NOAA Technical Memorandum ERL ARL-231

FISCAL YEAR 1998 SUMMARY REPORT OF THE NOAA ATMOSPHERIC SCIENCES MODELING DIVISION TO THE U.S. ENVIRONMENTAL PROTECTION AGENCY

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(Editors)

Atmospheric Sciences Modeling Division
Research Triangle Park, North Carolina

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PREFACE

This document summarizes the Fiscal Year 1998 research and operational activities of the Atmospheric Sciences Modeling Division (ASMD), Air Resources Laboratory (ARL), working under Interagency Agreements EPA DW13938483, 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 (NERL) 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 (OAQPS). 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 G. 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 or email: francis.schiermeier@noaa.gov.

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ABSTRACT. During Fiscal Year 1998, the Atmospheric Sciences Modeling Division provided meteorological and modeling assistance 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 and results were the publication and distribution of Models-3/Community Multiscale Air Quality system; estimation of the nitrogen deposition to Chesapeake Bay; continued evaluation and application of air quality models for mercury, dioxin, and heavy metals; continued conduct of deposition velocity field studies over various major categories of land-use; conduct of the Ozark Isoprene Experiment to investigate biogenic isoprene emissions; analysis and modeling of dust resuspension data; continued study of buoyant puff dispersion in the convective boundary layer; and development of a standard practice for an objective statistical procedure for comparing air quality model outputs with field data.

1. INTRODUCTION

In Fiscal Year 1998, 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 23rd NATO/CCMS International Technical Meeting held in Varna, Bulgaria, from September 28 to October 2, 1998; the proceedings will be published by Plenum Press as were the proceedings from the 22nd ITM held in Clermont-Ferrand, France, during June 1997 (*Air Pollution Modeling and Its Application XII*, 1998). The NATO/CCMS Scientific Committee selected Boulder, Colorado, as the site for the 24th (Millennium) International Technical Meeting to be held during May 15-19, 2000.

2.1.1.2 Regional/Transboundary Transport of Air Pollution

The Division Director serves as the United States representative on the International Oversight Committee for the NATO/CCMS Pilot Study on Regional/Transboundary Transport of Air Pollution. The aim of the pilot study, sponsored by Greece and approved by NATO in March 1998, is to improve the exchange of views and experience among participating countries in the field of regional/transboundary transport of air pollution. The initial organizing meeting was held in Varna, Bulgaria, during September 1998 in association with the NATO/CCMS ITM. The framework for the pilot study is now being revised to reflect inputs of the meeting participants.

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-1998, 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-1998. The annual Working Group meeting at the Main Geophysical Observatory in St. Petersburg, Russia, was held during June 1998.

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, 1998). 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. BASC members recently completed a landmark publication that sets forth recommendations intended to strengthen atmospheric science and services, and to enhance benefits to the nation (National Research Council, 1998). This report is intended for those who share the responsibility for maintaining the pace of improvement in the atmospheric sciences, including leaders and policy makers in the public sector; legislators and executives of the relevant federal agencies; decision makers in the private sector of the atmospheric sciences; and university departments that include atmospheric science.

2.1.6 Committee on Computing, Information, and Communications

The Division Director served 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, until its dissolution in FY-1998. The mission of the Committee was 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). The Committee also served as the National Coordination Office for the High Performance Computing and Communications (HPCC) program in which the Division has a major role. The functions of this Committee were transferred to the NSTC Committee on Technology.

2.1.7 Standing Air Simulation Work Group

The Division Director serves as the EPA Office of Research and Development 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 a 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 participated 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, the AMS reviewed existing entries in the 1959 edition of the Glossary and revised and updated 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.

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 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 prospective assessment of the benefits and costs of the Clean Air Act Amendments (CAAA) of 1990, assuming full implementation. Work in FY-1998 emphasized development of revised assessment emission 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) to link atmospheric deposition with watershed models, and in dealing with the potential role 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-1998 focused on creation of RADM/RPM predictions at 20-km resolution of the estimated effects of 1990 CAAA controls as defined by the 812 Prospective Study on the nitrogen deposition to the Chesapeake watershed basins and to the Bay. The FY-1998 work was in support of the 1997 Chesapeake Bay Agreement Re-evaluation.

2.1.12 Megacity Impact on Regional and Global Environments

A Division scientist was asked to serve as a member of the External Advisory Panel on the Megacity Impact on Regional and Global Environments (MIRAGE) project at the National Center for Atmospheric Research (NCAR). The MIRAGE project is expected to become an official NCAR program in the next year and is jointly directed by the NCAR Research Aviation Facility and the Atmospheric Chemistry Division. The advisory panel is composed of 11 scientists from academia and federal agencies, who are presently involved in urban environmental research. The panel is expected to review the overall program inception, review progress of various studies, and participate in the planning of field experiments. The objective of the project is to study how megacities affect the environment on local, regional, and global scales. The study will be carried out through field study data collection to better understand the physical processes and use of models to help diagnose how human activities in megacities produce their impacts. The initial focus will be on two megacities, Mexico City, Mexico, and Beijing, People's Republic of China. In FY-1998, the panel met to review the overall development of the project and comment on project structure and complementarity with other research programs in the universities and agencies.

2.1.13 North American Research Strategy for Tropospheric Ozone

The North American Research Strategy for Tropospheric Ozone (NARSTO) program was established in FY-1995 to address ozone research and coordinate 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. The Subcommittee on Air Quality Research of the Committee on Environment and Natural Resources within NSTC facilitates the coordination of NARSTO Federal research activities. Four technical teams were established: Analysis and Assessment; Observations; Modeling and Chemistry; and Emissions. A major goal of NARSTO is to produce a scientific assessment of the state of tropospheric ozone science. A draft of the 1998 NARSTO scientific assessment was written. A Division scientist was chosen to co-author 1 of the 15 critical review papers that were commissioned to provide technical background to the NARSTO assessment group. During FY-1998, a revised draft of the critical review paper on modeling and evaluation of advanced models was completed for journal review.

During FY-1998, the NARSTO Executive Assembly considered expanding its activities to include fine-particle research under its purview. It decided to include fine-particle research activities. Once the organization made this decision, the question became what to call the *new* NARSTO. Although the preference is for program names or acronyms to describe the program's activities, the organization chose to retain the program name, NARSTO, as the organization's name.

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. Three planned workshops were held at the International Institute for Applied Systems Analysis in Laxenburg, Austria. Internal reviews were completed, and a draft monograph of the workshop discussions will be finished in FY-1999.

2.1.15 RADM Application Studies

Efforts during FY-1998 concentrated on completing several RADM application studies related to the 1997 Chesapeake Bay Agreement Re-evaluation and on analyzing RADM/RPM results for acidic deposition, fine particulate matter, and visibility in support of the Regulatory Impact Statement for the EPA NO_x SIP (State Implementation Plan) Call. 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. A new estimate of the airshed affecting the Bay was completed and is under review. Other EPA regional offices are requesting similar information.

In FY-1998, 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 completed during FY-1998 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 the nitrogen load to the Bay (U.S. Environmental Protection Agency, 1996). In FY-1998, in response to requests by the EPA Regional Offices 1, 2, 3, and 4 and EPA Great Waters Program, the number of source regions modeled by RADM was doubled to support definition of airsheds for coastal watersheds along the East and Gulf Coasts. The analyses to estimate the airsheds will continue into FY-1999. This work will be coordinated with the NOAA assessment of atmospheric deposition to coastal estuaries now underway.

In FY-1998, a new version of RADM was created that incorporates fine particle physics directly into the model for full dynamic coupling of all particulates involved in nitrogen deposition. The full coupling is required to account for ammonia deposition and partitioning of total ammonia into gaseous ammonia and particulate ammonium. The new model, still undergoing testing, will be able to address deposition of both oxidized and reduced nitrogen to the eastern United States and will allow the extension of the estimation of airsheds to ammonia.

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 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 (HyperText Markup Language) documents of the FY-1997 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 (CAA) provides a societal mandate to assess and manage air pollution levels to protect human health and the environment. 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 dioxide. 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. 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 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 air quality modeling component within Models-3 is called the Community Multiscale Air Quality (CMAQ) system. The Models-3/CMAQ system is designed as a multipollutant, multiscale Eulerian 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.

The first Models-3/CMAQ version was released in June 1998. It contains options representing different model descriptions for some of the major science processes. Among the processes included are a choice of two gas-phase chemistry mechanisms, RADM2 and Carbon Bond IV (CB-IV); two numerical solvers for the chemistry mechanisms, a vectorized Gear (SMVGEAR) solver and a quasi-steady state approximation (QSSA) solver; three options for horizontal and vertical advection schemes (piece-wise parabolic, Bott, and Yamartino-Blackman cubic schemes); a vertical diffusion routine based on eddy-diffusion theory; a modal approach aerosol algorithm for fine and coarse particulate matter predictions; a photolysis rate treatment; and an optional plume-in-grid method explicitly accounting for major elevated point sources. Process analysis routines are included to reveal individual effects of each science process on pollutant concentrations. In addition, an integrated reaction rate analysis routine reveals the detailed contribution of each gas-phase reaction. An aggregation technique for estimating annual average concentrations and deposition fields from a smaller sample of simulation runs was tested. The system does not yet include tools for systematic sensitivity and uncertainty analyses, although these are planned for future versions.

The first released version of Models-3/CMAQ was tested against a photochemical ozone episode in the northeastern United States for the period July 12–15, 1995. The preliminary results were very promising when compared with observed surface ozone concentrations. The model is not fully evaluated; rigorous evaluation efforts will continue through FY-1999. The user's guide was completed and released with the Models-3/CMAQ system (Atmospheric Modeling Division, 1998b). A complete science documentation for the CMAQ system is being prepared. The document will be available on the Models-3/CMAQ web site (http://www.epa.gov/asmdnerl/models3/CMAQ/index.html).

2.2.1.2 Development of the Community Multiscale Air Quality Modeling System

To simulate weather and air quality phenomena realistically, adaptation of a *one-atmosphere* perspective based mainly on *first principles* science descriptions of the atmospheric system is necessary. This perspective emphasizes the interactions among multiple air pollutants at different dynamic scales. For example, the description of processes critical to producing oxidants, acid and nutrient depositions, and fine particles are too closely related to be treated separately. Proper modeling of these air pollutants requires the broad range of temporal and spatial scales of multipollutant interactions be considered simultaneously. Another key aspect of the one-atmosphere perspective is the dynamic description of the atmosphere. Air quality modeling should be viewed as an integral part of atmospheric modeling and the governing equations and computational algorithms should be consistent and compatible.

As a priority, the CMAQ design adopted the one-atmosphere concept for air quality modeling. The Models-3/CMAQ air quality 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 environmental studies that 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 single model, but rather a modeling system that allows users to build customized CTMs for solving air quality problems.

Science submodels in the CMAQ system are the Mesoscale Model Version 5 (MM5), Models-3 Emissions Processing and Projection System (MEPPS), and the CMAQ chemical-transport model (CCTM). There are several interface processors that link other model input data to the CCTM. The Meteorology-Chemistry Interface Processor (MCIP) processes MM5 output to provide a complete set of meteorological data needed for CCTM. MCIP is designed in such a way that other meteorological models can be linked with minimal effort. Initial and boundary conditions are processed with the processors, ICON and BCON, respectively, and the Emissions-Chemistry Interface Processor (ECIP) combines area and point source emissions to generate three-dimensional gridded emission data for CCTM. 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 of taking into account the total ozone column (from TOMS satellite 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 within CMAQ.

With this version of CMAQ, the level of modularity is influenced by the way the science process codes are archived in the system. Here class is defined as a collection of different modules for a given science process. The science classes are identified with the grouping of the terms in the governing conservation equation. Nine science process classes are defined:

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

Here emissions are not defined as a separate science process, because they can be either a part of the vertical diffusion or the gas-phase chemical reaction process. In addition to nine science process modules, CMAQ includes routines computing photolysis rates and aerosol particle size-dependent dry deposition velocities.

2.2.1.3 Transport Processes within CMAQ

Governing set of equations in generalized coordinates.

In CMAQ, the governing equations for the dynamic processes are expressed in terms of the generalized coordinates to facilitate linkage of the CCTM to many different types of meteorological models. The generalized CCTM 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, Lambert, and Polar Stereographic projections. Vertical coordinates supported are height and pressure coordinates and terrain-following coordinates, such as time-dependent hydrostatic pressure (Sigma-p), time-independent reference hydrostatic pressure (Sigma-p_o), and time-independent scale height (Sigma-z) coordinates.

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 that the transport of pollutants in the atmospheric turbulent flow field can be described by means of differential equations and appropriate initial and boundary conditions. Numerical schemes for solving the transport equation must meet a convergence condition and correctly model the conservative, dissipative, and dispersive properties of the governing equation. Numerical algorithms for the advection and diffusion processes implemented in CMAQ satisfy these properties. In CMAQ

CCTM, advection is represented in flux form. Advection algorithms implemented are the Bott scheme based on a polynomial description of subgrid concentration, Yamartino-Blackman cubic scheme, and piecewise parabolic method. Atmospheric mixing processes are represented in Reynolds flux terms. Depending on the atmospheric stability conditions, local and non-local mixing schemes are used in CCTM. The eddy diffusion (K-Theory) is used for the vertical mixing. Other algorithms under study are a turbulent kinetic energy method, and nonlocal schemes, such as the Blackadar scheme, asymmetric convection model, and transilient turbulence method. The deposition flux is represented as the bottom boundary condition in the vertical mixing algorithms. An eddy diffusion algorithm is used for the horizontal diffusion process in the CCTM.

2.2.1.4 Aerosol and Visibility Module

The aerosol and visibility module was enhanced by the addition of new methods to estimate the reduction of visual range by the presence of particles. The first method uses an approximation to Mie extinction efficiency, which is valid for all size parameters (Evans and Fournier, 1990). This approximate expression is integrated over the lognormal size distribution using a Gauss-Hermite numerical quadrature procedure. If the same numerical quadrature procedure is used with the Mie expression for extinction efficiency, the resulting values for extinction coefficient at various values of the geometric mean diameter of the size distribution are very close. In some cases, for typical values of the real part of the refractive index, the curves are indistinguishable. A second method is that used in the Interagency Monitoring of PROtected Visual Environments (IMPROVE) program (Malm *et al.*, 1994). Both methods are implemented in CMAQ and provide hourly estimates of extinction coefficient and visual range expressed in deciview units (Pitchford and Malm, 1994).

2.2.1.5 Photolysis Rates

The photolysis rate model included in the 1998 release of Models-3/CMAQ uses a table-interpolation method. Photolysis rates are calculated for different times of day, latitudes, and heights. Photolysis rates for individual grid cells of CMAQ are then computed by interpolating values from the precomputed table. Refinements to the photolysis rate model continued during this year. A more robust method for calculating cloud transmissivity was added to the model. In addition, a method is being developed for linking the radiative transfer calculations with aerosol model predictions from CMAQ. Development and evaluation will continue into FY-1999.

2.2.1.6 Cloud Dynamics and Aqueous-Phase Chemistry Module

A cloud dynamics and chemistry module was incorporated into Models-3/CMAQ. The cloud module consists of a subgrid cloud model and a grid-resolved cloud model. The subgrid cloud model, which is based on the RADM cloud module (Dennis *et al.*, 1993; Chang *et al.*, 1990; Walcek and Taylor, 1986), simulates convective precipitating and non-precipitating clouds. The grid-resolved cloud model simulated clouds occupying the entire grid cell and resolved by the meteorological model. The implementation of the cloud model in CMAQ will be evaluated in FY-1999 using available wet deposition data sets.

