Air Pollution Modeling and Its Application I

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Foreword

This is the first in a new series of publications arising out of the work of the Committee on Challenges of Modern Society of the North Atlantic Treaty Organization.

The CCMS was established in 1969 with a mandate to examine practical ways of improving the exchange of experience among member nations of the Alliance in the task of creating a better environment for their societies. It was charged with considering "specific problems of the human environment with the deliberate objective of stimulating action by member governments".

It may come as a surprise to some that NATO - generally thought of as being an organization devoted solely to matters of defence - should concern itself with the environment at all. But this is to overlook Article 2 of the North Atlantic Treaty of 1949, which expressly provides that member countries should contribute towards the further development of peaceful and friendly international relations by promoting conditions of stability and well-being. This concern is reflected in many non-military areas, in addition to the environmental one.

I wish the present volume, which has been edited by the Belgian Prime Minister's Office for Science Policy Programming, every success.

Robert Chabbal
Assistant Secretary
General for Scientific and
Environmental Affairs

Preface

In 1969 the North Atlantic Treaty Organisation established the Committee on the Challenges of Modern Society. Air Pollution was from the start one of the priority problems under study within the framework of the pilot studies undertaken by this Committee. The organisation of a yearly symposium dealing with air pollution modelling and its application is one of the main activities within the pilot study in relation to air pollution.

After being organised for five years by the United States and for five years by the Federal Republic of Germany, Belgium, represented by the Prime Minister's Office for Science Policy Programming, became responsible in 1980 for the organisation of this symposium.

This volume contains the papers presented at the 11th International Technical Meeting on Air Pollution Modeling and its Application held at Amsterdam, The Netherlands from 24th to 27th November 1980. The meeting was jointly organized by the Prime Minister's Office for Science Policy Programming, Belgium and the Ministry of Health and Environmental Protection, The Netherlands. The conference was attended by 139 participants and 45 papers have been presented. The members of the selection committee of the 11th I.T.M. were A. Berger (Chairman, Belgium), W. Klug (Federal Republic of Germany), L.E. Niemeyer (United States of America), L. Santomauro (Italy), J. Tikvart (United States of America), M.L. Williams (United Kingdom), S. Zwerver (The Netherlands), C. De Wispelaere (Coordinator, Belgium).

The main topic of this 11th I.T.M. was Interregional Transport of Air Pollution up to several hundreds of kilometers. On this topic three review papers were presented: one paper dealing with model types and results by W.B. Johnson, SRI International, USA, another paper, "Probability prediction of wet deposition of airborne pollution," by F.B. Smith, Meteorological Office, United Kingdom and finally a paper in relation to the transport of air pollutants over Western Europe, in particular the Netherlands-German case by N. van Egmond, Dutch National Institute of Public Health, The Netherlands.

Other topics of the conference were: meterological parameters for use in advanced diffusion models, advanced techniques in air pollution modelling to take into account complex terrain, heavy gasses, light wind conditions, forecasting of pollutant concentration under episodic conditions and finally regulatory applications.

On behalf of the selection committee and as organizer and editor I should like to record my gratitude to all participants who made the meeting so stimulating and the book possible. Among them I particularly mention the chairmen and rapporteurs of the different sessions. Thanks also to the local organizing committee, especially Mr. S. Zwerver and Mr. J. van Ham, and Mrs. P.W.A.M. Venispols who was the Conference Secretary. Finally it is a pleasure to record my thanks to Miss A. Vandeputte for preparing the papers, and Miss C. Bonnewijn and Miss L. Vandersmissen for typing the papers.

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Chairman: W. Klug **Rapporteur: J. Tikvart**

INTERREGIONAL EXCHANGES OF AIR POLLUTION:

MODEL TYPES AND APPLICATIONS

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INTRODUCTION

During the last two decades there has been a simultaneous growth in awareness of the quality of the environment, in the ability to measure its chemical constituents with greater accuracy and precision, and in the widespread use of mathematical models for estimating the transport and diffusion of air pollutants. In recent years, special attention has been given to problems resulting from long-range transport of air pollutants over large regional- or continental-scale areas. Air concentrations and ground deposition of sulfur compounds have been of particular concern.

The OECD-sponsored study of Long-Range Transport of Air Pollutants (LRTAP) conducted in Europe (Ottar, 1978; OECD, 1977) and the Sulfate Regional Experiment (SURE) in the United States (Perhac, 1978), typify recent major environmental assessments of the problems posed by aggregated emissions over large areas. In many of these studies, theoretical models have been developed and applied to simulate the transport, diffusion, transformation, and removal of SO_x released into the atmosphere from the multitude of sources located within a given region.

The development of suitable models for this application is a difficult task, considering the very large geographical areas involved. This is because of the need to strike an appropriate compromise between two equally desirable but conflicting model characteristics--accuracy and practicality. The achievement of additional accuracy in a model requires additional sophistication in the physical formulations, as well as additional detail in the controlling input variables. These in turn require additional computer time for running the model and additional effort for preparing the input data, which together result in a less economical and thus less practical model.

