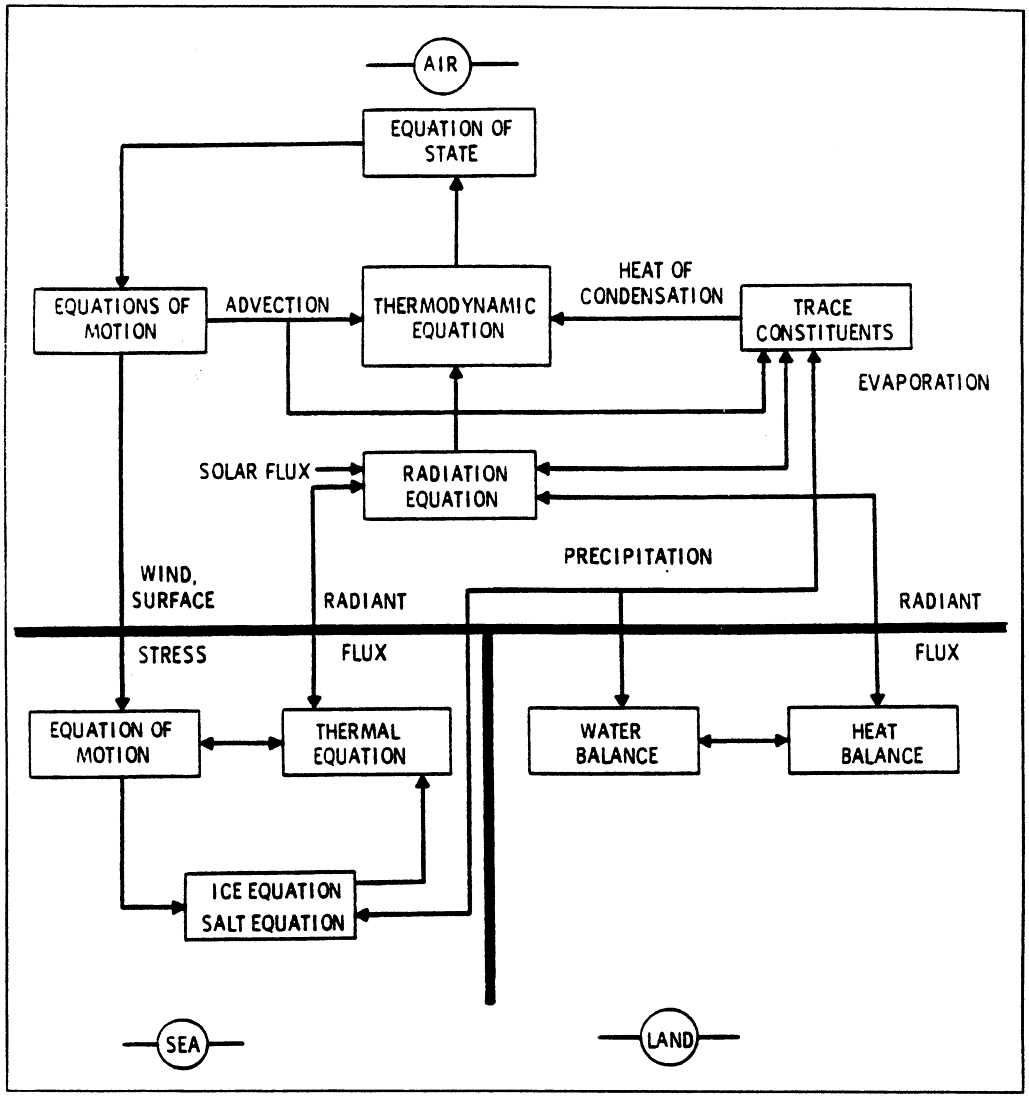

Figure 2–2. *Processes comprising weather, climate and the fate of pollutants (from Drake, 1979). [Reprinted with permission from the Electric Power Research Institute.]*

atmospheric turbulence and air pollution, while Dutton (1976) and Pielke (1984) have provided full discussion of meteorological equations and modeling. Seinfeld (1986) and Finlayson-Pitts and Pitts (1986) discuss atmospheric chemistry in great detail.

2.4 SOME PRACTICAL CONSIDERATIONS

Practical application of deterministic air quality models requires

- analysis of the problem
- selection of the appropriate model(s)
- application of the selected model(s)

The analysis of the problem requires, as a minimum, the identification of

- the type of pollutant (reactive or nonreactive)
- the averaging time of interest (e.g., instantaneous concentrations, for odor problems; one-hour averages, for short-term cases; or annual averages, for long-term analyses)
- the characteristics of the domain (e.g., simple flat terrain cases or complex orography)
- the computational limitations (e.g., simple assumptions or more complex formulations, depending on the available computational facilities)

Model selection should be performed by taking into account the above factors, as illustrated in Figure 2-3.

