NOAA Technical Memorandum ERL ARL-226

FISCAL YEAR 1997 SUMMARY REPORT OF THE NOAA ATMOSPHERIC SCIENCES MODELING DIVISION TO THE U.S. ENVIRONMENTAL PROTECTION AGENCY

E.M. Poole-Kober
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(Editors)

Atmospheric Sciences Modeling Division
Research Triangle Park, North Carolina

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UNITED STATES DEPARTMENT OF COMMERCE

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Secretary

NATIONAL OCEANIC AND ATMOSPHERIC ADMINISTRATION

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PREFACE

This document summarizes the Fiscal Year 1997 research and operational activities of the Atmospheric Sciences Modeling Division (ASMD), Air Resources Laboratory, working under Interagency Agreements EPA DW13937039, DW13937252, and DW13947769 between the U.S. Environmental Protection Agency (EPA) and the National Oceanic and Atmospheric Administration (NOAA). The summary includes descriptions of research and operational efforts in air pollution meteorology, air pollution control activities, and abatement and compliance programs.

Established in 1955, the Division serves as the vehicle for implementing the agreements with the EPA, which funds the research efforts in air pollution meteorology. ASMD conducts research activities internally and through contract and cooperative agreements for the National Exposure Research Laboratory and other EPA groups. With a staff consisting of NOAA, EPA, and Public Health Service Commissioned Corps personnel, ASMD also provides technical information, observational and forecasting support, and consulting on all meteorological aspects of the air pollution control program to many EPA offices, including the Office of Air Quality Planning and Standards. The primary groups within ASMD are the Atmospheric Model Development Branch, Modeling Systems Analysis Branch, Applied Modeling Research Branch, and Air Policy Support Branch. The staff is listed in Appendix F. Acronyms, publications, and other professional activities are listed in the remaining appendices.

Any inquiry on the research or support activities outlined in this report should be sent to the Director, Atmospheric Sciences Modeling Division (MD-80), Environmental Protection Agency, Research Triangle Park, NC 27711.

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FISCAL YEAR 1997 SUMMARY REPORT OF THE NOAA ATMOSPHERIC SCIENCES MODELING DIVISION TO THE U.S. ENVIRONMENTAL PROTECTION AGENCY

ABSTRACT. During Fiscal Year 1997, the Atmospheric Sciences Modeling Division provided meteorological and modeling support to the U.S. Environmental Protection Agency. This ranged from the conduct of research studies and model applications to the provision of advice and guidance. Research efforts emphasized the development and evaluation of air quality models using numerical and physical techniques supported by field studies. Among the significant research studies were the continued development and evaluation of Models-3; development of a community multiscale air quality modeling system; continued development and application of air quality models for mercury, dioxin, and heavy metals; evaluation of enhanced human exposure models; analysis and modeling of dust resuspension data; study of buoyant puff dispersion in the convective boundary layer; and development of methodologies to estimate the drift of airborne agricultural pesticides.

1. INTRODUCTION

In Fiscal Year 1997, the Atmospheric Sciences Modeling Division (ASMD) continued its commitment for providing goal-oriented, high-quality research and development, and operational support to the U.S. Environmental Protection Agency (EPA). Using an interdisciplinary approach emphasizing integration and close cooperation with the EPA and public and private research communities, the Division's primary efforts were studying processes affecting dispersion of atmospheric pollutants, modeling pollutant dispersion on all temporal and spatial scales, and developing multimedia model frameworks in a high performance computing and communications environment. The technology and research products developed by the Division are transferred to the public and private national and international user communities. Section 2.1 discusses Division participation in international activities, while Sections 2.2 through 2.4 outline the Division research activities in support of the short- and long-term needs of the EPA and the environmental community. Section 2.5 discusses Division support to the operational programs and general air quality model user community.

2. PROGRAM REVIEW

2.1 Office of the Director

The Office of the Director provides direction, supervision, program management, and administrative support in performing the Division's mission and in achieving its goals of advancing the state of the atmospheric sciences and enhancing the protection of the environment. The Director's Office also engages in several domestic and international research exchange activities.

2.1.1 NATO Committee on Challenges of Modern Society

The North Atlantic Treaty Organization (NATO) Committee on Challenges of Modern Society (CCMS) was established in 1969 with the mandate to examine how to improve, in every practical way, the exchange of views and experience among the Allied countries in the task of creating a better environment for their societies. The Committee considers specific problems of the human environment with the deliberate objective of stimulating action by member governments. The Committee's work is carried out on a decentralized basis through pilot studies, discussions on environmental issues, and fellowships.

2.1.1.1 International Technical Meetings

The Division Director serves as the United States representative on the Scientific Committee for International Technical Meetings (ITMs) on Air Pollution Modeling and Its Application, sponsored by NATO/CCMS. A primary activity within the NATO/CCMS Pilot Study on Air Pollution Control Strategies and Impact Modeling is organizing a symposium every eighteen months that deals with various aspects of air pollution dispersion modeling. The meetings are rotated among different NATO and Eastern Bloc countries, with every third ITM held in North America and the two intervening ITMs held in European countries.

The Division Director served as sponsor and session chairman of the 22nd NATO/CCMS International Technical Meeting held in Clermont-Ferrand, France, during June 2–6, 1997; the proceedings will be published by Plenum Press. The NATO/CCMS Scientific Committee selected Varna, Bulgaria, as the site for the 23rd International Technical Meeting to be held during September 28–October 2, 1998.

2.1.1.2 Coastal Urban Air Pollution Study

The Division Director served as the United States representative on the International Oversight Committee for the NATO/CCMS Pilot Study on Urban Pollutant Dispersion near Coastal Areas. This pilot study, sponsored by Greece, originated in a workshop held in Athens during February 1992. The purpose was to understand the causes of high air pollution episodes in coastal urban areas and to devise strategies to mitigate pollution problems caused by vehicular and industrial emissions in these areas. A NATO/CCMS advanced research workshop was held during May 1993 to design a reference experiment in a coastal urban area to collect relevant ambient measurements and emissions for use in evaluation of existing urban dispersion models and for understanding the atmospheric boundary layer at the interface of land and water. A final report of the pilot study was presented at a NATO/CCMS Plenary Meeting in Brussels, Belgium, in April 1997 (Kambezidis, 1997).

2.1.2 United States/Japan Environmental Agreement

The Division Director serves as the United States Co-Chairman of the Air Pollution Meteorology Panel under the United States/Japan Agreement on Cooperation in the Field of Environment. The purpose of this 1975 agreement is to facilitate, through mutual visits and reciprocal assignments of personnel, the exchange of scientific and regulatory research results pertaining to control of air pollution. Although no reciprocal visits were made in FY-1997, interactions were maintained through correspondence and exchange of research findings.

2.1.3 United States/Russia Joint Environmental Committee

The Division Director serves as the United States Co-Chairman of the United States/Russia Working Group 02.01-10 on Air Pollution Modeling, Instrumentation, and Measurement Methodology, and as Co-Leader of the United States/Russia Project 02.01-11 on Air Pollution Modeling and Standard Setting. The purpose of the 1972 Nixon-Podgorny Agreement forming the US/USSR Joint Committee on Cooperation in the Field of Environmental Protection is to promote, through mutual visits and reciprocal assignments of personnel, the sharing of scientific and regulatory research results related to the control of air pollution. Activities under this agreement have been extended to also comply with the 1993 Gore-Chernomyrdin Agreement forming the United States/ Russia Commission on Economic and Technological Cooperation. There are four Projects under Working Group 02.01-10:

Project 02.01-11: Air Pollution Modeling and Standard Setting
Project 02.01-12: Instrumentation and Measurement Methodology
Project 02.01-13: Remote Sensing of Atmospheric Parameters
Project 02.01-14: Statistical Analysis Methodology and Air Quality Trend Assessment.

Progress under this Working Group continued during FY-1997. The annual Working Group meeting at the Main Geophysical Observatory in St. Petersburg, Russia, was held during July 1997.

2.1.4 Meteorological Coordinating Committees

2.1.4.1 Federal Meteorological Committee

The Division Director serves as the Agency representative on the Federal Committee for Meteorological Services and Supporting Research (FCMSSR). The Committee is composed of representatives from 14 Federal government agencies and is chaired by the Under Secretary of Commerce for Oceans and Atmosphere, who is also the NOAA Administrator. FCMSSR was established in 1964 with high-level agency representation to provide policy guidance to the Federal Coordinator for Meteorology, and to resolve agency differences that arise during coordination of meteorological activities and the preparation of Federal plans in general.

2.1.4.2 Interdepartmental Meteorological Committee

The Division Director serves as the Agency representative on the Interdepartmental Committee for Meteorological Services and Supporting Research (ICMSSR). The Committee. composed of representatives from 14 Federal government agencies, was formed in 1964 under Public Law 87-843 and OMB Circular A-62 to provide the Executive Branch and the Congress with a coordinated, multi-agency plan for government meteorological services and for those research and development programs that directly support and improve these services. The Committee prepared the annual Federal Plan for Meteorological Services and Supporting Research (U.S. Department of Commerce, 1997). Other Division members serve on the ICMSSR Working Group for Atmospheric Transport and Diffusion and the Working Group for Climate Services.

2.1.5 Board on Atmospheric Sciences and Climate

The Division Director serves as the Agency liaison to the Board on Atmospheric Sciences and Climate (BASC) of the National Research Council, National Academy of Sciences. The BASC activity that most closely relates to the work of the Division is the Panel on Atmospheric Aerosols. Specifically, the panel is reviewing existing and new evidence regarding anthropogenic and natural aerosol-producing processes; their sources, characteristics, and distribution; their transport and removal; and their quantified effects on atmospheric processes and on the global and regional radiation forcing of the climate system. The panel will advise regarding the observation, monitoring, and research strategies needed to understand atmospheric processes and aerosol characteristics important in weather and air pollution research.

2.1.6 Committee on Computing, Information, and Communications

The Division Director serves as the alternate Agency member to the Committee on Computing, Information, and Communications of the National Science and Technology Council (NSTC), Office of Science and Technology Policy. The mission of the Committee is to "accelerate the evolution of existing technology and nurture innovation that will enable universal, accessible, and affordable application of information technology to enable America's economic and national security in the 21st century" (U.S. Office of Science and Technology Policy, 1995). This mission is achieved through six strategic focus areas: global-scale information infrastructure technologies; high performance/scalable systems; high confidence systems; virtual environments; user-centered interfaces and tools; and human resources and education. The Committee serves as the National Coordination Office for the High Performance Computing and Communications (HPCC) program in which this Division has a major role.

2.1.7 Standing Air Simulation Work Group

The Division Director serves as the Agency Office of Research and Development (ORD) representative to the Standing Air Simulation Work Group (SASWG), which serves as a forum for issues relating to air quality simulation modeling of criteria and other air pollutants from point, area, and mobile sources. Its scope encompasses policies, procedures, programs, model development, and model application. The work group fosters consensus between the Agency and the state and local air pollution control programs through semi-annual meetings of members representing all levels of enforcement.

2.1.8 AMS Glossary of Meteorology

The Division is participating in multi-agency funding of the updating and revision of the *Glossary of Meteorology* by the American Meteorological Society (AMS). Under sponsorship of the National Science Foundation (NSF), the AMS will review the existing entries in the 1959 edition of the Glossary and revise and update the listings resulting in a potential doubling of the number of entries. The new Glossary will be published in both print and CD-ROM formats in mid-1998.

2.1.9 European Monitoring and Evaluation Program

A Division scientist serves as the United States representative to the European Monitoring and Evaluation Program (EMEP) that oversees the cooperative program for monitoring and evaluation of the long-range transmission of air pollutants in Europe. The primary goal of EMEP is to use regional air quality models to produce assessments evaluating the influence of one country's emissions on another country's air concentrations or deposition.

The emphasis has shifted from acidic deposition to ozone. The United States and Canadian representatives report on North American activities related to long-range transport. The Division scientist also evaluates European studies of special relevance to the program, providing technical critiques of the EMEP work during formal and informal interactions; and develops and coordinates such programs with EMEP as the modeling studies of the Modeling Synthesizing Center West (MSC-W) at the Norwegian Meteorological Institute in Oslo, Norway.

2.1.10 Section 812 Assessment Work Group

A Division scientist is a member of the 812 Assessment Work Group, in coordination with the EPA Office of Program Assessment and Review and the EPA Office of Policy, Planning, and Evaluation, with responsibility for developing approaches to assess regional air quality and acidic deposition. The responsibilities of this working group are to produce a retrospective assessment of the benefits and costs of the Clean Air Act (CAA) of 1970 and a prospective assessment of the benefits and costs of the Clean Air Act Amendments (CAAA) of 1990, assuming full implementation. Work in FY-1997 emphasized peer review of the prospective assessment emissions projections and development of regional model predictions for the years 2000 and 2010 assuming both full implementation and no implementation of the 1990 CAAA.

2.1.11 Chesapeake Bay Program Air Subcommittee and Chesapeake Bay Program Modeling Subcommittee

A Division scientist is a member of the Air Subcommittee, a working subcommittee of the Chesapeake Bay Program. Previously this subcommittee was an advisory group to the Implementation Committee. The subcommittee has responsibility for advice and leadership on issues of atmospheric deposition to the watershed and the Bay, on overseeing application of the Regional Acid Deposition Model (RADM), and in dealing with the influence of atmospheric deposition on Bay restoration efforts. The Air Subcommittee also works with other Chesapeake Bay committees to define the top priority air quality scenarios to be simulated by RADM. The Division scientist is also an ex officio member of the Modeling Subcommittee of the Implementation Committee. This subcommittee has responsibility for overseeing the application of water quality models and coordinating the linkage of RADM with those models and the interpretation of the findings. Work in FY-1997 focused on creation of RADM predictions at 20-km resolution of the estimated effects of 1990 CAAA potential oxidant-related controls and of a limit-of-technology set of feasible controls on the nitrogen deposition to the Chesapeake watershed basins and to the Bay. The FY-1997 work was in support of the 1997 Chesapeake Bay Agreement Re-evaluation.

2.1.12 Consortium for Advanced Modeling of Regional Air Quality

A Division scientist serves as an Agency representative to the Consortium for Advanced Modeling of Regional Air Quality (CAMRAQ). This consortium is composed of representatives from the Electric Power Research Institute, American Petroleum Institute, Pacific Gas and Electric, California Air Resources Board, Department of Energy, National Oceanic and Atmospheric Administration, Environmental Protection Agency, Department of Defense, Atmospheric Environment Service of Canada, Ontario Ministry of the Environment, and EUROTRAC (EUROpean experiment on the TRAnsport and transformation of trace atmospheric Constituents). The members of CAMRAQ share a mutual interest in making regional-scale atmospheric models usable tools for air quality and emergency response planning. They also share an interest in bringing the emerging power of high performance computing to regional air quality modeling. The goals of the consortium are to coordinate research and to form a basis for collaboration on projects that will enhance the ability of each to achieve their respective goals regarding atmospheric modeling. In FY-1997, CAMRAQ decided to tentatively adopt the Models-3 framework, pending final development of the EPA Third Generation Modeling System, Models-3.

2.1.13 North American Research Strategy for Tropospheric Ozone

The North American Research Strategy for Tropospheric Ozone (NARSTO) is a research program with the goal of addressing outstanding issues regarding the understanding and management of tropospheric ozone and coordinating collaborative research among all North American organizations performing and sponsoring tropospheric ozone studies. Sponsors include the private sector and State, Provincial and Federal governments of the United States, Canada and Mexico. NARSTO was formally established in FY-1995. The Subcommittee on Air Quality Research of the Committee on Environment and Natural Resources within the NSTC will facilitate the coordination of NARSTO Federal research activities. Four technical teams have been established: Analysis and Assessment; Observations; Modeling and Chemistry; and Emissions. A first major goal of NARSTO is to produce in 1998 a scientific assessment of the state of tropospheric ozone science.

During FY-1997, the process for the 1998 NARSTO scientific assessment was implemented. A Division scientist was chosen to co-author one of the fifteen critical review papers that were commissioned to provide technical background to the NARSTO assessment group. During FY-1997, a draft of the critical review paper on modeling and evaluation of advanced models was completed for NARSTO review.

2.1.14 International Task Force on Forecasting Environmental Change

A Division scientist is a member of the International Task Force on Forecasting Environmental Change that addresses the methodological and philosophical problems of forecasting under the expectation of significant structural changes in the behavior of physical, chemical or biological systems. The three planned workshops have been held at the International Institute for Applied Systems Analysis in Laxenburg, Austria. A monograph of the workshop discussions is being prepared by individual task force members. A new publisher for the monograph was identified.

