Air Pollution Modeling and Its Application II

Edited by
C. De Wispelaere

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Prime Minister's Office for Science Policy
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Brussels, Belgium

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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 12th International Technical Meeting on Air Pollution Modeling and its Application held at SRI International, Menlo Park, California in the USA from 25th to 28th August 1981. The meeting was jointly organized by the Prime Minister's Office for Science Policy Programming, Belgium and SRI International, USA. The conference was attended by 109 participants and 51 papers have been presented. The members of the selection committee of the 12th 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), H. Van Dop (The Netherlands), C. De Wispelaere (Coordinator, Belgium).

The main topic of this 12th I.T.M. was Physical-chemical reactions in plumes. On this topic two review papers were presented : one paper dealing with "Chemical transformation in plumes" by C.S. Burton, M.K. Liu, P.M. Roth, C. Seigneur and G.Z. Whitten, Systems Applications, Inc.,U.S.A. and another one "A comparison between chemically reacting plume models and windtunnel experiments by P.J.H. Builtjes, T.N.O., The Netherlands.

Other topics of the conference were: air trajectory models for air pollution transport, advanced mathematical techniques in air pollution modeling, evaluation of model performance in practical applications and finally particular studies in the field of air pollution modeling.

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. W.B. Johnson and Miss Valerie Ramsay who was the Conference Secretary. Finally it is a pleasure to record my thanks to Miss A. Vandeputte for preparing the papers, and Misses C. Bonnewijn, M.L. Koekelbergh and L. Mongaré for typing the papers.

C. De Wispelaere
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CONTENTS

I : PHYSICAL-CHEMICAL REACTIONS IN PLUMES

1. Chemical transformation in plumes 3
C.S. Burton, M.K. Liu, P.M. Roth, C. Seigneur and G.Z. Whitten

2. A comparison between chemically reacting plume models and windtunnel experiments 59
P.J.H. Builtjes

3. Air pollutant reactions in major plumes transported over the North Sea 85
I.T. Schneider

4. Solutions to the equation for surface depletion of a gaussian plume 107
R.J. Yamartino

5. Mathematical modeling of chemically reactive plumes in an urban environment 121
C.Seigneur, P.M. Roth and R.E. Wyzga

6. Chemical modeling studies of the long-range dispersion of power-plant plumes 137
A.T. Cocks, I.S. Fletcher and A.S. Kallend

7. A comparison of the regional scale effects on in-cloud conversion of SO_2 to $SO_4^=$ in an eight layer diabatic model with a single layer model 159
W.E. Davis

8. The washout of hydrogen fluoride 175
F.M. Bosch and P.M. De Keyser

9. Performance evaluation of the empirical kinetic modeling approach (EKMA) 199
J.R. Martinez, C. Maxwell, H.S. Javitz and R. Bawol

10. Urban visual air quality : modeled and perceived 213
P. Middleton, R.L. Dennis, and T.R. Stewart

2 : AIR TRAJECTORY MODELS FOR AIR POLLUTION TRANSPORT

11. A gaussian trajectory model for hazard evaluation for prolonged releases from nuclear reactors 231
E. Doron and E. Asculai

12. Application of trajectory model to regional transport characterization 245
B. Weisman

13. Refined air pollution model for calculating daily regional patterns and transfrontier exchanges of airborne sulfur in central and western Europe 265
C.M. Bhumralkar, R.M. Endlich, K. Nitz, R. Brodzinsky, J.R. Martinez and W.B. Johnson

14. On a method of evaluation of performance of a trajectory model for long-range transport of atmospheric pollutants 277
J.L. Walmsley and J. Mailhot

15. The pseudo-spectral technique in the computation of seasonal average concentrations and its comparison with the trajectory technique 285
B.D. Murphy

16. A mesoscale air pollution transport model : outline and preliminary results 303
H. van Dop and B.J. De Haan

17. Initial evaluation of Canadian and United States regional models for transboundary air pollution 317
J.W.S. Young and B.L. Nieman

18. Comparison of an eulerian with a lagrangian type numerical air pollution dispersion model 335
N.D. Van Egmond and H. Kesseboom

19. Analysis of particles trajectories during a land-sea breeze cycle using two-dimensional numerical mesoscale models 349
C. Blondin and G. Therry

20. Verification of a three-dimensional transport model using tetroon data from projects state and neros 361
T.T. Warner and R.R. Fizz