A detailed grid-resolved cloud model is being developed. This model will include a microphysical submodel for following the evolution of the cloud (*i.e.*, cloud droplet formation, growth of rain droplets, and descent through model layers to the ground). It will also consider cloud lifetimes extending beyond the CMAQ synchronization time step, thus, maintaining the partition between gas- and aqueous-phase pollutants during the gas-phase chemistry calculations. Development and testing of this model will continue in FY-1999.

2.2.1.7 Plume-in-Grid Effort for Models-3

The plume-in-grid (PinG) algorithms were successfully incorporated and tested within the Models-3/CMAQ modeling system and were included in the first public release in June 1998. The PinG algorithms were designed to rectify overdilution of major elevated point source emissions within Eulerian grid models for air quality. The PinG approach provides a realistic scientific treatment of the subgrid scale physical and chemical processes affecting chemical species within pollutant plumes. An overview of the plume-in-grid technique implemented in CMAQ CCTM is described by Gillani *et al.* (1998).

The key modeling components used to simulate the relevant processes at the proper spatial and temporal scales for pollutant plumes include a PDM processor, designed to generate the position and physical dimensions of individual plume sections by simulating plume rise, vertical and horizontal plume growth, and plume transport (Godowitch *et al.*, 1995); and a Lagrangian reactive plume model, which serves as the PinG module by simulating the relevant processes of a moving array of attached cells representing a vertical plume cross-section. The data file generated by PDM, the CCTM three-dimensional concentration field, and meteorology data files are used to drive the PinG module during the subgrid scale phase for each pollutant plume. Test simulations were successfully performed with the RADM2 and CB-IV gas-phase chemistry mechanisms, the same chemistry mechanisms used with the CCTM grid cells. CCTM/PinG is being applied to case study days from the Southern Oxidant Study's Nashville 1995 field experiment in preparation for an evaluation of the model results against plume data. Results of the PinG evaluation are anticipated in FY-1999.

2.2.1.8 Meteorology-Chemistry Interface Processor

The Meteorology-Chemistry Interface Processor (MCIP) links such meteorological models as MM5 with CCTM, to provide a complete set of meteorological data needed for air quality simulation. Because most meteorological models are not built for air quality modeling purposes, MCIP deals with issues related to data format translation, conversion of units of parameters, diagnostic estimations of parameters not provided, extraction of data for appropriate window domains, and reconstruction of meteorological data on different grid and layer structures. To support the multiscale generalized coordinates implementation of CCTM, MCIP provides appropriate dynamic meteorological parameters to allow mass-consistent air quality computations. The implementation of MCIP links MM5 meteorological data to CCTM. Because its code has a streamlined modular computational structure, adapting the system to other meteorological model outputs only requires inclusion of a reader module and a description of the coordinates used in the model.

2.2.1.9 Aggregation Research for Models-3/CMAQ

In support of studies mandated by the 1990 CAAA, Models-3/CMAQ will be used to estimate deposition and air concentrations associated with specified levels of emissions. Assessment studies require CMAQ-based distributional estimates of ozone, acidic deposition, $PM_{2.5}$, as well as visibility, on seasonal and annual time frames. Unfortunately, it is too resource intensive to execute CMAQ over such extended time periods. Therefore, CMAQ must be executed for a finite number of episodes or events, which are selected to represent a variety of meteorological classes. A statistical procedure called aggregation, must then be applied to the outputs from CMAQ to derive the required seasonal and annual estimates.

The objective of this research was to develop an aggregation approach and a set of episodes that would support model-based distributional estimates, over the continental domain, of the air quality parameters mentioned above. The approach utilized cluster analysis and the 700 mb u and v wind-field components over the time period 1984–1992 to define homogeneous meteorological clusters. A total of 20 clusters, 5 per season, were identified by the technique. A stratified sample of 40 events were selected from the clusters, using a systematic sampling technique.

This stratified sample was then evaluated through a comparison of aggregated estimates of the mean extinction coefficients (b_{ext}) to the actual mean b_{ext} observed at 201 stations nationwide. The b_{ext} was selected as a surrogate for $PM_{2.5}$ because it had been used successfully in a similar study involving RADM (Eder and LeDuc, 1996a; 1996b). Results from the evaluation revealed a high level of agreement ($r^2 = 0.988$) indicating that the aggregation and episode selection scheme was indeed representative (Cohn *et al.*, in press).

2.2.2 Models-3/Air Management Version

With the release of the first version of Models-3/CMAQ in June 1998, an Air Management Version (AMV) was configured for use by the EPA Office of Air Quality Planning and Standards (OAQPS) and other groups involved in policy and regulatory analyses for air quality management. In CMAQ/AMV, particular modules were chosen for use and the resulting model was tested against data from a July 1995 ozone episode during the North American Research Strategy for Tropospheric Ozone – NorthEast (NARSTO-NE) field study in the northeastern United States. CMAQ was configured in a one-way nested grid mode, with grid resolutions of 36 km, 12 km, and 4 km, telescoping on the northeastern United States and the Washington-New York corridor. Initial tests were conducted with the RADM2 chemical mechanism in CMAQ. Results indicated that the model was performing reasonably well for ozone in the northeast, although there were problems seen in the midwest and south in the 36-km domain. A problem in the emissions inventory was discovered later, and the simulations are being repeated with corrections to the emission inventory. Also, during FY-1999, the CB-IV chemical mechanism will be tested in CMAQ/AMV on the same July 1995 episode.

2.2.3 Aerosol Research and Modeling

The CMAQ aerosol module was independently evaluated under contract with the Coordinating Research Council in Atlanta, Georgia. The thermodynamic component was compared with SCAPE (Simulating Composition of Atmospheric Particles at Equilibrium) (Kim *et al.*, 1993), EQUISOLV (Equilibrium Solver) (Jacobson *et al.*, 1996), SEQUILIB (Sectional Equilibrium) (Pilinis and Seinfeld, 1987), and AIM (Aerosol Inorganic Model) (Wexler *et al.*, 1990). The CMAQ thermodynamic module, identified in this work as MARS-A (Model for an Aerosol Reacting System-A) predicts results comparable to the more complex models for the sulfuric acid, ammonia, nitric acid, and water system. A journal article describing this work is being prepared.

The aerosol dynamics codes were also compared with other aerosol models. The CMAQ aerosol model was the only modal model; all of the others used the sectional method. The recommendation of this evaluation was that the original CMAQ approach of using a fixed standard deviation was inadequate, and that a variable standard deviation should be used. Work has begun to include a variable standard deviation in the June 1999 version of CMAQ.

The question of how to model the interaction of particulate matter emitted as primary particles with particulate matter formed by chemical transformation or secondary particulate was studied with a prototype box-model extension of the CMAQ aerosol module. Results showed that coagulation of accumulation mode primary and secondary particles will result in a mixed particle even for periods as short as 12 hours. Condensation of secondary material on primary particles produces mixed particles at a much faster rate, as expected. The approach developed in the prototype is being considered for inclusion in a later version of 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 were completed and published during FY-1998. The first study considers atmospheric mercury exposure from all major anthropogenic sources; the second study considers 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-1998 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 review of the mercury study report to the U.S. Congress (U.S. Environmental Protection Agency, 1997a). A revised air emission inventory for total mercury mass was provided by the EPA OAQPS, which included additional information about the air pollution control devices in use at particular industrial point sources. These new source definition data were used to develop a modified estimate of the chemical and physical forms of mercury emitted by pertinent industrial sources to reflect the estimated mercury collection efficiencies of the air pollution control devices in use.

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 final mercury study report to the U.S. Congress (U.S. Environmental Protection Agency, 1997b; 1997c; 1997d; 1997e; 1997f; 1997g; 1997h; 1997i), and a final report to the U.S. Congress on the electric utility steam generating units hazardous air pollutant study (U.S. Environmental Protection Agency, 1998b; 1998c).

A study was completed during FY-1998 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 published (Bullock *et al.*, 1998).

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 was traditionally 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.

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. The results obtained from this modeling study were used in developing the *Study of Hazardous Air Pollutant Emissions from Electric Utility Steam Generating Units —Final Report to Congress* (U.S. Environmental Protection Agency, 1998b; 1998c).

To provide the EPA Office of Solid Waste (OSW) 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 to complete a one-year simulation during FY-1998 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. Model simulation results were delivered to OSW to be used in the development of its Hazardous Waste Combustion Rule due in December 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, the 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 *Study of Hazardous Air Pollutant Emissions from Electric Utility Steam Generating Units — Final Report to Congress* (U.S. Environmental Protection Agency, 1998b; 1998c).

2.2.5 Meteorological Modeling Studies

The fifth-generation Penn State/NCAR Mesoscale Model (MM5) is the primary tool for providing meteorological input for the Models-3/CMAQ system. MM5 is also widely used for providing meteorological characterization generally throughout the air quality modeling community. For Models-3/CMAQ, MM5 is applied to several case studies at a variety of spatial scales using a series of one-way nested domains. MM5 is run retrospectively using four-dimensional data assimilation (FDDA) for a dynamic analysis of the observations through the simulation period. The output represents a dynamically consistent multiscale meteorology simulation for continental scale (horizontal grid spacing of 108 km), regional scale (36 km), mesoscale (12 km), and urban scale (4 km). The three finest resolutions are then run through the emissions and chemistry (CMAQ) models.

2.2.5.1 Meteorology Modeling for Models-3/CMAQ Applications

For the Models-3/CMAQ demonstration, MM5 was configured and run for the July 6–15, 1995, high-ozone episode for the northeastern United States. The demonstration included a series of one-way nested domains (108 km, 36 km, 12 km, and 4 km) for two 120-hour periods. The output from this demonstration was compared at various scales to independent hourly radar wind profiler observations that were not assimilated in the model. Although all simulations generated reasonable results, the comparison with the profilers illustrated the benefit of higher-resolution meteorology simulations for air quality studies. Through the lowest 2.5 kilometers of the atmosphere, a model-generated sounding from the 4-km domain best depicted the speed and directional shear associated with the low-level jet for this episode. The 12-km simulation had a lesser depiction of these features, and the 36-km domain showed hints of a weaker low-level jet. Further evaluation of the urban-scale simulations will occur in FY-1999 in conjunction with the CMAQ evaluation.

The local baseline of MM5 was upgraded from MM5v2.6 to MM5v2.10 with minor modifications. This change enables the Division to use the most current NCAR release of MM5 tailored for air quality simulations. Some of the more significant changes from v2.6 to v2.10 include use of a single source code base for serial and parallel processing, inclusion of several surface parameters in the MM5 standard binary output file, and correction of minor software bugs throughout the model. The inclusion of the parallel directives in the same source code enables the use of more sophisticated high-performance computers, while minimizing the potential for human error. This change should have pronounced impact in the coming years. The local modifications to MM5 include a standardized earth radius (for consistency with CMAQ), a new output file containing additional two-dimensional parameters, modifications to the Blackadar planetary boundary layer scheme that are consistent with MCNC[1] and Penn State[2] versions, improved representation of urban areas, a 1-km land-use database, and a correction to enable FDDA and initialization from one-way nesting in the same simulation. The Division's version of MM5 was installed in a CVS (Concurrent Versions System) repository to allow scientists, contractors, and grantees access to the same baseline for research and production runs.

Preliminary work was completed to implement observation nudging in the version of MM5 used with Models-3/CMAQ. While observation nudging was a part of MM5 for several years (*e.g.*, Stauffer and Seaman, 1990), some changes were made to the observation preprocessing to ease the transition of the software to a wider user base, *e.g.*, Models-3. It is anticipated that the implementation of observation nudging in MM5 for Models-3/CMAQ will occur in the June 1999 release.

2.2.5.2 Advanced Land-Surface and Planetary Boundary Layer Modeling in MM5

MM5 was coupled to an advanced land-surface and planetary boundary layer (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. The modified version of MM5 is called MM5PX (Pleim and Xiu, 1995) in which a new land-

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[1]MCNC, Research Triangle Park, NC.

[2]Pennsylvania State University, College Park, PA.

surface model, including explicit representation of soil moisture and vegetative evapotranspiration along with the Asymmetric Convective Model, replaces the standard surface and PBL schemes available in the MM5 system. The FY-1998 work involved both applications of MM5PX to air quality modeling and further development and evaluation.

The first application of MM5PX to a major air quality study was made in conjunction with the Lake Michigan Mass Balance Project (see Section 2.4.2). The MM5PX was run for the entire spring and early summer of 1995 to provide meteorology and surface conditions, including soil moisture and temperature, to estimate atrazine emissions in eastern North America. This project necessitated the development of a seasonal vegetation growth scheme to simulate the change of vegetation characteristics during the modeling period. Planting dates by state were provided as input to the model, and crop growth was modeled simply by using days after plants emerged. Natural vegetation growth, particularly deciduous leaf-out, was parameterized as a function of deep soil temperature. The model-simulated spatial evolution of leaf area showed remarkable agreement with biweekly Normalized Difference Vegetative Index (NDVI) composite maps. Since soil temperature and moisture were modeled continuously for the 4-month period (April–July), this comparison to NDVI data also provided an indirect evaluation of the deep soil temperature, the entire land-surface model, and the soil moisture nudging scheme.

To this point, applications of the MM5PX were based on MM5v1.0. The system is being updated to include the PX PBL-Surface model as an operational option in MM5v2.10. The Division collaborated with the MM5 group at NCAR to modify the terrain preprocessor to read and process more detailed and up-to-date land use data from the U.S. Geological Survey (USGS). The goal is to have the PX PBL-Surface model in the NCAR mid-1999 release of MM5v3 and the next release of Models-3/CMAQ.

2.2.6 Dry Deposition Studies

There were many activities in FY-1998 concerning dry deposition that cut across several parts of the Division and involved other groups in NOAA and EPA. These include a field measurement program, dry deposition modeling associated with the Clean Air Status and Trends Network (CASTNet), development of improved models for dispersion modeling, and new modeling techniques for Models-3/CMAQ. The synergy between modeling and field measurements has proven to be very valuable for evaluation and development of the models and analysis of the measurements.

2.2.6.1 Field Measurements

A field research program was started several years ago to systematically measure deposition velocity over the major land use categories, and to use those data to evaluate and improve deposition velocity models. Extensive field studies were completed over such crops as corn, soybeans, and pasture, and over pine, deciduous, and mixed deciduous and coniferous forests. Other studies that were completed include an intercomparison study in which the Division's measurements were compared with those from other co-located research groups, and a study of deposition over open salt water. The common suite of measurements includes the fluxes of HNO_3, O_3, SO_2, H_2O, CO_2, heat, and momentum, as well as a full set of meteorological and plant observations. Using these data, model evaluations were completed on point deposition velocity models used in CASTNet, and regional deposition velocity models used in Models-3/CMAQ. The FY-1998 study took place in a mixed conifer and deciduous forest in the Adirondack Mountains of New York State. A 120-foot tower was erected in the forest in the early spring, and data were collected from late April to the middle of October. Analysis of the data is ongoing. This completes the terrestrial portion of the dry deposition monitoring research plan. The next phase will measure fluxes to a salt-water marsh in the Chesapeake Bay, in a study involving NOAA ARL-HQ, ASMD, and EPA.