2.1.15 RADM Application Studies

Efforts during FY-1997 concentrated on completing several RADM application studies related to the 1997 Chesapeake Bay Agreement Re-evaluation and analyzing RADM results in support of Regulatory Impact Statements mandated in the 1990 CAAA for ozone and visibility. Other applications are in progress, principally for the Chesapeake Bay and other coastal estuaries. The EPA Region 3 Office and the Chesapeake Bay Program Office need nitrogen deposition and source attribution information to address the atmospheric component of loading of nitrogen to the Chesapeake Bay. Estimates of the airshed affecting the Bay were completed and reviewed.

In FY-1997, the 80- and 20-km versions of RADM were coupled with the Regional Particulate Model (RPM) to take into account the partitioning of total nitrate into nitric acid and particulate nitrate, and to develop more accurate estimates of deposition gradients and deposition to the water surfaces of the Bay. The new RADM/RPM duo was used to estimate the nitrogen deposition reductions possible from ozone-driven regional- and national-nitrogen oxide emission reductions under the 1990 CAAA. These estimates were made available to the Chesapeake Bay Water Quality Model. This work provided technical input to discussions regarding renewal of the Bay Agreement by the Bay States and EPA. A RADM study was underway during FY-1997 to more accurately estimate source region responsibility for the nitrogen deposition to the different water basins of the Bay as part of a cost analysis of air controls relative to their ability to reduce nitrogen load to the Bay (U.S. Environmental Protection Agency, 1996). This work is being extended into FY-1998 and will form the basis of estimates for airsheds of coastal estuaries other than Chesapeake Bay for the EPA Region 3 Office and the EPA Great Waters Program of the 1990 CAAA.

2.1.16 ASMD Library Home Page

The ASMD Library maintained a world-wide web (WWW) home page (http://www.epa.gov/asmdnerl/library/library.htm), which provides a brief overview of the Library's history and location. The purpose of the home page is to make accessible information about the Library's collection, policies, and services to the Division staff and other users in

Research Triangle Park, North Carolina, and other locations. The home page provides Telnet and WWW interface connections to the EPA and NOAA on-line catalogs in which the Library's book and journal collections are cataloged. In addition, the page provides links to other information resources through the agencies' home pages and to other WWW resources that reflect the Library's collection and staff needs. Division library staff provided HTML documents of the FY-1996 annual report and publication citations for inclusion on the Division's home page (http://www.epa.gov/asmdnerl).

2.2 Atmospheric Model Development Branch

The Atmospheric Model Development Branch develops, evaluates, and validates analytical and numerical models that describe the transport, dispersion, transformation, and removal/resuspension of atmospheric pollutants on local, urban, and regional scales. These are comprehensive air quality modeling systems that incorporate state-of-science formulations describing physical and chemical processes.

2.2.1 Models-3 Advanced Air Quality Modeling

2.2.1.1 Introduction

Air quality simulation models are important tools for use by regulatory, policy, and research communities. The Clean Air Act provides a societal mandate to assess and manage air pollution levels to protect human health and the environment. The EPA established National Ambient Air Quality Standards (NAAQS), requiring the development of effective emission control strategies for such pollutants as ozone, particulate matter, and nitrogen species. National and regional policies are needed for reducing and managing the amount and type of emissions that cause acid, nutrient, and toxic pollutant deposition to ecosystems at risk and for enhancing the visual quality of the environment. Air quality models are used to develop emission control strategies that achieve these objectives. Control strategies must be both environmentally protective and cost effective. However, effectiveness depends upon recognizing that air pollution problems and strategies for their mitigation are very complex, and the linkages between sources, meteorology, natural sources, and landscapes are highly varied, complex, and not very well understood. The goal of developing cost-effective control strategies is challenging, and the effectiveness is very limiting if air pollution issues are handled in isolation rather than holistically. Emissions from chemical, manufacturing, and such industrial activities as power generation, transportation, and waste treatment activities contribute to a variety of air pollution issues, including ozone, particulate matter (PM), acid, nutrient and toxic deposition, and visibility in complex ways, and at a variety of spatial and temporal scales. The residence times of pollutants in the atmosphere can extend to multiple days; thus, transport consideration must be at least regional in scale. NAAQS requirements and other goals for a cleaner environment vary over a large range of time scales, from peak hourly to annual averages.

To meet the challenges posed by the 1990 CAAA, the Division embarked upon the development of an advanced modeling framework, Models-3. It was designed to perform environmental modeling, utilizing state-of-science representation of atmospheric processes in a high performance computing environment. The science components in Models-3 are called the Community Multiscale Air Quality (CMAQ) system. The Models-3/CMAQ system is designed as a multipollutant, multiscale Eulerian framework air quality and atmospheric deposition modeling system. It contains state-of-science parameterizations of atmospheric processes affecting transport, transformation, and deposition of such pollutants as ozone, particulate matter, airborne toxics, and acidic and nutrient pollutant species. With science in a continuing state of advancement and review, an important design feature in the Models-3 framework and CMAQ is the capability to integrate and test future formulations in an efficient manner, without needing to develop a completely new modeling system.

Efforts were undertaken to provide in June 1998 the first released version of CMAQ-98, which will contain options representing different model descriptions of the major science processes. The science options available to the user will include the gas phase chemistry mechanisms, RADM2, and CB-IV; a set of numerical solvers for the mechanisms; options for horizontal and vertical advection schemes; algorithms for fine and coarse particulate matter predictions; photolysis rates; and a plume-in-grid approach. Capabilities to perform model evaluation, sensitivity, and uncertainty analyses include provisions for process and integrated reaction rate-mass balance analyses. Aggregation techniques for developing annual average concentration and deposition fields from a smaller sample of 5-day simulation runs were performed. A brief summary of several key science processes and specific model advances achieved during the year follows.

2.2.1.2 Development of Community Multiscale Air Quality Modeling System

The Models-3/CMAQ system is composed of two major components: a system framework (Models-3) and an air quality system (CMAQ). Models-3 is a computational system framework for multimedia environmental studies, which contains a variety of tools that facilitate scientific computations and analyses. CMAQ is the first major implementation of a science model in the Models-3 system framework for a single medium application (i.e., air quality simulation). Models-3/CMAQ integrates emissions processing, meteorological modeling, chemistry-transport models (CTMs), and analyses of inputs and outputs. It is not a monolithic model, but rather a modeling system that allows users to build customized CTMs for solving air quality problems. One of the priorities of the CMAQ design was to realize the one-atmosphere concept for air quality modeling.

Key science submodels in the CMAQ system are the Mesoscale Meteorological Model Version 5 (MM5), Models-3 Emissions Processing and Projection System (MEPPS), and chemical-transport models. There are several interface processors that link other model input data to the CTMs. The Meteorology-Chemistry Interface Processor (MCIP) processes MM5 output to provide a complete set of meteorological data needed for a CTM. MCIP is designed in such a way that other meteorological models can be linked with minimal effort. Initial and boundary conditions are processed with processors named ICON and BCON, respectively, and the Emissions-Chemistry Interface Processor (ECIP) combines area and point source emissions to generate three-dimensional gridded emissions data for CTMs. A photolytic rate constant processor, which is based on RADM's JPROC, computes species specific photolysis rates for a set of predefined zenith angles and altitudes. An alternative detailed-science version adopts state-of-the-science radiative transfer models with a possibility to take into account the total ozone column (TOMS data) and turbidity. In addition, a plume dynamics model (PDM) is used to provide major elevated point-source plume dispersion characteristics for driving the plume-in-grid processing in CMAQ. The science processes implemented in CMAQ are defined by the way one or a collection of the terms are grouped in the governing atmospheric diffusion equation. The key science process classes defined in CMAQ are as follows:

DRIVER: controls model data flows and synchronizes fractional time steps,
HADV: computes horizontal advection,
VADV: computes vertical advection,
ADJCON: adjusts mass conservation property of advection processes,
HDIFF: computes horizontal diffusion,
VDIFF: computes vertical diffusion,
CHEM: computes gas-phase chemical reactions
CLOUD: computes aqueous-phase reactions and cloud mixing
AERO: computes aerosol dynamics and size distributions
PING: computes the effects of plume chemistry

CMAQ/CTM does not classify emissions as a separate science process because emissions can belong either in the vertical diffusion or the gas-phase chemical reaction process. In addition to the regular science process classes, a PHOT routine, which computes attenuation of photolytic constants by cloud, is included as an atypical science process class, a so-called data-provider module. Several other modules provide necessary functionalities for CMAQ; these are grouped as auxiliary routines in the UTIL class. Modularity of CMAQ embodies practicality rather than strictly following a design paradigm. In the future, the definition of the modularity will be at a user-defined granularity level.

2.2.1.3 Transport Processes

Governing set of equations in generalized form. In Models-3, the governing equations for the dynamic processes are expressed in terms of the generalized coordinates to facilitate linkage of CTM to many different types of meteorological models. The generalized governing equations for the CTM were derived using tensor algebra. The generalized CTM can deal with several different conformal map projections as horizontal coordinates, and many popular vertical coordinates used for atmospheric modeling studies. Conformal maps supported are Mercator, Lambent, and Polar Stereographic projections. Vertical coordinates supported are Sigma-p hydrostatic coordinate, Sigma-z coordinate, and height coordinate. The governing atmospheric diffusion equations include conservation equations for air and trace gases, and other diagnostic equations for contravariant wind components. Vertical mixing is presented with Reynolds flux terms that can be implemented whether using local or non-local closure parameterizations.

Advection and mixing algorithms. The transport process, in principle, consists of advection and diffusion that cause the movement and dispersion of pollutants in space and with time. It is assumed the transport of pollutants in the atmospheric turbulent flow field can be described by means of differential equations and appropriate initial and boundary conditions. In Eulerian air quality models, the transport process is solved using appropriate numerical algorithms. These numerical algorithms for the advection and diffusion processes must satisfy several properties that are essential for making useful air quality simulations. As with all numerical methods, the numerical schemes for solving the transport equation must meet the convergence condition and correctly model the conservative, transportive, dissipative, and dispersive properties of the governing equations.

In Models-3 CTM, advection is represented in flux form and an additional divergence term for non-divergent flow. Advection algorithms implemented are the Bott scheme based on polynomial description of subgrid concentration; Smolarkiewicz iterative upwind scheme; and Piecewise Parabolic Method. The atmospheric mixing process is represented in Reynolds flux terms. Depending on the atmospheric stability conditions, local and non-local mixing schemes are used in CTM. The vertical mixing algorithms under study are eddy diffusion; turbulent kinetic energy method; and Asymmetric Convection Model. The results are compared with atmospheric mixing predicted by the transilient turbulence method. The deposition flux is included as the bottom boundary condition in the vertical mixing algorithms available in Models-3. Also, the quantification of numerical horizontal diffusion of advection schemes is under study. This information will be used to assess the need for a horizontal diffusion process in CTM.

2.2.1.4 Aerosol and Visibility Module

The aerosol and visibility module of the Regional Particulate Model (RPM) was expanded and entered into the Models-3 system as part of CMAQ. The new aerosol module now predicts species mass and number for three lognormal modes (Aitken, accumulation, and coarse). The visibility module was incorporated into CMAQ. Primary emissions of fine ($PM_{2.5}$) and coarse (PM_{10} minus $PM_{2.5}$) particles were also included. The number of chemical species was increased. Inorganic species in the Aitken and accumulation modes are the same as in RPM (sulfate, nitrate, ammonium, water). However, the organic species were refined to include secondary organic aerosols of both anthropogenic and biogenic origins. The primary emissions for $PM_{2.5}$ are speciated into elemental carbon, organic carbon, and others. The speciation algorithm is temporary, and better speciation will come from a better emissions inventory.

2.2.1.5 Photolysis Rates

Development and testing continued on the photolysis rate module for Models-3/CMAQ (Roselle *et al.*, 1997). The model combines advanced radiative transfer models (Madronich 1987; Zeng *et al.*, 1996) with detailed spatial and temporal data. Photolysis rates are computed for gridded modeling domains by performing explicit radiative transfer calculations on all grid cells of a modeling domain using modeled temperature and pressure profiles from MM5, modeled cloud fields, gridded surface albedo, and total ozone column data (TOMS). The model also offers a generalized framework for specifying different sets of absorption cross section and quantum yield data, to allow generation of photolysis rates for any chemical mechanism (e.g. RADM2, CB-IV, etc.). The model can perform radiative transfer calculations using either simple two-stream approximations or a more complex multistream discrete ordinates method. The major enhancements incorporated into the model included a method for incorporating satellite cloud data into the radiative transfer calculation, and a method of linking the cloud transmissivity/optical properties directly with MM5 calculations. Many sensitivity tests were conducted, including comparisons of results with (1) the explicit scheme and simpler interpolation schemes, (2) two-stream and multistream radiative transfer models, (3) TOMS data and the U.S. Standard Atmosphere total ozone column value (U.S. Standard Atmosphere, 1976), and (4) MM5 specified albedo and a spatially uniform albedo. Testing and evaluation will continue during FY-1998.

2.2.1.6 Cloud Dynamics and Aqueous-Phase Chemistry Module

Two modules were incorporated into Models-3/CMAQ. The RADM cloud module (Walcek *et al.*, 1986) from MCNC's[1] EDSS/MAQSIP was modified to conform with Models-3 coding standards and incorporated into the system. In addition, the aqueous-phase chemistry module was replaced with a version from the Engineering Aerosol Model Version 1.0, which included treatment of both gas and aerosol species. Because the aqueous chemistry module was specifically designed for the RADM2 chemical mechanism, a translator was developed to map chemical and aerosol species from CMAQ to those expected by the aqueous chemistry module. This translator was required to enable the use of the cloud/aqueous chemistry module with different gas-phase chemical mechanisms (i.e. RADM2, CB-IV, and SAPRC). A generalized Henry's Law Constant routine was developed to remove other hardwiring of the cloud module to the RADM2 mechanism. Development and testing will continue during the next fiscal year, including development of a resolved-scale cloud module and incorporation of in-cloud scavenging of Aitken-mode aerosols.

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[1] MCNC, Research Triangle Park, NC.

2.2.1.7 Plume-in-Grid Effort for Models-3

Results of simulations from an Eulerian grid model and a Lagrangian plume model with high NO_x emissions from a major point source indicated the downwind maximum ozone to be sensitive to the grid cell size of the Eulerian model and differed from the plume model concentrations (Godowitch, 1996), which is an undesirable feature when assessing impacts of point source emissions on secondary pollutant concentrations. Consequently, a development and testing effort of plume-in-grid algorithms was conducted to provide a realistic treatment of the subgrid scale physical and chemical processes impacting pollutant species in plumes emitted from selected major elevated point sources.

The key modeling components developed to simulate the relevant processes at the proper spatial and temporal scales for pollutant plumes include a plume dynamics model (PDM) processor designed to provide the location and physical dimensions of individual plume sections by simulating plume rise, plume vertical/horizontal growth, and plume transport (Godowitch *et al*., 1995); and a Lagrangian reactive plume module (LRPM), which simulates the relevant processes of a moving array of attached cells representing a vertical plume cross-section. The LRPM was adapted and incorporated into CTM to simulate the processes governing reactive pollutants for multiple plume sections released from selected major point sources during the Eulerian grid model simulation. The data file generated by PDM, as well as the three-dimensional gridded concentration field provided by CTM, are used to drive the LRPM module during the subgrid scale phase for each pollutant plume. Test simulations are underway to identify the physical and chemical criteria for transferring the plume concentrations to the gridded concentration array at the proper time and location. The same chemistry mechanism and solver algorithms used for the CTM grid cells are applied to perform the chemical processes in the plume-in-grid module. An overview of the plume-in-grid technique is described by Gillani *et al*. (in press). The plume-in-grid approach will undergo evaluation as part of the overall Models-3 algorithms with the Southern Oxidant Study's Nashville 1995 field experimental data.

2.2.1.8 Meteorology-Chemistry Transport Model Interface Processor

The Meteorology-Chemistry Transport Model Interface Processor (MCIP) links output of MM5 with Models-3 CTM. Its major function is translating meteorological parameters output of MM5 to the format suitable for CTM operation. Those necessary meteorological parameters not provided by MM5 are estimated using appropriate algorithms in the program. MCIP reads output files from MM5 and processes meteorological parameters suitable for the CTM simulation. The processor produces comprehensive meteorological information for the CTM domain, some of which are directly passed through from MM5 parameters, and others parameters are computed using appropriate diagnostic formulas. The output files generated are in Models-3/EDSS Input/Output Applications Program Interface (I/O API) format (Coats, 1996). Key functions of MCIP are:

- Reading meteorological model output files for the entire meteorology model domain. The enhanced MM5 version (Pleim *et al.*, 1997) generates not only the standard MM5 output but also additional files that contain detailed PBL and surface parameters and cloud information. MCIP reads these files and stores the information in the memory for further processing. Essential header information is passed to the Models-3 I/O API file header.

