AA Technical Memorandum OAR ARL-245

FISCAL YEAR 2001 SUMMARY REPORT OF THE NOAA ATMOSPHERIC SCIENCES MODELING DIVISION TO THE U.S. ENVIRONMENTAL PROTECTION AGENCY

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Atmospheric Sciences Modeling Division
Research Triangle Park, North Carolina

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noaa NATIONAL OCEANIC AND ATMOSPHERIC ADMINISTRATION / Oceanic and Atmospheric Research Laboratories

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UNITED STATES DEPARTMENT OF COMMERCE

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Secretary

NATIONAL OCEANIC AND ATMOSPHERIC ADMINISTRATION

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PREFACE

This document summarizes the Fiscal Year 2001 research and operational activities of the Atmospheric Sciences Modeling Division (ASMD), Air Resources Laboratory, working under Interagency Agreements EPA DW13938483 and DW13948634 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, atmospheric modeling, air pollution control activities, and abatement and compliance programs.

Established in 1955, the Division serves as the vehicle for implementing the agreements with EPA, which funds the research efforts in air pollution meteorology and atmospheric modeling. ASMD conducts research activities in-house and through contract and cooperative agreements for the EPA's National Exposure Research Laboratory and other EPA groups. With a staff consisting of NOAA and EPA, ASMD also provides technical information, observational and forecasting support, and consulting on all meteorological aspects of the air pollution control program to many EPA offices, including the Office of Air Quality Planning and Standards. The primary groups within ASMD are the Atmospheric Model Development Branch, Modeling Systems Analysis Branch, Applied Modeling Research Branch, and Air Policy Support Branch. The staff is listed in Appendix 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-E-243-02), U.S. Environmental Protection Agency, 109 T.W. Alexander Drive, Research Triangle Park, NC 27711.

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FISCAL YEAR 2001 SUMMARY REPORT OF THE NOAA ATMOSPHERIC SCIENCES MODELING DIVISION TO THE U.S. ENVIRONMENTAL PROTECTION AGENCY

ABSTRACT. During Fiscal Year 2001, the Atmospheric Sciences Modeling Division provided meteorological and air quality modeling assistance to the U.S. Environmental Protection Agency. This ranged from research studies and model applications to the provision of advice and guidance. Research efforts emphasized the development and evaluation of air quality simulation models. Among the research studies and results were the release of the FY-2001 version of the Community Multiscale Air Quality (CMAQ) modeling system, the integration of the Sparse Matrix Operator Kernel Emissions model into CMAQ, the inclusion of the aerosol algorithm into the Plume-in-Grid (PinG) model, the preliminary evaluation of the CMAQ particulate matter module, the continued evaluation and modification of CMAQ-Hg, development of the Multi-Layer Bio-Chemical dry deposition model, continuation of compartmental multimedia modeling, and development of a method for estimating the vertical flux of resuspended particles.

1. INTRODUCTION

In Fiscal Year 2001, 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 EPA and public and private research communities, the Division's primary efforts focused on studying processes affecting dispersion of atmospheric pollutants, modeling pollutant dispersion on all temporal and spatial scales, and developing multi-media modeling frameworks in a high performance computing and communications environment. The 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 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 the Challenges of Modern Society

The North Atlantic Treaty Organization (NATO) Committee on the 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 corrective action by member governments. The Committee's work is carried out on a decentralized basis through pilot studies, discussions on environmental issues, and fellowships.

The Division Director serves as the U.S. 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 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 former Division Director served as the Conference Chairman of the Millennium (24th) NATO/CCMS International Technical Meeting held in Boulder, Colorado, during May 15–19, 2000. The proceedings were published by Kluwer Academic/Plenum Publishers (*Air Pollution Modeling and Its Application XIV*, 2001).

2.1.2 United States/Russia Joint Environmental Committee

The former Division Director served 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 was 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-2001. An annual Working Group meeting was held during November 2000 at the Main Geophysical Observatory in St. Petersburg, Russia. The Russian scientists presented information regarding the development of a new version of the Russian regulatory dispersion model, which will be introduced next year as a national guideline. They informed the group about current work aimed at developing and generalizing a methodology for the computational and hybrid monitoring jointly using the results of measurements and computations. The Russian work in forecasting urban air pollution was outlined. An English version of the official report, *Air Quality in Major Russian Cities for Ten Years*, was presented.

The U.S. Co-Chairman informed his Russian counterparts about the latest developments in the implementation of the Models-3/Community Multiscale Air Quality (CMAQ) model. A computer demonstration was presented, which visualized the results of several application runs with Models-3/CMAQ. These runs illustrated the relative efficacies of different emission control strategies in improving ozone, visibility, acid deposition, and $PM_{2.5}$ in the eastern United States.

In recognition of the impending retirement of the U.S. Working Group Co-Chairman, a letter from the Head of the Russian Federal Service for Hydro-meteorology and Environmental Monitoring was presented by the Director of the Voeikov Main Geophysical Observatory. The letter acknowledged the organization and promotion of cooperation between Russian and American scientists working in the area of air pollution modeling and monitoring during the last fifteen years.

2.1.3 Interdepartmental Meteorological Committee

The Division Director serves as the U.S. Environmental Protection 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, 2001).

The Division Director also serves on the ICMSSR Committee for Cooperative Research. Other Division members serve on the ICMSSR Working Group for Atmospheric Transport and Diffusion and on the ICMSSR Working Group for Climate Services.

2.1.4 Board on Atmospheric Sciences and Climate

The Division Director serves as the Agency liaison to the Board on Atmospheric Sciences and Climate (BASC) of the National Research Council, National Academy of Sciences. The BASC seeks to advance our understanding of the atmosphere and climate, and to improve our ability to apply this knowledge for our benefit. The Board (1) reviews in broad perspectives both basic and applied research dealing with the atmosphere and with the geophysical systems influencing weather and climate; (2) provides advice and guidance to appropriate government agencies on problems and programs within the Board's interest and expertise; and (3) counsels the United States participation in international research and application programs relating to the atmosphere and climate such as the World Climate Program and its research activities.

2.1.5 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.

2.1.6 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 and there is now interest in fine particulates and toxic chemicals. 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.

2.1.7 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. The subcommittee has responsibility for advice and leadership on issues of atmospheric deposition to the watershed and the Bay, on overseeing application of the Extended Regional Acid Deposition Model (Extended RADM) to link atmospheric deposition with Bay watershed models, and in dealing with the potential role of atmospheric deposition reductions anticipated by the 1990 Clean Air Act Amendments (CAAA) 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 the Extended 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 their linkage with the Extended RADM and interpretation of the findings.

Work in FY-2001 with the Extended RADM focused on a re-evaluation of the potential magnitude of reductions in oxidized nitrogen deposition stemming from the CAAA and possible additional reductions from point sources beyond requirements of the CAAA. The CAAA reductions were associated with the new heavy duty diesel rule being promulgated by EPA for 2020 and the additional point source reductions were those being examined by the EPA Office of Air Programs, Clean Air Markets Division. The Extended RADM was also used to estimate the relative contribution each of the six Bay states' (Maryland, Pennsylvania, Virginia, New York, Delaware, and West Virginia) nitrogen oxide emissions make to the oxidized nitrogen deposition to the Chesapeake Bay major tributaries.