2.2.6.2 Dry Deposition Modeling

As part of the CMAQ development, a new method for modeling dry deposition of gaseous chemical species was developed to take advantage of the more sophisticated surface model implemented in the MM5PX. Since the MM5PX now has a parameterization for 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 conductance estimates resulting from the integrated surface energy calculation where the soil moisture is continually adjusted to minimize model errors of temperature and humidity. The dry deposition model was evaluated for ozone deposition by comparing model results with field measurements at Bondville, Illinois, and Keysburg, Kentucky, being made for the MM5PX (Pleim *et al.,* 1996; Pleim *et al.,* 1997). The impact of the new dry deposition model and the MM5PX on the simulation of air chemistry by the CMAQ system is being tested as part of the NARSTO-NE evaluation studies.

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 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 are also participating in the continental NARSTO program. During FY-1998, 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 first NARSTO-sponsored state-of-science assessment for tropospheric ozone was underway. 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-1998 and are due to be completed by the end of FY-1999. Several Division members are participating in the assessment as co-authors of certain critical review papers and the assessment report.

2.2.7.2 Southern Oxidants Study

FY-1998 was the eighth year of the multi-year Southern Oxidants 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 aerometric data archiving. The last major SOS field study occurred in the Nashville/middle Tennessee region during June and July 1995. During FY-1998, a major activity within the Division was to obtain data sets of interest from this study and to begin configuring the Models-3/CMAQ in a nested grid configuration on this area for model application and evaluation. The CMAQ model simulations for Nashville will begin in FY-1999.

2.2.7.3 Seasonal Modeling of Regional Air Quality Project

A regional-scale modeling project, Seasonal Modeling of Regional Air Quality (SMRAQ), for 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 Multiscale Air Quality SImulation Platform (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 advisory group for the project.

2.2.7.4 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 with the EPA, U.S. Forest Service, U.S. Fish and Wildlife Service, and National Park 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 CAA. As part of the IWAQM activity, a full year of hourly gridded (80-km spatial resolution) modeled meteorological fields from MM4 with FDDA, as pseudo radiosonde data, were compared with interpolated meteorological fields from actual radiosondes for use in local and mesoscale dispersion models. The preliminary results indicated that the modeled meteorology produced significantly more accurate results than that using the interpolated fields from radiosonde data alone. This led to the production of a second year of modeled meteorology (1992) for use in dispersion models. In FY-1998, hourly gridded (80 km) modeled meteorological fields were produced for 1992 using MM5 with FDDA for the purpose of extending the basis of comparison against the interpolated radiosonde database. This database was sent to the National Park Service.

2.2.7.5 Total Column Ozone

The spatial and temporal variability of total column ozone obtained from the Total Ozone Mapping Spectrometer (TOMS) during the period 1980-1992 was examined through the use of a multivariate statistical technique called Rotated Principal Component Analysis (RPCA) (Eder, 1998). This work was performed in support of the EPA Global Change Program. Due to the copious amount of data resulting from such a large scale investigation, it proved advantageous to employ an analysis method that would identify, through a reduction in data, the recurring and independent modes of variation within the larger data set. Such analysis was achieved with RPCA, which allowed for the reduction of the original data set, containing 1872 5° latitude by 5° longitude grid cells, down to 14 uncorrelated variables (the principal components) while still explaining more than 70% of the total variance. Application of Kaiser's Varimax rotation led to the identification of 14 mostly contiguous subregions, each of which exhibited statistically unique total column ozone characteristics.

The first RPC identified an area north of 40° N that was dynamically driven, linked to the mass transport of ozone from the equator to the middle northern latitudes and to the tropopause effect. The second RPC, encompassing much of the remainder of the Northern Hemisphere from 5° to 30° N, was controlled by photochemical processes, although the Quasi-Biennial Oscillation (QBO) appeared to have some influence here. The third RPC, an area encompassing much of the Southern Hemisphere stretching from 5° to 45° S, was controlled by a combination of dynamical and photochemical processes. The fourth RPC clearly defined the area most influenced by the QBO, a slightly asymmetrical region extending a little further north (15° N) than south (10° S). The QBO signal was also slightly stronger from 70° E to 80° W.

The fifth through ninth RPCs identified five similar subregions in the southernmost section of the study area between 45° and 65° S that are centered at 170° W (5), 100° W (7), 40° W (9), 20° E (6) and 90° E (8). Although separate, the subregions are thought to be driven by the same dynamic force; namely, medium-scale baroclinic waves. These waves have also been called the *wave number 5* or *pentagonal waves* associated with the Antarctic polar jet stream, which advects ozone, both vertically and horizontally. The 10th RPC was thought to be an extension of RPCs five and nine, and therefore may be responding to the same physical processes previously discussed.

The 11th RPC identified a small area in the Southern Hemisphere from New Guinea in the Western Pacific to central South America that is clearly associated with the El Nino - Southern Oscillation (ENSO). This analysis showed that association is strongest in the equatorial Pacific from 5° to 15° S and from 110° to 160° W. The 12th RPC was unusual in that it identified two separate regions, the first extending from Brazil eastward into the South Atlantic, and the second extending from the Middle East, across northern Africa into the Atlantic Ocean. The phenomenon responsible for these signals was thought to be the result of a data retrieval problem associated with aerosol interference, as both regions are subject to great aerosol loading, Brazil due to biomass burning and Africa due to Saharan dust. The 13th and 14th RPCs each defined small areas over the North Atlantic Ocean, and over eastern sections of the Pacific Ocean and western sections of North America, respectively. It was thought that the two areas, which are downstream from intense jet stream cores, are favored areas for the advection of ozone into the Northern Hemisphere from lower latitudes.

This analysis has allowed an examination of the spatial and temporal variability of total column ozone across a wide range of scales, identifying and quantifying characteristics that might otherwise go undetected. For instance, the data processing artifact found in an earlier analysis performed by the authors on version 6.0 TOMS would likely have gone unnoticed using most other analysis techniques. This artifact was not found in this most recent analysis, leading to the conclusion that its influence was reduced in version 7.0 TOMS. The identification and subsequent characterization of areas of homogeneous total column ozone have other benefits as well. It can be used in the evaluation of numerical global models where it will hopefully stimulate theoretical analysis. It can also aid the steering committee of the International Tropospheric Ozone Years in the placement of 50 future ozonesonde stations around the globe.

2.2.7.6 Climatological and Regional Analyses of CASTNet Data

The CASTNet monitoring program was analyzed using rotated principal component analysis and spectral density analysis. This approach provides an objective, statistically based technique designed to identify and characterize *influence regimes* associated with ambient air concentrations of SO_2, SO_4^{2-}, NO_3^-, HNO_3, NH_4^+ and O_3. This approach was 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). Depending on the species, either two (NO_3^-), three (SO_2, SO_4^{2-}, NH_4^+, O_3) or four (HNO_3) influence regimes or subregions were identified by the analysis (Eder and Sickles, 1998). Examination of the climatological-scale variability of these homogeneous subregions revealed periodicities ranging from weeks to years, as well as several trends. The identification of homogeneity across sites has added to the weight of evidence supporting regionality of behavior of species, likely due to a commonality of emission and/or meteorological patterns. Subsequent analysis will attempt to provide additional insight into the physical mechanisms shaping the spatial and temporal morphology of the subregions.

2.2.7.7 Statistical Modeling of Ozone in the Houston Area

A statistical study, performed in conjunction with the EPA National Center for Environmental Statistics, compared the results from a single-stage clustering technique (average linkage) with those of a two-stage technique (average linkage then k-means) (Eder *et al.*, 1993) as part of an objective meteorological classification scheme designed to better elucidate ozone's dependence on meteorology in the Houston, Texas, area (Davis *et al.*, 1998). 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 supports 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- and multi-stressor human and ecosystem problems.

2.3.1 Emission Modeling

The Models-3 Emission Processing and Projection System (MEPPS) was enhanced and tested within the Models-3 framework for the first public release of Models-3 on June 30, 1998. Also, MEPPS began to produce processed emission data on a regular basis for the rest of the Models-3 system. Specifically:

- MEPPS was used to generate large emission data sets for July 2-15, 1995, with spatial domains covering more than half of the United States and Canada, for use in demonstration and evaluation of the rest of the Models-3 system, including CMAQ. The emission data sets were produced at 36-km, 12-km, and 4-km spatial resolution.

- An Inventory Data Analyzer (IDA) was designed and implemented for the Models-3 framework. IDA is not embedded in MEPPS, but operates in conjunction with a new generic File Converter to import, quality control, and aid in analysis of unprocessed emission data, including new emission inventories. File Converter imports or exports files in SAS®[3], ASCII, or netCDF (network Common Data Form) I/O API formats, performs basic quality control, and allows the user to reorder the file fields and convert to one of the other supported formats. IDA accepts emission-related files from File Converter, including emission inventories, hourly continuous emission monitoring data or other hourly emission data, temporal allocation profiles, emission control factor files, etc. IDA performs more quality control functions specific to emission data, and automatically computes corrections where possible, or applies default values. IDA also allows the user to visualize the data through a geographic information system tool.

- The EPA Highway Vehicle Particulate Emission Modeling Software — PART 5 — is being incorporated into MEPPS. PART 5 computes hourly particulate emissions for a range of vehicle categories using atmospheric temperature as an input. It operates as a companion to the Mobile 5a model, which computes hourly gaseous emissions from vehicles. PART 5 is important because of the increasing need for accurate particulate emission inventory data for air quality modeling to support the new, more stringent, particulate NAAQS.

- Work has begun to incorporate the Sparse Matrix Operator Kernel Emissions (SMOKE©) modeling system in the Models-3 framework. SMOKE© was developed by the MCNC-North Carolina Supercomputing Center[4] over the past four years. Its matrix approach to the repetitive computations involving very large emission databases improves processing performance by at least an order of magnitude. In addition, SMOKE© can be fully

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

[4]MCNC-North Carolina Supercomputing Center, Research Triangle Park, NC

incorporated and compliant within the Models-3 framework, unlike MEPPS, which is a SAS®-based system that can only be semi-compliant. Because SMOKE© is not SAS®-based, the emission file space demands ought to be much less than for MEPPS. MEPPS often fills large disk drives with tens of gigabytes of intermediate processing data that will not be needed by SMOKE©.

2.3.2 Biogenic Emissions

During the past ten years, new emission measurements and vegetation cover inventories have resulted in rapid changes in isoprene emission estimates, causing some to question the legitimacy of isoprene emission estimates in photochemical grid model simulations. Pierce *et al.* (1998a) examined the sensitivity of regional ozone model predictions with the first and second versions of the Biogenic Emissions Inventory System (BEIS). BEIS2 isoprene emissions are a factor of five higher than BEIS1. Pierce *et al.* (1998a) documented the methods used in BEIS2, presented modeling results for a high ozone period during 1998, and compared isoprene concentrations measured near Scotia, Pennsylvania, to concentrations estimated with the Regional Acid Deposition Model (RADM). While the paper supports the veracity of the BEIS2 isoprene emissions over central Pennsylvania, other modeled *hot spots* of isoprene, for example, south-central Missouri, deserve to be examined with observational data.

A team of biogenic emission experts, under the auspices of NARSTO, is completing a critical assessment of biogenic emissions. The assessment will be published. This effort is leading to the development of the next version BEIS. This new version, BEIS3, will include a 1-km resolved vegetation cover database, more detailed speciation of monoterpenes that are important for aerosol formation, and a refined leaf temperature canopy model. Release of BEIS3 is anticipated during FY-1999.

The OZark Isoprene Experiment (OZIE) has been investigating isoprene emissions and isoprene concentrations near the Ozark Plateau in Arkansas. This region is densely populated with oak trees, which are high emitters of isoprene. Furthermore, abnormally high isoprene concentrations have been predicted by various photochemical grid models as noted by Pierce *et al.* (1998a). OZIE participants include AMEREN (an energy company that sponsored some of the field measurements), Illinois Environmental Protection Agency, Indiana Department of Natural Resources, Lake Michigan Air Directors Consortium, Missouri Department of Natural Resources, National Center for Atmospheric Research, Boulder, Colorado, Purdue University, Lafayette, Indiana, U.S. Environmental Protection Agency (Office of Research and Development, Region V, and Region VII), Washington State University, Pullman, Washington, and Washington University, St. Louis, Missouri. A Division scientist was instrumental in organizing and coordinating the OZIE program. Field measurements occurred over a 2-week period during July 1998, which included one episode (July 18–22, 1998) when temperatures peaked in the middle 90's. Surface isoprene concentrations peaked around 50 ppbv. Since isoprene varies strongly with sunlight and temperature, with maximum emission rates occurring around 95° F, OZIE benefited from excellent sampling conditions during this 5-day period. The resulting data set will be valuable for evaluating photochemical grid models and isoprene emission flux estimates.

2.3.3 Improvements in Vegetation Cover Data

Progress continues on a 1-km vegetation cover data set for North America. Pierce *et al.* (1998b) demonstrated the usefulness of the data set for Missouri. This data set builds on features found in the 1-km USGS land characteristics data set, a 1-km U.S. Forest Service forest density data set, 1992 U.S. Agricultural Census, and forest inventory statistics from the U.S. Forest Service. Unlike data used in existing global and continental numerical weather prediction models, this data set will provide tree species and crop type information at a 1-km resolution. It is anticipated that this increased knowledge of vegetation cover may allow better simulations of energy and moisture fluxes, dry deposition, and biogenic emissions. The data set is being integrated into BEIS3 and will be tested with MM5v2 and Models-3/CMAQ.

2.3.4 Visualization and Analysis Tools

Visualization and analysis tools for integration into the Models-3 framework were developed, improved, and applied during FY-1998. Considerable progress was achieved to address preparation of data for viewing and analysis. Tools to visualize vertical wind profiles using IBM DX® and AVS® were improved. Modeled and observed winds were displayed simultaneously and then animated. Displays may consist of multiple sites shown at various geographic locations. The system was designed to handle missing data. The procedure was documented for preparing vertical wind profiles from the archived Doppler radar available from the National Climatic Data Center.

In addition, precipitation rates were processed and displayed simultaneously with MM5 model output. The precipitation rate data were derived from Doppler radar for 2-km grid cells across the continental United States. The precipitation rate was displayed as a texture map on the Earth's surface. Rainwater was displayed as an isosurface above the Earth's surface. Vis5D© was used for this display, and animation was used to examine changes over several days. The derived rainfall rate from MM5 can also be displayed as a two-dimensional field on the surface. The MM5 model output data require special preprocessing before they can be visualized with Vis5D©. An on-line tutorial has been developed to assist the user with these visualization tools (http://www.epa.gov/asmdnerl/models3/vistutor/vistoc.html).

2.3.5 Technology Transfer

The transfer of the Models-3/CMAQ system commenced with the public release on June 30, 1998. Informal in-house demonstration and training were provided to one group at the time of the release. Plans were developed to equip a classroom for future Models-3 training. The classroom will be equipped with a Sun™[5] workstation with Solaris 2.6 Operating Environment™[6], and PCs with Microsoft®[7] Windows NT® operating system. Several training courses are being developed.

2.3.6 Single Source Code Design

To better support multiple computer platforms, the Models-3 science modules were developed utilizing standardized code and preprocessing directives. This achieved a single set of source code compatible with all the supported computer platforms, including Sun™, DEC Alpha™[8], Cray C90™[9], and Microsoft® Windows NT®. Because these platforms use the same set of code, this design simplifies the management and maintenance of the software.

2.3.7 Models-3 Air Quality Modeling and Analysis System

The computer-based Models-3 framework was publicly released in June 1998. It was developed to simplify the use and continued enhancement of environmental models, by providing a user-friendly interface and flexibility for the evolution of environmental models. The initial release of Models-3 includes the Community Multiscale Air Quality (CMAQ) modeling system for urban to regional scale air quality simulation of tropospheric ozone, acid deposition, visibility, and fine particles. Two other modeling systems are also included with the initial release of Model-3: (1) the Penn State/NCAR MM5 system and (2) the MEPPS emission modeling system. The Models-3 framework manages and enhances the coordination of these three modeling systems (CMAQ, MM5, and MEPPS).