- Extracting meteorological model output for CTM window domain. In general, CTM has a smaller computational domain than MM5. Because MM5 predictions in the cells near the boundary may not be suitable for use in air quality simulation, MCIP extracts only the portion of the MM5 output data that falls within the CTM's main domain and boundary cells.

- Interpolating coarse meteorological model output for finer grid when necessary. When a user requests meteorological data on a finer resolution grid than that simulated in the meteorological model, MCIP interpolates profile data using simple bilinear interpolation.

- Collapsing meteorological profile data if coarse vertical resolution data is requested. MCIP performs a mass-weighted averaging of data in the vertical direction. For example, 30-layer meteorological data may be lumped into CTM 15 layers, or 6 layers.

- Computing or passing through surface and PBL parameters. Depending on the user options, MCIP either passes through surface and PBL parameters through parameters simulated by the meteorology model directly or diagnoses them using the mean wind, temperature, and humidity profile data, surface data, and detailed land-use information.

- Diagnosing cloud parameters. When important parameters related with clouds are not provided by the meteorological model, MCIP diagnoses such cloud information as cloud top, cloud base, liquid water content, and cloud coverage, using a simple convective parameterization. The information can be used in CTM to process aqueous-phase chemistry and cloud mixing as well as to modulate photolysis rates reflecting the effects of cloud.

- Computing species-specific dry deposition velocities. MCIP computes dry deposition velocities for important gaseous species using either diagnosed PBL parameters or the surface/PBL information passed through from the meteorological model.

- Generating coordinate-dependent meteorological data for the generalized CTM simulation. In MCIP, many coordinate-related functions traditionally treated in CTM were incorporated as a part of the preprocessor functions. This change was necessary to maintain modularity of Models-3/CMAQ CTM regardless of the coordinates used, thus, removing many coordinate-dependent processor modules in CTM. By incorporating dynamically consistent interpolation methods and associated subroutines in CTM, the dynamic and thermodynamic consistencies among the meteorological data can be maintained even after the temporal interpolations.

- Outputting meteorological data in Models-3 I/O API format. MCIP writes the bulk of its two- and three-dimensional meteorological and geophysical output data in a transportable binary format using the Models-3 I/O API library.

2.2.1.9 Aggregation Research for Models-3/Community Multiscale Air Quality System

The most scientifically credible and reliable tool for estimating air quality change for large regions, both past and future, are such regional air quality models as the Models-3/CMAQ system. Application of such models requires massive resources, both human and computer, for each policy and/or meteorological scenario. The benefits analyses proposed for the 1990 CAAA require annual time scales. Unfortunately, CMAQ, like most Eulerian models, challenges the practical limits of computer resources and the ability to collect the pertinent input data on annual scales. As a result, applications to determine the long-term relationship between changing emissions patterns and ambient air concentrations are limited.

To circumvent this problem, an aggregation method, initially developed for RADM acid-deposition applications, will be utilized to provide estimates of long-term (seasonal or annual) ambient air concentrations as well as wet and dry deposition amounts. The aggregation method is based on the premise that at any given location, ambient air concentrations (as well as deposition) are governed by a finite number of different, though recurring meteorological regimes. Identification of these patterns facilitates selection of time periods, i.e. the sample, for simulation by CMAQ. Model output from the sample will then be used in the aggregation approach.

The aggregation approach is based on weights determined for meteorological categories that account for a significant proportion of the variability, and for variation in the air quality measures. Within and between clusters, variability of air quality measures will be examined. The extinction coefficient will be used first as was done for RADM (Eder and LeDuc, 1996; LeDuc *et al.*, in press). Other air quality characterizations will be evaluated with available air quality data sets. With weights based on strata of wind, the transport mechanisms involved in the associated atmospheric processes are considered. This will facilitate source-attribution analyses. This requires that clusters reflect wind flow parameters, since wind field patterns in essence describe frontal passages, along with their meteorological properties. Evaluation of aggregation results may require additional parameters in defining clusters.

2.2.2 Photochemical Modeling

A Models-3 Air Management Version (AMV) is being prepared for use in regulatory and policy applications within the overall framework of the Models-3 system. This version will have a pre-selected specific configuration of the air quality model, CMAQ, that will be tested on a July 1995 case from the NARSTO-NE (North American Research Strategy for Tropospheric Ozone-NorthEast) field study. The test demonstration of Models-3/AMV will include a nested domain configuration of three grids; one with 36-km resolution covering the eastern United States; one with 12-km resolution covering the northeastern United States; and one with 4-km resolution covering the New Jersey-New York-Connecticut area. It is anticipated that the Models-3/AMV will be used by OAQPS and the states for regional/urban ozone and $PM_{2.5}$ assessments against the NAAQS beginning around FY-2000. This demonstration project became operational near the end of FY-1997.

2.2.3 Aerosol Research and Modeling

During the summer of 1997, the EPA announced a new NAAQS, the PM fine standard, and adopted a Regional Haze Rule. Implementation of these requirements to promulgate a new standard and rule requires urban to regional scale modeling of the PM fine concentration fields. The Division continued a program of model development evaluation and refinement capable of addressing environmental issues associated with aerosols. These issues incorporate all the known major physical and chemical processes affecting the concentration distribution, chemical composition, and physical characteristics of atmospheric aerosols.

Using the Regional Particulate Model (RPM), a base case scenario was examined and the results compared with observations. In general, sulfate mass was well predicted. Nitrates were less well predicted, and organic aerosols were underpredicted. The nitrate result was expected. Primary emissions of organics and an explicit representation of biogenic precursors were not included. Further, RPM only included the hydroxyl radical attack on the precursors. Ozone is a strong oxidant of these precursors, and nitrate radicals are strong attackers at night. The reactions are included in the Models-3/CMAQ.

2.2.4 Atmospheric Toxic Pollutant Deposition Modeling

Prompted by Congressional mandates, three atmospheric modeling assessments of human exposure to toxic pollutants in the environment are continuing. The first study considers atmospheric mercury exposure from all major anthropogenic sources; the second study handles dioxin-like compounds from electric power generating utilities and hazardous waste incinerators; and the third study focuses on exposure to toxic particulate metals from the air emissions of electric power generating utilities.

2.2.4.1 Mercury Modeling

The first study was a cooperative effort with other research laboratories; multimedia model results were provided to the Agency. The REgional Lagrangian Model of Air Pollution (RELMAP) (Eder *et al.*, 1986) was previously adapted to simulate the emission, transport, dispersion, atmospheric chemistry, and deposition of mercury across the continental United States (Bullock *et al.*, 1997). The atmospheric chemistry algorithm, based on formulations of Petersen *et al.* (1995), considers the aqueous reaction of elemental mercury with ozone to produce inorganic mercury in precipitation. This mercury wet deposition is augmented by adsorption of inorganic mercury to carbon soot particles in cloud water and is moderated by the catalytic reduction of inorganic mercury to elemental mercury by ubiquitous sulfite ions also in cloud water. Model adaptation and testing continued during FY-1997 in response to scientific critiques of model results presented at various conferences and workshops, organized peer reviews of journal articles submitted for publication, and specifically to address comments from an EPA Science Advisory Board Report on the Mercury Study Report to Congress (U.S. Environmental Protection Agency, 1997a). Assumptions about the chemical and physical form of the air emissions from various source types were modified to reflect new information from source testing and to account for expected changes in the chemical and physical forms of mercury emissions due to various air pollution control equipment known to be installed at certain large industrial operations.

The updated RELMAP Mercury Model was applied to calculate annual mean air concentrations and wet and dry depositions of mercury across 40-km grid cells covering the lower 48 States using 1989 meteorological forcing and current air emissions estimates. Division personnel participated with EPA managers and researchers throughout the United States in the interpretation of these regional-scale air modeling results, which were integrated with modeling results obtained for other environmental media to produce a revised Mercury Study Report to Congress (U.S. Environmental Protection Agency, 1997b; 1997c; 1997d; 1997e; 1997f; 1997g; 1997h; 1997i) and a revised Report to Congress on Electric Utility Steam Generating Units Hazardous Air Pollutant Study (Utility Report). Submission of the Mercury Study Report to Congress is anticipated in December 1997 following final review by the White House Office of Management and Budget. Submission of the Utility Report is expected soon thereafter.

The RELMAP Mercury Model was previously applied for NorthEast States for Coordinated Air Use Management (NESCAUM) to simulate concentrations and wet and dry depositions of atmospheric mercury attributable to various source types using updated emission rates for sources within the boundaries of the NESCAUM member states. NESCAUM corrected errors in the site specific mercury emissions data previously used and performed new simulations with RELMAP during FY-1997. RELMAP was applied using the EPA emissions estimates for non-NESCAUM states and the updated NESCAUM data from its member states to estimate a general mass balance of mercury transport to and from the NESCAUM states. This modeling assessment indicated that the majority of atmospheric mercury that is deposited to the NESCAUM states is probably emitted from sources located within the NESCAUM region, with municipal waste combustion being the largest source type. However, the RELMAP simulation showed a significant fraction of the mercury deposited to the NESCAUM states can be attributed to air emissions from coal-fired electric utility boilers outside the NESCAUM region. NESCAUM has worked with eastern Canadian provinces to develop a report entitled *Northeast States/Eastern Canadian Provinces Mercury Study,* which describes the results of this RELMAP modeling assessment. This report is undergoing scientific peer review from outside experts and Division personnel are participating in the review process.

A study was continued during FY-1997 to evaluate the sensitivity of the RELMAP Mercury Model wet deposition results to uncertainty in the chemical and physical forms of atmospheric mercury emissions. Estimates of the fractions of mercury emitted as elemental mercury gas (Hg^0), divalent mercury gas (Hg^{2+}), and particulate mercury (Hg_P) were used for each of the major anthropogenic source types modeled. These estimates of the mercury emission speciation are quite uncertain for most source types. Engineering principles suggest that actual emission speciations will vary from source to source based on the composition of the feedstock, the mechanics of the combustion or reaction process used, and the air pollution control technology applied to the exhaust stream. To evaluate model sensitivity, seven major source types were each modeled with four widely varying emission speciation profiles, (1) a base-case approximation, (2) all Hg^0, (3) all Hg^{2+}, and (4) all Hg_P. Due to the linear chemistry of the RELMAP Mercury Model, the results of the individual source-type simulations could be compiled for each of the 16,384 (4^7) possible combinations and a distribution of possible model outcomes obtained. The distributions of total wet deposition of mercury versus total atmospheric emission of Hg^0, Hg^{2+} and Hg_P indicated a strong sensitivity of the RELMAP Mercury Model in each case. Based on these results, it was concluded that precise and accurate modeling of atmospheric mercury is dependent on a good understanding of mercury emission speciations and any chemical and/or physical transformations that might take place in the atmosphere after emission. Preliminary results from this study were first presented at an international conference in Hamburg, Germany, in 1996. A journal article describing model sensitivity for both wet and dry deposition of mercury was accepted for publication in a special issue of *Science of the Total Environment* (Bullock *et al., 1997*).

2.2.4.2 Modeling Dioxin and Other Semi-Volatile Toxics

For the second study, RELMAP was modified and applied to simulate the transport and deposition of 17 separate congeners of polychlorinated dibenzo-p-dioxin (PCDD) and polychlorinated dibenzofuran (PCDF). This version was used to provide estimates of average annual concentration and wet and dry deposition attributable to air emissions from electric utility boilers and hazardous waste incinerators. Human exposure to all PCDD and PCDF compounds has traditionally been quantified in terms of a summed toxic equivalent (TEQ) to 2,3,7,8-tetrachlorodibenzo-*p*-dioxin, the most toxic of all PCDD and PCDF congeners. However, the various congeners of dioxin and furan have different vapor pressures and gas/particle mass partitioning ratios in the atmosphere. Thus, a scientifically credible treatment of the transport and deposition of total dioxin toxicity required that each congener be modeled explicitly. Once the exposures to each of the 17 congeners was estimated by RELMAP, TEQ was calculated based on prescribed toxic equivalency factors for each congener. The results of this application suggested that some variation does indeed exist in the transport and deposition characteristics of the various PCDD and PCDF congeners. There is significant uncertainty regarding the dry deposition of the gaseous fraction of the more chlorinated congeners. Although their gaseous fraction is thought to be quite small, preliminary field experiments show greater assimilation of these compounds in some plant species than can be explained by particulate dry deposition alone. These experimental results have not yet been subject to formal scientific peer review. It is certainly possible that the understanding of particulate PCDD and PCDF deposition to vegetation is flawed and/or incomplete and that significant gaseous deposition is not required to account for observed assimilation rates of these compounds in plant material.

To provide OAQPS some model-derived estimates of PCDD and PCDF air concentrations and wet and dry depositions from electric utility boilers, the RELMAP Dioxin Model was applied during early 1997. It was assumed that gaseous dry deposition of these compounds is negligible because PCDD and PCDF are hydrophobic, incapable of dissolving on or chemically reacting to underlying terrain, water surfaces, or vegetation in the gas phase. The results obtained from this modeling study were used in developing the Report to Congress on Electric Utility Steam Generating Units Hazardous Air Pollutant Study.

To provide EPA Office of Solid Waste and Emergency Response nationwide estimates of exposure to atmospheric dioxin and furan compounds from hazardous waste incineration, the RELMAP Dioxin Model was modified to incorporate the latest scientific evidence of dry gaseous deposition of dioxin and furan compounds to vegetated surfaces. This updated version of the model was used during FY-1997 to assess the average concentration and total wet and dry deposition patterns of PCDD and PCDF congeners over the lower 48 States from these sources. This work is ongoing and final results are not expected until FY-1998.

2.2.4.3 Modeling of Toxic Particulate Metals

In the third study, RELMAP was modified and applied to simulate the transport and deposition of particulate emissions of nickel and chromium compounds. RELMAP was previously applied for particulate arsenic, cadmium, and lead. Using an expanded and updated air emissions inventory, this expanded particulate metals version of RELMAP was applied to estimate average concentration and deposition patterns for the lower 48 States specifically from electric power generating utilities. The results from these simulations were also used in developing the Report to Congress on Electric Utility Steam Generating Units Hazardous Air Pollutant Study mentioned in the previous section.

2.2.5 Meteorological Modeling Studies

The Penn State/NCAR Mesoscale Meteorological Model Version 5 (MM5) is the primary tool for providing meteorological input data for air quality modeling studies, including Models-3. MM5 is run in retrospective mode using four-dimensional data-assimilation. The model is being applied to several case studies at a variety of scales using a series of one-way nested domains. This technique produces consistent meteorological characterizations from continental scale (with 108-km grid resolution) through regional scale (36-km resolution), and mesoscale (12 km) down to urban scale (4 km).

MM5 was coupled to an advanced land-surface and PBL model to improve simulation of surface fluxes and PBL characterization. Such surface and PBL quantities as surface air temperature and PBL height are critical to realistic air quality modeling. Therefore, model development efforts have concentrated in this crucial area. This version of MM5, referred to as MM5PX after developers Pleim and Xiu, is only being used in-house; collaboration is underway with NCAR to include this module in the NCAR supported system.

The new land-surface model is based on a simple surface energy and moisture parameterization, including explicit representation of soil moisture and vegetative transpiration (Noilhan and Planton, 1989), and the Asymmetric Convective Model, which was originally developed for RADM by Pleim and Chang (1992). The coupled surface/PBL model performs integrated simulations of soil temperatures and soil moisture in two layers as well as PBL evolution and vertical transport of heat, moisture, and momentum within the PBL. Its more sophisticated treatments of soil hydrology and vegetative processes require additional soil texture and land-use data sets that include more detailed characterization of vegetation properties. An important component of the surface model is indirect nudging of soil moisture based on errors in air temperature and humidity predictions when compared to analyses of surface observations. A description of the surface/PBL model and initial testing in a one-dimensional prototype was presented by Pleim and Xiu (1995).

Evaluation through comparison to field measurements has been ongoing for several years in cooperation with the flux monitoring experiments. These studies have lead to many refinements in the stomatal conductance parameterization. MM5PX results were compared to field measurements of surface fluxes and PBL heights taken in the summer of 1994 at Bondville, Illinois (Pleim *et al.*, 1996); measurements of surface fluxes and temperatures from FIFE taken in the summer of 1987 in Kansas; and measurements of surface flux taken in 1995 at Keysburg, Kentucky (Pleim *et al.*, 1997). The Keysburg study, in particular, shows that the model is well able to simulate the effects of changing moisture conditions over a several week period.