Finally, the optimal application of a deterministic model for control strategy analysis should incorporate its calibration and evaluation with local air quality monitoring data, in order to determine its applicability and minimize forecasting errors, as illustrated in Figure 2-4. Only models that have been verified by past data should be used for future forecasting. Calibration and evaluation are, however, difficult in many cases, when sufficient air quality and meteorological data are not available, and impossible in others, when, for example, models are used to simulate the impacts of possible *future* new sources.

Since ideal model application conditions are seldom found, air quality models are often used beyond their theoretical and practical limits of applicability. It is, therefore, not surprising that several model validation studies (e.g., Reynolds et al., 1984a,b; Lewellen and Sykes, 1983; Ruff et al., 1984) have shown unsatisfactory performance, especially when steady-state representations are used to simulate complex, time-dependent atmospheric phenomena.

2.5 MODELING FROM A PHILOSOPHICAL STANDPOINT

Phenomena such as turbulent diffusion can be viewed as stochastic processes; i.e., processes whose dynamics are so complicated that they can only be

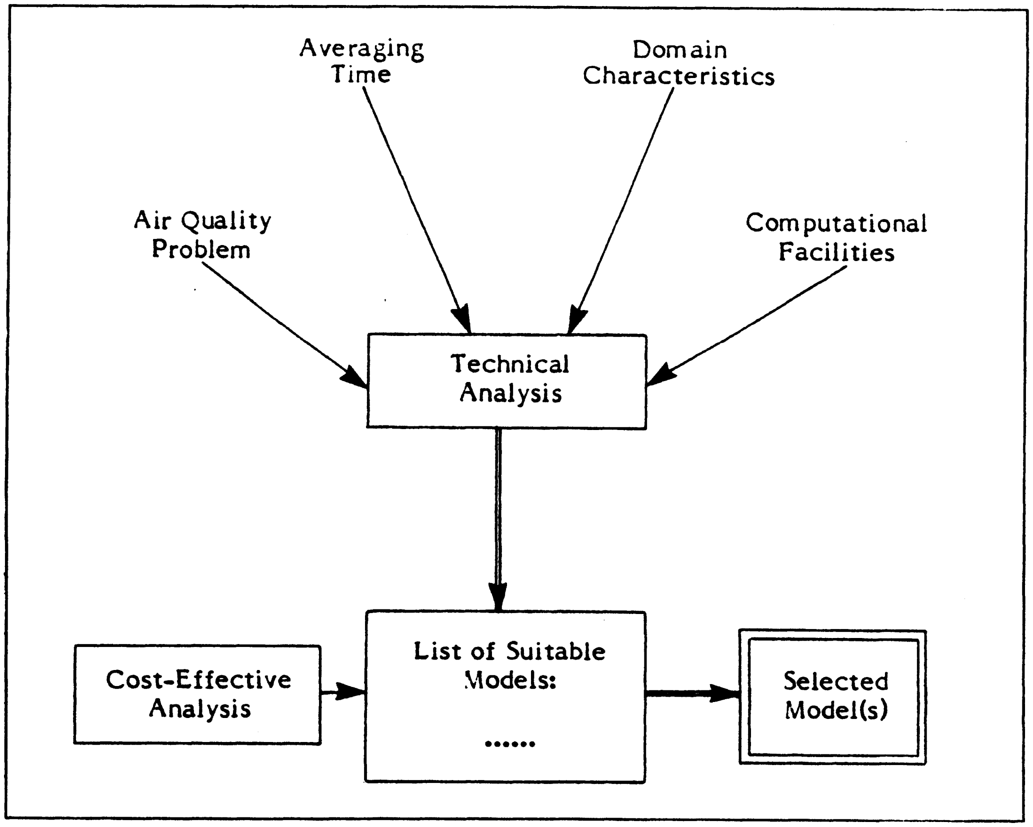

Figure 2-3. Model selection.

treated as if they were affected by random components. Wyngaard (from Nieuwstadt and van Dop, 1982) clarified this point by asking simple questions: "Why is it necessary to *model* them [the equations of motion in the atmospheric boundary layer] before solving them numerically? Why can't we solve them directly on today's large, fast computers?" The answer is provided by his length-scale analysis of the atmospheric turbulent flow, showing that typical boundary layer situations are associated with scales of turbulent motion from 300 m down to 1 mm. Therefore, a numerical grid, for example on a 10 km x 10 km region, would require about 10^{20} grid points to (hopefully) solve all fluctuations. Moreover, initial and time-varying boundary conditions should be exactly specified. This task is clearly impossible at present.