2.1.8 Regional Acid Deposition Model Application Studies

During FY-2001, an operational version of the Extended RADM, which operates on the Cray® T3D™[1] massively parallel computer, was finalized for use with adjusted ammonia emissions, using a primitive model inversion. The Extended RADM incorporates the full dynamics of secondary inorganic fine particle formation and is, therefore, able to simulate ammonia (reduced nitrogen) deposition in addition to oxidized nitrogen deposition, simulate the partitioning of total ammonia into gaseous ammonia and particulate ammonium, and the partitioning of total nitrate into gaseous nitric acid and particulate nitrate. The Extended RADM represents a step in the transition to Models-3/CMAQ for application simulations.

A Division scientist is participating in an integrated assessment of Shenandoah National Park that is being coordinated by the U.S. National Park Service. The first purpose of the assessment is to estimate how air pollution stressors will be reduced due to ozone and acid rain controls on air emissions that stem from CAAA and how ecosystem damage from ozone and acid

[1]Cray is a registered trademark and Cray T3D is a trademark of Cray Research.

rain will be changed or mitigated and second, and how air quality related values connected to visibility degradation will be affected. The second purpose of the assessment is to provide an approximate sense of how much farther air emissions would need to be reduced to provide full protection of the ecosystems from ozone and acid rain damage. During FY-2001, the Extended RADM was run in aggregation mode for a set of four future emission scenarios to define the changes in seasonal ozone, annual acidic deposition, and annual inorganic fine particulates relative to an updated 1990 base case consistent with the future scenarios. Extensive use of the EPA National Environmental Supercomputing Center (NESC) Cray® T3D™ computer resource was made. Two of the scenarios represented estimates of the effects of, first, acid rain controls and, second, acid rain mobile source Tier II standards, and new heavy duty diesel vehicle regulations. Two of the scenarios represented potential cases with extreme emissions reductions beyond those called for in the 1990 Amendments to the Clean Air Act (CAAA). The changes in air pollution stressor metrics over Shenandoah were then passed to the ecosystem modelers. In addition, the range of influence mappings from the RADM and Extended RADM were used to define airsheds for the Shenandoah National Park associated with sulfur deposition, oxidized-nitrogen deposition and sulfate air concentrations. The airsheds were further subdivided to characterize from where and how far away the emissions emanate that have the greatest importance to stressing the ecosystems of the Shenandoah National Park. Work in FY-2002 will focus on writing the Shenandoah assessment.

2.1.9 Nitrogen Deposition to Coastal Estuaries

Using the procedure developed for the Chesapeake Bay and outlined in Dennis (1997), airsheds for 20 coastal watersheds along the East and Gulf Coasts were developed. These oxidized nitrogen airsheds are expected to be available on the Division's multi-media web site in FY-2002. This work is presented in the NOAA assessment of atmospheric deposition to coastal estuaries (Paerl *et al.*, 2001).

Ammonia deposition is a major new focus of assessment for deposition to the Chesapeake Bay watershed and Bay surface waters, and to the Neuse River Estuary and Pamlico Sound of North Carolina. In FY-2001, reduced nitrogen range of influence mapping with the Extended RADM was completed for 12 emission source subregions, bringing the total to 56 subregions, to support the development of airshed estimates for ammonia. Reduced nitrogen airsheds for Chesapeake Bay, Neuse River Estuary, and Pamlico Sound, Apalachee Bay, and Long Island Sound watersheds were developed. These reduced nitrogen airsheds will be available on the Division's multi-media web site in FY-2002.

2.1.10 Community Multiscale Air Quality Model Evaluation Studies

Ozone continues to be a pollutant of concern because national standards are still being violated. CMAQ represents a new, multi-pollutant tool to support development of ozone-related controls on emissions. Division scientists conducted an initial, operational evaluation of CMAQ for ozone using databases from two field studies. The scientists evaluated model performance in terms of bias and gross error for averaging periods associated with the form of the ozone standard and of interest to regulators, particularly the ability to reproduce the 1-hour peak and 8-hour average daily maximum ozone levels. To better challenge CMAQ, a two-week period from July 5–18, 1995, that included some of the highest and lowest daily maxima observed in that year at approximately 560 ozone monitoring sites in the eastern United States was used. Initial evaluation of the model indicates that CMAQ is functioning satisfactorily for ozone. CMAQ performed quite well for high-ozone days, but less satisfactorily for low-ozone days and for days with larger mean-to-maximum ranges. However, CMAQ is operating in a range consistent with other large ozone models in the United States, while predicting a full suite of multiple pollutants. The model evaluation results support CMAQ's wide-spread use (Arnold and Dennis, 2001).

Fine particulate matter was found to have a significant impact on human health. Sulfate is a dominant constituent of fine particulate mass across the eastern United States and Canada. In 1995, sulfur dioxide (SO_2) emissions were reduced in accordance with the CAAA. Trend analysis of the Clean Air Status and Trends Network (CASTNet) ambient data showed that reduction of sulfate air concentrations was smaller than reduction of SO_2 concentrations by a significant amount. Division scientists evaluated the ability of CMAQ to replicate the nonlinear response of sulfate. A sulfate tracking version of CMAQ was specially constructed for the analysis and was able to successfully replicate the main features of the sulfate changes due to reductions in SO_2 emissions. Preliminary results of the study were presented at the NARSTO International Symposium on Particulate Matter in Querétaro, Mexico, in October 2000. Sensitivity analyses with the CMAQ sulfate tracking model show that both meteorology and chemical nonlinearity contribute to the less-than-proportional response of sulfate and that, for the June 1990 to 1995 period studied, meteorology has by far the larger influence on sulfate non-proportionality. However, the role of oxidant limitation is seen to be quite important to the production of sulfate fine particulate matter, particularly when meteorology is held constant in the model comparisons, and is much larger than its role in acidic deposition.

2.1.11 Ozone Forming Potential of Organic Emissions

Volatile organic emissions (VOC) have different reactivities or potentials for producing ozone in the atmosphere. They are classified into negligibly reactive (exempt from ozone regulations), reactive, and highly reactive, the latter two classes being subject to inventory and control regulations. Evidencing and documenting negligible reactivity is a highly sensitive and often controversial subject as it determines the outcome of petitions submitted to EPA by industry for exempting new VOC emission products or processes from ozone regulations. This, and also the large uncertainties of the reactivity-based VOC control strategies currently in place and the substantial costs of such strategies, led the U.S. Congress to earmark monies for and direct EPA to undertake a substantial research/development effort to advance the reactivity science and generate improved reactivity data. Through its National Exposure Research Laboratory (NERL), EPA responded by enhancing its in-house reactivity program, by founding a national Reactivity Research Work Group (RRWG) composed of Government, industry, and university research institutions, and by awarding several cooperative agreements and contracts for reactivity research to universities. Work in FY-2001 focused on in-house reactivity modeling studies and reviewing of industry petitions, on building a new generation smog chamber facility for improved reactivity testing of VOCs at the University of California, Riverside, on completing through RRWG a substantial effort to identify scientific and policy issues and develop responsive research plans in the reactivity area, on initiating cooperative and contract research programs, and on drafting an Ozone Criteria Document Section on VOC Reactivity. In the reactivity modeling area, a fixed parameter version of the SAPRC99 chemical mechanism and the SMOKE©[2] emissions processor were incorporated into the Models3/CMAQ modeling system. Such a system will be used eventually for substantially improved model-computation of reactivity. Overall, the FY-2001 activities are of benefit in that they sensitize the scientific and regulatory communities to uncertainties and gaps in reactivity science and will lead ultimately to the development of scientific basis for reactivity-based VOC control policies.