2.2.6 Dry Deposition Studies

A new method for modeling dry deposition of gaseous chemical species was developed to take advantage of the more sophisticated surface model implemented in MM5PX. Since the modified MM5 now has a parameterization of evapotranspiration, the same stomatal and canopy conductances can be used to compute dry deposition velocities of gaseous species. This technique has the advantage of using more realistic estimates of these conductances resulting from the integrated surface energy calculation in which the soil moisture is continually adjusted to minimize model errors of temperature and humidity. Other surface resistances needed for the estimation of dry deposition velocity are parameterized according to relative solubility and reactivity in a similar manner to the scheme used in ADOM, CALPUFF, and ISC3 (Pleim *et al.*, 1984). Additional updates to this model include revision of many empirical parameters according to more recent experimental data, as well as an additional deposition pathway through the canopy to the ground.

The dry deposition model is being evaluated for ozone deposition by comparing the model results with the comparisons to field measurements taken at Bondville and Keysburg. Preliminary results from both studies are presented by Pleim *et al.* (1996) and Pleim *et al.* (1997). The new model is also compared to the MultiLayer Model (MLM) that was used for CASTNet (Clean Air Status and Trends Network). Results from both studies show better agreement with ozone deposition velocity measurements for the new model than for MLM particularly during daytime hours when evapotranspiration is important.

2.2.7 Technical Support

2.2.7.1 North American Research Strategy for Tropospheric Ozone

The North American Research Strategy for Tropospheric Ozone (NARSTO) is a plan for a coordinated 10-year research strategy to pursue the science-based issues that will lead to better management of the North American tropospheric ozone problems. It includes a management plan for performing this coordination across the public and private sector organizations sponsoring ozone research, as well as those groups performing the research, including the university community. Canada and Mexico also are participating in the continental NARSTO plan. During FY-1997, two Division representatives were involved in co-chairing key teams for the continental NARSTO program: the modeling team and the analysis and assessment team. Also, the NARSTO-sponsored tropospheric ozone state-of-science assessment was in high gear. It is composed of a series of critical review papers on particular areas of the science, as well as an assessment report that indicates how the science can address outstanding policy issues in tropospheric ozone. The critical review papers and assessment report were being written during FY-1997 and are due to be completed by the end of 1998. As part of EPA's contribution to NARSTO, all non-effects scientific aspects of tropospheric ozone research, including atmospheric chemistry, modeling, monitoring and field studies, methods development, emissions research, and emissions control technology are being coordinated and managed by a Division member.

2.2.7.2 Southern Oxidant Study

FY-1997 was the seventh year of the multiyear Southern Oxidant Study (SOS), a major field and modeling project concerned with the generation and control of ozone and photochemical processes in the southeastern United States. A consortium of Southeastern universities is coordinating the study. Division personnel are involved in providing technical leadership on aspects of air quality simulation modeling and emissions inventory development on various cooperative agreements. During FY-1997, the focus of activities was on the analysis and interpretation of data obtained from a major field study in and around Nashville, Tennessee, during the summer of 1995. The principal objective of the study was the physical and chemical interaction of power plant plumes and the Nashville urban plume with the regional environment. Besides intensive measurements obtained at the surface, observations aloft were also made by several aircraft, including the NOAA/ARL Twin Otter and the NOAA/ARL P3. An SOS data analysis session was held in conjunction with the Fall 1996 American Geophysical Union meeting. Papers were presented and submitted for publication on many aspects of the Nashville study. Results showed several stagnation events had occurred in the Nashville area during the field campaign. Ozone episodes in the Nashville area were a part of a larger pattern of elevated ozone concentrations in the eastern United States during the period. It was found that ozone production efficiencies were surprisingly low within the Nashville and nearby power plant plumes. NO_y was lost within the plumes more rapidly then expected, possibly due to heterogeneous conversion.

2.2.7.3 Federal Advisory Committee Act Subcommittee on Ozone, Particulate Matter, and Regional Haze

New air quality standards for ozone and fine particulate matter were announced during FY-1997. The EPA is considering a joint implementation of assessments for the new standards regarding the interactions between ozone and fine particulates. A Federal Advisory Committee Act (FACA) Subcommittee on Ozone, Particulate Matter, and Regional Haze was established to help guide the EPA in developing guidelines and procedures to facilitate this implementation. Several working groups exist to serve the Subcommittee, including groups for Base Programs Analyses and Policies, National and Regional Strategies, Science and Technical Support, and Communications and Outreach. One Division member assisted the Science and Technical Support Group in developing a conceptual model of the science underpinning the new joint implementation. Comments are being prepared on the proposed use of scientific methods and tools advocated in policy-oriented issue papers that the other working groups are writing.

2.2.7.4 Seasonal Modeling of Regional Air Quality

A large-scale Seasonal Modeling of Regional Air Quality (SMRAQ) over the eastern United States from May through September 1995 is being conducted jointly by MCNC, Research Triangle Park, North Carolina; Georgia Institute of Technology, Atlanta, Georgia; and Duke University, Durham, North Carolina. The project is sponsored by the Southeast States for Air Resource Management and is aimed at studying useful air quality management options for the southeastern United States, applicable over seasonal time scales. The project uses MM5 and the MAQSIP ozone air quality model at 36-km horizontal resolution. One member of the Division participates on the SMRAQ Technical Liaison Committee, a peer-review and advisement group for the project.

2.2.7.5 Interagency Work Group on Air Quality Modeling

The Interagency Work Group on Air Quality Modeling (IWAQM) was formed in FY-1991 through a Memorandum of Understanding between the EPA, U.S. Forest Service, U.S. Fish and Wildlife Service, and National Parks Service. IWAQM seeks to develop the modeling tools needed to conduct assessments of individual and cumulative impacts of existing and proposed sources of air pollution on local and regional scales with special emphasis on the protection of Class I areas as defined by the Clean Air Act. In FY-1996, the production of a comparable data set for a second year (1992) was begun using MM5 with FDDA. The goal is to obtain, as a minimum, a three-year database of modeled meteorology fields making possible the implementation of the IWAQM recommendation to perform assessments of source impact to Class I areas using local- and regional-scale dispersion models. The transition for the MM5 system from Version 1 to Version 2 in FY-1997 necessitated a significant delay in completing the second-year data set.

2.2.7.6 Total Column Ozone

The global distribution of total column ozone is attracting great international attention as concerns escalate about reduced global amounts. Detection of a trend is an arduous task, made difficult by numerous natural inter- and intra-annual fluctuations, many of which are not well understood. Accordingly, the purpose of this analysis is to develop a better understanding of these natural variations across all spatial and temporal scales. This is being achieved through the application of a multivariate statistical technique called rotated principal component analysis (PCA) to the total column ozone data derived from Version 7.0 TOMS (Total Ozone Mapping Spectrometer) for the period 1980 through 1992.

TOMS is a nadir (downward-looking) instrument, launched onboard the Nimbus 7 satellite in 1978. It consists of a single monochromator that rapidly scans wavelengths from 312 to 380 nm while spatially scanning across the orbital track, producing global maps of total column ozone on a daily basis with a resolution of 1° lat. by 1.25° long. The data, in Dobson Units [1 DU = 2.69 x 10^{16} molecules cm^{-2}], were obtained on a CD-ROM from NASA National Satellite Service Data Center located at the Goddard Space Flight Center.

The objective in using PCA is to identify, through a reduction of data, the significant recurring and independent modes of variation (signals) within this large data set. This technique will summarize the essential information of that data set so that meaningful and descriptive conclusions can be made. This technique is very appropriate for application to the TOMS data set where the total number of observations exceed 1 x 10^8. Utilization of Kaiser's varimax orthogonal rotation will allow delineation of homogeneous subregions; that is, areas of the globe that experience unique total ozone characteristics. Examination of the time series associated with each unique subregion will be based on spectral density analysis. This will allow further elucidation (across all possible wavelengths) of the physical phenomena (i.e. Quasi-Biennial Oscillation, El Nino-Southern Oscillation, annual and semi-annual oscillations) responsible for the natural variability of total column ozone.

2.2.7.7 Climatological and Regional Analyses of Clean Air Status and Trends Network Data

The Clean Air Status and Trends Network (CASTNet) monitoring program is being analyzed using rotated principal component analysis and spectral density analysis. This is being done to regionalize the CASTNet stations into *influence regimes* or subregions whose fluxes, concentrations, and deposition velocities exhibit statistically unique, homogeneous characteristics, presumably in response to a commonality of forcing factors (i.e. meteorology, emissions, geography). This approach has been used successfully in the examination of other aerometric data, including $SO_4^=$ concentrations in precipitation (Eder, 1989) and ambient air concentrations of O_3 (Eder *et al.*, 1993).

2.2.7.8 Statistical Modeling of Ozone in Houston

A two-stage statistical clustering approach (average linkage and k-means) designed by Eder *et al.* (1994) for Birmingham, Alabama, was applied to Houston, Texas (Davis *et al.*, in press), in an effort to refine the approach and simultaneously account for the variability observed in ozone attributable to meteorology. When applied to 12 years of meteorological data (1981–1992), each clustering technique identified 7 statistically distinct meteorological regimes. The majority of these regimes exhibited significantly different daily 1-hour maximum ozone (O_3) concentrations, with the two-stage approach resulting in a better segregation of the mean concentrations when compared to the single-stage approach. Both approaches indicated that the largest mean daily 1-hour maximum concentrations are associated with migrating anticyclones that occur most often during spring and summer, and not with the quasi-permanent Bermuda High that often dominates the southeastern United States during the summer. As a result, maximum ozone concentrations are just as likely during the months of April, May, September, and October as they are during the summer months. Generalized additive models were then developed within each meteorological regime in order to identify those meteorological covariates most closely associated with O_3 concentrations. Three surface wind covariates, speed, and the *u* and *v* components, were selected nearly unanimously in those meteorological regimes dominated by anticyclones, indicating the importance of transport within these O_3 conducive meteorological regimes.

2.3 Modeling Systems Analysis Branch

The Modeling Systems Analysis Branch interacts with the other Branches in the Division by providing routine and high performance computing support needed in the development, evaluation, and application of environmental models. The Branch is the focal point for modeling software design and systems analysis in compliance with stated Agency requirements of quality control and assurance, and for conducting research in the High Performance Computing and Communications (HPCC) program, which includes parallel processing, visualization, and advanced networking. Under the HPCC program, the Branch is developing a flexible environmental modeling and decision support tool to deal with multiple scales and multiple pollutants simultaneously, thus facilitating a more comprehensive and cost effective approach to related single-stressor and multistressor human and ecosystem problems.

2.3.1 High Performance Computing and Communications Program

The High Performance Computing and Communication (HPCC) program is a cross-agency coordinated program under the leadership of the National Science and Technology Council (NSTC) Committee on Computing, Information, and Communications, which conducts long-term research and development in advanced computing, communications, and information technologies and applies those technologies to achieve Agency missions. The Agency is moving toward community-based environmental management involving stakeholders, local industry, state and local governments, and people in the community whose health, environment, and jobs are most impacted. The primary goal of the HPCC program is to improve the stakeholders' capability to access data, reliable environmental models, and visualization and analysis tools to make informed decisions involving risks to human health, ecosystems, and the economics of local industry and surrounding community. This goal is also consistent and supportive of the goals and objectives of the NSTC Committee on Environment and Natural Resources. The HPCC technology research focuses on three areas: environmental assessment framework development; high performance numerical methods for scalable parallel architectures; and public data access and visualization and analysis techniques.

2.3.1.1 Models-3 Framework

In FY-1997, the HPCC program continued work on the first version of Models-3, a flexible software system designed to facilitate the development and use of environmental assessment and decision support tools. The initial version of Models-3 focuses on urban to regional scale air quality simulation of ground-level ozone, acid deposition, visibility, and fine particulates. The Models-3 framework provides interfaces between the user and operational models, between the scientist and developing models, and between the hardware and software. This enhances the user's ability to perform environmental management tasks ranging from regulatory and policy analysis to understanding the interactions of atmospheric chemistry and physics, while rapidly adapting to emerging technology. Models-3 is intended to serve as a community framework for continual advancement of environmental assessment tools.

To adapt to changing hardware and software, the framework uses specialized object libraries and a standardized interface design that isolates critical system components. This minimizes the impact of hardware and software upgrades. A client-server architecture, in conjunction with a standardized data interface and object-oriented database containing metadata, enables transparent use of multiple computing platforms and access of data across the network. The object-oriented database contains such shared data as model domain, map projections, grid resolution, and chemical species that enable the interchange of science codes while maintaining user control of the specifics of a model application. A library-based graphical user interface facilitates ease of use for model executions and access to a variety of visualization and analysis packages. Components of Models-3 assist in design and preparation of source emissions inventories compatible with a variety of air quality modeling capabilities.

2.3.1.2 Models-3 Extension for Cross-Media Modeling

The primary purpose of this research is to facilitate the development of a community environmental modeling framework to serve as a foundation upon which the scientific and technical communities can build, component by component, complex multidiscipline and multipollutant assessment tools. This effort depends upon emerging technology that enables Federal agencies, academia, and research institutions to participate in a collaborative approach to multidiscipline environmental modeling. To test the feasibility of this approach, three models were linked into Models-3 and data conversions were performed to facilitate the exchange of data among the models. The models were RADM for atmospheric deposition, the Hydrological Simulation Program - FORTRAN model for Chesapeake Bay nutrient flow in the watershed to the Bay, and the Chesapeake Bay Water Quality Model with its embedded hydrodynamic model for the Bay response to nutrient loading.

2.3.1.3 Models-3 Emissions Data Processing

The Models-3 Emission Processing and Projection System (MEPPS) portion of the Models-3 air quality modeling system was operational in a stand-alone mode throughout FY-1997, and was integrated into the Models-3 framework during the spring. MEPPS provides emissions data to the CTM module of Models-3. Principal developments in MEPPS include:

- Installing a basic reader for continuous emissions monitoring data. The data are hourly emissions measurements from large industrial facilities, initially electric utilities. These data are combined with estimated hourly emissions inventory data from other point sources to substantially improve inventory quality and modeling results. An improved reader is planned for FY-1998.

- Completing and linking the Models-3 Emission PROjection processor (MEPRO) system to the Models-3 framework. Based on a modified version of the EPA Multiple Projection System (Monroe *et al.*, 1994), MEPRO runs under Microsoft® Windows NT™ operating system.[2] MEPRO projects emissions for future years from point- and area-emission sources using economic projection factors developed by the Economic Growth Analysis System (Young, 1994) and applied by specific categories of sources. Emissions from biogenic and mobile sources are adjusted to the future by anticipated land-use changes and travel- demand projections. MEPPS processes the resulting projected emissions inventories for air quality modeling for future years.

- Installing geographic information system coverage for major highways in the United States (Federal Highway Administration data), and local roads (Tiger/Line data from the U.S. Census Bureau). These coverages are used to provide accurate spatial allocation of emissions data from mobile sources modeled by the U.S. EPA Mobile 5a (U.S. Environmental Protection Agency, 1994). Political boundary, census, and land-use coverages also are in place for Mexico and Canada because regional modeling geographic domains often overlap national borders.

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[2] Microsoft and Miscrosoft Windows NT are registered trademarks of Microsoft Corporation; TN is a registered trademark of Northern Telecom Limited.

- Creating graphical user interface screens including selectable, user-modifiable icons within the Models-3 framework study planner to allow relatively easy modification and batch execution of the MEPPS emissions data processors. The screens appear as simplified processing plan layouts corresponding to point, area, biogenic, and mobile source data processing. This greatly simplifies processing for the user. Without the use of the graphical interface screens, interactive emissions data processing requires several dozen SAS®[3] screens and hundreds of smaller programs.

- Expanding and completing analysis and query functions, in both tabular and geographical information system formats, for the initial version of MEPPS. These tools allow both quality control and analysis of the contents of emissions inventories.

2.3.2 Visualization and Analysis Tools

The primary goal of the visualization and analysis effort is to provide a desktop-accessible integrated software system that assists Federal, state, and industrial groups in performing environmental research, modeling, assessment, and decision-making activities. New visualization capabilities were integrated into the Models-3 framework. Enhancements in Vis5D,© an interactive three-dimensional visualization package developed at the University of Wisconsin-Madison, added capability to look at vertical profiles and multiple side-by-side five-dimensional visualizations.[4]

Capability for visually exploring the relationship of vertical winds from model output to vertical winds from NEXRAD VAD and wind profilers was developed. The visualization software packages used are IBM DX®[5] and AVS®[6].

2.3.3 Technology Transfer

A cooperative agreement with North Carolina State University (NCSU), Raleigh, North Carolina, to conduct research facilitating the transfer of advanced air quality models in Models-3

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[3]SAS is a registered trademark of SAS Institute Inc.

[4] Developed through cooperation between the EPA and the Space Science and Engineering Center of the University of Wisconsin-Madison.