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[5]Sun in a trademark of Sun Microsystems.

[6]Solaris Operating Environment is a trademark of Sun Microsystems.

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

[8]Alpha is a trademark of the Digital Equipment Corporation.

[9]Cray C90 is a trademark of Cray Research, L.L.C., a wholly owned subsidiary of Silicon Graphics, Inc.

Many components were developed as part of the Models-3 framework to build and apply environmental models, visualize and manipulate data, manage model source code, and perform system administrative duties. Through these components, CMAQ and MEPPS can be used to develop modeling simulations for specific domains and time periods. In addition, visualization tools can be accessed through the Models-3 framework to analyze model results and compare data without the need to export or convert data formats. Another advantage to using the Models-3 framework components is that models can be customized without having to modify model source code, which provides quality assurance and removes complexity.

A three-volume document was published for the public release of Models-3 (Atmospheric Modeling Division 1998a; 1998b; 1998c). The installation and operations manual details the installation procedures for the Models-3 framework. The user manual serves as a reference for the Models-3 software system; includes instructions for using the Models-3 components to develop, manage, and analyze model simulations; and presents an overview of the CMAQ, MM5, and MEPPS modeling systems, and CMAQ science options. The tutorial includes step-by-step exercises to develop a CMAQ simulation using Models-3 components and advanced exercises for developing new projected emissions and a customized CMAQ model.

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 to 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. Another activity of FMF is the study of resuspension mechanics and wind erosion, primarily through experimental field measurements. Research is coordinated with other agencies and researchers.

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. It has an airflow speed range of 0.5 to 10 m/s, and 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 CBL capped by an overlying inversion.

During FY-1998, FMF experienced a number of significant changes, requiring some restructuring of research goals and schedules. Primary research efforts were refocused into three areas: (1) continuation of analysis and reporting on results from studies of buoyant puff and plume dispersion in a convective boundary layer, (2) initial evaluations of instrumentation for investigating the physics of particle resuspension from grass-like surfaces, and (3) fundamental measurements of flow and dispersion within, over, and around an array of buildings.

2.4.1. Multimedia Modeling Component for Endocrine Disruptor Exposure

The study of chemicals identified as having the ability to disrupt the function of human and ecological endocrine systems (EDCs) continued during FY-1998. 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-1998, a one-week hands-on multimedia modeling training seminar was held. The course included a general introduction to dynamic, multimedia mass balance modeling as well as detailed instruction in the use of the MEND-TOX model. Several case studies were explored by the class. In response to class comment, the MEND-TOX model was modified to respond more realistically to heavy rainfall events (mass transfer, runoff, and soil mechanics). Model output options were greatly expanded to facilitate detailed analysis of intermedia transfer processes and mechanisms. Two applications for Benzo[*a*]pyrene (B[*a*]P), a suspect endocrine disruptor, were developed for the Middle Neuse Basin of North Carolina. B[*a*]P is a common atmospheric pollutant derived from the partial combustion of hydrocarbons. In urban areas, its concentration is closely related to vehicle traffic patterns. In the study area, the dominant source is agricultural open field burning and wildfires. The first application highlighted the use of the dynamic, hybrid modeling approach to facilitate endocrine disruptor methods development research. The second application examined the multimedia impact of regional precipitation frequency and intensity changes on the local movement of atmospheric Benzo[*a*]pyrene to land and water surfaces.

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.

Research performed during FY-1998 identified several additional ORTECH model modifications that were needed to clearly establish MM5 and the soil emissions model linkage. These changes included initialization of the soil temperature and moisture profiles of the emissions model, modification of soil temperature and moisture profile lower boundary estimation techniques, and the resolution of the impact of scale differences (field emissions versus 36 km^2 grid cell meteorology) on energy and moisture flux estimates. Research questions raised during model development include the response of atrazine emissions to naturally occurring, regional patterns of wet and dry weather. This issue is particularly critical to the estimation of regional emissions during the mid-Atlantic drought of spring and summer 1995. The fate and transport modeling portion of this research is being actively coordinated with related activities in the NOAA Air Resources Laboratory.

2.4.3 Solar UV and Total Column Ozone Modeling

Daily average total column ozone data collected from four mid-Atlantic states monitoring stations in the EPA Brewer Spectrophotometer Network were compared with satellite-monitored total column ozone from the NOAA SBUV/2 instrument for the same latitude and longitude. Statistics of data comparison included correlation, bias, comparability, precision, and completeness. Further analyses were achieved through regression with a seasonal model. Model parameters — mean, amplitude, and phase — were optimized separately for Brewer and satellite data at each location. Data comparison indicated an overall small positive bias of the Brewer over the SBUV/2. Comparison of model parameters confirmed an overall greater Brewer mean ozone. A mid-Atlantic states regional total column ozone model was developed from the data sets. The basic modeling approach applied to each location separately was extended regionally by further parameterizing model mean, amplitude, and phase, as functions of latitude and longitude. Gridded data were generated using spacial interpolation/extrapolation of the local model parameters using a normalized (1/r)-weighted Krieging scheme. Regional mean, amplitude, and phase parameters were then regressed against latitude and longitude. An approach to temporal-averaging for characterization of continuously varying modeled spectral UV radiation was developed to support UV-stressor profile characterization of the mid-Atlantic region. A seasonal mean spectral flux was calculated for the solar zenith angle corresponding to the seasonal mean broadband flux for a mid-season day.

2.4.4 Hazardous Waste Identification Rule

The EPA Office of Solid Waste is developing a proposed amendment to its regulations under the Resource Conservation and Recovery Act (RCRA) by establishing constituent-specific exit criteria for low-risk solid wastes that are designated as hazardous because they are listed, or have been mixed with, derived from, or contain listed hazardous wastes. Listed waste with concentrations below the exit concentrations would no longer be regulated by RCRA Subtitle C. The methodology under development for the Hazardous Waste Identification Rule (HWIR) will estimate risks through an integrated multimedia, multiple pathway, and multiple receptor assessment that characterizes potential human health, and ecological exposure and risk. The characterization of exposures and risks are intended to provide a national distribution of individual risk for individual constituents released from the following types of waste management units: industrial landfills, waste piles, land application units, surface impoundments, and tanks.

The air concentration and deposition estimates needed for the assessment will be determined using the Industrial Source Complex - Short Term (ISCST3) model. ISCST3 is typically run using hourly meteorological data. For HWIR, the runtime for the ISCST3 model is prohibitively long. Therefore, an approach for using a subset of the complete meteorological database was investigated. The meteorological data were reduced through the sampled chronological input method whereby the data were sampled at regular intervals (*e.g.*, every 25 hours) and model estimates were scaled up based on the number of hours sampled. Testing showed that the sampled data produced annual average concentration and annual dry deposition estimates that were comparable to those obtained from the full data set even at an interval as large as 193 hours (eight days). However, as expected, the wet deposition estimates were considerably more sensitive to the sampling interval. The method was expanded to allow the inclusion of a second sampling interval for modeling the wet hours. At intervals up to 8 hours, the sampling for wet hours produced comparable results to the full data set.

2.4.5 Correlation Study of Particulate Matter with Gaseous Pollutants

A statistical study was undertaken to address the general question of the magnitude of the correlation between ambient particulate matter (PM) concentrations and ambient gaseous pollutant concentrations. Ambient PM has been associated in epidemiologic studies with mortality and morbidity, but questions have arisen about the role of gaseous pollutants (CO, SO_2, NO_2, and O_3) ascribed to PM. To investigate the question of the general co-linear behavior of these gaseous pollutants in the United States, the EPA Aerometric Information Retrieval System (AIRS) database was examined for the years 1992 through 1996. Collocated PM and gaseous pollutant data were taken for the highest urban PM site and the lowest PM rural site in each state of the United States and the Pearson correlation coefficients between them were determined. These data, presented as histograms, showed that in general there was a distribution of correlation coefficients between PM and the gases of order 0.25 with a standard deviation of 0.2. However, the individual correlation coefficients ranged from -0.7 to +0.7. It was concluded that no generalization could be made about the correlation between PM and any particular gas that would justify *a priori* exclusion of its consideration as a confounder or an effect modifier in an epidemiologic study of the health effects of PM.

2.4.6 Hazardous Air Pollutant Exposure Model

2.4.6.1 Optimizing the Hazardous Air Pollutant Exposure Model Code

Major enhancements to the Hazardous Air Pollutant Exposure Model (HAPEM) were undertaken during FY-1998. To make the model run more efficiently, the model code underwent major revision, thus resulting in the development of a UNIX®[10]-workstation version of HAPEM. This revised version of the model was run for 14 cities in the United States to provide information on exposures to mobile source pollutants. This work was performed in support of the EPA Office of Mobile Sources, and the requirement under the 1990 CAAA to assess the impact of control programs on exposure to air toxic emissions from mobile sources.

2.4.6.2 Adding New Components to the Hazardous Air Pollutant Exposure Model

HAPEM was modified to utilize modeled data for its ambient air quality data inputs. This marked the first time that HAPEM could be used with anything other than measured ambient air quality data. This work was sponsored by the EPA OAQPS.

The 1990 CAAA requires EPA to identify sources of air toxic pollutants, assess risks associated with human exposure, and promulgate regulations to control emissions and reduce human exposure to these pollutants. In an effort to meet these requirements, the EPA Office of Policy, Planning, and Evaluation developed the Cumulative Exposure Project (CEP) model. Under this effort, the CEP model was imported to an in-house workstation for nationwide modeling assessments. The CEP model predicted nationwide air toxic concentrations at the

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[10] UNIX is a registered trademark of AT&T.

census tract level. These data were then coupled with HAPEM to assess human exposure to air toxics at the census tract level. This work will continue in FY-1999.

2.4.7 Human Exposure Microenvironmental Modeling

Research projects to support human exposure assessment of air pollutant within microenvironments is ongoing. A project to characterize human exposure to automobile emissions was started in collaboration with the EPA Mobile Sources Characterization research group. A van was instrumented to continuously measure total HC, NO, CO, O_3, particle-bound PAH and SF_6. The van also has a fifth wheel and laser rangefinder to monitor vehicle speed and distance from a lead vehicle. Ambient air is being measured alongside the roadway (parked van) and within the van (travel along the roadway) to characterize the pathway from source to personal exposures. Experimental studies of controlled SF_6 emissions from lead vehicles are being studied to characterize potential personal exposure from individual vehicles. These measurement studies will continue into FY-1999. A model of roadway emission sources, roadway dispersion, and penetration into moving vehicles along the roadway is being developed. The ongoing modeling activity includes development of a new *microfactor* emissions model, potential modifications to the CALINE models, and application of numerical simulation using Computational Fluid Dynamics (CFD) Fluent Inc. finite volume code. The goal is to model the pathway from the source to human exposure. In addition to these roadway microneviromental studies, planning for application of the CFD code to building microenvironments was started with major development expected during FY-1999. The intent is to use limited ambient measurements, wind tunnel measurements, and numerical simulation studies to construct simplified applied models in support of human exposure modeling in urban microenvironments of exposure.

2.4.8 Analysis of CO Trends for Several United States Cities

Statistical analyses were performed on ambient CO concentrations taken from the AIRS database for Denver, New York City, Los Angeles, and Phoenix. The spatial and temporal variability in ambient CO levels were characterized. This work extended an investigation of CO trends in the continental United States covering an 8-year period (1984-1991) (Glen *et al.*, 1996). This work provided information toward understanding the CO exposure profiles of the population and provided information for the next CO criteria document.

Data were collected for various numbers of monitoring sites in and around the cities of Denver, New York City, Los Angeles, and Phoenix. The AIRS database was used to retrieve hourly average CO data for each city's Metropolitan Statistical Area for the years 1986-1996. Statistics on central tendency and correlation were tabulated for all of the sites in each city for both the hourly and 8-hour running averages. The data were separated, and the statistics analyzed, by the year, season, day of week, and hour of day.

The analysis of the four geographically diverse cities showed that urban carbon monoxide, while generally decreasing in concentration, is still a major contributor to urban air pollution. From this work, it is clear that CO is not a pollutant that can be dismissed as unimportant. The number of violation days has declined for these cities. Although the seasonally averaged peak concentrations generally did not exceed 8 ppm, at least one case of 9 ppm for the maximum daily 8-hour average for CO occurred in either 1995 or 1996 in all four of these cities.

2.4.9 AMS/EPA Regulatory Model Improvement Committee

The AMS/EPA Regulatory Model Improvement Committee (AERMIC) continued its efforts in FY-1998 to complete the technical formulation and operational code for the AERMOD plume dispersion model. An extensive external peer review uncovered a number of formulation issues that were addressed by the committee. At the peer reviewers' request, the model was also evaluated with 2 additional complex terrain databases bringing the total to 10 field studies and one wind tunnel study. Reports on the final technical formulation, extensive model evaluations, sensitivity studies to meteorological inputs, and model user's guides are near completion. Additionally, issues related to the regulatory applicability of the model as a replacement for existing regulatory plume models are being addressed.

AERMOD is to be presented to the public for review and comment at the EPA Seventh Modeling Conference in early 1999 as required by the CAA. In FY-1999, the AERMIC development team expects to make improvements to the building downwash algorithm and the dry and wet deposition algorithms, and to develop a screening version of the model.

2.4.10 Buoyant Puff and Plume Dispersion in a Convective Boundary Layer

During FY-1995 and 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 of obsolete munitions at the Department of Defense and Department of Energy facilities.

During FY-1997, this modeling effort was extended to include an examination of the rise of buoyant puffs through a CBL, hence extending the applicability of the results to the more commonly encountered conditions. These laboratory experiments were the first on buoyant puff dispersion in a CBL, where a large number of experiments were conducted under near-identical conditions to obtain reliable ensemble statistics. They are particularly important for model development because of the difficulty of obtaining statistically stable field measurements in the CBL.

During FY-1998, the results of these experiments were presented (Lawson *et al.*, 1998; Thompson *et al.*, 1998; Weil *et al.*, 1998a; 1998b), and two additional manuscripts were prepared for journal publication. The articles will describe the convection tank, laser-induced fluorescence measurement system, and data-processing procedures; summarize statistics of mean and fluctuating concentration; and contrast the results with both field data and earlier laboratory experiments of Deardorff and Willis (1984). The lateral plume spread was found to be substantially larger than in the earlier laboratory experiments and more consistent with available field data.

To facilitate analysis of the buoyant puff experiments, digital images obtained during the experiments were processed to produce cross sectional images of both mean concentration and statistics of the concentration fluctuations, using pseudocolor enhancement to visually show the range of values in each case. These digital images were, in turn, used to produce a videotape showing the temporal development of each statistic for an ensemble of 33 experiments out to a time of 4t*, where $t^*=z_i/w^*$ is the convective time scale. This was repeated for each of the three buoyancy values used in the experiments. The summary video tapes allow for quick inspection and comparison of mean statistics as well as providing a fascinating view of the initial rise, inversion penetration, and subsequent entrainment into the mixed layer.

