Air Pollution Modeling and Its Application III

Edited by

C. De Wispelaere

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C. De Wispelaere
Prime Minister's Office for Science Policy
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PREFACE

In 1969 the North Atlantic Treaty Organization 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 organization of a yearly symposium dealing with air pollution modeling and its application is one of the main activities within the pilot study in relation to air pollution.

After being organized 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 organization of this symposium.

This volume contains the papers presented at the 13th International Technical Meeting on Air Pollution Modeling and its Application held at Ile des Embiez, France, from 14th to 17th September 1982. This meeting was jointly organized by the Prime Minister's Office for Science Policy Programming, Belgium, and the Ministère de l'Environnement, France. The conference was attended by 120 participants and 45 papers have been presented. The closing session of the 13th I.T.M. has been attended by Mr. Alain Bombard, French Minister of the Environment. The members of the selection committee of the 13th I.T.M. were A. Berger (Chairman, Belgium), W. Klug (Federal Republic of Germany), K. Demerjian (United States of America), L. Santomauro (Italy), M.L. Williams (United Kingdom), H. Van Dop (The Netherlands), H.E. Turner (Canada), C. De Wispelaere (Coordinator, Belgium).

The main topic of this 13th I.T.M. was Langrangian Modeling. On this topic a review paper was presented by Anton Eliassen (Norwegian Meteorological Institute). Other topics of the conference were : Modeling cooling tower and power plant plumes, Modeling the dispersion of heavy gases, Remote sensing as a tool for air pollution modeling, Dispersion modeling including photochemistry. Dr. J. Knox (Lawrence Livermore National Laboratory) presented a review paper as an introduction to the topic Modeling the dispersion of heavy gases

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 particulary mention the chairmen and rapporteurs of the different sessions. Thanks also to the local organizing committee, especially Dr. J.C. Oppenau and Miss J. Maréchal, who was the Conference Secretary. Finally it is a pleasure to record my thanks to Mrs Desees, Mrs Van Saen and Miss De Corte, for preparing and typing these papers.

C. De Wispelaere

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C. M. Bhumralker
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ASPECTS OF LAGRANGIAN AIR POLLUTION MODELLING

Anton Eliassen

The Norwegian Meteorological Institute
P.O. Box 320, Blindern
Oslo 3, Norway

INTRODUCTION

Lagrangian models are models in which parcels of air are followed as they blow with the wind. The models keep track of the pollutant content of the parcels. This is in contrast to Eulerian models, where the integration of the mass-balance equation is performed in a geographically fixed grid. Lagrangian models are popular, because their basic principle is easy to grasp also for non-professionals. In addition some numerical problems associated with the advection terms in the Eulerian mass-balance equation are avoided by Lagrangian models.

Considering the number of papers that have accumulated on Lagrangian air pollution models, a complete review of the subject represents a formidable task. This contribution is limited to a discussion of the basic principles of such models, and looks at typical examples of the main model types. The sensitivity of model calculations to some of the physical parameters is also discussed.

Lagrangian models for long range transport of air pollution

Consider a well-mixed parcel of air, with base area A(t) and height h(t), that moves with a certain height-independent advection wind. Assume further that the pollutant considered is depleted by dry deposition, and by a general first-order chemical decay. The mass balance equation for the pollutant within the air-parcel is

$$\frac{d}{dt}(Ahq) = v_d Aq - kAhq + \dot{Q}A \qquad (1)$$

where q is the pollutant concentration (mass per unit volume), v_d is the deposition velocity, k is the rate of the first-order decay, and Q is the pollutant emission per unit area and time. The time derivative is the total (Lagrangian) derivative. The equation above is the basic equation for Lagrangian models of air pollution.

The Lagrangian models fall into two main types : source-oriented and receptor-oriented. In a source-oriented model, the positions of puffs, consecutively emitted from each source, are traced as a function ot time. At any instant, the concentration field is given as the sum of concentrations due to each puff. For each puff, the source term in (1) acts only to give the puff a certain mass or concentration at the time of emission. In a receptor-oriented model on the other hand, the pollutant content of an air parcel is followed until the air parcel arrives at one of the selected receptor points. During its travel, the air parcel receives emitted material from the sources it passes over, i.e. the source term in (1) acts continuously.