[5] IBM Visualization Data Explorer is a registered trademark of International Business Machines Corporation.

[6] AVS is a registered trademark of Advanced Visual Systems, Inc.

was completed. Two workshops were broadcast by satellite from NCSU through the Air Pollution Distance Learning Network. The February 20, 1997, workshop, *How Models-3 Can Help You in Air Quality Management: Real Examples*, and the September 25, 1997, workshop, *Models-3 Beta Experience,* are available on videotape.

The technology transfer included conducting a beta test of the Models-3 framework during the summer of 1997. Prior to the beta test, a two-day workshop was held at Duke University School of the Environment, Durham, North Carolina. After the workshop, six external beta sites installed the Models-3 framework and provided feedback for framework developers. As an important quality assurance tool, the beta test feedback was captured and tasks were defined to modify the framework to respond to user feedback. In addition, a workshop was held to explore the community model aspect of Models-3.

2.3.4 Computing Infrastructure

2.3.4.1 Division World-Wide Web Home Page

The Division Home Page for the WWW was updated. The page includes an overview of the Division's mission; a staff directory with phone numbers and addresses; a link to the Division Library; a list of Division publications; the FY-1996 annual report; monthly highlights; and links to sites that provide computer models and databases. The Division's URL address is http://www.epa.gov/asmdnerl/. The Internet anonymous ftp site (monsoon.rtpnc.epa.gov) includes databases and air quality simulation modeling programs developed or supported by the Division. Computer files are available for the following: acid deposition modeling, photochemical oxidant (smog) modeling, hazardous release modeling, particulate modeling, toxic modeling, emissions modeling (biogenic and anthropogenic), and associated meteorological models and data. Statistics show that the number of hits to the web site increased during FY-1997 from 27,000 hits to 50,000.

2.3.4.2 Files and Tapes Management

The clean-up on the IBM®[7] mainframe continued. There were 17,300 old files deleted from the IBM. With new files being generated every day, the number of files slowly decreased from 80,000 to 60,000. The number of tapes decreased from 3,000 to 31.

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[7] IBM is a registered trademark of International Business Machines Corporation.

2.3.5 Biogenic Emissions

The air quality modeling community continued to show interest and concern about biogenic emissions, particularly for regional ozone and aerosol formation. A Division scientist helped plan and organize an AMS Symposium on Biogenic Hydrocarbons, which was held in Charlottesville, Virginia, in August 1997. Partly to address the controversy surrounding the high emissions of isoprene predicted by the Biogenic Emissions Inventory System (BEIS-2), research was undertaken to compare isoprene concentrations estimated with RADM2 against observations taken near Scotia, Pennsylvania, during the summer of 1988 (Pierce *et al.*, in press). Information from BEIS-2 continues to be used in the EPA's annual emissions trends report (U.S. Environmental Protection Agency, 1997j).

As a part of a team of biogenic emissions experts working under the auspices of NARSTO, a Division scientist continued to work on a critique of biogenic emissions research. This effort will lead to the development of the next version of BEIS (BEIS-3). The new version of BEIS will include a 1-km resolved vegetation cover data set, more detailed speciation of monoterpenes (important for aerosol formation), and a refined leaf temperature canopy model.

A Division scientist continued to analyze the data taken from a soil NO_x flux experiment conducted in Washington County in eastern North Carolina. The Natural Oxidant Emissions and Validation Experiment was a multi-agency and academic effort to measure NO_x fluxes from agricultural fields (Aneja *et al.*, 1996).

2.3.6 Improvements in Vegetation Cover Data

A 1-km vegetation cover data set is being prepared for North America. This data set will be an amalgamation of information, including the U.S. Geological Survey (USGS) 1-km land characteristics data set, urbanized areas from the 1990 U.S. Census, crop coverage from the 1992 U.S. Agricultural Census, and forest inventory statistics from the U.S. Forest Service. This data set will build on Kinnee *et al.* (1997) by providing tree-species and crop-type information at a 1-km resolution. The data set will be integrated into BEIS-3 and tested with Models-3/CMAQ, particularly with MM5.

2.3.7 Working Group for Climate Services

The Working Group for Climate Services is one of four working groups of the Interdepartmental Committee for Meteorological Services and Supporting Research sponsored by the Office of the Federal Coordinator for Meteorological Services and Supporting Research. This group met twice during FY-1997. The working group consists of representatives from nine Federal agencies. At meetings, representatives give agency status reports including information on available data sets and data sets under development. One issue of concern during the year was the quality of observational systems for climate characterization and change detection. The working group provided input to the North American Observing System regarding changes in the rawinsonde observations.

2.4 Applied Modeling Research Branch

The Applied Modeling Research Branch investigates and develops applied numerical simulation models of sources, transport, fate, and mitigation of air toxic pollutants in the near field and conducts research to develop and improve human exposure predictive models, focusing principally on urban environments where exposures are high. Databases are assembled and used for model development and research on flow characterization, dispersion modeling, and human exposure. Using the Fluid Modeling Facility (FMF), the Branch conducts simulations of atmospheric flow and pollutant dispersion in complex terrain, in and around such obstacles as buildings, in convective boundary layers and dense gas plumes, and in other situations not easily handled by mathematical models. The FMF consists of large and small wind tunnels, a large water channel/towing tank, and a convection tank. The large wind tunnel has an overall length of 38 m with a test section 18.3 m long, 3.7 m wide, and 2.1 m high, and an airflow speed range of 0.5 to 10 m/s. It is generally used for simulating transport and dispersion in the neutral-atmospheric boundary layer. The towing tank has an overall length of 35 m with a test section 25 m long, 2.4 m wide, and 1.2 m deep, and the towing carriage has a speed range of 1 to 50 cm/s. The towing tank is primarily used for simulation of strongly stable flow; salt water of variable concentration is used to establish a density gradient in the tank, which simulates the nighttime temperature gradient in the atmosphere. A convection tank measuring 1.2 m on each side and containing water to a depth of 0.4 m is used to study the convective boundary layer (CBL), and flow and dispersion under convective conditions. The tank is initially temperature stratified using an electrical heating grid. Convection is then initiated by heating the floor of the tank. This produces a simulated convective boundary layer capped by an overlying inversion. Another activity of the FMF is the study of resuspension mechanics and wind erosion, primarily through experimental field measurements. Research is coordinated with other agencies and researchers.

2.4.1 Development of a Multimedia Modeling Component for Endocrine Disruptor Exposure Research

Potential endocrine disrupting chemicals (EDCs) were identified as a new, relatively poorly understood source of environmental risk to biological health. An environmental endocrine disruptor was defined as an exogenous agent that interferes with the production, release, transport, metabolism, binding action, or elimination of natural hormones in the body responsible for the maintenance of homeostasis and regulation of developmental processes. In addition to the so-called environmental estrogens and anti-androgens, the term includes agents that affect the thyroid and pituitary glands and other components of the endocrine system. Potential EDCs include such used and banned agricultural chemicals as DDT/DDE, aldrin, dieldrin and atrazine, many PAHs (polycyclic aeromatic hydrocarbons), and PCBs (polychlorobiphenyls), and such trace metals as mercury, lead, and arsenic.

In FY-1997, a multimedia hybrid compartmental model, MEND-TOX, was identified as a state-of-the-science environmental media fate and transport model that might be appropriate for EDC media exposure research. An initial one-day multimedia modeling workshop was held and plans for model acquisition and application were developed. Linkages between endocrine disruptor modeling and monitoring activities were established. Plans were made to explore the value of the selected multimedia model to the design and execution of a pilot multimedia EDC monitoring program for the Neuse River Basin.

2.4.2 Lake Michigan Mass Balance Project

The Lake Michigan Mass Balance (LMMB) project utilizes a mass balance approach to develop a lake-wide management plan to address toxics in Lake Michigan. The primary goal of the mass balance study is to develop a sound, scientific base of information to guide future toxic load reduction efforts at the state and Federal levels for Lake Michigan. The principal objectives of the modeling portion of this effort are to estimate the atmospheric deposition and air-water exchange of priority toxic pollutants. This includes the description of the spatial and temporal variability over Lake Michigan; evaluation of the magnitude and variability of toxic chemical fluxes within and between lake compartments, especially between the sediment and water column and between the water column and the atmosphere; development of contaminant concentration forecasts in water and sediment throughout Lake Michigan, based upon meteorological forcing functions and future loadings using load reduction alternatives; and the quantification of the uncertainty in estimates of tributary and atmospheric loads of priority toxic pollutants and model predictions of contaminant concentrations.

During FY-1997, an atrazine emissions model, developed at the Canadian Global Emissions Interpretation Centre, Mississauga, Ontario, was modified to respond to short-term episodic meteorological conditions. MM5 was modified to include a spatially detailed vegetation- and land-cover module. This will improve the description of transient seasonal meteorological features. Input data sets required for MM5 and emissions model application were prepared; the linked modeling system is ready for application to the 1995 growing season data in the United States and in Canada east of the Rocky Mountains.

A preliminary climatological analysis was also completed during FY-1997. It was used to evaluate proposed baseline atrazine load estimates based on data collected during 1995. It is clear from the analysis that 1995 cumulative monthly (28-day collection periods) atrazine estimates are unlikely to be either temporally or spatially representative of baseline meteorologically driven atrazine emissions and transport throughout the upper midwestern United States. Complex interactions between emission, transport, and removal processes preclude similar statements at the seasonal or annual scale until after full fate and transport model execution occurs during FY-1998. The climatological analysis will be used to assist the analysis and interpretation of these application results.

2.4.3 Air Toxics Human Exposure

The Division supports the development of multimedia, multipollutant human exposure models. These models provide the Agency with the tools needed to assess and manage the risks associated with exposures to toxic pollutants. There is a realization within the regulatory components of EPA that a more holistic approach to limiting emissions and managing risks across all media is needed to ensure human health. This shift in philosophy is fostering a demand for intensified development of multimedia, multipollutant human exposure models to understand processes, investigate complex and non-linear systems, and assist in exposure assessments at various scales and for both prognostic and diagnostic applications. The Branch is responsive to the needs of the program offices for modification, evaluation, and possibly improvements to existing human exposure models.

Development has begun of an urban-scale human exposure model for air toxics having known emissions and air chemistry. This program involves (a) development of models for key human exposure microenvironments, (b) air concentration measurement studies to support model development/evaluation, and (c) development of databases and integration of all data, including demography, geography, meteorology, human activity patterns, source emissions, and regional/urban/microenvironmental scale concentrations. The past year focused primarily on improving and applying the annual-averaged exposure model, HAPEM-MS (Hazardous Air Pollutant Exposure Model for Mobile Sources). In the long run, a short term (1-hour averaged) model similar to the probabilistic NAAQS Exposure Model (pNEM) is needed. Work has begun on modeling and measuring human exposure inside a motor vehicle and in measuring the air exchange rates. The vehicle cabin was selected as a key microenvironment for urban air toxics. A population of motor vehicles will be examined. A passenger van is being instrumented to measure air toxic and particulate matter inside and outside the van. These measurements will be used to support the development of an on-road model for major roadways and measure spatial variation of concentrations along minor roadways downwind of major roadways.[8] The goals for these studies are to provide better exposure factors related to roadway emissions and integrate them into a human exposure modeling framework.

2.4.4 Development and Evaluation of Enhancements to Human Exposure Models

The Clean Air Act, as amended in 1990, requires the EPA to promulgate regulations containing reasonable requirements to control hazardous air pollutants from motor vehicles and their fuels. The EPA regulations must contain standards that reflect the greatest degree of

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[8] Major roadways interconnect major population centers, carrying commuter and business traffic; minor roadways are tributary roads from residences, connecting to major roadways.

emissions reductions achievable through the application of best available technology and, at a minimum, apply to emissions of benzene and formaldehyde. In support of this regulatory requirement, the Office of Mobile Sources must assess the impact of control programs on exposure to air toxic emissions from mobile sources. To this end, HAPEM-MS3 will be used to predict human exposures to mobile source carbon monoxide emissions.

In a typical application of HAPEM-MS3, the population of a study area is subdivided into a comprehensive set of cohorts. Each cohort is defined by a home location, a demographic group, and a work location. A set of exposure districts are defined for the purpose of specifying home and work locations. A set of environmental settings, defined by microenvironment and exposure district, are specified to account for movements of the cohorts. Activity diary data are used to determine the fraction of time spent by each cohort in each environmental setting. An annual average concentration is determined for each environmental setting based on assumed indoor/outdoor ratios and proximity to emission sources. These estimates are combined with estimates of population of each cohort to determine the distribution of exposures within the study area population. The user is able to treat the activity pattern and pollutant concentration associated with each environmental setting as parameters that vary with season and hour of the day or night. In HAPEM-MS3, the time spent by each cohort in an environmental setting is specified as an annual average. The pollutant concentration associated with each environmental setting is also specified as an annual average. Thirty-seven predetermined microenvironments are being used to define the environmental settings; the number of exposure districts varies with the study area.

2.4.5 Modeling Pesticide Applications

In FY-1997, Division scientists continued their involvement in a program to develop methodologies for estimating the drift of airborne pesticides from agricultural pesticide applications. This model development program involves a cooperative research and development agreement (CRADA) with the agricultural chemical industry's Spray Drift Task Force (SDTF). The overall goals of the program are to expand our understanding of the important atmospheric and application mechanisms that affect off-target drift of pesticides and to develop improved models of transport, dispersion, and deposition of pesticides within, above, and beyond the target canopy.

The CRADA participants are expected to complete Version 1.0 of the AGDRIFT spray-drift modeling system in January 1998. This PC-based modeling system is designed to predict the motion of sprayed material released from aircraft, tractor booms, and/or orchard air-blast equipment in scenarios relevant to agricultural pesticide applications. AGDRIFT consists of a screening tier for aerial applications where only the released drop-size distribution is selected by the user with the model providing realistic, yet conservative, estimates of off-target impacts. The screening tier model parameters were selected as those associated with the 90th percentile of downwind deposition as determined in three major field studies. The data from the field studies was reviewed by Bird and Perry (1996). In higher tier levels of the model, the user has full flexibility in establishing application scenarios. AGDRIFT includes data libraries of aircraft types (aircraft type greatly influences the initial mixing of spray droplets), physical properties of pesticide materials, spray nozzle types and orientations, and associated drop-size distributions. And finally, the meteorological parameters can be specified by the user.

The algorithms in AGDRIFT that serve as the kernel for the drift and deposition calculations were first proposed by Bilanin *et al.* (1989). The model is based on a Lagrangian approach to the solution of the equations of motion governing the flow field in which the spray material is released. Passive droplets released into a turbulent flow are assumed to behave as fluid elements and travel with the local velocity. AGDRIFT includes simplified algorithms for simulating the effects of aircraft wake as well as ambient turbulence. The model is undergoing evaluation against the SDTF field study data. The model and its documentation will undergo external peer review in FY-1998.

2.4.6 AMS/EPA Regulatory Model Improvement Committee

For a number of years, the AMS and EPA joined in a formal collaborative effort to advance the scientific basis of regulatory dispersion models. The AMS and EPA formed AERMIC (AMS/EPA Regulatory Model Improvement Committee) to introduce changes in the scientific components of the models and evaluate and implement the new methodologies. AERMIC focused on near-field impacts from industrial source types and developed a prototype model called AERMOD, which is under evaluation. A general overview of the model and its preliminary comparisons with field data are contained in Perry *et al.* (1994), and Cimorelli *et al.* (1996). Additional papers on AERMOD will be published (Lee *et al.,* in press; Venkatram *et al.*, in press).

In FY-1997, AERMIC concluded the prototype model formulation and addressed some specific issues with urban boundary layers and with near surface parameterizations of turbulence and dispersion. Additionally, the committee developed algorithms for blending the surface and elevated formulations. A major effort was placed on beta testing of the code and detailed documentation of the model algorithms and their bases. In the process, a draft model formulation document was developed that contains every equation that appears in the code and an explanation for its selection. This document, critical for future model improvement efforts, is expected to be completed in FY-1998 and delivered with the evaluated model. In FY-1998, the model will go through rigorous testing against three independent field study databases, a sensitivity analysis, and an evaluation of issues related to the regulatory applicability of the model.

2.4.7 Industrial Source Complex - Short Term Model

The Industrial Source Complex - Short Term (ISCST) model has long been the regulatory tool for estimating pollutant concentrations resulting from point, area, and volume source emissions in simple terrain. In recognition of the need for a state-of-the-science model for estimating pollutant dry and wet deposition, as well as concentrations, the released ISCST3 integrates the algorithms for modeling simple terrain found in previous versions of the ISCST model and the algorithms found in the COMPLEX I model, an EPA screening model for complex terrain applications (U.S. Environmental Protection Agency, 1995a; 1995b). In addition, ISCST3 includes an algorithm for modeling dry deposition of particulates, an algorithm for modeling wet deposition of gases and particles, a new algorithm for modeling area sources, and algorithms for treating open-pit source types.