2.4.11 Measurements of Flow and Dispersion in and Around an Array of Buildings

FMF is working with the Energy and Environmental Analysis Division of the Los Alamos National Laboratory to perform physical modeling studies of the flow and dispersion in and around an idealized urban area. The thrust of the effort is to develop a database for evaluation and refinement of state-of-the-art three-dimensional fluid dynamic codes used to predict the transport and fate of chemical and biological releases in an urban complex. Since the model must address scales of motion from the regional down to individual structures or interiors of structures, wind-tunnel studies provide the only practical means to obtain an adequate database. The urban building array model is complete as well as installation of the wind-tunnel boundary-layer simulation apparatus. Initial boundary-layer velocity and turbulence measurements were completed, as well as a series of flow visualization experiments, where the array geometry (two-dimensional versus three-dimensional), approaching wind direction, and dimensions of the individual structures were systematically varied while observing and recording the effect on flow over and through the array.

The results of these flow-visualization experiments will be used to determine under what conditions the flow penetrates the array as opposed to the flow skimming over the top of the array; two sets of conditions that are expected to result in drastically different rates of ventilation for pollutants released within the array. This will be followed by quantitative measurements to fully document the flow and provide the initial database for model evaluation. A follow-on project with Lawrence Livermore National Laboratory will provide additional flow measurements and tracer concentration data for inclusion in the database.

2.4.12 Research into the Mechanics of Resuspension: Modeling of PM_{10} and $PM_{2.5}$ from Soil and Vegetative Surfaces

FMF initiated a study to examine the fundamental physical processes underlying the resuspension of particles from grass and grass-like surfaces. The initial efforts are centered around evaluation of two SENSIT™[11] instruments that are to be used to distinguish the ways grass blades interact, hence how energy is transferred from wind to grass blades and ultimately to small particles that can be dislodged from the grass blades. An electronic interface for the instruments was completed and data acquisition software written. Initial measurements were made to characterize the SENSIT™ instrument's response to background turbulence and vibration.

2.4.13 Effect of Soil Crusting on Resuspension

Protection against resuspension of particles by the wind for natural soils is provided primarily by the presence of vegetation. Another important protector of bare soil surfaces is the presence of soil crusts. Thick and hard surface crusts are protective of the surface for almost all winds. However, thin surface crusts are weak and destroyed by winds that are occasionally experienced in most environments.

Research was conducted on the effect of soil crusting on resuspension. Owens (dry) Lake near Olancha, California, was the sampling site. The objective was to measure the sand drift — that is the horizontal flux of sand — at a given point on a crusted dry lake area and to relate it to the potential sand drift from a crust-free surface. This potential sand drift was derived from wind and sand flux measurements at the same location when no soil crust was observed on the surface. The difference between the actual sand drift and the potential sand drift was related to observations of the surface, measurements of the minimum wind required to initiate movement of sand drift, roughness of the surface, and change of that roughness. Individual crusts were defined as lying between two soaking rain events separated by a thorough drying of the soil.

Unbroken crusting with no loose surface particles caused a halt of any local wind erosion. When the surface was crusted with a thin layer of loose particles on the surface, the sand flux rates were about the same as for non-crusted soils. In some cases, however, the loose particle layer became sufficiently depleted to decrease the mass flux rates versus wind friction velocity ratios. These supply limited cases are especially interesting since they represent differences between the potential flux, supply unlimited, where the only limitation is of the wind energy and non-erodible, unbroken crust having no loose particles on the surface. These cases are relevant to many kinds of resuspension problems. A paper is being written discussing the results of the study.

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[11]SENSIT is a trademark of Sensit Company.

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 evaluating models and simulation techniques that are used to assess, develop, or revise national, state, and local 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 Notice of Final Rulemaking

Section 110 (a) 2 (d) of CAA 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. EPA issued a Notice of Proposed Rulemaking (NPR) in November 1997, which proposed that 22 States and the District of Columbia each controls emissions that significantly contribute to nonattainment of the ozone NAAQS in other *downwind* States. This proposal was based on air quality modeling results from the Ozone Transport Assessment Group.

After issuing the SIP Call NPR, EPA received numerous public comments calling for a more refined set of air quality modeling to provide the technical basis for determining the States that contribute significantly to ozone in other States. In response to these comments, EPA performed State-specific modeling to support the final determination of the significant contributions. This included both *zero-out* model runs using the UAM-V model and *source apportionment* model runs using the CAMx model. In *zero-out* modeling, all manmade emissions were removed from each State in separate runs. The ozone predictions from each of these runs were compared to a base case to estimate the impact of emissions from the zero-out State on ozone predictions in other States in the modeling domain. In source apportionment modeling, ozone formed from manmade emissions in each State was tracked during the model simulation to determine the hourly contributions to selected nonattainment receptor areas in other States.

The results of both types of State-by-State model runs were determined using several *metrics*, or measures of contribution. The metrics were selected to provide quantitative information for three key contributing factors: the magnitude of the contribution, frequency of the contribution, and amount of the contribution relative to the level of nonattainment in the receptor area. Metrics were prepared for specific *upwind State to downwind area* linkages (*e.g.*, Ohio's contribution to nonattainment in New York City). The results were evaluated to determine whether the contributions — estimated for each linkage — were significant. The findings of this State-specific assessment confirmed 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. The Notice of Final Rulemaking was signed by EPA on September 24, 1998, and States named as significant contributors have one year to develop and submit emission control plans that will reduce nitrogen oxide emissions to levels prescribed by EPA.

2.5.1.2 Assessments of Air Toxics on Urban and National Scales

The EPA Urban Air Toxics strategy is in response to a Congressional mandate in CAA to reduce public exposure to air toxics in urban areas. Air toxics are those pollutants known to cause, or suspected of causing, cancer or other serious health effects. To support the strategy, the Branch conducted a study to determine ambient concentrations of five pollutants — Benzene, 1,3 Butadiene, Formaldehyde, Polycyclic Organic Matter, and Chromium (U.S. Environmental Protection Agency, 1998a) — and to estimate ambient air toxics concentrations in two pilot cities, Phoenix and Houston, using the Industrial Source Complex (ISC) model. The advantage of using the ISC model is its ability to estimate concentration gradients near point and area sources (Figure 1). A statistical technique was developed to reduce the number of receptors in the urban areas. A simplified approach was tested for estimating the impact of secondary production of formaldehyde based upon the pollutant half-life. Study results showed that air toxics impacts are very localized and that models should be able to estimate concentrations as close as plant fence line distances when the commensurate emissions inventory input is available. The draft report underwent a technical peer review and peer reviewer comments will be incorporated before releasing the study. Results from the study are being used to develop guidance to state and local air pollution agencies on air toxics model applications in urban areas.

EPA also developed a new air quality model, the Cumulative Exposure Project (CEP) that could provide a screening-level estimate of toxic air pollutant concentrations across the nation. The Branch successfully tested CEP, developed a user's guide, and provided training to state and local air pollution control agencies (Systems Applications International, 1998). Efforts are now underway to develop an emission preprocessing system that can be easily used to test the EPA control strategy options. Future activities include enhancing the scientific basis of the model by adding improved deposition algorithms and addressing the impact of secondary transformations.

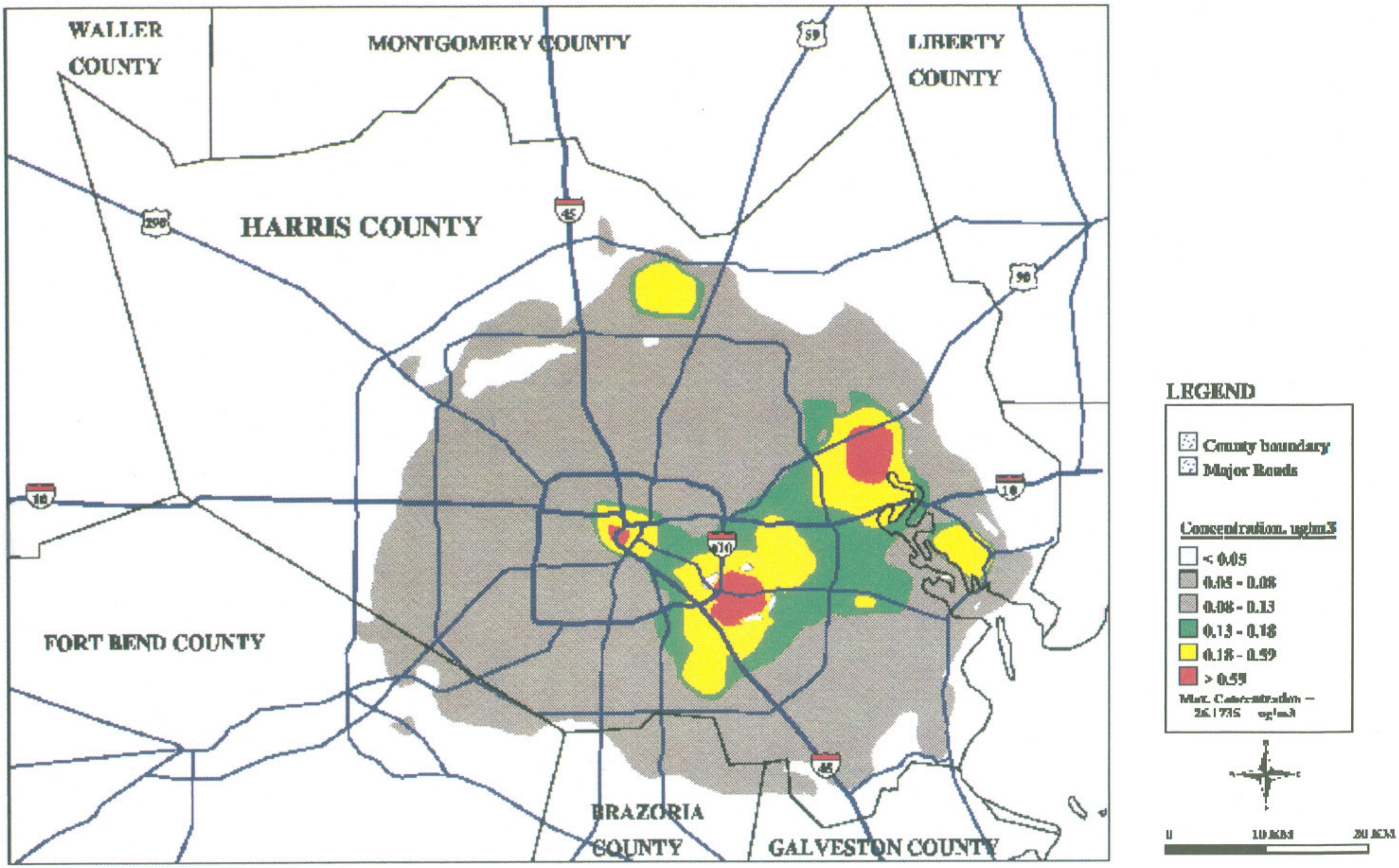

Figure 1 Isopleths of Annual Average Concentrations of 1,3 Butadiene in Houston, Texas, 1987-1991

2.5.1.3 Statistical Evaluation of Model Performance

Within the American Society for Testing and Materials (ASTM) a Standard Practice (Z6849Z) is being developed to provide an objective statistical procedure for comparing air quality simulation modeling results with tracer field data. The practice is limited to steady-state local-scale transport from isolated point sources in simple terrain. Statistical evaluation of model performance is viewed as part of a larger process that collectively is referred to as model evaluation. Two major considerations in developing the statistical comparison measures are that deterministic steady-state dispersion models provide estimates of the average concentration for the specified meteorological conditions, and that the large differences seen in comparisons 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 the variance is considered inherent because it cannot be reduced significantly by improving the physics of the air quality models. The goal of the practice is to select a model whose results are the closest to the observed average result, and to determine which results of other models are significantly different from the selected model using an objective statistical significance test.

To compare simulation results with an observed average result, the practice begins by stratifying the experimental observations into regimes, in which the physical processes affecting the dispersion are similar. A regime is an estimate of an ensemble that refers to the infinite population of all possible realizations and is developed from a set of experiments having similar external conditions. Model performance is then assessed by its ability to replicate without bias the regime's characteristics (such as the average maximum, average lateral extent, or average crosswind integrated concentration). For each regime, comparisons can be made of the average of a model's estimates with the average derived from the group of observations. From a summary of these results across all the regimes, the model with the smallest combined value of the average absolute fractional bias and variance can be determined.

To illustrate how the evaluation methodology would work, the draft practice describes how comparisons could be made of model performance in estimating the average maximum centerline concentration. Irwin and Rosu (1998) tested various aspects of the draft practice up to and including the manner in which the experimental data should be processed to select receptors suitably close to the observed center of mass such that one could assume the observed concentration is representative of the centerline concentration. It was determined that a robust way to combine observed concentrations along arcs within a given regime was to use the computed center of mass from each arc as a common reference point, and by expressing the receptor positions relative to the center of mass seen for each experiment, the results from all the experiments within the regime could be combined. Once grouped in this manner, a lateral dispersion can be computed for all the results in the regime. This regime lateral dispersion, σ_y, can then be used to define for each experiment the receptors close (within $\pm 0.67\sigma_y$) to the center of mass. The statistical properties derived from these receptor concentration values are considered representative of centerline concentration values.

Irwin (1998) tested the remaining aspects of the draft practice, the summarization across all regimes such that one can conclude which of several models most consistently simulates the observed average result; the summarization to determine if the difference seen between models is significant; and the effect on conclusions reached in model performance of the differences seen in the resampling results when individual samples are taken versus a pair. In Irwin (1998), centerline concentrations measured during three field studies were compared with estimates from three steady-state plume models. From these results it was concluded that the evaluation methodology is capable of objectively discerning differences in the models' ability to estimate the centerline maximum concentration at the surface downwind from a point source release.

The results presented in Irwin (1998) and Irwin and Rosu (1998) provided a complete examination of the draft ASTM Standard Practice under development. The next steps include revising the practice to be consistent with the results and developing a numerical algorithm that can generate pseudo modeling results with known statistical properties. This last step will allow direct investigation of how discerning the developed evaluation procedures are, and provide a means for testing whether proposed future changes to the methodology are significant and therefore should be adopted.

The grouping of the data is a valuable and important feature of the draft practice, and yet it is inherently subjective and will likely cause concern. Stratifying the data into groups is a standard statistical technique to provide greater discernment in statistical significance tests. The data grouping allows the computation of an average characteristic (such as the centerline maximum concentration), for comparison with what the steady-state model is simulating. By making the basic statistical comparisons within each regime, model estimates and observations that have ostensibly similar meteorological conditions are compared. Since it is known how the models perform in each regime, it becomes obvious under what conditions the dispersion characterizations need improvement. Employing bootstrap resampling within each regime provides summary statistics for each regime. These summary statistics provide a means for performing an objective test of whether the differences between models in one or more of the regimes are statistically significant. Preliminary testing of alternative grouping criteria suggests that the relative ranking of performance between models remains the same. As promising as these preliminary results are, concern may be raised regarding the criteria used in selecting and grouping the data for analysis. For instance, the methodology assumes average characteristics of data grouped together are representative of a steady-state meteorological condition. If conditions were not steady-state over the sampling time of one or more of the experiments, should these experiments be used? It is believed that as the methodology receives broader use, experience will provide guidance on acceptable practices in grouping data for analysis.