<u>Source-oriented Models</u> For a source-oriented model, (1) takes the form

$$\frac{d}{dt}(Ahq) = -v_d Aq - kAhq, \qquad \text{for } t>0 \qquad (2)$$

Introducing the pollutant mass M of the puff

$$M = Ahq \qquad (3)$$

we obtain simply

$$\frac{dM}{dt} = -\frac{v_d}{h}M - kM \qquad (4)$$

where, in principle, v_d, h and k can be functions of t. If (4) is integrated to give M(t), then the concentration q can be found using (3), if the horizontal area A(t) and the height h(t) of the puff are prescribed. Note that if the three-dimensional divergence of the velocity field is assumed to be zero, then A(t) and h(t) can both change either by turbulence or by systematic horizontal divergence. However, the volume A(t)h(t) will only change due to turbulence.

A good example of a model of this type is the EURMAP/ENAMAP model (Johnson et al. 1978, Bhumralkar et al. 1979). This model has been used to calculate the transport and deposition of airborne sulphur pollution over Europe and over Eastern North America.

The original EURMAP-1 model was designed to predict long-term ($\sim$ annual) deposition and concentration pattern. The radius r of the cylindrical puffs was specified as a function of travel time t as

$$r = (r_o^2 + t.10^4 m^2 s^{-1})^{1/2} \quad (5)$$

where r_o is an initial radius of $\sim$ 30 km. In the vertical, instantaneous mixing up to a constant mixing height of 1000 m was assumed. A refined scheme for vertical mixing has been adopted in EURMAP 2, designed for episode studies. Here, the mixing height is estimated as a function of time and space, from 00 and 12 GMT radiosonde data. The vertical extent of the puff is prescribed as a function of travel distance and stability. When the puff penetrates the mixing height, its vertical growth rate is reduced by means of an assumed stability increase.

The MESOS model (ApSimon and Goddard 1976, Wrighley et al., 1979), is designed to estimate the dispersion of radioactive material over Europe. This model has now been used together with a meteorological data base covering the year 1976, to obtain dispersion statistics for releases from a single source of duration 3 hours, 6 hours, 12 hours, 1 day, 3 days and 7 days. In the MESOS model, a well-mixed turbulent boundary layer is assumed to be surmounted by a series of stably stratified layers, each 100 m thick, and with relatively little mixing between these layers. Vertical dispersion of a puff in the well-mixed layer is based on local Pasquill dispersion parameters and stability categories. Eventually the material fills the mixing layer completely. If then the mixing layer becomes deeper, the pollutant is diluted and mixed up to the new height. If the mixing layer becomes shallower, some of the material becomes isolated in the stable layers aloft and cannot be depleted by dry deposition. This vertical stratification of the puff represents a refinement compared to other operative Lagrangian models, since it allows for the isolation of pollutants from the surface by stable stratification. The isolated pollutants are not subject to dry deposition.

The next logical step is to allow for wind shear, so that each of the stably stratified layers is advected by a different horizontal wind. The puff model discussed by Pack et al. (1978) has been modified (Draxler and Taylor, 1982) to include this effect. The model has been tested against data for the dispersion of Kr-85, released from the Idaho National Engineering Laboratory in 1974 (Draxler, 1982). In this model, no vertical mixing is assumed during the night, when a puff splits into five equal sublayers, each of 300 m height. These sub-layers are followed as separate trajectories for all subsequent calculations. During the next daytime phase the elevated layers are permitted to mix downward and upward at a rate of 300 m per 3 hours. This procedure results in an increase in the number of trajectories by a factor of 5 each day.

The wind shear/vertical diffusion mechanism causes an instantaneous puff release to be gradually elongated. The mechanism has been studied theoretically by Taylor (1982). He shows that at long travel times ($\sim 10^5$s) the spread of material in the long direction of the puff is dominated by the shear effect, except in very light winds or very large values of the horizontal diffusivity. Across the puff, however, the effect of horizontal diffusion on the spread of material is always comparable to that of shear, and eventually dominates it for very long travel times.

Clearly, the wind shear effect is important for instantaneous releases. However, model predictions are often compared with measurements that are averages over a certain sampling time. During the sampling time trajectories consecutively emitted from a source will take different paths, and cause a horizontal spread of the plume. This effect is further discussed in Section 3.

Table 1. The average spread of an instantaneous puff release σ_h as a function of travel distance d, compared to the mode Θ of the angular spread and the width of the plume Θd for a sampling time of 24 hours. Values for σ_h given by the theory of Taylor (1982), with a geostrophic wind speed of 11 ms^{-1} and horizontal and vertical diffusivities of 10^4 m^2s^{-1} and 10^2 m^2s^{-1}. The material presented by Gifford (1982) gives similar values for σ_h. Values of Θ taken from Figure 2, reproduced from Smith (1979).

d (km)	σ_h(km)	Θ(radians)	Θd (km)
100	10	0.63	63
250	20	0.58	144
500	30	0.52	260
1000	60	0.49	490
2000	110	0.43	860