A study was performed to examine the sensitivity of maximum predicted concentrations and dry and wet deposition to input parameters related to the deposition of particles from point sources (Schwede and Paumier, 1997). Tests included considering the effects of dry and wet plume depletion, shape and resolution of the particle size distribution, the particle density, scavenging coefficients, and use of gridded terrain data. Results from the tests were compared for three effective plume heights and four meteorological data sets.

For the model sensitivities explored, the results of the study showed that the predicted maximum concentrations and deposition responded in a manner that is supported by the technical basis of the model. In general, changing any of the input parameters had a greater effect on the maximum hourly deposition values than on the maximum hourly concentration. Modeled deposition values were particularly sensitive to the shape and the resolution of the particle size distribution and use of the depletion option.

2.4.8 Resuspension

An active research topic in the field of resuspension is the quantification of the emission of PM_{10} related to the total mass flux of all particles moved in the resuspension episode. The interest in this relationship is due to the comparatively well-tested models of total particle mass fluxes. Part of the total mass flux moves in a hopping motion along the ground and exchanges momentum from the wind to the ground. This momentum transfer allows a theoretical expression of mass flux as a function of measurable wind properties. One theory relating vertical flux of PM_{10} to total horizontal mass flux is that of Shao *et al.* (1993). Another theory is that of Alfaro *et al.* (1997).

PM_{10} fluxes generated by soil emissions are of considerable interest. The scientific community has acknowledged the crucial role that mineral dust aerosols play in climate forcing (Tegen *et al.*, 1996; Sokolik and Toon, 1996). However, attempts to integrate dust production into global climate and general circulation models simplify dust production rates of mineral aerosols from disturbed lands as a function of meteorological conditions. For these models to become more realistic, they must incorporate advanced PM_{10} emission models. PM_{10} emission models must be developed using outdoor measurements of total particle flux (q_{tot}) and simultaneous measurements of PM_{10} vertical flux (F_a).

Such a data set was presented by Gillette *et al.* (1997). Figure 1 shows the ratio of F_a/q_{tot} (in units of m^{-1}) for data obtained during the Lake Owens Dust Experiment conducted in California, and during earlier campaigns for wind-erodible soils of different textures in west Texas. The figure shows that the F_a/q_{tot} results for the loam texture and sand textures falls within the same range; sandy loam and loamy sand textures are higher and clay textures are lower. The

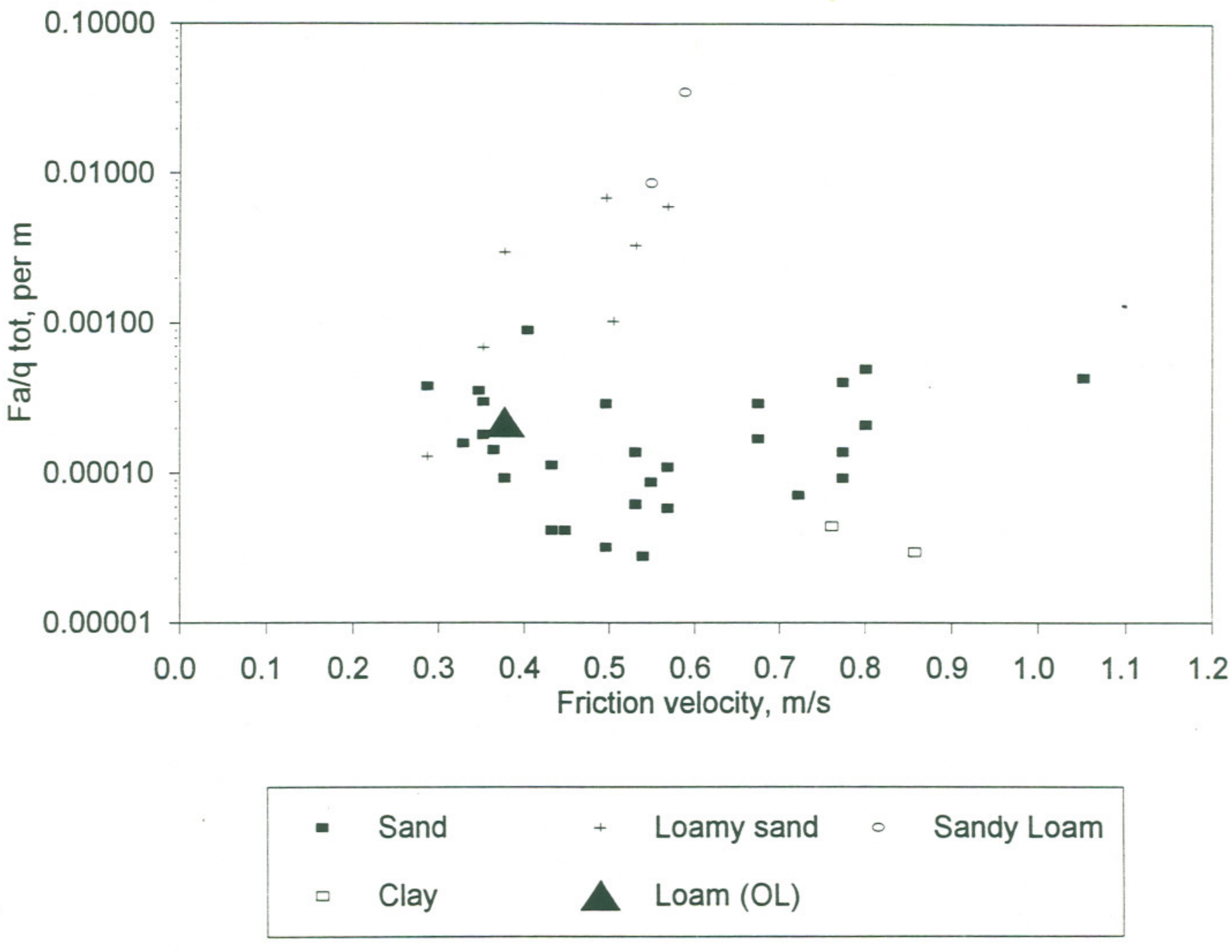

Figure 1. Ratio of vertical flux of PM_{10} to horizontal flux of total particle mass versus friction velocity for experiments corresponding to different soil texture.

F_a/q_{tot} data point for the loam soil (a soil having a large proportion of mass in particles from 2 to 50 μm) is close to the values for the F_a/q_{tot} data points of sand soils (having a small proportion of mass in particles smaller than 50 μm). This closeness of loam and sandy soils may be interpreted as having almost the same kinetic energy for sandblasting of PM_{10}. This is probably caused by similarity in both size of the saltating grains and binding energies for all the soils tested. The higher values of F_a/q_{tot} for sandy loam and loamy sand is provisionally interpreted as reflecting weaker binding energies for those two textures of soil. The clay soil, formed of hard cubical pellets of dried clay, is interpreted as having quite high binding energies and large particle sizes delivering large kinetic energies in single particle collisions.

2.4.9 Buoyant Puff Dispersion in a Convective Boundary Layer

During FY-1996, extensive experiments were performed in the FMF water channel to investigate the rise of buoyant puffs through a neutral environment capped by a stable layer (Thompson and Snyder, 1996a; 1996b). These initial experiments were motivated by the need to develop better models for predicting the transport and fate of pollutants released during the open burning and open detonation (OBOD.) of obsolete munitions at Department of Defense and Department of Energy facilities. Since OBOD generates substantial quantities of noxious gases, facilities using this method must demonstrate that such releases will not pose a risk to human health or result in environmental degradation. Appropriate dispersion models for such releases must provide physically realistic estimates of pollutant distribution, including dosage, surface deposition, and estimates of peak ground-level concentrations for averaging times ranging from a few minutes to an hour. During FY-1997, this modeling effort was extended to include an examination of the rise of buoyant puffs through a convective boundary layer (CBL). These laboratory experiments are the first on buoyant puff dispersion in the CBL and are particularly important for model development in view of the difficulty of obtaining statistically stable field measurements in the CBL.

The CBL is the dominant form of the planetary boundary layer in weak-gradient high pressure areas where subsidence dries the air, allowing for strong surface heating. The strong surface heating, in turn, generates turbulent eddies that are *capped* by the overlying subsidence inversion. As long as the wind remains light, these buoyancy-generated eddies are the primary source of turbulence in this *mixed* layer, which is characterized its depth z_i and the convective velocity scale, w_*.

During an open detonation or explosion under conditions where convection is dominant, the sudden release of heat generates an essentially instantaneous puff of buoyant material. This puff rises through the CBL, spreading under the action of the ambient turbulence until its buoyancy is greatly diluted and/or it reaches the top of the CBL, where vertical motion is strongly inhibited by the inversion. The greater the amount of material burned or exploded, the greater the amount of heat released and, hence, the more buoyant the ensuing puff. Strongly buoyant puffs rise quickly to the base of the inversion, minimizing the opportunity for initial dispersion in the mixed layer and resulting in most of the puff material being spread laterally at the base of the inversion, subsequently fumigating downward to the surface as the material is entrained into the mixed layer. Weakly buoyant puffs rise more slowly, offering the convective turbulence ample time to mix the plume material as it rises. Very weakly buoyant puffs will quickly become mixed uniformly through the vertical extent of the CBL.

In the convection tank, buoyant puffs were simulated by using a mixture of water, methyl alcohol, and fluorescent dye to obtain a desired puff buoyancy. Three mixtures were used, representing weak, moderate, and strongly buoyant puffs, roughly comparable to detonations of 1.5, 6, and 24 tons of obsolete ordnance. The instantaneous release was simulated by a small cylindrical container with sliding top and bottom. The tank was initially stratified to produce an elevated inversion similar to that which typically exists above the fair-weather CBL. Convection was then initiated by heating the floor of the tank with electrical heaters. After the simulated CBL was established, the source cylinder was moved into place near the center of the tank and just above the surface. The top and bottom covers of the source cylinder were then quickly slid aside, releasing the dye mixture. As the puff began to rise and spread, Centerplane cross sections of the puff were obtained by illuminating the puff with a sheet of light from an argon-ion laser. The laser light induced fluorescence in the plume in proportion to the dye concentration, and the resulting fluorescence was recorded by a video camera and subsequently converted to dye concentration. Measurements were made for times up to 4t*, where $t^*=z_i/w_*$ is the convective time scale.

Because of the inherent variability of puff dispersion in the CBL, an ensemble of experiments is typically required in order to obtain stable plume statistics for each puff buoyancy. Automation of the entire measurement process allowed an ensemble of 33 realizations to be measured under as near identical conditions as possible. Figure 2 shows typical results obtained at t=0.5t* from the moderate-buoyancy (6-ton detonation) experiment for 4 realizations along with the ensemble average of all 33 realizations. Figure 3 shows the dimensionless mean puff height as a function of dimensionless time obtained from ensembles for the three puff buoyancies, indicated by the non-dimensional buoyancy, F_{T*}. Note that, even for the weakest buoyancy, there is substantial lofting of the puff near t/t*=1. The solid lines are model results (Weil *et al.*, 1996) and are seen to agree rather well with the data in the initial rise region.

2.4.10 Doppler Sodar Comparison Studies

This study is a compilation of the results obtained from various Doppler sodar comparison experiments conducted over the last 20 years (Crescenti, 1997). These studies attempted to quantify the uncertainties in sodar-derived values of the horizontal wind speed, wind direction, standard deviation of the vertical wind speed, σ_w, and standard deviation of the horizontal wind direction, σ_θ. Doppler sodar configurations examined in these studies included

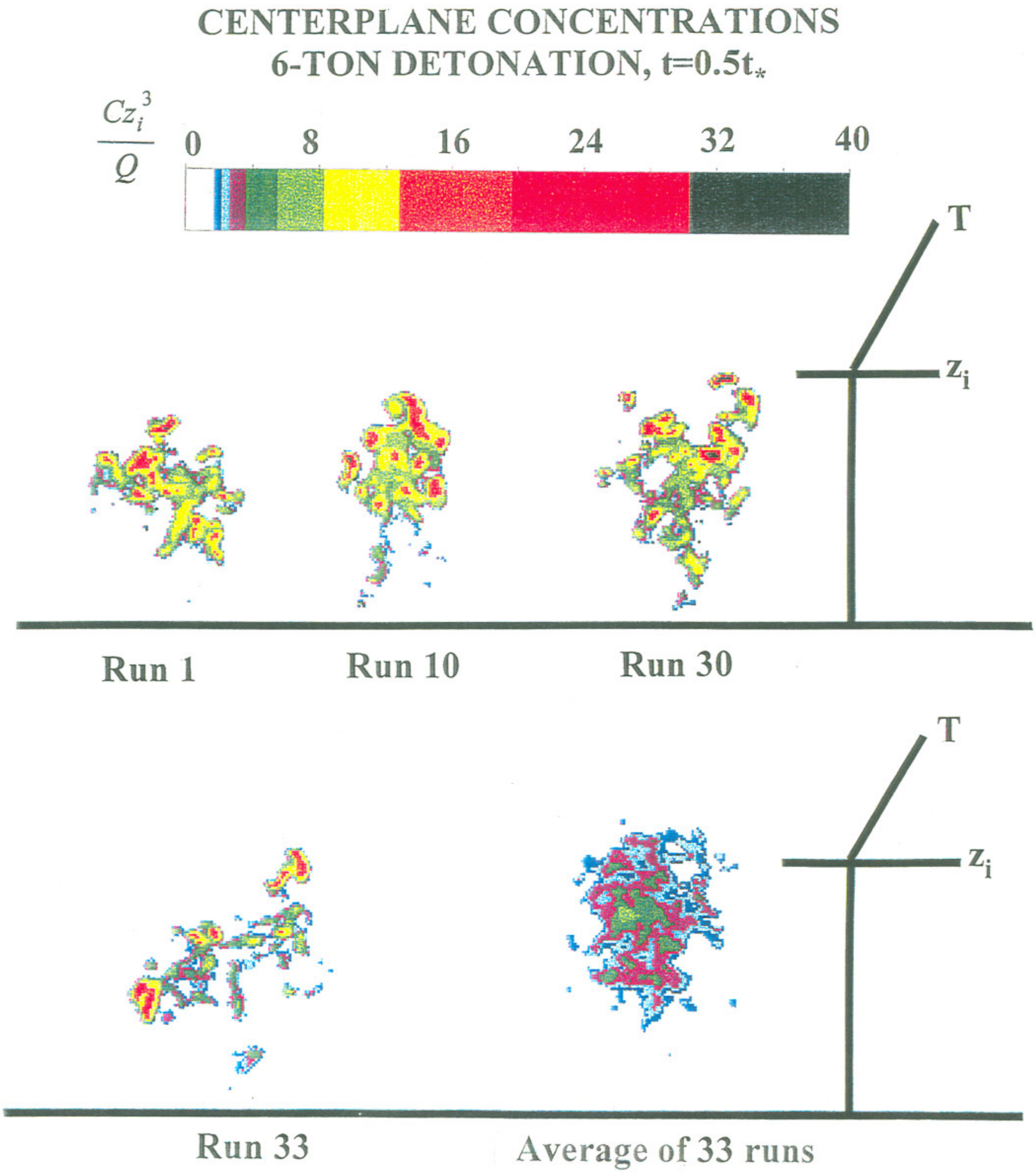

Figure 2. Centerplane concentrations for 4 realizations of a 6-ton detonation contrasted with the ensemble average of 33 realizations.