2.1.12 United States-Germany Environmental Agreement

The United States-Germany Environmental Agreement for information exchange was initiated in 1988. Information exchange is effected mainly through participation in biennial Workshops organized jointly by the two countries. To date, there have been six Workshops. Workshop scope was initially limited to the photochemical ozone pollution problem, but was recently expanded to include also photochemical aerosols. Participation also was expanded recently to include countries from Eastern Europe and non-European countries. The Workshop agenda is designed so as to include presentations on subjects of mutual interest. In past years, United States interest was mainly in European atmospheric chemistry studies, particularly those at the newly built, large, ultra-modern outdoor smog chamber facility in Valencia, Spain. European interest was mostly in modeling studies and regulatory policies and strategies in the United States. Efforts in FY-2001 included completing the Proceedings from the 6th Workshop, and planning of the 7th Workshop scheduled for the second week of October 2002 in Germany. Anticipated benefit from 7th Workshop is new information leading to updating of the chemical mechanisms for ozone and fine particulate matter species and models used in the United States.

2.1.13 Atmospheric Sciences Modeling Division Library

The Division supports a research library that originated in 1958 at the Robert S. Taft Sanitary Engineering Center in Cincinnati, Ohio. In 1971, the Library became part of the EPA at Research Triangle Park, North Carolina, and NOAA at Silver Spring, Maryland, when the EPA and NOAA were established in the Executive Branch by Reorganization Plans Nos. 3 and 4 of 1970. The Library is unique in that its collection is included in both the EPA and NOAA library networks.

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[2]Copyright 2000 MCNC–Environmental Modeling Center

The Library is part of the ASMD Office of Director. Its mission is to serve the NOAA Division assigned to support EPA's National Exposure Research Laboratory, Office of Air Quality Planning and Standards, and Environmental Research Center staff located in Research Triangle Park, North Carolina, and EPA and NOAA nationwide. Because the Library is a participating member of OCLC (Online Computer Library Center), it provides services to all members of that organization. The major field of interest is the meteorological aspects of air pollution, including numerical and physical model development and application. The Library is a member of American Meteorological Society.

2.1.13.1 International Association of Aquatic and Marine Science Librarians and Information Centers

The Division Librarian participated in the 26th International Association of Aquatic and Marine Science Libraries and Information Centers (IAMSLIC) Annual Conference, September 28–October 6, 2000, in Victoria, British Columbia, Canada. At the conference, the Librarian presented an informational poster on the membership representation of the Atmospheric Science Librarians International (ASLI) organization. The Librarian introduced the Director of the Law Library and Professor of Law at the University of North Carolina at Chapel Hill, who led a two-hour copyright workshop. The Librarian served on the officers nomination committee.

2.1.13.2 Southeast Affiliate of IAMSLIC Librarians

The Division Librarian attended the SAIL 2001 Conference, May 2–4, 2001, in Sarasota, Florida, at the Mote Marine Laboratory. The Mote scientists, library professors, and librarians presented relevant topics for the attendees. SAIL members made other presentations about activities in their areas. The 35 attendees included NOAA Librarians, and librarians and scientists from the academic and municipal community, and a non-profit laboratory. The ASMD Librarian was elected SAIL archivist.

2.1.13.3 Atmospheric Science Librarians International

The Division Librarian attended the Fourth Annual Conference of the Atmospheric Science Librarians International (ASLI), which was held in conjunction with the 81st Annual Meeting of the American Meteorological Society, January 9–14, 2001, in Albuquerque, New Mexico. At the third annual conference in Long Beach, California, the Librarian was elected Chair of ASLI for 2000; therefore, as Chair, the Librarian planned the 2001 program and acted as moderator of the meeting (http://www.lib.noaa.gov/asli/asli2001ag.htm). At the conference, the Librarian also served at the ASLI exhibit booth and at the Air Resources Laboratory (ARL) booth in the exhibit hall. During 2001, the Librarian served as a member of the ASLI Executive Board and Membership Chair.

2.1.13.4 Atmospheric Sciences Modeling Division Library Web Page

The ASMD Library maintains a world-wide web (WWW) page (http://www.epa.gov/asmdnerl/library/library.htm), which provides information about the Library's history, location, 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. The Librarian provides PDF documents of publication citations for inclusion on the Division's home page (http://www.epa.gov/asmdnerl/) and publication citations for the NOAA Air Resources Laboratory home page (http://www.arl.noaa.gov/). During the year, the process of updating the web site to be in compliance with Section 508 of the Rehabilitation Act of 1973 was completed.

2.2 Atmospheric Model Development Branch

The Atmospheric Model Development Branch develops and evaluates 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 Community Multiscale Air Quality Modeling System

2.2.1.1 Introduction

EPA released the Community Multiscale Air Quality (CMAQ) modeling system, initially in June 1998, and several subsequent revisions in FY-1999, FY-2000, and FY-2001. Models-3/CMAQ is a numerical modeling system that can simultaneously simulate the transport, physical transformation, and chemical reactions of multiple pollutants across large geographic regions. The system is useful to states and other government agencies for making regulatory decisions on air quality management, as well as to research scientists for performing atmospheric research. Models-3, a flexible software framework, and the CMAQ modeling system, support air quality applications ranging from regulatory issues to scientific research on atmospheric processes. A modular science design of CMAQ allows the user to build different chemistry-transport models for various air quality problems. The CMAQ models can be operated independently of the Models-3 system framework, providing more flexibility for advanced research and applications. The CMAQ models were tested for several air quality studies, including photochemical ozone and particular matter episodes in 1995 in the northeastern United States (NARSTO-NorthEast field study) and southeastern United States (Nashville, Tennessee, Southern Oxidants Study (SOS)) for the period July 2–18, 1995. The test results are very promising when compared with observed surface ozone concentrations and aircraft measurements. Preliminary model assessments for particulate matter indicate that the CMAQ model is performing quite well for modeling particulate sulfate, but is overpredicting nitrate, and underpredicting organic aerosols. Work continued through FY-2001 in diagnosing the reasons for these biases in the model.

2.2.1.2 Research and Development Scope of the Community Multiscale Air Quality Modeling System

After the initial release of the Models-3/CMAQ modeling system, development continued to improve its science content and expand the operational platforms. The Models-3/CMAQ science paradigm embodies the one-atmosphere concept for air quality modeling. To simulate weather and air quality phenomena realistically, adaptation of a one-atmosphere perspective based mainly on first principle science descriptions of the atmospheric system is necessary. This perspective emphasizes the interactions among multiple air pollutants at different dynamic scales. For example, processes critical to producing oxidants, acid and nutrient depositions, and fine particles are too closely related to be treated separately.