21. A new trajectory model and its practical application for accident and risk assessments 373
K.J. Vogt, H. Geiss and J. Straka

22. A finite element flow model over the Alsace plain 393
P. Racher, F.X. Le Dimet, J.F. Roussel, P. Rosset, and P. Mery

23. Modifications of trajectory models needed for pollutant source-receptor analysis 403
P. Michael and G.S. Raynor

24. Sensitivity analysis of a climatological air trajectory model 415
P.J. Samson, R.J. Fox and R.A. Foltman

3 : ADVANCED MATHEMATICAL TECHNIQUES IN AIR POLLUTION MODELING

25. A model for pollutant concentration prediction in complex terrain 429
H.N. Lee, W.S. Kau and S.K. Kao

26. Pollutant dispersion in the Ekman layer using moment-reduced transport equations 437
D. Eppel, J. Häuser, H. Lohse, and F. Tanzer

27. A simple model for dispersion of non-buoyant particles inside a convective boundary layer 451
P.K. Misra

28. Dispersion from fugitive sources 459
C. Demuth, P. Hecq and A. Berger

29. A comparison with experimental data of several models for dispersion of heavy vapor clouds 477
J.L. Woodward, J.A. Havens, W.C. McBride and J.R. Taft

30. Application of the sulfur transport eulerian model (STEM) to a sure data set 501
G.R. Carmichael and L.K. Peters

31. Particle simulation of inhomogeneous turbulent diffusion 527
L. Janicke

32. The apt computer program for the numerical solution of problems in atmospheric dispersion 537
A. Ghobadian, A.J.H. Goddard and A.D. Gosman

33. A three dimensional, finite element model for simulating heavier-than-air gaseous releases over variable terrain . 555
R.L. Lee, P.M. Gresho, S.T. Chan and C.D. Upson

34. Numerical solution of three-dimensional and time-dependent advection-diffusion equations by "orthogonal collocation on multiple elements" 575
H. Wengle

35. Analysis of a finite release of a pollutant followed by an abrupt change of wind direction 591
D. Skibin

36. Two-dimensional unsteady gravity currents 603
A.P. van Ulden and B.J. de Haan

37. Lagrangian modeling of air pollutants dispersion from a point source 617
E. Runca, G. Bonino and M. Posch

38. Physical and mathematical simulation of Pb dispersion in and around a Pb industry in an urbanized area 631
P. Hecq, C. Demuth and A. Berger

4 : EVALUATION OF MODEL PERFORMANCE IN PRACTICAL APPLICATIONS

39. Observations and simulations of carbon monoxide concentrations in the wake of an urban garage 651
U. Pechinger, H. Kolb, H. Mohnl and R. Werner

40. Influence of meteorological input data on the comparison between calculated and measured aerosol ground level concentrations and depositions 663
I. Mertens, J. Kretzschmar and B. Vanderborght

41. EPRI plume model validation project results for a plains site power plant 675
R.J. Londergan and H. Borenstein

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1: PHYSICAL-CHEMICAL REACTIONS IN PLUMES

Chairmen: W. Klug
P. Roth

Rapporteurs: R. Stern
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CHEMICAL TRANSFORMATION IN PLUMES

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INTRODUCTION

It is now recognized that a variety of chemical transformations occurs in plumes. The types of transformations, their rates of occurrence, and the magnitudes of the resultant pollutant concentrations depend on the chemical composition of a plume and of the ambient air entrained in a plume, the elevation and temperature of a plume, and the meteorological conditions (including solar intensity) experienced by a plume. It is postulated that these transformations contribute to atmospheric haziness and discoloration, atmospheric acidity, and extended sulfate and ozone concentrations in rural areas. In addition, it is postulated that transformations in plumes contribute to brief, elevated ground-level concentrations of nitrogen dioxide.

The topic of chemical transformations in plumes, taken literally, is broadly encompassing; we cannot hope to cover all aspects of it--not even all the principal aspects. Thus,we have adopted some guidelines as to the areas that we will cover.

> Attention is primarily given to a review of chemistry and chemical transformations. The physical processes, such as transport and dispersion, are discussed only in terms of their influence on the chemistry. Deposition and scavenging processes are not considered.

> Emphasis is given to the review and synthesis of topics. Reporting of specific research studies is minimized.

> Topical areas are segmented as follows :

- Knowledge gained through observational (field) programs--section 2.
- Knowledge of atmospheric chemical reactions--section 3.
- The encoding of known chemical and physical processes in plume models--section 4.
- Research and development needs--section 5.