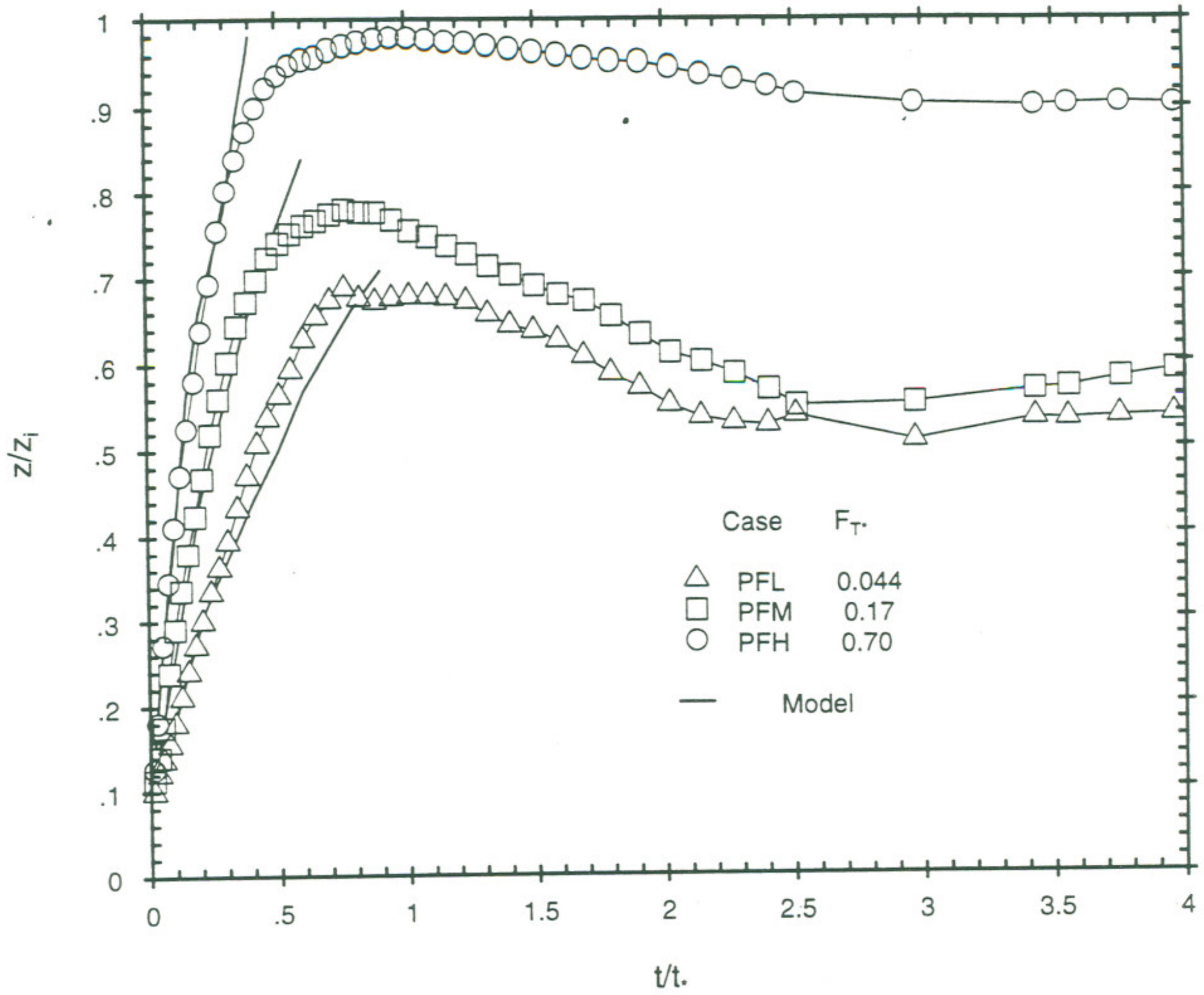

Figure 3. Dimensionless mean puff height as a function of dimensionless time for weak (PFL), moderate (PFM) and strongly (PFH) buoyant puff releases, corresponding to detonation of 1.5, 6, and 24 tons of obsolete ordnance.

bistatic, monostatic, and phased-array. In most cases, reference measurements used for comparison were made by tower-based *in situ* sensors. Many investigators have used such simple linear regressions and other statistical measures as the correlation coefficient, bias (mean difference), comparability (root-mean-square difference), and precision (standard deviation) in an attempt to quantify those errors. The sodar-derived wind speed and wind direction are highly correlated against reference measurements (~0.92) with a precision of 1.06 m s^{-1} and 21.5°, respectively, for the entire data set. Correlations of sodar-derived values of σ_w were not quite as good (~0.81) with an average precision of 0.18 m s^{-1}. Past studies have shown that σ_w accuracies vary significantly from day (convective conditions) to night (stable conditions). Very few data values were available for σ_θ, which had a poor correlation of 0.57 and a precision of 10.7°. The conclusions from many of these studies have shown that Doppler sodars can accurately obtain the mean wind speed and wind direction. Values of σ_w have larger uncertainties while estimates of σ_θ have errors that are considered unacceptable for any practical use. Much of the observed scatter in sodar wind measurements can be attributed to a number of factors. These include, but are not limited to, instrument configuration, spatiotemporal variability, noise, and processing techniques.

2.4.11 Degradation Of Doppler Sodar Performance Due To Noise

Selecting a site for a Doppler sodar is perhaps the greatest challenge to ensure acquisition of reliable wind profiles. The limiting factor in wind velocity determination is usually the amount of environmental noise included with the backscattered signal. Noise sources can be classified as active or passive and as broad-band or narrow-band. Artificial sources include highway traffic, heavy machinery, industrial facilities, power plants, and aircraft. Natural sources include insects and birds. Rainfall and wind-generated noise resulting from flow through and/or around various structures also lead to data degradation. A carefully designed noise survey that covers diurnal and weekly patterns can aid in the decision for site selection. A qualitative survey should identify all active noise sources. A quantitative survey can be conducted with minimal cost and effort with the use of a simple noise meter. A portable laptop computer, a sound card, a microphone, and spectral analysis software can be used to identify the amplitudes and frequencies of the background noise. In addition, a site should be relatively clear of obstacles that could act as fixed-echo reflectors. The antennae tilted at an oblique angle from the vertical should be pointed in a direction away from those objects. Some commercially available sodars have algorithms that identify and remove backscattered frequencies with zero Doppler shift that remain constant in space and over time.

Selection of acoustic transmit frequency has implications on the maximum sounding range and the potential for noise interference. Because molecular and excess attenuation are much smaller for lower acoustic frequencies, greater sounding ranges can be achieved. However, most ambient background noise tends to have lower frequencies, thus the potential for noise interference increases. More side lobe energy exists for lower frequencies. If unshielded, these side lobes can be an irritating source of noise pollution. Higher frequency acoustic pulses have an increased antenna directivity and smaller side lobes at angles of 70° to 90° from the main beam. Sodars that use higher frequencies have a reduced response to ambient noise because of the increased side lobe suppression and also because of the characteristic spectrum of ambient noise, which decreases in amplitude as frequency increases. However, the biggest disadvantage of using higher acoustic frequencies is the very limited sounding range due to the strong effects of molecular attenuation.

A significant reduction in both radiated and received side lobe acoustic energy can be achieved with anechoic shields. Past studies have demonstrated that these shields significantly reduce the amount of ambient noise being received by the sodar while at the same time reducing the transmitted side lobe energy that is a source of noise pollution. Using a sufficiently large isolation radius also ensures that the sodar will not be a source of irritation to residential neighborhoods.

2.5 Air Policy Support Branch

The Air Policy Support Branch supports activities of the EPA Office of Air Quality Planning and Standards (OAQPS). The Branch responsibilities include evaluating, modifying, and improving atmospheric dispersion and related models to ensure adequacy, appropriateness, and consistency with established scientific principles and Agency policy; preparing guidance on applying and evaluating models and simulation techniques that are used to assess, develop, or revise national, regional, state, and local air pollution control strategies for attainment and maintenance of National Ambient Air Quality Standards (NAAQS); and providing meteorological assistance and consultation to support OAQPS in developing and enforcing Federal regulations and standards and assisting the EPA Regional Offices.

2.5.1 Modeling Studies

2.5.1.1 Ozone Transport Assessment Group

The EPA and Environmental Council of States established the Ozone Transport Assessment Group (OTAG) in 1995 to develop strategies that address the interstate transport of smog-forming pollutants and make recommendations for reducing nitrogen oxide emissions and other major sources of smog-forming pollutants. OTAG includes the 37 eastern-most States and the District of Columbia. The technical aspects of OTAG included (a) extensive modeling analyses to assess the relative benefits of alternative regional strategies, (b) development of emissions inventories of man-made and natural emissions as well as meteorological databases to drive model simulations, and (c) analyses of ambient measurements to characterize the spatial and temporal extent of high ozone concentrations and transport.

During FY-1997, the *OTAG EPA Modeling Centers* (http://www.iceis.mcnc.org/OTAGDC/modeling_centers.html) simulated over 50 emissions scenarios to look at the effects of geographic variations in control strategies; previous *rounds* of OTAG modeling looked at controls applied throughout the eastern United States modeling domain. This work included developing emission inputs reflecting the controls in these scenarios; performing model simulations; and analyzing and interpreting the results in terms of strategy-relevant issues. The tasks were coordinated with the other Centers through weekly conference calls and bi-monthly meetings. Results were presented to the EPA management and OTAG Policy Group, comprised of the Environmental Commissioners from the 37 participating states.

The fundamental findings from the work are regional reductions in NO_x emissions would provide large reductions in ozone transport across the region; regional reductions in VOC emissions would provide relatively small reductions in ozone transport; emission reductions in a given portion of the region would provide the greatest benefit in that same area although there would be benefits in other *downwind* areas; and the spatial scale of upwind/downwind transport in the East is generally on the order of 150 to 500 miles. Based on these findings and other technical results, the Policy Group developed specific regional control strategy recommendations and provided them to EPA for regulatory action. Figure 4 provides an example of some of the findings. This figure displays the impacts on 1-hour ozone concentrations of applying fairly stringent controls on utilities in nine states: Alabama, Kentucky, Michigan, North Carolina, Ohio, South Carolina, Tennessee, Virginia, and West Virginia. The results indicate that the largest ozone reductions (14 ppb or more) are predicted within these States. However, impacts of 2 ppb or more are evident in other states as far downwind as the central parts of Maine.

2.5.1.2 Notice of Proposed Rulemaking

Section 110 (a) 2 (d) of the Clean Air Act requires States to control emissions that contribute to nonattainment of a NAAQS in another State. Once EPA makes a finding that a State contributes *significantly* to nonattainment in another State, the contributing State must develop a State Implementation Plan (SIP) committing to adopt and implement controls to mitigate this contribution. Because OTAG modeling results indicate that emissions in many eastern States may contribute to ozone nonattainment in other States in the region, EPA proceeded to develop the technical information and arguments necessary for a section 110 *SIP call* to a number of States. This included (a) analyses of the OTAG modeling data to quantify the contributions from each State to nonattainment of the ozone NAAQS in other States, and (b) a *weight-of-evidence* analysis to determine, based on a number of pieces of technical information, which states are contributing *significantly* to nonattainment in other states.

The information considered in making the *significance* determination included air quality model simulations, the magnitude and spatial density of man-made nitrogen oxide emissions, trajectory analyses of source-receptor relationships, and analyses of ambient ozone measurements. The results indicate that the following States and the District of Columbia make a significant contribution to nonattainment of the ozone NAAQS in other states: Alabama, Connecticut, Delaware, District of Columbia, Georgia, Illinois, Indiana, Kentucky, Maryland, Massachusetts, Michigan, Missouri, New Jersey, New York, North Carolina, Ohio, Pennsylvania, Rhode Island, South Carolina, Tennessee, Virginia, West Virginia, and Wisconsin. EPA intends to issue these findings in the Federal Register as a Notice of Proposed Rulemaking in early November 1998.

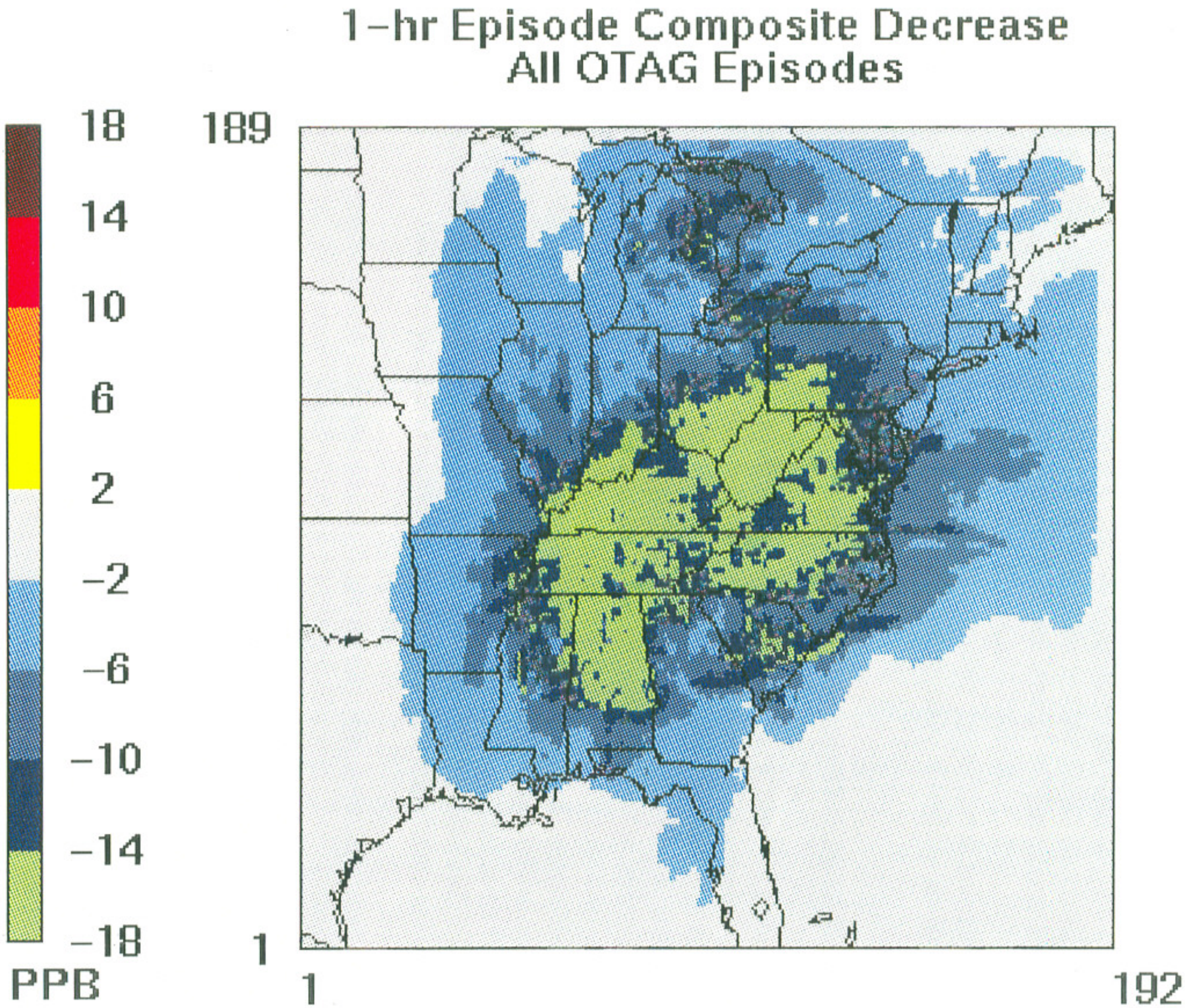

Figure 4. Impact of utility NO_x controls in nine midwest and southeast States.

2.5.1.3 AMS/EPA Regulatory Model Improvement Committee

In 1991, the AMS and EPA initiated a formal collaboration with the goal of modifying applied dispersion models to include scientific advances in understanding the planetary boundary layer. A working group, AERMIC, was formed to facilitate this collaborative effort. The initial focus of the AERMIC group has been on applied models designed for estimating near-field impacts from industrial source types. The primary products of the ongoing AERMIC development work are the AERMOD, the AERMIC plume dispersion model; AERMET, the meteorological preprocessor; and AERMAP, the terrain preprocessor. Previous papers (Perry *et al.*, 1994; Cimorelli *et al.*, 1996) described the general structure and the technical basis of AERMOD, AERMET, and AERMAP, and revisions made during the development of the modeling system. Lee *et al.* (1996) and Lee and Irwin (1995) reported evaluation studies on earlier draft versions of the AERMOD system. An evaluation study was completed of this version of the AERMOD system.

AERMOD is being developed as a regulatory tool; thus, it is intended to handle a variety of pollutant source types (i.e., surface and buoyant elevated sources) in a wide variety of modeling situations (i.e., rural, urban, flat terrain, and complex terrain). With this in mind, data from five diverse field studies were selected for the developmental evaluation: the Prairie Grass near-surface SO_2 releases (Barad, 1958; Haugen, 1959); the Kincaid SF_6 and SO_2 tall stack releases (Liu and Moore, 1984; Bowne *et al.*, 1983); the Indianapolis SF_6 medium-tall stack releases (Murray and Bowne, 1988); and the Lovett Power Plant SO_2 medium-tall stack in complex terrain releases (Paumier *et al.*, 1992).

The developmental evaluation is diagnostic as well as descriptive of the model performance. Highlights of some of the evaluation results for this model are presented in Figure 5 using residual plots and quantile-quantile (Q-Q) plots. All concentrations are normalized by emission rate. For the intensive data sets (Prairie Grass, Kincaid SF_6, and Indianapolis), concentration residuals of the form $<C_p/C_o>$ were plotted as a function of downwind distance for each of two stabilities (convective and stable). Here C_o is the maximum observed concentration and C_p the maximum predicted on an arc at a given time. The brackets, $<C_p/C_o>$, indicate the median of the ratio. These data were paired in time and downwind distance. For the other data sets (Kincaid SO_2 and Lovett), where the sampler array was not sufficiently dense to arrange the data in arcs, the concentration measures used were the maximum observed and predicted over the entire receptor array at a given time. For these, residual plots by distance are not meaningful.