Figures 1, 2, 3, and 4 demonstrate the one-atmosphere modeling concept and illustrate Models-3/CMAQ simulation results for ozone and fine particulate matter ($PM_{2.5}$), sulfates, and visibility for July 6, 1999, for the contiguous United States at 32-km horizontal grid dimension, a period of widespread ambient pollution in the nation. Figure 1 illustrates maximum 1-hr average ozone concentration (ppmV) in each grid cell between 7:00 AM and midnight EDT. Figure 2 illustrates 24-hr averages of sulfate concentrations (micrograms/m^3). Figure 3 illustrates 24-hr averages of $PM_{2.5}$ concentrations (micrograms/m^3) in each 32-km grid cell. Figure 4 illustrates noontime EDT visibility (deciview, note insert) in each grid cell.

Science modules in the CMAQ system are the Fifth Generation Pennsylvania State University/National Center for Atmospheric Research (NCAR) Mesoscale Meteorological Model (MM5), the Sparse Matrix Operator Kernel Emissions (SMOKE)©[3] system, and the CMAQ Chemical Transport Model (CCTM). There are several interface processors that link other model input data to CCTM. The Meteorology-Chemistry Interface Processor (MCIP) processes MM5 output to provide a complete set of meteorological data for CCTM. Initial and boundary conditions are processed with the processors, ICON and BCON, respectively. 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. 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. The continued improvement of many elements of the CMAQ system is described below.

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[3]Copyright 2000 MCNC–Environmental Modeling Center

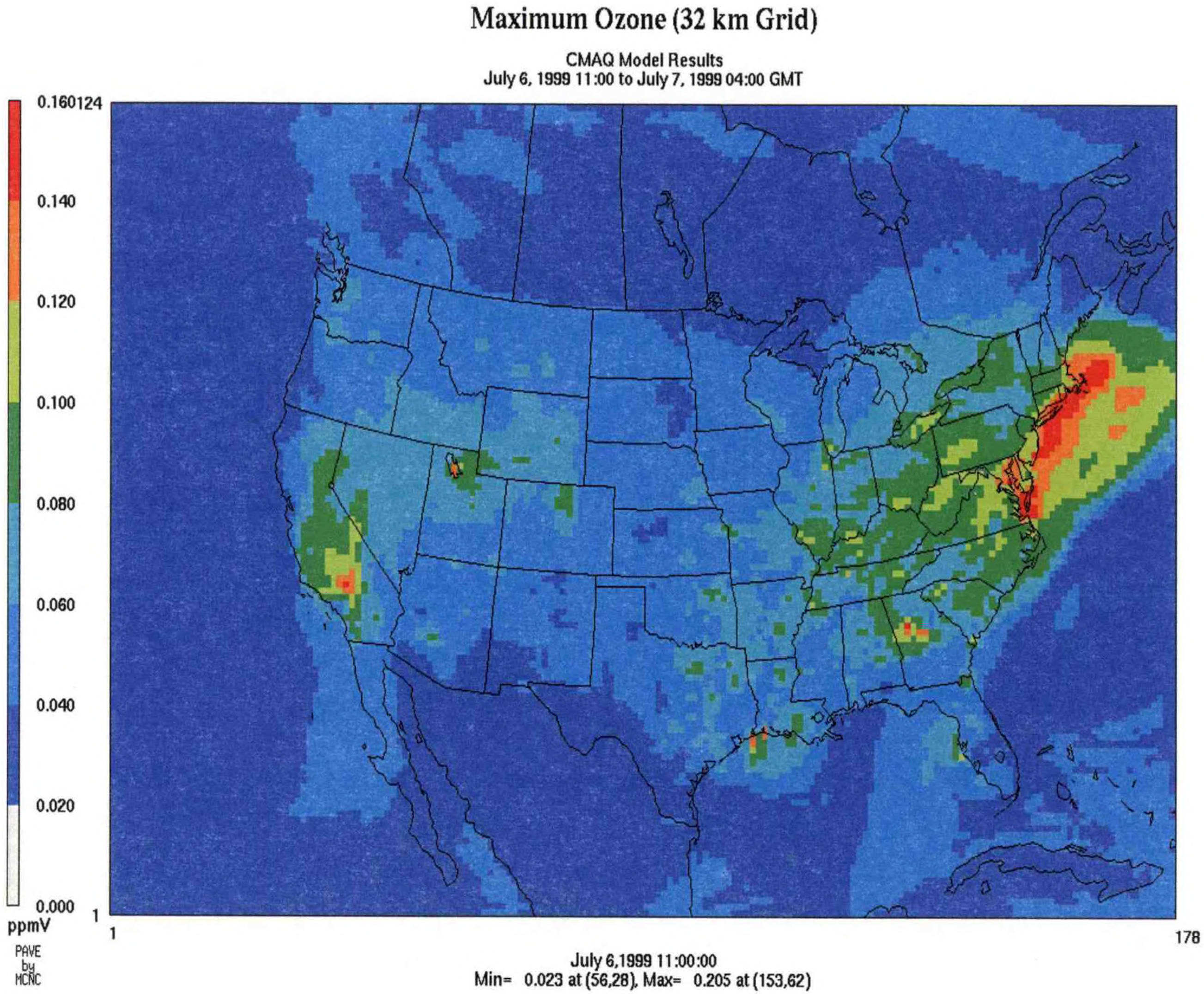

Figure 1. Models-3/CMAQ simulation results for July 6, 1999, for the contiguous United States at 32-km horizontal grid spacing showing maximum 1-hr average ozone concentration (ppmV) in each grid cell between 7:00 AM and midnight EDT.