> The examination of atmospheric chemistry is organized according to the following groupings :

- Atmospheric SO_2 oxidation.
- The chemistry of nitrogen oxides in plumes.

> The focus, in terms of air quality impacts and thus reaction products, includes

- Ozone, NO_2, and photochemical oxidation products.
- Species potentially involved in visibility reduction.
- Precursors to the formation of acid precipitation.

Following the list of references at the end of the paper we have included a list of recommended readings that, taken together, constitute a comprehensive discussion of the topics treated in the paper.

OBSERVATIONAL PROGRAMS

This section presents an overview of observational programs that have as their focus the study of chemical transformations in plumes and the environmental effects of pollutants found in plumes. The section does not present an exhaustive review of plume field programs. Rather, it summarizes the findings of some of the primary programs that have provided the observational bases for improving the knowledge of plume chemistry and for developing and evaluating mathematical models. Table 1 lists some of these programs. Each program and the corresponding findings are briefly described in the remainder of this section.

Project MISTT (Midwest Interstate Sulfur Transformation and Transport)

The main objective of Project MISTT was to study the transformation of SO_2 to sulfate in plumes emitted from a power plant--the Labadie power plant, from refineries--the Wood River complex, and from an urban area--the St. Louis area. This study, sponsored by the U.S. Environmental Protection Agency (EPA), involved a large number of participants including academic institutions, private firms, and government agencies. The program took place during July and August of 1973 and 1974, February, July, and August, 1975, and July and August, 1976. It involved the use of two instrumented aircraft, an instrumented van, and three mobile, single-theodolite pilot balloon units.

The main results of Project MISTT can be summarized as follows:

1. Secondary pollutants, such as sulfates and ozone formed in plumes, may be transported over distances of 50 to 200 kilometers.

2. Ground-level concentrations of SO_2 emitted from tall stacks are less than those emitted from short stacks. However, SO_2 emissions from tall stacks lead to higher sulfate formation than do SO_2 emissions from short stacks because of diminished SO_2 deposition on the ground.

3. Visibility impairment is mainly due to secondary aerosol formation.

4. Because of adverse weather conditions that occurred during field studies, the processes involved in heterogeneous SO_2 oxidation could not be quantitatively assessed. However, homogeneous SO_2 oxidation processes could be studied with satisfactory accuracy.

Project CARB (California Air Resources Board)

In a study sponsored by the State of California Air Resources Board, ground-level measurements of plume concentrations of nitrogen oxides, ozone, sulfur dioxide, sulfates, nitrates, and SF_6 tracer were conducted within 19 km downwind of the Haynes steam plant and the Alamitos generating station. This field study differs from most of the others described here, in that it is concerned with power plant plumes in an urban environment. The principal conclusions of the study are :

1. The photostationary-state relationship among NO, NO_2 and O_3 was in agreement with the measurements.

2. Secondary sulfate formation was negligible during the first 90 minutes of plume transport.

3. Sulfuric acid formed in the plume probably displaced the ammonia/nitric acid/ammonium nitrate equilibrium, since lower ammonium nitrate concentrations were observed in the plume than in the background.*

Project EPRI (Electric Power Research Institute)

The Electric Power Research Institute contracted with Meteorology Research, Inc. (MRI), Systems Applications, Inc. (SAI), and the University of Washington Cloud and Aerosol Research Group to study (from 1975 to 1977), by means of airborne measurements, the chemical transformations that occur in coal- and gas-fired power plants. The power plants studied were the Four Corners near Farmington, New Mexico; Cunningham, at Hobbs, New Mexico; Wilkes near Lor view, Texas; Centralia in Washington; and a power plant near Jefferson, Texas.

The conclusions drawn from the results of these field studies are discussed in the references given in table 1. They are summarized here :

> Net formation of ozone in power plant plumes is not common. The entrainment of ambient ozone and ozone precursors into the plume accounts for the observed plume ozone levels.

> The photostationary-state relationship among NO, NO_2 and O_3 was verified within the degree of uncertainty of the measurements.

> Conversion of SO_2 to aerosol sulfate was on the order of a few tenths of one percent for the Centralia power plant and a few percent for the Four Corners power plant. No conclusions were drawn as to the mechanisms that govern gas-to-particle conversion.