Air quality modeling specialists have made substantial progress in recent years in developing new techniques to meet the challenges of simulating long-range pollutant transport and deposition. A number of excellent comprehensive reviews of the modeling work in this field have been prepared recently, such as those of Eliassen (1980), Bass (1980), Smith and Hunt (1979), Niemann et al. (1980), Hosker (1980), MacCracken (1979), Fisher (1978), Demerjian (1980).

In view of the above, it was not intended that this paper be another comprehensive review of long-range transport (LRT) modeling. Rather, the purpose of this paper is to briefly review some of the general characteristics and problems associated with air quality models on this scale, particularly interregional-type models (to be defined below), and to illustrate the various kinds of results that can be obtained by application of a sample model of this type.

CAPABILITIES AND CHARACTERISTICS OF INTERREGIONAL MODELS

The focus of this paper is on interregional air quality simulation models, which are defined as those long-range transport/ deposition models having the following characteristics:

- Multiple-source
- Scale: hundred to thousands of kilometers (moving pollutants undergo at least one diurnal cycle)
- Averaging time: hourly to yearly
- Can determine contributions from individual sources or source areas.

The most important factor in this definition of interregional models is the last one above, namely the ability of interregional models to quantitatively assess the pollutant exchanges between individual source-receptor pairs. Therefore, interregional models should consider all (or as many as possible) of the pollutant emissions from both area and point sources in the entire geographical area of interest.

The capabilities and applications of models in this general category have been summarized well by Venkatram (1980):

- Determine contributions of various sources to receptors of interest

- Estimate consequences of projected emissions changes
- Fill in gaps between observations
- Help plan field studies
  - -- which variables to measure?
  - -- where to site stations?
- Help interpret data
  - -- e.g., infer transformation or deposition rates (this will be discussed further in a later section)

Note that most of these useful tasks can only be accomplished through the use of models--measurements by themselves are not adequate to provide the necessary information.

MAJOR TYPES OF LRT/INTERREGIONAL MODELS

The following general features of LRT/interregional models are to be considered highly desirable:

- Easy to understand and use
- Suitable for both short and long terms
- Spatial resolution 100 km or better
- Require only readily available input data
- Well evaluated against measurements
- Physically realistic and accurate
- Well documented
- Easily adapted for running on typical computers
- Efficient in computer running time
- Treat wet and dry deposition separately for different chemical species.

Unfortunately, some of these features are mutually contradictory, and thus the design of every model involves a number of compromises. Modeling skill becomes most important here, in determining which portions or features of a model are least important, and thus can be compromised with the least degradation in the usefulness of the model for its intended application.

As listed in Table 1, the LRT/interregional models that have been developed to date can be classed into three main types:

Eulerian grid, statistical trajectory, and Lagrangian trajectory. Each of these model types and their advantages and disadvantages will be briefly discussed next.

Table 1. Major Types of LRT/Interregional Models, and Some of the Investigators Who Have Developed Models of These Types

EULERIAN GRID	STATISTICAL TRAJECTORY	LAGRANGIAN TRAJECTORY
A. MOMENT METHOD	Rodhe (1972, 1974)	A. RECEPTOR-ORIENTED
Carmichael and Peters (1979)	Bolin and Persson (1975)	Eliassen and Saltbones (1975)
Egan et al. (1976)	McMahon et al. (1976)	Eliassen (1978)
Pedersen and Prahm (1974)	Fisher (1975, 1978)	Ottar (1979)
Nordø (1974, 1976)	Scriven and Fisher (1975)	Szepesi (1978)
Lavery et al. (1980)	Shannon (1979)	Olson et al. (1979)
	Shieh (1977)	
B. PSEUDOSPECTRAL METHOD	Mills and Hirata (1978)	B. SOURCE-ORIENTED
Fox and Orszay (1973)	Venkatrom et al. (1980)	Wendell et al. (1976)
Christensen and Prahm (1976)	Fay and Rosenzweig (1980)	Johnson et al. (1978)
Prahm and Christensen (1977)		Mancuso et al. (1979)
Berkowicz and Prahm (1978)		Bhumralkar et al. (1980)
		Heffter (1980)
C. PIC METHOD		Powell et al. (1979)
Sklarew et al. (1971)		Maul (1977)
Lange (1978)		
		C. HYBRID
		Draxler (1977, 1979)
		Meyers et al. (1979)

Eulerian Grid Models

This type of model breaks up the geographical area or volume of interest into a two- or three- dimensional array of grid cells. The advection, diffusion, transformation, and removal (deposition) of pollutant emissions in each grid cell is simulated by a set of mathematical expressions, generally involving the K-theory assumption (assumption that the flux of a scalar is proportional to its gradient). Some type of finite-differencing technique is usually employed in the numerical solution of these equations.

The major advantages and disadvantages of the Eulerian grid approach are summarized below:

Advantages:

- Capable of sophisticated 3-D physical treatments
- Can handle nonlinear chemistry
- Data input is simplified on Eulerian grid.