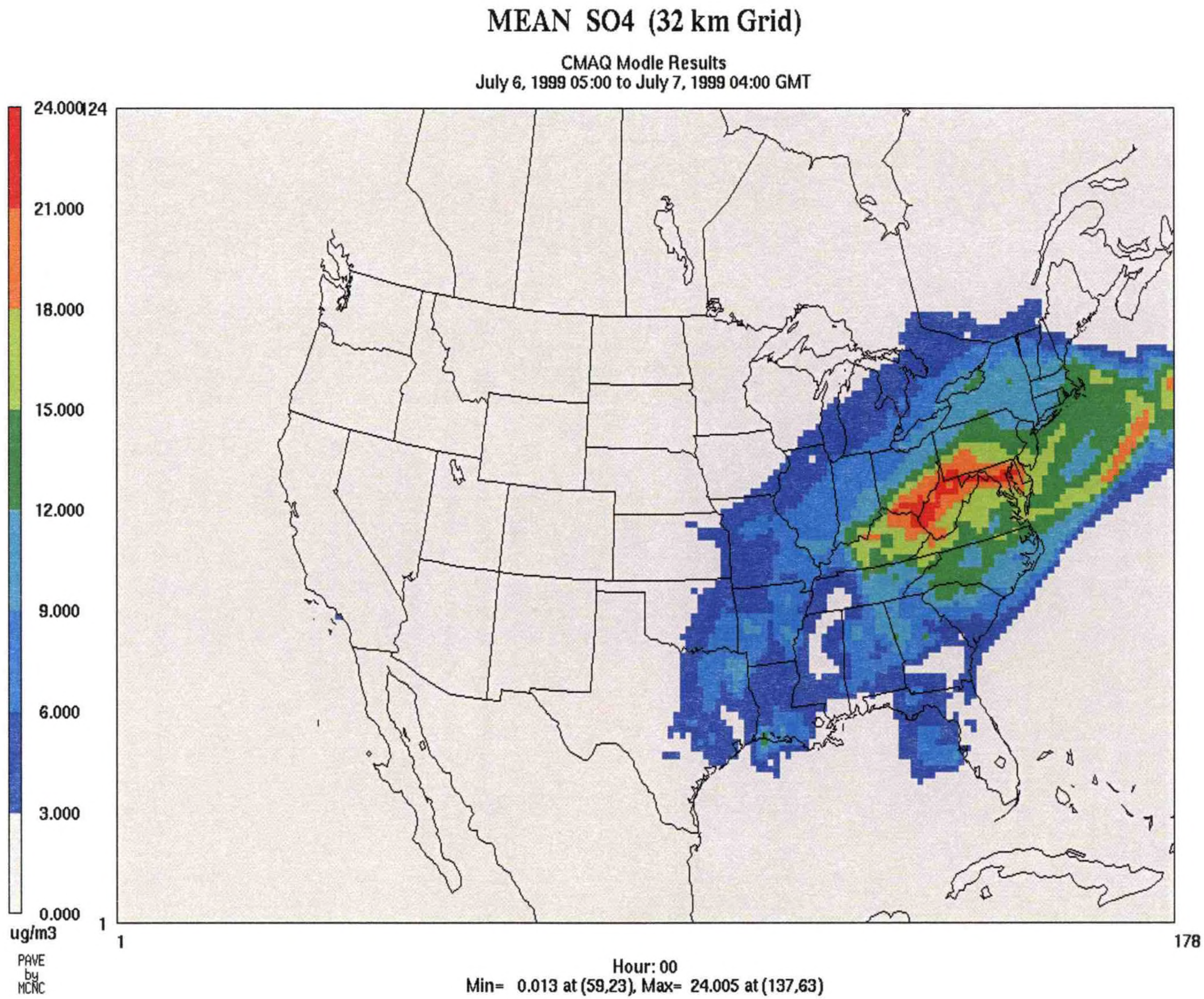

Figure 2. Models-3/CMAQ simulation results for July 6, 1999, for the contiguous United States at 32-km horizontal grid spacing showing 24-hr averages of sulfate concentrations (micrograms/m^3).

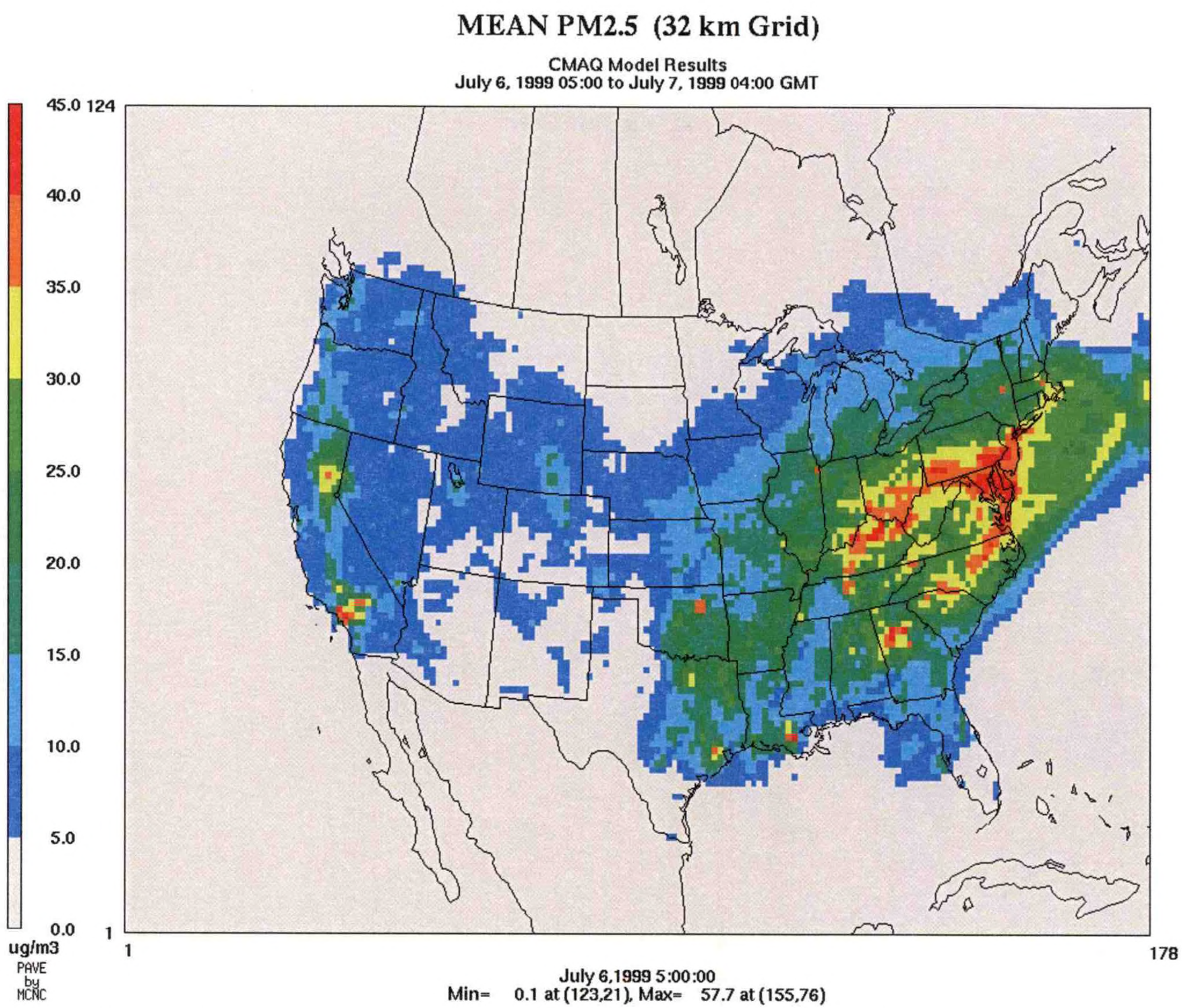

Figure 3. Models-3/CMAQ simulation results for July 6, 1999, for the contiguous United States at 32-km horizontal grid spacing showing 24-hr averages of $PM_{2.5}$ concentrations (micrograms/m^3) in each 32-km grid cell.