Project TREATS (Tennessee Regional Atmospheric Transport Study)

Project TREATS was sponsored by the EPA as part of the Federal Interagency Energy/Environmental Research and Development program and was initiated by the Tennessee Valley Authority. The main objectives of this project were to study the phenomena that affect regional pollutant levels and interregional transport of sulfur dioxide and sulfates. The first studies were conducted during the spring of 1976 and the summer of 1977. Seven coal-fired power plants are located in the region studied, i.e., the Tennessee valley region.

* Sulfuric acid formed in the plume reacts with the gas-phase ammonia to form ammonium sulfate. Then, the product of the HNO_3 and NH_3 partial pressures is less than the saturation value, and particulate ammonium nitrate decomposes.

Table 1. Some Observational Programs Focusing on Plume Chemistry, Physics, and Optics

Program	Date of Field Program	Plumes Studied	Principal Processes Studied	Sponsor	References
MISTT	1973-1976	Labadie power plant Wood River refinery complex St. Louis urban plume	Sulfate and ozone formation Secondary aerosol formation	EPA	Wilson (1978) White et al. (1976)
CARB	September 1974			CARB	Richards, Avol, and Harker (1976)
EPRI	1975-1977	Four Corners power plant Cunningham power plant Jefferson power plant Centralia power plant Wilkes power plant	Ozone-nitrogen oxides chemistry SO_2-sulfate chemistry	EPRI	Ogren et al. (1976) Hegg, Hobbs, and Radke (1976) Hegg et al. (1977) Hobbs et al. (1979)
TREATS	Spring 1976, Summer 1977	Seven power plants in the Tennessee valley region	Regional data--sulfur and sulfates	EPA	Crawford and Reisinger (1980)
STATE	August 1978	Cumberland steam plant	Sulfate formation	EPA	Schiermeier et al. (1979)
VISTTA	1978-1981	Four Corners power plant San Manuel smelter Navajo power plant Kincaid power plant LaCygne power plant Labadie power plant Douglas smelter	Plume chemistry Aerosol dynamics Plume visual effect	EPA	Zwicker et al. (1981) Blumenthal et al. (1981) Richards et al. (1981) Seigneur et al. (1980)
SEAPC	August 1980	Navajo power plant	Plume chemistry Aerosol dynamics Plume dispersion Plume visual effects	SRP	
MAP3S	1976-1981	Oak Creek power plant St. Louis urban plume	Sulfate and nitrate formation	DOE	Miller et al. (1978) MAP3S (1979)

Several conclusions regarding the long-range transport of sulfur compounds were drawn from these field programs. The principal findings can be summarized as follows :

1. Measurements of SO_2 concentrations generally showed lower values in the afternoon than in the morning. No such trend was observed for sulfate, nitrate, or ammonium ions.

2. The emissions from power plants located in the Tennessee valley region did not account for the total sulfur budget. Evidence strongly suggests that upwind anthropogenic sources and, possibly, biogenic sources contribute to the sulfur concentrations measured.

3. Sulfur dioxide, sulfate, nitrate and ammonium concentrations depend on mean direction of wind flow, time of day, and atmospheric stability.

Project STATE (Sulfur Transport And Transformation in the Environment)

The goal of the EPA-sponsored Project STATE was to investigate the effect on air quality of pollutants released far upwind and to relate the emissions of sulfur dioxides to the observed ambient levels of sulfates. Field measurements conducted during the program included sulfur dioxide, sulfates, ammonia, ammonium ion, total acidity, hydrocarbon species, nitrogen oxides, ozone, primary aerosols, and meteorological parameters. The first phase of the program--the Tennessee Plume Study (TPS)--which took place in August 1978, was designed to study the air quality impact of the Cumberland steam plant located at Cumberland City, Tennessee. Data analysis has not yet been completed. Plume transport, dispersion, transformation and removal processes will be analyzed and the data will be used for air quality model evaluation.

The second phase of the STATE program was concerned with the analysis of a Prolonged Elevated Pollution Episode (PEPE) caused by the stagnation of a high-pressure center over the northeastern United States. Although it was mainly a regional field study program, it involved the study of urban and large point source plumes for one to two days of transport.

Project VISTTA (Visibility Impairment due to Sulfur Transport and Transformation in the Atmosphere)

The EPA-sponsored VISTTA field programs were designed to study the relative contributions of natural and anthopogenic sources to visibility impairment and to provide a detailed data base that could be used for the evaluation of visibility models. The June-July and December 1979, field programs were conducted in the vicinity of a coal-fired power plant--the Navajo Generating Station near Page,