2.5.1.4 Comparisons of CALPUFF Modeling System with Tracer Field Data

To assist EPA in proposing the CALPUFF modeling system (U.S. Environmental Protection Agency, 1995a; 1995b) for routine use in regulatory assessments, a series of studies are underway. This modeling system is composed of two parts: a meteorological processor, CALMET, and a puff dispersion model, CALPUFF. The diagnostic wind model in CALMET adjusts an initial guess field for terrain effects and divergence minimization to produce a three-dimensional wind field for each hour. CALPUFF is a multi-layer, multi-species non-steady-state puff dispersion model that simulates the effects of time- and space-varying meteorological conditions on pollutant transport, transformation, and removal. CALPUFF can be applied on scales from tens of meters from a source to hundreds of kilometers. It includes algorithms for such near-field effects as building downwash; a transitional buoyant and momentum plume rise; partial plume penetration; subgrid-scale terrain and coastal-interaction effects; and terrain impingement; and for such long-range effects as pollutant removal due to wet scavenging and dry deposition; chemical transformation; vertical wind shear; overwater transport; plume fumigation; and visibility effects of particulate matter concentrations.

There are very few intensive tracer field experiments available for investigating model simulations of mesoscale transport and dispersion. During FY-1998, comparisons were made for two field studies, one conducted in 1975 at the Savannah River Laboratory and a second conducted in 1980 near Norman, Oklahoma (Paumier and Brode, 1998).

CALPUFF dispersion model results were compared to observed tracer concentrations from a short-term field experiment conducted at the Savannah River Laboratory in South Carolina on December 10, 1975 (U.S. Department of Energy, 1978). The distance to the monitoring arc was approximately 100 kilometers. Two separate CALPUFF model runs were made using Pasquill-Gifford (PG) dispersion parameters, and dispersion coefficients from internally-calculated σ_v and σ_w from the micrometeorological variables calculated in CALMET (hereafter referred to as similarity dispersion). With only one realization from a 4-hour release for comparison, general conclusions regarding model performance were not possible. But the simulation results were in reasonable accord with the simulated maximum being within 40% of that observed and the location of the simulated maximum being within 20 degrees of that observed. These results were encouraging given that only routine National Weather Service (NWS) observations were employed in developing the meteorological fields.

Figure 2 shows the plots of the concentration estimates at the receptors (continuous curves) and the observed concentrations at the receptors (labeled points). The modeled peaks are 10° to 20° further to the south than the observed peak. It appears that the CALMET meteorology derived using routine NWS data was not able to characterize this initial difference in wind direction sufficiently to transport the plume more toward the north.

With only one realization for comparison, general conclusions regarding model performance are not possible. But the simulation results are in reasonable accord and do not suggest severe problems in the modeling system. It is encouraging that the correspondence is close since only routine NWS observations were employed in developing the meteorological fields.

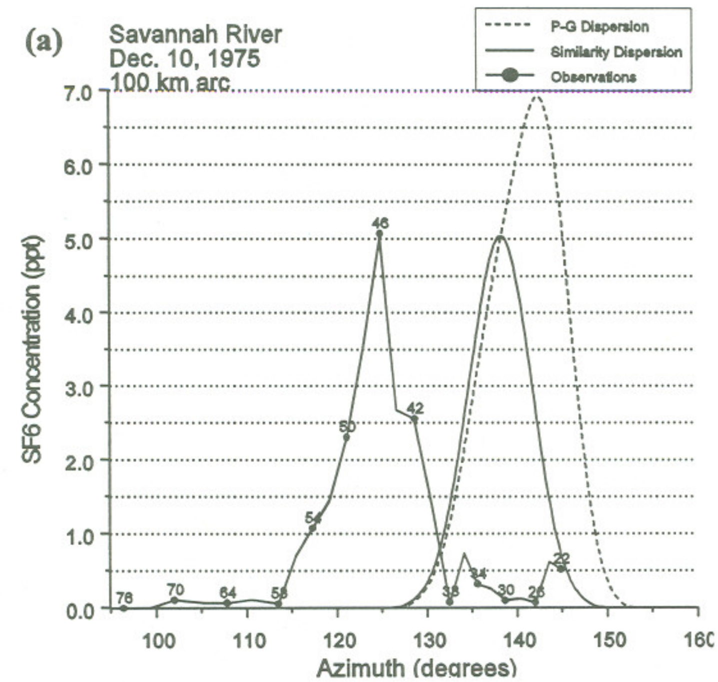

Figure 2. Simulated and observed seven-hour average concentration values along the sampling arc for the Savannah River Laboratory December 10, 1975, tracer field experiment.

CALPUFF dispersion model results were compared to observed tracer concentrations from a short-term field experiment (the Great Plains experiment) near Norman, Oklahoma (Ferber *et al.*, 1981) on July 8 and 11, 1980. This experiment examined long-range transport of inert tracer materials to demonstrate the feasibility of using other tracers as alternatives to the more commonly used SF_6. Several tracers were released for 3 to 4 hours and the resulting plume concentrations were recorded at an array of monitors downwind from the source. For the Great Plains experiment, arcs of monitors were located 100 and 600 kilometers from the source. For the July 8 experiment, sampling was conducted using two arcs of monitors: 100 km and 600 km. For the July 11 experiment, sampling was conducted on only the 100-km arc. Two separate CALPUFF model runs were made using PG dispersion parameters, and similarity dispersion. For both releases, the simulations overestimated the concentrations on the 100-km arc and underestimated the concentrations on the 600-km arc. Previous dispersion simulations for these experiments employing sophisticated meteorological modeling and Lagrangian particle simulation have encountered similar difficulties. It has been hypothesized that the effects of the nocturnal jet, which can be quite strong in this region of the United States, is not being properly simulated in the characterization of the dispersion meteorology. Even so, the CALPUFF simulations were encouraging in that they were similar to those obtained by the more sophisticated modeling.

2.5.1.5 CALPUFF Screening Model

For most of the modeling situations where a refined modeling technique is recommended by EPA for regulatory assessments, a screening analysis is also provided, which is meant to be easy to conduct and provide a worst-case maximum impact estimate. If the results of the screening analysis show compliance with existing regulatory requirements, then no further modeling is required. One of the most demanding tasks in performing refined puff model simulations is to develop a valid time and space varying characterization of the meteorological conditions. The processors that format and organize the input data to CALMET are not presently user-friendly and demand strong computer skills. CALPUFF has a built-in mode whereby it can use the meteorological data file generated for the ISCST3 model, which bypasses the need to run CALMET. Therefore, a study was conducted to see if screening estimates could be generated by CALPUFF through the use of ISCST3 meteorology. This screening methodology was designed for cases involving an isolated source, which is anticipated to have possibly large impacts on a protected Class I area that is at least greater than 50 km from the source.

A screening methodology was devised and tested in two ways: five years of hourly meteorology were used to develop data for assessing the year-to-year variability, and one year of hourly meteorology was fully processed through CALMET to assess whether the screening methodology devised provided greater concentration impacts than would be developed using a fully developed set of meteorology. There were reasonably large variations in the SO_2 concentration maxima from one year to the next. There are limitations to the conclusions that can be reached, because comparisons of results obtained using the new screening methodology versus results obtained using fully developed CALMET meteorology has only been conducted for one location and for one year. In all cases examined, situations could be found where the CALPUFF screening results underestimated the maximum impacts simulated using more fully developed (CALMET) meteorology as input to CALPUFF. However, it was concluded that the screening method that was tested does not guarantee that the pollutant impacts will always be greater than those obtained using refined meteorology. Whether this precludes its use is a judgement decision. There is a certain degree of conservatism inherent in the screening procedure tested, because the screening procedure requires use of receptor rings that completely surround the source being assessed, and it requires use of the maximum impact found anywhere along the receptor ring. In an actual situation, it is unlikely that the Class I area will completely surround the source being analyzed. It is more likely that the actual Class I area is limited to a small segment of a receptor ring. Thus, if actual refined (fully developed) meteorology were developed and used, along with actual source locations and receptors limited to the Class I area, the impacts simulated within the Class I may be considerably lower than those derived from the screening procedure for receptors that encircle the source.

2.5.2 Modeling Guidance

2.5.2.1 Support Center for Regulatory Air Models

During FY-1998, several activities were accomplished on the Support Center for Regulatory Air Models (SCRAM) Web site. The most significant activity was establishment of a new area, the *Regional Modeling Center* (RMC). RMC allows users to upload materials to an FTP area for exchange and dissemination of the latest regional modeling materials. Also, a general FTP area was added to the SCRAM Web site to facilitate the downloading of any SCRAM file. Two new areas were added to the SCRAM Model Support page. These areas are for Frequently Asked Questions (FAQs) and a Public Forum. The FAQ area addresses some of the more common questions, while the Public Forum area allows the user to pose questions or comments to other users. SCRAM downloads average about one thousand per week.

2.5.2.2 Workshop on Remote Sensing

A workshop to finalize guidance for on-site, upper-air meteorological monitoring was conducted July 20–22, 1998, in Research Triangle Park, North Carolina. The primary focus of the workshop was to create a draft document providing guidance on ground-based remote sensing of the atmospheric boundary layer. Workshop participants were provided copies of a mock-up for review prior to the workshop, and finalization of the document during the workshop. Participants in the workshop were selected for their expertise in ground-based remote sensing (*i.e.*, Doppler sodar and radar wind profilers) and use of upper-air data in regulatory applications. All relevant interest groups were represented: remote sensing equipment vendors; local, state, and Federal regulatory staff; the NOAA laboratories; university staff; and private consultants. The end product of the workshop was a revised Chapter 9 to the *On-Site Meteorological Program Guidance for Regulatory Modeling Applications*. This revised chapter is scheduled to be published in January 1999. A summary of the workshop is being prepared for a peer-reviewed journal.

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APPENDIX A: ACRONYMS, ABBREVIATIONS, AND DEFINITIONS

AERMIC	AMS/EPA Regulatory Model Improvement Committee
AERMOD	AMS/EPA regulatory model
AIM	Aerosol Inorganic Model
AIRS	Aerometric Information Retrieval System
AMS	American Meteorological Society
AMV	Air Management Version of Models-3 air quality model
ARL	Air Resources Laboratory (NOAA)
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
CALINE	CAlifornia LINE Source Dispersion model
CALMET	CALifornia METeorological model
CALPUFF	CALifornia PUFF model
CAMx	Comprehensive Air quality Model with eXtensions
CASTNet	Clean Air Status and Trends Network
CB-IV	Carbon Bond IV
CBL	Convective Boundary Layer
CCTM	CMAQ Chemistry-Transport Model
CD-ROM	Compact Disk - Read Only Memory
CEP	Cumulative Exposure Project
CFD	Computational Fluid Dynamics
CMAQ	Community Multiscale Air Quality model
CTM	Chemistry-Transport Model
CVS	Concurrent Versions System
ECIP	Emissions-Chemistry Interface Processor
EDC	Endocrine Disrupting Chemical
EMEP	European Monitoring and Evaluation Program
ENSO	El Nino - Southern Oscillation
EPA	Environmental Protection Agency
EQUISOLV	Equilibrium Solver
FAQ	Frequently Asked Questions
FCMSSR	Federal Committee for Meteorological Services and Supporting Research
FDDA	Four-Dimensional Data Assimilation
FMF	Fluid Modeling Facility

FTP	File Transfer Protocol
FY	Fiscal Year
HAPEM	Hazardous Air Pollutant Exposure Model
HPCC	High Performance Computing and Communications program
HTML	HyperText Markup Language
HWIR	Hazardous Waste and Identification Rule
ICMSSR	Interdepartmental Committee for Meteorological Services and Supporting Research
ICON	Initial CONditions processor
IDA	Inventory Data Analyzer
I/O API	Input/Output Applications Program Interface
IMPROVE	Interagency Monitoring of PROtected Visual Environments
ISC	Industrial Source Complex model
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
MARS-A	Model for an Aerosol Reacting System - A
MAQSIP	Multiscale Air Quality SImulation Platform
MCIP	Meteorology-Chemistry Interface Processor
MEND-TOX	Multimedia hybrid compartmental model
MEPPS	Models-3 Emission Processing and Projection System
MIRAGE	Megacity Impact on Regional And Global Environment
MM5	Mesoscale Meteorological Model - Version 5
MM5PX	Modified MM5 for land-surface effects
Models-3	Third generation air quality modeling system
NAAQS	National Ambient Air Quality Standards
NARSTO	North American Research Strategy for Tropospheric Ozone
NARSTO-NE	NARSTO-NorthEast
NATO/CCMS	North Atlantic Treaty Organization Committee on Challenges of Modern Society
NCAR	National Center for Atmospheric Research
NDVI	Normalized Difference Vegetative Index
NERL	National Exposure Research Laboratory (EPA)
netCDF	network Common Data Form
NOAA	National Oceanic and Atmospheric Administration
NPR	Notice of Proposed Rulemaking
NSTC	National Science and Technology Council
NWS	National Weather Service
OAQPS	Office of Air Quality Planning and Standards (EPA)
OMB	Office of Management and Budget
OSW	Office of Solid Waste (EPA)

OZIE	OZark Isoprene Experiment
PAH	Polycyclic Aeromatic Hydrocarbon
PBL	Planetary Boundary Layer
PC	Personal Computer
PCB	PolyChloroBiphenyl
PCDD	PolyChlorinated Dibenzo-p-Dioxin
PCDF	PolyChlorinated DibenzoFuran
PDM	Plume Dynamics Model
PG	Pasquill-Gifford dispersion parameters
PinG	Plume-in-Grid algorithm
PM	Particulate Matter
QSSA	Quasi-Steady State Approximation
RADM	Regional Acid Deposition Model
RCRA	Resource Conservation and Recovery Act
RELMAP	REgional Lagrangian Model of Air Pollution
RMC	Regional Modeling Center
RPC	Rotated Principal Component
RPCA	Rotated Principal Component Analysis
RPM	Regional Particulate Model
SASWG	Standing Air Simulation Work Group
SBUV	Solar Backscattered Ultra-Violet radiometer
SCAPE	Simulating Composition of Atmospheric Particles at Equilibrium
SCRAM BBS	Support Center for Regulatory Air quality Models Bulletin Board System
SEQUILIB	Sectional EQUILIBrium
SIP	State Implementation Plan
SMOKE©	Sparse Matrix Operator Kernel Emission
SMRAQ	Seasonal Modeling of Regional Air Quality
SMVGEAR	A vectorized gear solver
SOS	Southern Oxidant Study
TEQ	Toxic EQuivalent
TOMS	Total Ozone Mapping Spectrometer
UAM-V	Urban Airshed Model - Variable grid
USGS	U.S. Geological Survey
US/USSR	United States/Union of Soviet Socialists Republics
UV	Ultraviolet
WWW	World-Wide Web

APPENDIX B: PUBLICATIONS

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APPENDIX C: PRESENTATIONS

Atkinson, D.A. Meteorological data issues. Presentation via telephone at the Region IV State/Local Modeling Workshop, Atlanta, GA, November 18, 1997.

Atkinson, D.A. Meteorological data issues. Presentation at the 1998 Regional, State, and Local Modelers Workshop in Orlando, FL, May 6, 1998.

Binkowski, F.S. Particulate matter modeling within the EPA Models-3 system. Presentation at the International Specialty Conference on $PM_{2.5}$: A Fine Particle Standard, Long Beach, CA, January 28, 1998.

Binkowski, F.S. Modeling particulate matter with the Models-3/CMAQ. Presentation of a series of four invited lectures at the Fraunhofer Institute for Atmospheric Environmental Research, Garmisch-Partenkirchen, Bavaria, Germany, March 30, March 31, April 1, and April 2, 1998.

Binkowski, F.S. Toward external mixtures using a modal approach. Presentation at the 17th Annual Conference of the American Association for Aerosol Research, Cincinnati, OH, June 24, 1998.

Bullock, O.R., Jr. Lessons learned from Lagrangian modeling of atmospheric mercury and their implications for a South Florida field study. Presentation at the South Florida Mercury Research Planning Meeting, Tallahassee and Wakulla Springs, FL, December 18, 1997.