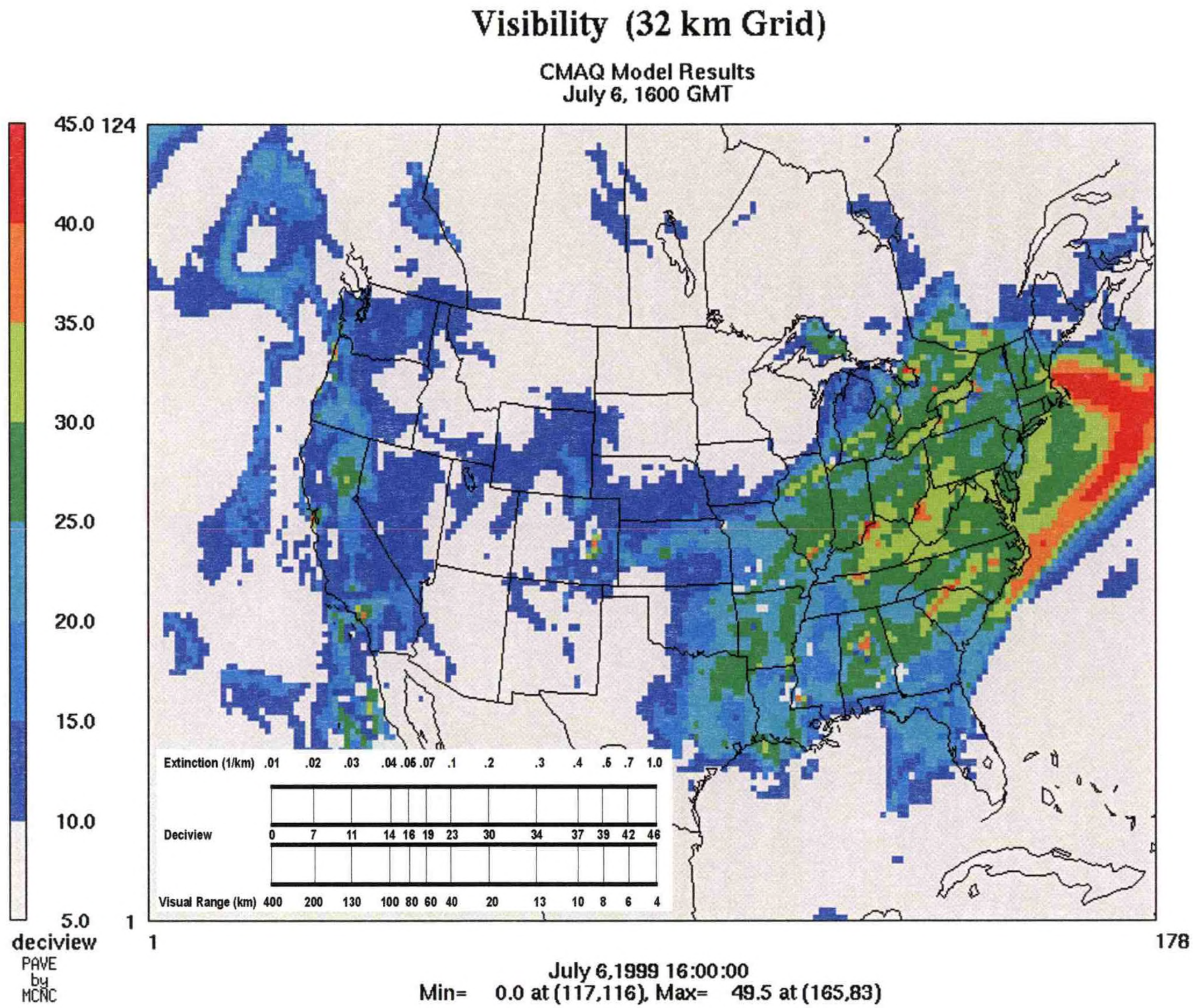

Figure 4. Models-3/CMAQ simulation results for July 6, 1999, for the contiguous United States at 32-km horizontal grid spacing showing noontime EDT visibility (deciview, note insert) in each grid cell.

The latest public release of the CMAQ modeling system occurred in February 2001. In this version, the computationally-efficient SMOKE© emissions model replaced the older Models-3 Emissions Processing and Projection System. A new efficient numerical solver for the gas-phase chemistry, a modified Euler backward iterative technique, was implemented. Model testing and evaluation will continue in FY-2002, and will include examining the impacts of using new land-surface, deposition, and turbulence schemes in the modeling system, as well as using a new chemical kinetic mechanism to treat gas-phase reactions.

2.2.1.3 Photolysis Rates

The photolysis rate model in CMAQ computes rates for various altitudes, latitudes, and hours from local noon using a radiative transfer model, typical atmospheric conditions, detailed satellite ozone data (if available), modeled cloud fields, a standard aerosol profile, and surface albedo. In FY-2001, development continued in coupling aerosols and gas-phase chemistry to include the effects of using dynamically-calculated aerosol profiles as an adjustment to photolysis rate estimates (Park, 2001). Alternative methods for treating cloud cover in the radiative transfer calculations are being developed and tested, including the use of GOES satellite data as an alternative source for cloud fields. Testing and evaluation will continue in FY-2002.

2.2.1.4 Cloud Dynamics and Aqueous-Phase Chemistry Module

The cloud module in CMAQ consists of a sub-grid cloud model and a grid-resolved cloud model. The sub-grid cloud model, which is based on the RADM cloud model (Walcek and Taylor, 1986; Chang *et al.*, 1990; Dennis *et al.*, 1993), simulates convective precipitating and non-precipitating clouds. The grid-resolved cloud model simulates clouds that occupy the entire grid cell and were resolved by the meteorological model. Development and evaluation continued on the CMAQ cloud module, referred to as the Sulfate-Tracking Model. The cloud module tracks the sources of sulfate (gas-phase production, aqueous-phase production, initial and boundary conditions, and emissions) at any location and at any time. Alternative models for deep convective, shallow convective, and grid-resolved clouds will be examined and considered for incorporation into CMAQ. Research will be initiated to re-examine and update the model for aqueous chemistry in CMAQ.

2.2.1.5 Sub-grid Scale Plume-in-Grid Modeling in the CMAQ Modeling System

The plume-in-grid (PinG) approach provides a realistic scientific treatment of the physical and chemical processes affecting pollutant concentrations in elevated, major-point source plumes in the CCTM. The PinG algorithm simulates the gradual growth of sub-grid scale plumes due to dispersion processes that are important factors impacting the temporal evolution of photochemistry in plume cells during the sub-grid scale phase. The description of the capabilities of the CMAQ/PinG model treatment and its technical formulation are described in

Gillani and Godowitch (1999). The key modeling components include a plume dynamics model (PDM) processor and a Lagrangian reactive plume model (PinG module), which are designed to simulate the relevant plume processes at the proper spatial and temporal scales. The PDM processor determines the position and physical dimensions of individual plume sections by simulating plume rise, vertical and horizontal plume growth, and plume transport. The PinG model simulates the relevant plume processes with a moving array of attached cells representing a plume horizontal cross-section. The PinG treatment is capable of simulating a single plume or multiple point-source plumes with hourly emission releases. The PinG module is fully integrated into the CCTM grid model. PinG is executed concurrently during a CCTM simulation and employs appropriate grid concentrations as boundary conditions for various plume sections. An important feedback occurs when a plume section reaches the grid cell size as the sub-grid plume treatment ceases and plume concentrations are incorporated into the Eulerian grid system.