Space- and time-averaging of boundary layer parameters have been considered to provide a valid practical solution, at least for large-scale meteorological phenomena. However, the recent numerical and philosophical analysis of

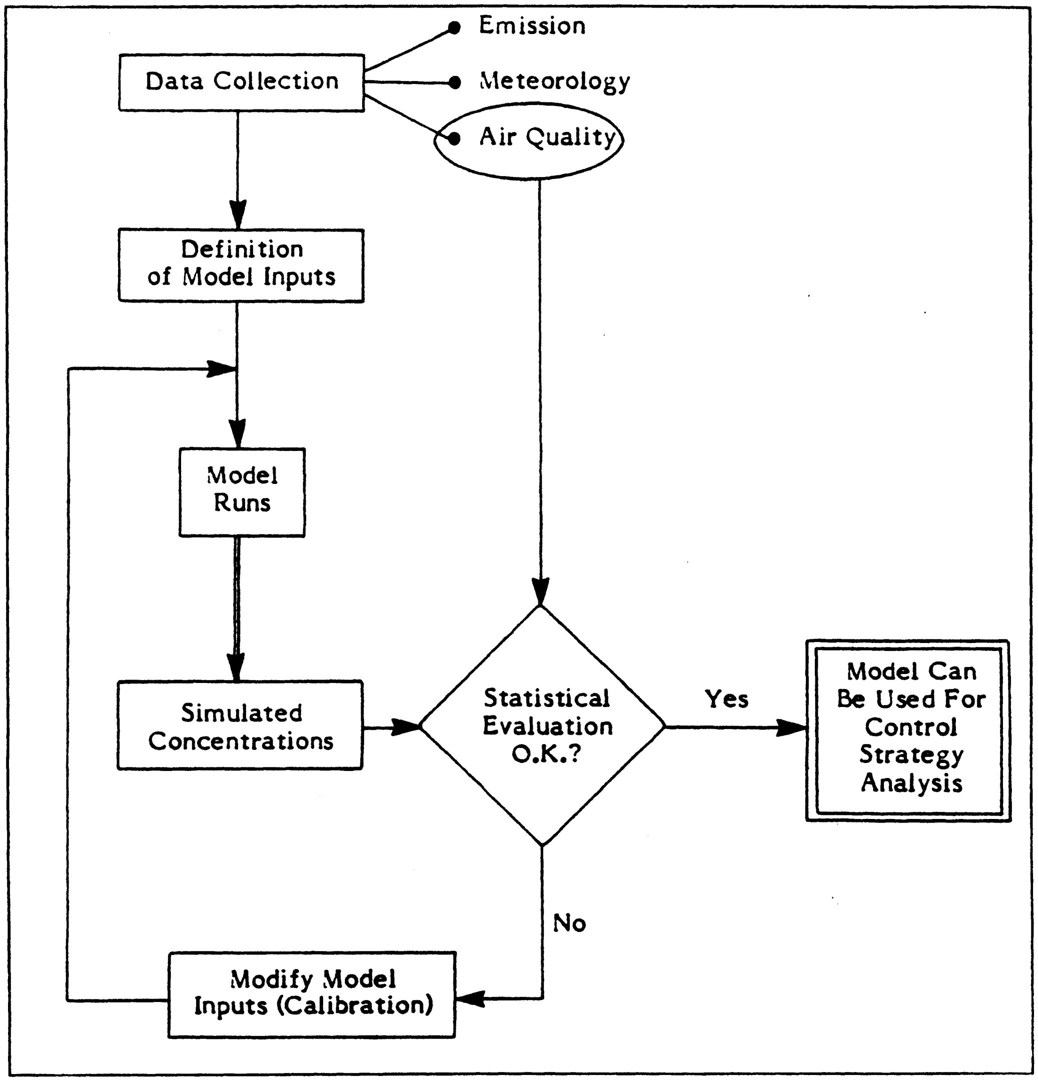

Figure 2-4. Optimal model application.

Lamb (1984) concludes that "due to a combination of our inability to quantify the precise state of the atmosphere and its boundary and to the inherent instability of atmospheric motion, not even large-scale meteorological phenomena can be rendered deterministic." He concludes that even a perfect model, using error-free input data and observations, will provide predicted quantities that still differ from the observed ones. Benarie (1987) provides additional interesting comments on the limits of air pollution modeling. The newly developed theories of chaos (Berge, 1984; Grebogi et al., 1987) seem promising for the understanding of these limits.