Bullock, O.R., Jr. A strategy for using the Models-3/CMAQ for atmospheric mercury and atrazine modeling. Presentation at the Lake Michigan Mass Balance Science Review, Detroit, MI, June 23, 1998.

Bullock, O.R., Jr. Atmospheric reactions of mercury and other heavy metals. Presentation at the Workshop on Atmospheric Transport and Fate of Metals in the Environment, International Council on Metals and the Environment, Antwerp, Belgium, September 10, 1998.

Bullock, O.R., Jr. Science issues regarding the modeling of atmospheric mercury transport and deposition. Presentation at the Scientist-to-Scientist Meeting on Mercury and Dioxin Modeling Uncertainty, the EPA Office of Solid Waste, Crystal City, VA, September 24, 1998.

Byun, D.W. Models-3/Community Multiscale Air Quality modeling system. Presentation at the NCAR Development Group Meeting, Boulder, CO, August 24, 1998.

Ching, J.K.S. Models-3 Community Multiscale Air Quality modeling system for regional urban scale modeling of fine particulates. Presentation at the International Specialty Conference on $PM_{2.5}$: A Fine Particle Standard, Long Beach, CA, January 28, 1998.

Cooter, E.J. Estimations of contaminant emissions and relevant meteorological conditions for the Lake Michigan Mass Balance Study modeling effort. Presentation at the Fourth Annual Lake Michigan Mass Balance Technical Meeting, Milwaukee, WI, December 3, 1997.

Cooter, E.J., T. Scholtz, and O.R. Bullock, Jr. Methodology and framework for modeling atrazine and mercury deposition. Presentation at the Lake Michigan Mass Balance Project Science Review Panel, Detroit, MI, June 23, 1998.

Dennis, R.L. Improving air quality model evaluation capabilities. Seminar presented at the Brookhaven National Laboratory, Brookhaven, NY, October 29, 1997.

Dennis, R.L. Acid rain and beyond. Seminar presented at Duke University, Durham, NC, November 10, 1997.

Dennis, R.L. The atmospheric component of multimedia modeling of pollutants at regional scales. Seminar presented at North Carolina State University, Raleigh, NC, February 23, 1998.

Dennis, R.L. Atmospheric transport and fate and links to water resources. Presentation at the Water Resources Research Institute Annual Meeting, Raleigh, NC, April 1, 1998.

Dennis, R.L. Systems-level sensitivity analysis, response surface comparisons, and diagnostic testing for evaluation of Eulerian air quality models. Presentation at the Sensitivity Analysis of Model Output Meeting, Venice, Italy, April 20, 1998.

Dennis, R.L. The Models-3 framework and the Community Multiscale Air Quality Model. Presentation at the Photochemical Reactivity Workshop, Durham, NC, May 12, 1998.

Dennis, R.L. Overview of computer simulation in the improvement of environmental management. Presentation at the Environmental Summit 98, Research Triangle Park, NC, May 12, 1998.

Gillette, D.A. Resuspension research. Presentation at the Carlsbad Environmental Monitoring and Research Center, Carlsbad, NM, October 13, 1997.

Gillette, D.A. Possible wind erosion contributions to South Florida aerosol deposition of phosphorus. Presentation at the South Florida Water Management District, West Palm Beach, FL, October 22, 1997.

Gillette, D.A. Review of Columbia Plateau PM_{10} Project. Presentation at Washington State University, Pullman, WA, November 29, 1997.

Gillette, D.A. Effects of soil crusting on dust emissions at Owens Lake. Presentation at the Great Basin Unified Air Pollution Control District, Bishop, CA, May 1, 1998.

Gillette, D.A. A strategy to compute dust concentrations in Kuwait during the Gulf War, 1991. Presentation at the Aberdeen Proving Grounds, U.S. Army, MD, June 7, 1998.

Godowitch, J.M. Modeling tall stack pollutant plumes for air quality simulations. Presentation at the Department of Civil & Environmental Engineering, Duke University, Durham, NC, October 17, 1997.

Huber, A.H. Contributions to human exposure of air pollutants from motor vehicles within an urban area. Presentation at the Annual Meeting of the International Society of Exposure Analysis, Research Triangle Park, NC, November 3, 1997.

Huber, A.H. Trends in urban CO. Presentation at the International Conference on Atmospheric Carbon Monoxide and its Environmental Effects, Portland, OR, December 3, 1997.

Irwin, J.S. AERMOD developments. Presentation at the Second Annual GMU/DSWA Transport and Dispersion Modeling Workshop, Fairfax, VA, July 29, 1998.

Irwin, J.S. The CALPUFF modeling system and use of mesoscale meteorological products. Presentation at the Second Annual GMU/DSWA Transport and Dispersion Modeling Workshop, Fairfax, VA, July 30, 1998.

Irwin, J.S. Use of mesoscale meteorological output by CALMET. Presentation at the WESTAR Mesoscale Model Workshop, Salt Lake City, UT, August 18, 1998.

LeDuc, S., and J.S. Irwin. Overview of regulatory approaches and current issues in air pollution meteorology. Short Course on Air Pollution Meteorology at the Annual Meeting of the American Meteorological Society, Phoenix, AZ, January 11, 1998.

Novak, J.H. Data management in Models-3. Presentation at the EPA Office of Research and Development, Scientific Information Management Coordination Board Meeting, Washington, DC, December 9, 1997.

Novak, J.H. Multimedia integrated modeling system architectural concepts. Presentation at the Software Engineering Institute, Pittsburgh, PA, March 27, 1998.

Novak, J.H. Current development of Models-3 and plans for a Multimedia Integrated Modeling System. Presentation to NOAA ARL Headquarters, Washington, DC, April 14, 1998.

Novak, J.H. Multimedia Integrated Modeling System development. Presentation at the Second Annual NERL Research Planning Meeting, Research Triangle Park, NC, March 30, 1998.

Novak, J.H. Current development of Models-3 and plans for a Multimedia Integrated Modeling System. Briefing for the Assistant Administration, National Weather Service, National Oceanic and Atmospheric Administration, Research Triangle Park, NC, May 22, 1998.

Novak, J.H. The EPA HPCC program budget plans. Presentation at the Computing, Information, and Communication Research and Development Committee Meeting, Washington, DC, September 16, 1998.

Novak, J.H., and J.M. Johnston. A community basis for complex system modeling: Evolution and involvement using problem solving environments. Keynote address at the Complex Systems Modeling Conference, New Orleans, LA, July 13, 1998.

Novak, J.H., and F.A. Schiermeier. Status of NERL HPCC and Models-3 research programs. Briefing for the Deputy Assistant Administrator for Science, Office of Research and Development, U.S. Environmental Protection Agency, Washington, DC, December 10, 1997.

Perry, S.G. Description and evaluation of AgDrift Spray Drift Model. Presentation to the Science Advisory Panel, Washington, DC, December 12, 1997.

Perry, S.G. Description and training on AERMOD model. Presentation at the Regional/State Modelers Workshop, Orlando, FL, May 5, 1998.

Perry, S.G. Division modeling activities. Presentation at the Regional/State Modelers Workshop, Orlando, FL, May 7, 1998.

Petersen, W.B. Physical modeling of atmospheric flows. Presentation at the Second Annual GMU/DSWA Transport and Dispersion Modeling Workshop, Fairfax, VA, July 29, 1998.

Pleim, J.E. Recent developments in meteorological modeling for AQ modeling. Presentation at the Second NOAA Mesoscale Modeler's Workshop, Boulder, CO, October 22, 1997.

Pleim, J.E. Modeling and field measurements of surface fluxes of heat, moisture, and pollutant dry deposition. Seminar presented at Huntsville, AL, December 16, 1997.

Pleim, J.E. Modeling springtime vegetation green-up in a Mesoscale Meteorology Model. Presentation at the American Geophysical Union Spring Meeting, Boston, May 27, 1998.

Poole-Kober, E.M. Sharing cultural information through collaboration in the era of high tech. Presentation at the Eighth Annual Meeting of SAIL, Nova Southeastern University Oceanographic Center, Dania, FL, April 15–17, 1998.

Poole-Kober, E.M. Sharing cultural differences to support collaborative learning. Panel presentation at the ASIS '98 Mid-Year Meeting, Orlando, FL, May 16–20, 1998.

Schere, K.L. Interface of atmospheric sciences and air quality management. Presentation at Duke University, Durham, NC, November 4, 1997.

Schere, K.L. Status of the NARSTO assessment. Presentation at the NARSTO Science Symposium, West Palm Beach, FL, November 17, 1997.

Schere, K.L. Status of NARSTO assessment. Presentation at No_x/VOC Science Symposium at Atmospheric Environment Service/Environment Canada, Toronto, Canada, December 3, 1997.

Schere, K.L. Research implications of new air quality standards. Presentation at the DOE Atmospheric Chemistry Meeting, Tysons Corner, VA, February 26, 1998.

Schere, K.L. Status of the NARSTO assessment. Presentation at the NARSTO Executive Assembly, the White House Conference Center, Washington, DC, March 2, 1998.

Schere, K.L. Status of NARSTO assessment. Presentation at the National Research Council Meeting, Washington, DC, March 3, 1998.

Schere, K.L. Status of Models-3. Presentation to SASWG/SAEWG by teleconference, April 2, 1998.

Schere, K.L. Status of the NARSTO assessment and a Models-3/CMAQ update. Presentation at the MARAMA Regional Modeling and Data Analysis Workshop, Silver Spring, MD, May 28, 1998.

Schiermeier, F.A. Proposed upgrade and location of the EPA high performance computing equipment to meet Agency needs. Briefing for the Acting Assistant Administrator, Office of Research and Development, U.S. Environmental Protection Agency, Washington, DC, October 9. 1997.

Schiermeier, F.A. Models-3 beta test and community modeling system. Presentation at the Standing Air Simulation Work Group Meeting, Grand Rapids, MI, October 24, 1997.

Schiermeier, F.A. Demonstration of the EPA Supercomputer Visualization Laboratory. Briefing for U.S. Congressional staffers, House Committee on Science, and Senate Committee on Environment and Public Works, Research Triangle Park, NC, January 6, 1998.

Schiermeier, F.A. Overview of Atmospheric Modeling Division research programs. Briefing for surveys and investigations staff, U.S. House Appropriations Committee, Research Triangle Park, NC, February 2, 1998.

Schiermeier, F.A., and E. Baldridge. Status of Models-3 community modeling and analysis systems. Presentation at the Standing Air Simulation Work Group Meeting, Point Clear, AL, April 3, 1998.

Schiermeier, F.A. Overview of Atmospheric Sciences Modeling Division research programs. Briefing for the Directors of the NOAA Office of Air and Radiation, Environmental Research Laboratories, and Air Resources Laboratory, Research Triangle Park, NC, May 22, 1998.

Schiermeier, F.A. Description of Atmospheric Modeling Division regional and mesoscale modeling activities. Presentation at the Twentieth US/Russia Working Group Meeting on Air Pollution Modeling, Instrumentation, and Measurement Methodology, Main Geophysical Observatory, St. Petersburg, Russia, July 1, 1998.

Schiermeier, F.A. Atmospheric Modeling Division budgets and programs. Briefing for the Office of Management and Budget, Office of Research and Development Examiner, Research Triangle Park, NC, July 23, 1998.

Schiermeier, F.A. Overview of support and planning of future ITMs. Presentation at the Twenty-Third NATO/CCMS International Technical Meeting on Air Pollution Modeling and Its Application, Varna, Bulgaria, September 30, 1998.

Streicher, J.J. Air concentrations and inhalation exposure to pesticides in the AHS. Presentation at the Human Exposure Program Peer Review, Research Triangle Park, NC, October 30,1997.

Streicher, J.J. A comparison of total column ozone from EPA's Brewer spectrophotometer network with SBUV/2 satellite data: Applications to mid-Atlantic UV stressor profiles. Presentation at the SETAC Symposium, Seattle, WA, August 17, 1998.

Zelenka, M.P. Air toxics. Presentation at the Human Exposure Program Peer Review, Research Triangle Park, NC, October 30, 1997.

Zelenka, M.P. Human exposure modeling. Presentation to the Human Exposure Program Peer Review, Research Triangle Park, NC, October 30, 1997.

Zelenka, M.P. Urban carbon monoxide concentrations and trends in Denver, CO. Presentation to the EPA Science Advisory Board for latest edition of the *Air Quality Criteria Document for Carbon Monoxide*, Research Triangle Park, NC, December 16, 1997.

APPENDIX D: WORKSHOPS AND MEETINGS

Data or Information: the Fading Boundaries, 23rd Annual IAMSLIC (International Association of Aquatic and Marine Science Libraries and Information Centers) Conference, College of Charleston, Charleston, SC, October 5–6, 1997.

E.M. Poole-Kober

Atmospheric Deposition into South Florida – Measuring Net Atmospheric Inputs of Nutrients, South Florida Water Management District, October 20–22, 1997.

D.A. Gillette

NOAA Mesoscale Modelers Workshop, Boulder, CO, October 22–23, 1997.

D.W. Byun
J.K.S. Ching
J.E. Pleim

Gulf of Mexico Modeling Meeting, Stennis Space Center, MS, October 28, 1997.

O.R. Bullock, Jr.

Meeting on South Florida Mercury Study, Ann Arbor, MI, November 6–7, 1997.

O.R. Bullock, Jr.

NOAA Assessment of Atmospheric Contribution to Coastal Nitrogen, Sarasota, FL, November 16–20, 1997.

R.L. Dennis

NARSTO 1997 Science Symposium, West Palm Beach, FL, November 16–20, 1997.

J.E. Pleim
K.L. Schere

Wildland Fire and Air Quality Workshop, Nebraska City, NE, November 17–21,1997.

J.K.S. Ching

ORD Workshop II – Hearing the Voice of ORD, Williamsburg, VA, December 1–4, 1997.

T.L. McDuffie
E.M. Poole-Kober
S.J. Roselle

Fourth Annual Technical Meeting for Lake Michigan Mass Balance Study, Milwaukee, WI, December 2–3, 1997.

O.R. Bullock, Jr.
E.J. Cooter

International Conference on Atmospheric Carbon Monoxide and its Environmental Effects, Portland State University, December 3–6, 1997.

A.H. Huber

Presidential Advisory Committee Meeting on High Performance Computing and Communications, Information Technology, and the Next Generation Internet, Washington, DC, December 9–10, 1997.

J.H. Novak
F.A. Schiermeier

South Florida Mercury Research Planning Meeting, Tallahassee, FL, December 17–21, 1997.

O.R. Bullock, Jr.

Eco Assesment/Eco Indicators STAR Grant Program Review Meeting, Las Vegas, NV, February 2–6, 1998.

O.R. Bullock, Jr.

CRC Air Quality Modeling Group Meeting, Washington, DC, February 5–6, 1998.

J.E. Pleim

EPA Panel Discussion with Presidents of Historically Black Colleges and Universities, Research Triangle Park, NC, February 18, 1998.

F.A. Schiermeier

DOE Atmospheric Chemistry Program Meeting, Tysons Corner, VA, February 26–27, 1998.

K.L. Schere

Workshop on the User Requirements of a Regional Re-analysis, Norman, OK, February 26–27, 1998.

D.W. Byun

NARSTO Executive Assembly Meeting, Washington, DC, March 2–3, 1998.

K.L. Schere

National Research Council Committee Meeting, Washington, DC, March 3, 1998.