The quantile-quantile (Q-Q) plots are simple ranked pairings of predicted and observed concentrations, such that any given quantile of the predicted concentration is plotted against the same quantile of the observed concentration. A solid line was added to the Q-Q plots to indicate an unbiased prediction and two dotted lines were added to indicate a factor of two under- and over-prediction. The Q-Q plot is an effective method for comparing the frequency distributions of two data sets.

In the six-panel Figure 5, the Q-Q and residual comparisons are shown for the daytime convective releases at Prairie Grass, Kincaid, and Indianapolis. Comparisons are shown for both AERMOD and the Industrial Source Complex Short-Term (ISCST3) dispersion model (U.S. Environmental Protection Agency, 1995a; 1995b). The residual plot for the Prairie Grass data (Figure 5a) and the Q-Q plot for the same data (Figure 5b) show that AERMOD has avoided the over prediction shown by ISCST3. This reduced bias appears to be due to the ability of AERMOD to vary dispersion with height. AERMOD shows somewhat improved behavior over ISCST3 using the Kincaid SF_6 data set. Although AERMOD shows a consistent under prediction of about a factor of two for all distances in the residual plot (Figure 5c), this does not seem to have carried over to the high end of the frequency distribution (Figure 5d). Note, however, that AERMOD predicts the 50^{th} percentile point within about a factor of two, while ISCST3 predicts about an order of magnitude low at that point. This has been characteristic of ISCST3 and other Gaussian models in several model evaluation studies using power plant data. The Indianapolis data set provides a database on which to test the behavior of the models in an urban setting. Both models predict reasonably well under convective conditions (Figure 5e), although AERMOD is more consistent in providing nearly unbiased predictions. The Q-Q plots (Figure 5f) confirm this.

AERMOD shows noticeably less bias and appears to show more consistent behavior than the regulatory model, ISCST3, for all of the databases tested. This evaluation exercise, using these data sets, was performed several times during the development of the model. An independent evaluation is in progress, using additional data sets to provide confirmation of these conclusions

2.5.1.4 Draft Standard Practice for Statistical Evaluation of Plume Dispersion Models

Within the American Society for Testing and Materials (ASTM), there is a Standard Practice (Z6849Z) drafted by ASMD staff. The draft practice describes an objective statistical procedure for comparing air quality simulation modeling results with tracer field data. The draft practice is limited to local scale (first tens of kilometers) transport and dispersion from isolated point sources in simple terrain situations. The practice describes how comparisons might be made of simulated centerline concentration values with observed concentrations from receptors near the observed center of mass along sampling arcs. A major consideration in developing the statistical comparison measures was that differences seen in the comparison of model predictions and observations of atmospheric air concentrations may largely reflect an inherent uncertainty caused by the stochastic nature of turbulence within the atmosphere. This component of variance was considered inherent, because it cannot be reduced significantly by improving the physics of the air quality models. Most operational dispersion models employ characterizations of the ensemble average result to be expected of the various processes affecting the fate of pollutants released into the atmosphere. Therefore, a strategy was developed to stratify the evaluation data into ensembles, and to evaluate model performance on the ability of the model to replicate

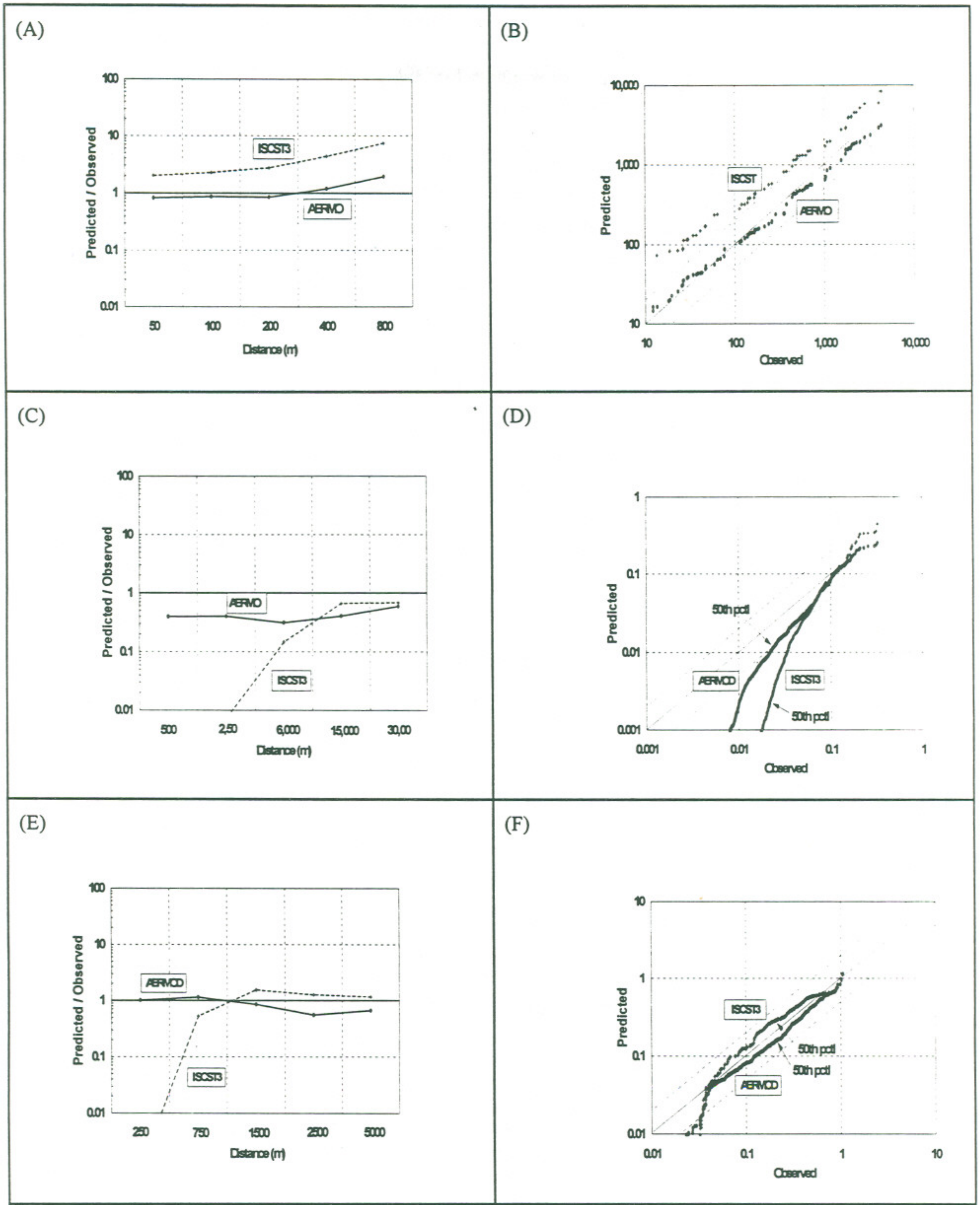

Figure 5. Median ratio of the residual versus distance plots, and Q-Q plots of C/Q for AERMOD and ISCST3 for (A,B) Prairie Grass, (C,D) Kincaid, and (E,F) Indianapolis.

without bias such ensemble characteristics as the ensemble maximum, average lateral extent, or average crosswind integrated concentration. An estimate of an ensemble can be developed from a set of experiments having very similar meteorological conditions, where the ensemble refers to the infinite population of all possible realizations.

The draft practice is being reviewed using tracer field data from the Project Prairie Grass and Kincaid experiments. It is concluded that receptor positions providing representative observations of the centerline concentration maximum are the receptor positions relative to the plume center of mass and can be defined using a lateral dispersion derived for the regime. This should be robust to counter slight inadequacies in sampling. The average of the centerline maximum concentration values and the bootstrap-derived standard deviation were seen to be well behaved, versus results obtained for individual percentile values of the frequency distribution of centerline concentration values. It was concluded that the average is a better statistic to use in the evaluation procedures in comparison to the draft's suggestion to use percentile values. A numerical experiment was developed to assess how many bootstrap samples may be needed. The results suggested bootstrap sample sizes ranging from 70 to 400. In developing the bootstrap samples, two replicate sampling methods were tested: sample of one versus sample of a pair. This was done to assess whether observations from adjacent receptors could be treated as independent. Significant differences in the results obtained were observed. Further testing is needed to assess the effect of these differences when using these sampling techniques within the context of the draft ASTM practice to assess model performance.

Future actions include constructing software that others can use to test the practice, and testing how results obtained from each regime can usefully be summarized over all regimes. Once this is accomplished, how well the procedures assess differences between models will be tested. Once these tests are completed, the practice can be redrafted and resubmitted for ASTM committee review and balloting.

2.5.2 Modeling Guidance

2.5.2.1 Support Center for Regulatory Air Models

During FY-1997, several activities were accomplished on the Support Center for Regulatory Air Models (SCRAM) Bulletin Board System and SCRAM web site. The most significant activity was a switch from maintaining both an electronic bulletin board system and Internet web site to only the SCRAM web site. The SCRAM web site is located on the central EPA web server at URL <http://www.epa.gov/scram001>. In addition, three new areas were added to the SCRAM menu structure. They are (1) Supporting Reports, under the Modeling Reports/Guidance section; (2) Non-EPA models, under the Air Quality Models section of the Models area; and (3) a Frequently Asked Questions section, under the Public Forum area. State environmental agency contact *hot links* were provided for quick and convenient access to State

EPA contacts. Links to State environmental web sites and other related information were also established.

2.5.2.2 National Speciality Workshop on Technical Tools for Air Toxics Assessment

On June 17-19, 1997, the Branch conducted the First National Speciality Workshop on Technical Tools for Air Toxics Assessment. This workshop was held in Raleigh, North Carolina, and designed for senior environmental scientists, engineers, chemists, meteorologists, and toxicologists with experience in toxic and risk assessments. The workshop was attended by 53 individuals: 35 from state offices, 9 from EPA regional offices, and 9 from county and other offices. In preparation for the workshop, six panels were organized on such selected topics as air toxics emissions inventories, dispersion modeling, exposure assessment techniques, etc. These panels conducted telephone conference calls during May and June of 1997, drafting discussions on the adequacy of tools, where deficiencies exist, and possible solutions. Following invited presentations from experts on these six focus topics, the panels reconvened, revised and extended their discussion papers, and drafted final recommendations. The conclusions and recommendations are being summarized in a technical report that will be presented to senior EPA management to aid in directing the future development of air toxics assessment tools.

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APPENDIX A: ACRONYMS, ABBREVIATIONS, AND DEFINITIONS

ACM	Asymmetric Convective Model
ADOM	Acid Deposition and Oxidant Model
AERMAP	AERMOD terrain height processor
AERMET	AERMOD meteorological processor
AERMIC	AMS/EPA Regulatory Model Improvement Committee
AERMOD	AMS/EPA regulatory model
AGDRIFT	AGricultural spray DRIFT model
AMS	American Meteorological Society
AMV	Air Management Version of Models-3 Air Quality Model
ARL	Air Resources Laboratory
ASMD	Atmospheric Sciences Modeling Division
ASTM	American Society for Testing and Materials
BASC	Board on Atmospheric Sciences and Climate (NAS/NRC)
BCON	Boundary CONditions processor
BEIS	Biogenic Emissions Inventory System
CAA	Clean Air Act of 1970
CAAA	Clean Air Act Amendments of 1990
CALPUFF	CALifornia PUFF model
CAMRAQ	Consortium for Advanced Modeling of Regional Air Quality
CASTNet	Clean Air Status and Trends Network
CB-IV	Carbon Bond IV
CBL	Convective Boundary Layer
CD-ROM	Compact Disk - Read Only Memory
CMAQ	Community Multiscale Air Quality model
CRADA	Cooperative Research And Development Agreement
CREME	Cooperative REgional Model Evaluation project
CTM	Chemistry-Transport Model
DOE	Department of Energy
ECIP	Emissions-Chemistry Interface Processor
EDC	Endocrine Disrupting Chemical
EDSS/MAQSIP	Environmental Decision Support System/Multiscale Air Quality Simulation Platform
EMEP	European Monitoring and Evaluation Program
EPA	Environmental Protection Agency
EUROTRAC	EUROpean experiment on the TRAnsport and transformation of trace atmospheric Constituents
FACA	Federal Advisory Committee Act
FAQ	Frequently Asked Questions
FCMSSR	Federal Committee for Meteorological Services and Supporting Research

FDDA	Four-Dimensional Data-Assimilation
FMF	Fluid Modeling Facility (EPA)
FY	Fiscal Year
GEMAP	Geocoded Emission Modeling And Projection
GIS	Geographical Information System
HAPEM	Hazardous Air Pollutant Exposure Model
HAPEM-MS	Hazardous Air Pollutant Exposure Model - Mobile Sources
HPCC	High Performance Computing and Communications program
ICMSSR	Interdepartmental Committee for Meteorological Services and Supporting Research
ICON	Initial CONditions processor
I/O API	Input/Output Applications Program Interface
IOV	Initial Operating Version
ISC3	Industrial Source Complex model - Version 3
ISCST	Industrial Source Complex - Short Term model
ITM	International Technical Meeting
IWAQM	Interagency Work Group on Air Quality Modeling
JPROC	Photolysis rate processor
LMMB	Lake Michigan Mass Balance project
LRPM	Lagrangian Reactive Plume Model
MCIP	Meteorology-Chemistry Interface Processor
MEND-TOX	Multimedia hybrid compartmental model
MEPPS	Models-3 Emission Processing and Projection System
MEPRO	Models-3 Emission PROjection processor
MLM	MultiLayer inferential dry deposition Model
MM4/5	Mesoscale Meteorological Model - Version 4/Version 5
Models-3	Third generation air quality modeling system
MPP	Massive Parallel Processor
MSC-W	Modeling Synthesizer Center - West
NAAQS	National Ambient Air Quality Standards
NARSTO	North American Research Strategy for Tropospheric Ozone
NARSTO-NE	NARSTO-NorthEast
NAS	National Academy of Sciences
NASA	National Aeronautical and Space Administration
NATO/CCMS	North Atlantic Treaty Organization Committee on Challenges of Modern Society
NCAR	National Center for Atmospheric Research
NCSU	North Carolina State University
NDDN	National Dry Deposition Network
NERL	National Exposure Research Laboratory (EPA)
NESCAUM	NorthEast States for Coordinated Air Use Management
NetCDFI/OAPI	Models-3 format
NEXRAD VAD	NEXt generation weather RADar Velocity Azimuth Display

NOAA	National Oceanic and Atmospheric Administration
NOVA	Natural emissions of Oxidant precursors: VAlidation of technique
NRC	National Research Council
NSF	National Science Foundation
NSTC	National Science and Technology Council
NWS	National Weather Service
OAQPS	Office of Air Quality Planning and Standards (EPA)
OBOD	Open Burning/Open Detonation
ORD	Office of Research and Development (EPA)
OTAG	Ozone Transport Assessment Group
PAH	Polycyclic Aeromatic Hydrocarbon
PAMS	Photochemical Assessment Monitoring Stations
PBL	Planetary Boundary Layer
PC	Personal Computer
PCA	Principal Component Analysis
PCB	Polychlorobiphenyl
PCDD	PolyChlorinated Dibenzo-p-Dioxin
PCDF	PolyChlorinated DibenzoFuran
PDM	Plume Dynamics Model
PM	Particulate Matter
pNEM	probabilistic NAAQS Exposure Model
PSU	Pennsylvania State University
Q-Q	Quantile-Quantile plot
QA	Quality Assurance
QC	Quality Control
RADM	Regional Acid Deposition Model
RELMAP	REgional Lagrangian Model of Air Pollution
RPM	Regional Particulate Model
SAPRC	State Air Pollution Control Research Center
SASWG	Standing Air Simulation Work Group
SCRAM BBS	Support Center for Regulatory Air quality Models Bulletin Board System
SDTF	Spray Drift Task Force
SIP	State Implementation Plan
SMRAQ	Seasonal Modeling of Regional Air Quality
SOP	Standard Operating Procedure
SOS	Southern Oxidant Study
SVOC	Semi-Volatile Organic Compound
TEQ	Toxic EQuivalent
TOMS	Total Ozone Mapping Spectrometer
UAM-V	Urban Airshed Model - Variable grid
URL	Uniform Resource Locator
USGS	U.S. Geological Survey