2.6 MODEL UNCERTAINTY

Air pollution models vary from simple methods, which possess only a few parameters, to complex ones, characterized by a large number of parameters. As illustrated in Figure 2-5, the larger the number of parameters, the lower the "natural" (or "stochastic") uncertainty associated with the model, and the smaller the errors in the model's representation of the physical reality. Unfortunately, however, the larger the number of input parameters to be specified, the larger the input data error. As indicated in Figure 2-5, there is an optimum number of parameters that minimizes the total model uncertainty. This simple interpretation explains why the performance of complex models is often equal or inferior to that of simpler methodologies. Complex models work well only when their extensive data input requirements are satisfied, which rarely occurs.

Attention must be paid to model evaluation efforts, whose results, because of the considerations above, can be misleading. Complex models can, in fact, because of their high number of parameters, be easily "tuned" or "calibrated" to well fit available measurements. This process does not, however, assure that

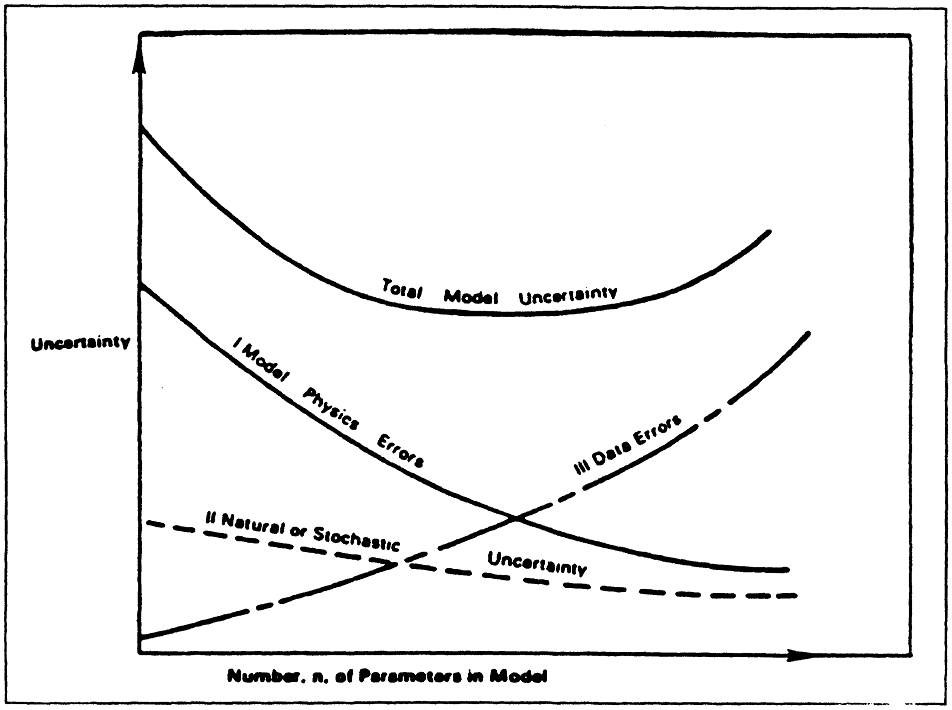

Figure 2-5. Optimal model application (from Hanna, 1989). [Reprinted with permission from Gulf Publishing Co.]

complex models perform better than simpler techniques, when applied on an "independent" data base (i.e., a data base different from the one used for model calibration). In other words, complex models can *fit* the data better than simpler techniques, but this does not necessarily indicate that complex models can *forecast* better than simpler ones.

2.7 SHORT-RANGE AND LONG-RANGE PHENOMENA

A preliminary distinction between the different transport scales of air pollution phenomena can be made as follows:

- near-field phenomena (<1 km from the source); e.g., downwash effects of plume caused by building aerodynamics
- short-range transport (<10 km from the source); e.g., the area in which the maximum ground-level impact of primary pollutants from an elevated source is generally found
- intermediate transport (between 10 km and 100 km); e.g., the area in which chemical reactions become important and must be taken into account
- long-range (or regional or interstate) transport (>100 km); e.g., the area in which large-scale meteorological effects and deposition and transformation rates play key roles.
- global effects; i.e., phenomena affecting the entire earth atmosphere; e.g., CO_2 accumulation

Until fifteen years ago, short-range problems were the major field of investigation, due to the lack of information about long-range atmospheric chemistry and, especially, because of the relatively low height of the emission stacks, so that pollutants were most noticeable only a few kilometers downwind. Moreover, calm, stagnant conditions were generally associated with the air pollution episodes under investigation, thus further restricting the length scale of the problem.