K.L. Schere

Environmental Multimedia Analysis of Chemical Distribution, National Exposure Research Laboratory, Research Triangle Park, NC, March 31–April 3, 1998.

E.J. Cooter
W.B. Petersen
D.B. Schwede

NARSTO Synthesis Meeting, Dallas, TX, March 30–April 1, 1998.

K.L. Schere

Water Resources Research Institute Annual Meeting, Raleigh, NC, April 1, 1998.

R.L. Dennis

Information Systems in the Electronic Age, Eighth Annual Meeting of SAIL (Southeast Affiliate of IAMSLIC Libraries), Nova Southeastern University Oceanographic Center, Dania, FL, April 15–17, 1998.

E.M. Poole-Kober

Sensitivity Analysis of Model Output Meeting, Venice, Italy, April 16–22, 1998.

R.L. Dennis

Annual ASTM Committee Meetings, Atlanta, GA, April 19–22, 1998.

J.S. Irwin

New Directions in Desert Surficial Processes and Landscape Dynamics on Military Lands, Zzyzx, CA, April 26–30, 1998.

D.A. Gillette

Fourth National Health & Environmental Effects Laboratory Symposium on Research Advances in Risk Assessment, Cary, NC, April 27–30, 1998.

D.W. Byun

Regional/State Modelers' Annual Meeting, Orlando, FL, May 4–8, 1998.

D.A. Atkinson
D.T. Bailey (Telephone Briefing)
J.S. Irwin
S.G. Perry
J.S. Touma (Telephone Briefing)

Photochemical Reactivity Workshop, Durham, NC, May 12–14, 1998.

D.W. Byun
J.K.S. Ching
R.L. Dennis
K.L. Schere

Collaboration Across Boundaries: Theories, Strategies, and Technology, ASIS (American Society for Information Science) Mid-Year 1998 Meeting, Orlando, FL, May 16–20, 1998.

E.M. Poole-Kober

$PM_{2.5}$ Monitoring Workshop, Cary, NC, May 20–21, 1998.

D.A. Gillette
R.E. Lawson
R.S. Thompson

PM_{10} Research, Fluid Modeling Facility, Research Triangle Park, NC, May 22, 1998.

D.A. Gillette

NARSTO Model Intercomparison Workshop, Washington, DC, May 27–28, 1998.

K.L. Schere

MARAMA Regional Modeling and Data Analysis Workshop, Silver Spring, MD, May 28–29, 1998.

K.L. Schere

Natural Mercury Emissions Workshop, University of Guelph, Guelph, Ontario, Canada, May 30– June 1, 1998.

O.R. Bullock, Jr.

MM5 Users, Real-Time Modeling, and Verification Workshop, Boulder, CO, June 15–19, 1998.

T.L. Otte

Planning meeting for new vertical transport and mixing initiative at PNNL, Richland, WA, June 23–24, 1998.

J.E. Pleim

Workshop on Remote Sensing of the Atmospheric Boundary Layer in Support of Air Quality Modeling, Research Triangle Park, NC, July 20–22, 1998.

D.T. Bailey
J.S. Irwin
K.L. Schere

PM Measurements Research Workshop, Chapel Hill, NC, July 22–23, 1998.

F.S. Binkowski
J.K.S. Ching
S.K. LeDuc
J.E. Pleim
K.L. Schere
F.A. Schiermeier

The Second Annual GMU/DSWA Transport and Dispersion Modeling Workshop, Fairfax, VA, July 29–30, 1998.

J.K.S. Ching
J.S. Irwin
W.B. Petersen

NARSTO Assessment Meeting, Albany, NY, August 17–18, 1998.

K.L. Schere

SETAC Symposium on Multi-Media Ecosystem Modeling, Seattle, WA , August 17–19, 1998.

O.R. Bullock, Jr.

AMS Conference on Cloud Physics, Everett, WA, August 17–22, 1998.

S.J. Roselle

WESTAR Mesoscale Model Workshop, Salt Lake City, UT August 19–20, 1998.

J.S. Irwin

Planning Meeting for the Integrated Mesoscale Observing and Prediction System Initiative, Boulder, CO, August 24–26, 1998.

D.W. Byun

Specialty Conference on Measurement of Toxic and Related Air Pollutants, Cary, NC, September 1–3, 1998.

F.S. Binkowski
O.R. Bullock, Jr.
D.W. Byun
J.K.S. Ching
E.J. Cooter
B.K. Eder
J.M. Godowitch
B.L. Orndorff
J.E. Pleim
S.J. Roselle
K.L. Schere
F.A. Schiermeier

WRAP (Western Regions Air Partnership) Workshop: Visibility and AQ Issues in the Western States, Albuquerque, NM, September 17–18, 1998.

J.K.S. Ching

NOAA Assessment of Atmospheric Contribution to Coastal Nitrogen, Block Island, RI, September 16–20, 1998.

R.L. Dennis

Megacity Impact on Regional and Global Environments Reviewers Meeting, Boulder, CO, September 30–October 2, 1998.

R.L. Dennis

APPENDIX E: VISITING SCIENTISTS

1. Dr. Ingmar Ackermann
   Ford Research Center
   Aachen, Germany

Dr. Ackermann visited the Division from October 21 to 24, 1997, to coordinate work on the CMAQ aerosol component, which he is using in his modeling studies of PM in Europe.

2. Dr. Arastoo Biazar
   University of Alabama – Huntsville
   Huntsville, AL

Dr. Biazar visited the Division from October 14 to 16, 1997, to collaborate on the Plume-in-Grid effort for Models-3.

3. Ms. Pam Brodowicz, and Mr. Rich Cook
   U.S. EPA, Office of Mobile Sources
   Ann Arbor, MI

Ms. Brodowicz and Mr. Cook visited the Division on February 25, 1998, to discuss human exposure modeling work being done in the National Urban Air Toxics Study.

4. Dr. Yoram Cohen
   University of California – Los Angeles
   Los Angeles, CA

Dr. Cohen visited the Division from March 30 to April 3, 1998, to teach a multimedia class and discuss research issues.

5. Dr. Chris Frey
   North Carolina State University
   Raleigh, NC

Dr. Frey visited the Division on March 5, 1998, to discuss the Model Uncertainty project.

6. Dr. Chris Fung
   Senior Environmental Protection Officer, Air Quality Group
   Hong Kong Government
   Hong Kong, People's Republic of China

Dr. Fung visited the Division from October 16 to 17, 1997, to discuss air quality modeling issues.

7. Dr. Heinz Hass
   Ford Research Center
   Aachen Germany

Dr. Hass visited the Division from March 26 to 27, 1998, for a meeting on air quality modeling at the Ford Research Center.

8. Dr. Shobha Kondragunta
   Department of Meteorology
   University of Maryland
   College Park, MD

Dr. Kondragunta visited the Division on November 14, 1997, and presented a seminar on the impact of aerosols on urban photochemical ozone production.

9. Drs. Marcelo Korc, and Robert Romano
   Pan American Health Organization
   Washington, DC

Drs. Korc and Romano visited the Division on August 31, 1998, to discuss modeling air quality in Latin America.

10. Sang-Mi Lee
    Department of Atmospheric Sciences
    College of Natural Science
    Seoul National University
    Kwanak-gu, Seoul, Korea

Ms. Sang-Mi Lee worked at the Division from January 15 to July 2, 1998, with Dr. D.W. Byun and focused on testing mass conservation properties of numerical advection algorithms used in the Models-3/CMAQ CTM.

11. Dr. Judy Nyquist
    National Research Council
    Washington, DC

    Dr. Martin Williams
    U.K. Department of Environment Transport and the Regions
    London, England

Drs. Nyquist and Williams visited FMF on November 19, 1997, for a tour of the facility.

12. Dr. Joe Friday
Director, OAR
NOAA
Silver Spring, MD

Dr. James Rasmussen
Director, ERL
NOAA
Silver Spring, MD

Mr. Bruce Hicks
Director, ARL
NOAA
Silver Spring, MD

Mr. Richard Artz
Deputy Director, ARL
NOAA
Silver Spring, MD

Drs. Friday and Rasmussen, and Messrs. Hicks and Artz visited the Division on June 15, 1998, for a tour of the facility and demonstrations.

13. Drs. W.H. Snyder, and Paul Hampton
University of Surrey
Guildford, Surrey
England

Drs. Snyder and Hampton visited FMF on December 1, 1997, to discuss fluid modeling studies.

14. Dr. Sugiyama
Japan Automobile Research Institute
Tsukuba, Japan

Dr. Sugiyama visited the Division on October 22, 1997, to exchange information on EPA research and the Japan Clean Air Program.

15. Dr. Itsushi Uno
National Institute for Environmental Studies
Onogawa, Tsukuba, Japan,

Dr. Uno visited the Division from February 12 to 13, 1998, to discuss air quality modeling issues.

16. Dr. Shinji Wakamatsu
National Institute for Environmental Studies
Onogawa, Tsukuba, Japan

Dr. Wakamatsu visited the Division from January 13 to February 3, 1998, to meet and discuss scientific issues.

17. Dr. J.C. Weil
Cooperative Institute for Research in Environmental Sciences
University of Colorado
Boulder, CO

Dr. W.H. Snyder
University of Surrey
Guildford, Surrey
England

Drs. Weil and Snyder visited FMF from October 9 to 10, 1997, to analyze and discuss results of convection lab experiments.

18. Dr. J.C. Weil
Cooperative Institute for Research in Environmental Sciences
University of Colorado
Boulder, CO

Dr. A. Venkatram
University of California
Riverside, CA

Mr. Robert Paine
ENSR
Acton, MA

Drs. Weil and Venkatram, and Mr. Paine visited the Division from December 17 to 19, 1997, to further develop the AERMOD model.

19. Dr. Julian Wilson
European Commission
Environment Institute TP 460
Ispra(Va), Italy

Dr. Wilson visited the Division on February 17, 1998, to discuss Models-3.

20. Professor Soon C. Yoon
Seoul National University
Kwanak-gu, Seoul, Korea

Dr. Yoon visited the Division on June 29, 1998, to discuss Ms. Sang-Mi Lee's research progress.

APPENDIX F: HIGH SCHOOL, UNDERGRADUATE, AND GRADUATE STUDENTS, AND POSTDOCTORAL RESEARCHERS

1. Dr. Jeffrey R. Arnold
   University Corporation for Atmospheric Research (UCAR)
   Boulder, Colorado

Dr. Arnold, a postdoctoral researcher, is in his second year with the Atmospheric Sciences Modeling Division. Dr. Arnold is developing more advanced methods to extend the state of the art of diagnostic model evaluation applicable to complex, nonlinear photochemical models, to codify the new evaluation techniques and make weight of evidence approaches objective.

2. Conan Morgan
   Garner High School
   Garner, NC 27529

Mr. Morgan, a senior high school student, was an intern from June 15 through August 26, 1998, in the Atmospheric Sciences Modeling Division under the EPA/Shaw University Research Apprenticeship Program for Culturally Diverse High School Students.

3. Lucy Reid
   School of Information and Library Science
   University of North Carolina at Chapel Hill
   Chapel Hill, NC

Mrs. Reid completed a field experience during the period from May 21 through June 25, 1998, observing in the Division's special library and assisting the Librarian with reference questions and interlibrary loans. For the field experience project, Mrs. Reid cataloged books and created a database of theses and dissertation titles held in the library's collection.

4. Dr. Qingyun Song
   Atmospheric Environment Service
   Ontario, Canada

Dr. Song worked as a postdoctoral researcher with the Division from August 1997 through August 1998. His research focused on development of a grid-resolved cloud model for CMAQ.

5. Dr. Gail S. Tonnesen
University Corporation for Atmospheric Research (UCAR)
Boulder, Colorado

Dr. Tonnesen, a postdoctoral researcher, completed her second year with the Atmospheric Sciences Modeling Division. Dr. Tonnesen investigated the identification of indicator ratios of ambient concentrations of photochemically active trace gases that might distinguish the sensitivity of the local production of ozone to NO_X and VOC emissions in the ambient atmosphere for the testing of air quality models. The tests were developed from theoretical considerations of atmospheric photochemistry.

APPENDIX G: ATMOSPHERIC SCIENCES MODELING DIVISION STAFF

All personnel are assigned to the U.S. Environmental Protection Agency from the National Oceanic and Atmospheric Administration, except those designated EPA, who are employees of the Environmental Protection Agency, or PHS, who are members of the Public Health Service Commissioned Corps.

Office of the Director

Francis A. Schiermeier, Supervisory Meteorologist, Director
Herbert J. Viebrock, Meteorologist, Assistant to the Director
Dr. Robin L. Dennis, Physical Scientist
Dr. Basil Dimitriades (EPA), Physical Scientist
Dr. Peter L. Finkelstein, Physical Scientist
Bruce W. Gay, Jr. (EPA), Program Manager
Evelyn M. Poole-Kober, Librarian
Julie Neal (EPA), Physical Science Technician (Summer)
Kent Parks (EPA), Library Technician (June)
Barbara R. Hinton (EPA), Secretary
B. Ann Warnick, Secretary

Atmospheric Model Development Branch

Kenneth L. Schere, Supervisory Meteorologist, Chief
Dr. Francis S. Binkowski, Meteorologist
O. Russell Bullock, Jr., Meteorologist
Dr. Daewon W. Byun, Physical Scientist
Dr. Jason K.S. Ching, Meteorologist
Dr. Brian K. Eder, Meteorologist
James M. Godowitch, Meteorologist
Dr. William Hutzell (EPA), Physical Scientist (Since September 1998)
Tanya Otte, Meteorologist (Since March 1998)
Dr. Jonathan A. Pleim, Physical Scientist
Shawn J. Roselle, Meteorologist
Jennifer Hehl (EPA), Physical Science Technician (Summer)
Tanya L. McDuffie, Secretary

Modeling Systems Analysis Branch

Joan H. Novak, Supervisory Computer Specialist, Chief
Dr. William G. Benjey, Physical Scientist
Steven C. Howard, Computer Specialist
Dr. Sharon K. LeDuc, Physical Scientist
Thomas E. Pierce, Meteorologist
John H. Rudisill, III, Equipment Specialist
Alfreida R. Torian, Computer Specialist
Gary L. Walter, Computer Scientist
Dr. Jeffrey O. Young, Mathematician
Jonathan Hill (EPA), Physical Science Technician (Summer)
Michael Keller (EPA), Computer Specialist (Summer)
Jamie Rhome (EPA), Physical Science Technician (Summer)
Carol C. Paramore, Secretary

Applied Modeling Research Branch

William B. Petersen, Supervisory Physical Scientist, Chief
Dr. Ellen J. Cooter, Meteorologist
Dr. Dale A. Gillette, Physical Scientist
Dr. Alan H. Huber, Physical Scientist
Robert E. Lawson, Jr., Physical Scientist
Dr. Steven G. Perry, Meteorologist
Donna B. Schwede, Physical Scientist
John J. Streicher, Physical Scientist
CDR. Roger S. Thompson (PHS), Environmental Engineer
Lawrence E. Truppi, Meteorologist
Robert Melvin (EPA), Physical Scientist (Summer)
Jonathan Petters (EPA), Engineering Technician (Summer)
Sherry A. Brown, Secretary

Air Policy Support Branch

Mark Evangelista, Supervisory Meteorologist, Chief (Since July 1998)
Dennis A. Atkinson, Meteorologist
Dr. Desmond T. Bailey, Meteorologist
John S. Irwin, Supervisory Meteorologist
Brian L. Orndorff, Meteorologist
Norman C. Possiel, Jr., Meteorologist
Jawad S. Touma, Meteorologist