Disadvantages:

- Require large amounts of computer time and storage
- Require large amounts of input data
- Cannot determine contribution from individual sources
- Artificial (computational) dispersion can be significant.

Although in principle this type of model is capable of incorporating more physical realism than some of the other model types, this advantage is largely offset in many applications by the high computational costs involved in its use.

A further problem is the artificial diffusion effect inherent in conventional finite-differencing techniques. This has led to the development of various modeling schemes to minimize this effect, such as the moment method, the pseudospectral method, and the particle-in-cell (PIC) method, as indicated in Table 1.

Statistical Trajectory Models

Although there are many different varieties of statistical trajectory models, these models have one or more of the following characteristic features that distinguish them as a type:

- Using climatological wind data, large numbers of air trajectories are calculated, either forward in time from source areas or backward in time from receptor areas, and the results are statistically analyzed to give average pollutant contributions, horizontal diffusion, etc.
- Meteorological variables are frequently averaged over long periods of time before application to calculate such parameters as concentrations and depositions.

Such models have the following advantages and disadvantages:

Advantages:

- Computational requirements are modest
- Well suited for repeated runs using alternative emissions scenarios
- No computational dispersion

- Can determine contributions from individual sources
- Pollutant mass balances can be determined.

Disadvantages:

- Most types not adaptable to short averaging times
- Dispersion and other processes are usually highly parameterized
- Dependence between meteorological variables (e.g., wind and precipitation) ignored in some types.

Statistical trajectory models enjoy a major advantage in having low computational costs, but this is sometimes obtained at the expense of physical realism.

Lagrangian Trajectory Models

A characteristic feature of these models is that calculations of pollutant diffusion, transformation, and removal are performed in a moving frame of reference tied to each of a number of air "parcels" as they are transported around the geographical region of interest in accordance with an observed or calculated wind field.

As indicated in Table 1, Lagrangian trajectory models can be either receptor-oriented, in which trajectories are calculated backward in time from the arrival of an air parcel at a receptor of interest, or source-oriented, in which trajectories are calculated forward in time from the release of a pollutant-containing air parcel from an emissions source. There are also a few hybrid approaches, in which a Lagrangian trajectory technique is used to simulate horizontal transport and diffusion, and an Eulerian grid technique is used to simulate vertical diffusion.

Most source-oriented Lagrangian trajectory models simulate continuous pollutant emissions by means of discrete increments or "puffs" of emission occurring at set time intervals, usually between 1 and 24 hrs, depending upon the designed averaging time of the model outputs. Such models simulate the movement and behavior of a pollutant plume from a continuous source (as shown in the upper left portion of Figure 1) by one of the three approaches illustrated in the other portions of the figure.

The "segmented plume" approach involves computational difficulties when variable wind fields cause convoluted plume geometries. The "puff superposition" approach avoids these problems, but can

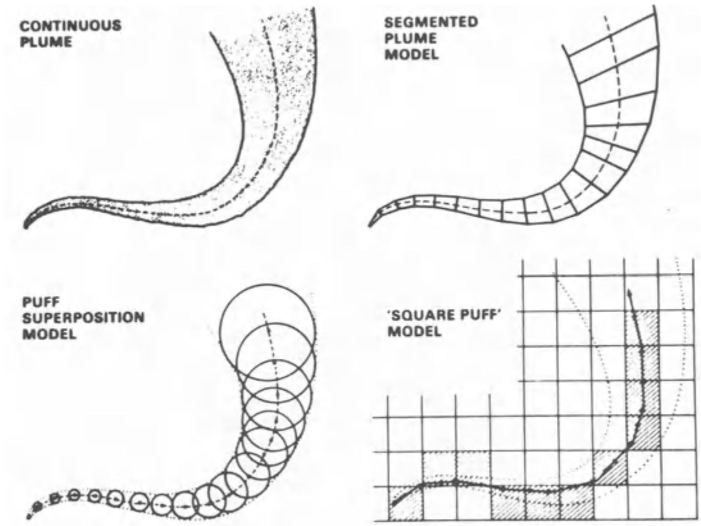

Fig. 1. Various trajectory modeling approaches (from Bass, 1980).

lead to errors when the product of wind speed and computational time-step duration is sufficiently high to cause puffs to travel long distances (relative to their size) between time steps. Under these circumstances, which are more likely to occur during the initial portion of its travel, a puff can skip over and make no (calculated) contribution of pollutant concentration or deposition to certain geographical areas, as illustrated in Figure 1. The "square puff" approach simply keeps track of the receptor cell containing the puff center at each time step, and assigns the entire contribution of the puff to this cell. This approach tends to ignore the effects of puff spread caused by horizontal diffusion.

Some of the advantages and disadvantages of Lagrangian trajectory models are listed below:

Advantages:

- Can determine contributions from individual sources
- Relatively inexpensive to run on a computer
- Easy to keep track of pollutant mass balances
- Realistic treatment of wet deposition
- No computational dispersion
- Individual sources or receptors can be run separately.