A notable, new extension for the PinG module is the inclusion of an aerosol/particulate modeling algorithm to treat particulate matter and aerosol species in the sub-grid plumes. The Binkowski (1999) aerosol treatment, which was the aerosol modeling component of the CCTM grid model, was adapted and integrated into the PinG module so that gas-phase chemistry and aerosols can be simulated in the same manner as in the grid model. Test simulations were underway with a group of major point sources exhibiting a wide range of NO_x and SO_x emission rates within a regional modeling domain encompassing the greater Nashville, Tennessee, area. Preliminary model test results reveal interesting differences in the formation of sulfate aerosol concentrations in plumes from the various point sources. Simulations are being conducted with the RADM2 and Carbon Bond-IV (CB-IV) gas-phase photochemical schemes to assess differences due to the choice of chemical mechanisms. For the gas-phase species, previous PinG results at various downwind distances were encouraging with the modeled plume NO_x and ozone concentrations exhibiting the same evolutionary pattern found in real-world plume measurements (Godowitch and Young, 2000). An initial, limited comparison of the PinG modeled plume concentrations against ozone, selected nitrogen species, and SO_2 data obtained from aircraft traverses across plumes was reported by Godowitch (2001). Further evaluation of the PinG module is underway with modeled gas and aerosol species comparisons with the observed plume data collected on various airborne platforms during the1995 and 1999 SOS field experiments. Additional simulations using CCTM/PinG and CCTM/NoPinG model versions are being performed over a two-week period to examine gridded concentration fields with PinG and without the PinG approach for the largest point-source emitters.

2.2.1.6 Air Quality Modeling of Particulate Matter and Air Toxics at Neighborhood Scales

Risks to human health from exposure to ozone, fine particulate matter ($PM_{2.5}$) and air toxics are undergoing rigorous scientific examination. Risk assessments from epidemiological and source-to-dose studies depend on exposure assessments, including exposure modeling, which are driven by data from central site monitors. Some types and classes of pollutants are characterized by high temporal and/or spatial variability; thus, for implementation of the National

Ambient Air Quality Standards of the CAAA, data and models used to drive human exposure-to-pollutants assessments will be required at commensurate scales. Further, the source contribution to exposure from biogenic and different anthropogenic sources (*e.g.*, transportation, industrial/commercial, residential activities) needs to be delineated in the assessments.

To support source-to-dose assessments as part of human population exposure modeling for EPA's risk assessment/risk management paradigm and also for assessment and management of risk associated with $PM_{2.5}$ and air toxics, an emissions-based modeling capability is being developed to provide air quality concentration fields and sub-grid variability characterization from regional to neighborhood scales. These modeled concentrations may augment and/or supplant observations from monitors that, by themselves, provide limited or negligible characterization of the requisite temporal variability and spatial features of the pollutant field. Additionally or as an alternative, model predictions may serve as a surrogate for pollutant compounds that are not measured.

With its multiscale modeling capability the CMAQ modeling system provides a powerful modeling platform for this effort. The interest is to extend the utility of CMAQ to grid sizes that exhibit gradients at fine scale. Modifications to MM5 were made to accommodate urban building morphological and detailed land-use data at fine scale resolution (Otte and Lacser, 2001). Additional modeling techniques are needed to describe the sub-grid scale variability, including those that are derived from turbulence-induced concentration fluctuations using large-eddy simulation (LES) techniques (Herwehe, 2000) and dispersion of point- and area-sources from street canyon flows, using a combination of computational fluid dynamics (CFD) and wind tunnel modeling techniques. This variability information, in the form of probability density functions (PDF), provides statistical information (*e.g.*, peak-to-mean ratios) and spatial structure functions of the variability as a function of the building morphology. The first application from this system is to provide ambient concentration fields to various micro-environments in the population-based Stochastic Human Exposure and Dose Simulation (SHEDS) model (Burke *et al.*, 2001).

Preliminary results from a proof-of-concept case study for the Philadelphia area (Ching *et al.*, 2001) show an example where the fine mode component of the $PM_{2.5}$ size distribution exhibited greater spatial variability than the $PM_{2.5}$ by mass. In addition, the extent of the resolved scale spatial variability is seen to vary with each pollutant and also, the grid-resolved variability does not necessarily increase monotonically with increased grid resolution. This means that the grid resolution selected for use in exposure modeling may need to be ascertained by numerical experiments. Results to date for the sub-grid modeling are from the use of a coupled LES with chemistry model (LESchem) in which the degree of the variability is governed by the chemical reactivity of the species, the atmospheric mixture, and the turbulent structure of the mixed layer.

2.2.1.7 Aggregation Research for Models-3/CMAQ

In support of studies mandated by the CAAA, the Models-3/CMAQ model is used by the EPA Program Offices 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. In practice, CMAQ may 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 is then applied to the outputs from CMAQ to derive the required seasonal and annual estimates (Cohn *et al.*, 2001).

The aggregation approach utilized cluster analysis of the 700 h Pa *u* and *v* wind field components over the time period 1984–1992 to define homogeneous meteorological clusters. Alternative schemes were compared using relative efficiencies and meteorological considerations. An optimal scheme was defined to include 20 clusters (five per season), and a stratified sample of 40 events was selected from the 20 clusters using a systematic sampling technique. The light-extinction coefficient, which provides a measure of visibility, was selected as the primary evaluative parameter for two reasons. First, this parameter can serve as a surrogate for $PM_{2.5}$, for which little observational data exist. Second, of the air quality parameters simulated by CMAQ, this visibility parameter has one of the most spatially and temporally comprehensive observational data sets. Results suggest that the approach reasonably characterizes synoptic-scale flow patterns and leads to strata that explain the variation in extinction coefficient and other parameters (temperature and relative humidity) used in this analysis, and, therefore, can be used to achieve improved estimates of these parameters relative to estimates obtained using other methods (Eder *et al.*, 2000a). Moreover, defining seasonally based clusters further improves the ability of the clusters to explain the variation in these parameters, and, therefore, leads to more precise estimates.

2.2.1.8 Collaborative Model Evaluation Studies for Particulate Matter

Three collaborative model evaluation projects are underway based upon utilization of the Models-3/CMAQ system:

Cooperative Agreement with University of Alabama-Huntsville.

A modeling center was started at the University of Alabama-Huntsville to develop a Models-3/CMAQ capability to serve present and future needs of the Southern Oxidant Study (SOS) community. As part of the functions of this Center for Models-3/CMAQ, some performance evaluation studies were conducted for specific episode simulations. The model-data intercomparisons were made for selected case studies using targeted data from aircraft, meteorological observations, and surface chemistry sites from the 1995 and 1999 Nashville SOS field experiments. The first set of studies conducted by the modeling team focused on the July 1995 SOS experimental period. Several modeling runs were made to study and evaluate the sensitivity of the use of the PinG approach in CMAQ, and to examine alternative methods for introducing initial and boundary conditions (IC/BCs). Experiments are being conducted to arrive at the most satisfying IC. Alternative runs with and without PinG are under study. Special attention is being given to the evaluation of the meteorology fields from MM5 as contrasted to the Regional Atmospheric Modeling System (RAMS), using as a basis wind profiler data for winds and satellite data for cloud predictions. One emphasis will be on the predictability of the nocturnal jets and their subsequent effects on plume dispersion. Statistical evaluations will provide the basis for an assessment and improvements to nudging coefficients used in MM5. These methods and evaluation studies are being conducted with different horizontal grid dimensions (*e.g.*, 36, 12 and 4 km).