Intermediate and long-range transport processes have received increasing attention in recent years, especially due to the following factors: (1) acidic deposition, (2) visibility degradation, and (3) U.S. environmental legislation, especially the Prevention of Significant Deterioration (PSD) doctrine. Also, the Chernobyl accident has strongly enhanced the interest in long-range studies.

In Europe, where the observed acidification of Scandinavian rivers and lakes was the major starting point for the research in this field, many studies have been performed to derive long-range numerical simulation models that better fit available air quality and meteorological measurements. Among the first studies were the OECD program on Long Range Transport of Air Pollutants (Ottar, 1978) and the Cooperative Program for Monitoring and Evaluation of the Long Range Transmission of Air Pollutants in Europe (EMEP, coordinated by the U.N. Economic Commission for Europe).

Similar interest in long-range dispersion grew also in the United States, primarily inspired by the acid rain problems in the northeastern United States and Canada. Large data bases were collected to study this problem, e.g., the Electric Power Research Institute (EPRI) Sulfate Regional Experiment, SURE (Perhac, 1978; McNaughton, 1980), the U.S. Department of Energy Multistate Atmospheric Power Production Pollution Study (MAP3S) precipitation chemistry network (Dana, 1979), and the Canadian regional study (Whelpdale, from Pack et al., 1978).

As a consequence of this new interest in long-range air pollution problems, the methodologies initially used for studying and simulating short-range phenomena were expanded to simulate long-range cases. Although the two transport situations obey the same physical laws, the following considerations indicate that they require different treatment:

- The time scale of long-range transport is sufficiently large to preclude using stationary homogeneous dispersion conditions. The entire process evolves on a continuous nonstationary basis, where totally different meteorological conditions affect the pollutant dispersion at each time. Consequently, only dynamic nonstationary dispersion models can generally be applied.
- Due to the time scale of long-range transport, factors like deposition and chemistry, which may not need to be taken into account for short-range dispersion, become important.
- Horizontal diffusion can often be neglected when the emission inputs are distributed over a large-scale area, so that the concentration field is initially smoothed out. However, when an Eulerian grid is chosen, the numerical error associated with the advection terms becomes the key factor, especially for point sources. In fact, in spite of the many numerical methods proposed for minimizing numerical error, this remains the major problem for long-range transport, since many advection steps are required to move pollutants

from the emission points to the receptors, and each step contributes to such error. (See Chapter 6 for further discussion on this subject.)

- Vertical diffusion can often be neglected, assuming a homogeneous mixing of pollutants in the entire boundary layer. Elevated plumes during persistent stable conditions cannot always be treated this way, however, as, for example, in the case described by Millan and Chung (1977) where an elevated plume, trapped beneath the subsidence inversion, was detected by a COSPEC remote sensor 400 km from the source. However, even when homogeneous vertical mixing is a reasonable assumption, the problem of understanding the mass flux across a temperature inversion, which often can be significantly higher than expected (Goodman and Miller, 1977), still persists.
- Pollutants transported over a long range often impinge on complex terrain, which generally enhances atmospheric dispersion. However, terrain complexities can sometimes create the opposite effect, where valleys suffer poor ventilation with consequent trapping of pollutants.

One of the major problems in modeling the long–range transport of air pollutants is the determination of the correct trajectory of plumes, since incorrect representations may carry pollutants tens or hundreds of kilometers from the actual point of impact. Pack et al. (1978), in particular, showed that available surface–based meteorological information is generally insufficient for a correct trajectory computation, so that large errors can occur. Moreover, these errors are not random but systematic, depending on the type of advection (cold or warm) and the type of surface (land or sea). They proposed empirical trajectory adjustments to fit existing measurements. Such adjustments require direction changes up to 40 degrees and wind speed changes by up to a factor of two, which indicates the gravity of the problem. Similar results have been obtained by Policastro et al. (1986), which show poor correlation between tracer concentrations and concentrations predicted by eight short–term long–range transport models, with plume trajectory direction errors in the range of 20–45 degrees.

The above results illuminate the importance of gathering detailed, precise wind information, both on the surface and aloft, for proper modeling treatment of regional–scale transport; without precise wind information, even the best dispersion model will fail. Such information can be provided either by interpolation of measurements or by application of numerical meteorological models, as discussed in Chapter 4.

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