Work is underway on a test case that will cover the period of June 22–August 17, 1999, and the simulation will use MM5. This period spans the major SOS field activities in Nashville (June 22–July 22) and Atlanta (August 1–August 31). The models will be run in two modes: a control run without satellite assimilation and a run with satellite assimilation. The satellite assimilation run will include insolation and soil moisture retrievals. Also, GOES visible broadband transmittance, surface albedo, and IR (infrared) cloud tops will be used in the CMAQ photolysis calculations. The MM5 control run was completed for the June 22–July 31 period. The satellite assimilation was carried out for June 22–29. Meteorological evaluation has started using the same techniques incorporated in the 1995 cases and include comparison against special observations such as profilers and standard National Weather Service observations.

Cooperative Agreement with the Washington University Center for Air Pollution Impacts and Trend Analysis (CAPITA) in St. Louis, Missouri.

A collaborative study between ASMD and the Center for Air Pollution Impacts and Trends Analysis (CAPITA), undertaken to evaluate the performance of Models-3/CMAQ, was completed. As part of this effort, CAPITA assessed the suitability of using visibility as a surrogate for $PM_{2.5}$ concentrations in the Models-3/CMAQ aggregation technique for producing annual- and long-term averages. Both efforts utilized CAPITA's consolidated database of PM data sets. CAPITA performed its evaluation of the CMAQ model using the IMPROVE (Interagency Monitoring of PROtected Visual Environments) mass and chemically speciated concentration data. The comparison period, July 4–18, 1995, was during a major ozone and PM episode covering much of the eastern United States. The daily average measured species concentrations were compared to the corresponding averages from the 36-km model grid. The model performance was evaluated based on the correlation of the model-data pairs. The model results were also examined on contour maps for each aerosol component to evaluate the spatial biases compared to the IMPROVE and AIRS (Aerometric Information Retrieval System) PM_{10} data. The measured and modeled $PM_{2.5}$ mass concentrations at the 18 eastern United States IMPROVE sites were found to be highly correlate (R^2= 0.84). There was an offset in the correlation, which implies an unaccounted background mass of about 4 mg/m^3. The model values were somewhat lower than the measured values (slope 0.84). There was no evidence of systematic spatial bias in the model-data $PM_{2.5}$ mass comparison. The modeled and measured fine particle sulfate concentrations over the eastern United States showed an excellent correlation

(R^2=0.86) and zero offset. The model sulfate was somewhat higher, but there was no evidence of systematic spatial bias in the model-data sulfate comparison.

The measured total organics in the IMPROVE data showed poor correlation with the model values (R^2= 0.03). In fact, the model organics were virtually constant at about 1.8 mg/m^3, while the corresponding measured values at the IMPROVE sites ranged from 2. 5 to 7 mg/m^3. The poor model-data comparison for organics is attributed to sources not considered in the model, such as biomass smoke. Qualitative biomass tracers in the IMPROVE data, (non-soil potassium), indicate that during the July 1995 summer episode, biomass smoke was a significant contributor to organic PM over the eastern United States. Unfortunately, the main quantitative features of biomass smoke emissions and ambient smoke composition are poorly understood. The IMPROVE data indicate that in July 1995, fine particle soil components contributed 2-10 mg/m^3 to the $PM_{2.5}$ over the eastern United States. The chemical fingerprints and transport also indicate that long-range transport of Sahara dust was a major fraction of fine dust over the eastern United States in July. Fine soil sources and intercontinental-scale transport are not included in the current model. The measured PM_{10} data from the extensive AIRS (600 sites) and IMPROVE networks are generally higher then the model values. The spatial pattern of the data-model difference shows large excess measured PM_{10} (up to ~30 ug/m^3) over the more arid western part of the domain, where windblown dust is significant. However, near urban areas the model exceeded the measured values, indicating that urban primary sources in the model were overemphasized.

<u>Interagency Agreement with the U.S. National Park Service</u>.

This collaboration involves the development, implementation, and utilization of Models-3/CMAQ to assess and develop strategic and tactical strategies to deal with existing and emerging pollution issues pertinent to the Class I natural areas in the West. This collaboration with the U.S. National Park Service includes principals from the Cooperative Institute for Research in the Atmosphere (CIRA) at the Colorado State University, Fort Collins, Colorado. After implementing Models-3/CMAQ at CIRA, the effort is developing and incorporating algorithms for advanced smoke emission processing from fires (prescribed, agricultural, and natural) into Models-3/CMAQ. This project will serve to facilitate the use of Models-3/CMAQ in the West to develop science-based strategic plans for dealing with smoke emission management issues and interstate transport affecting regional haze, $PM_{2.5}$, PM_{10}, and ozone. By design, the effort to develop the smoke emission processor will involve introducing several major components including:

- System to identify fire boundaries determined from the Geographic Information System (GIS) coverage generated for fires from various data sources. The basic output from this step is spatially identified fire boundaries as a function of time (daily or hourly). The National Fire Occurrence database, a spatial database with 1-km resolution that includes most fires for the period of record, 1986–1996, is being utilized for the first generation product.

- Fuel models that introduce vegetation coverage and fuel loading data associated with the fires using the EPA vegetation mapping coverage and the U.S. Forest Service risk analyses system. The emission production models require data about the amount and characteristics of fuel loading present on a piece of land. Generally, these are tied to the fuel models of the National Fire Danger Rating System, which includes handling of dead fuels moisture as well as live fuel moisture or greenness maps derived weekly from Normalized Difference Vegetation Index data observed by satellites.

- Fuel moisture model that compares the current fuel moisture content to the fuel moisture content threshold for flammability. Thus, the moisture content of each of the different fuel types is a critical determinant of flammability. The finer fuel moisture content will be calculated from the time weather conditions including temperature, relative humidity, and cloudiness data from the MM5 system.

- A fire generation processor based on spatial coverage of historical wildfires from satellite observations or individual fire records of a stochastic fire generator based on precipitation, humidity, drought determined from a drought index, strong convection as an index of lightning, indication of lightning or human ignition probability (might be based on population density).

- Processor for determining fire behavior or biomass consumption, and

- Processor for providing emissions profiles for speciated wildfire emission pollutants to be determined using current or recent research studies.

2.2.1.9 A Preliminary Evaluation of Models-3/CMAQ for Particulate Matter

Ambient air concentrations of particulate matter continue to be a major concern. High concentrations of fine particles were linked to detrimental health effects (including an increase in mortality) and visibility degradation. Accordingly, the 1990 Clean Air Act Amendments called for an assessment of current and future regulations designed to protect human health and welfare. The most reliable tool for carrying out such assessments are air quality models like the Models3/CMAQ, which simulate air concentrations and deposition of particulate matter as well as several measures of visibility associated with specified levels of emissions. These simulations can be used to support both regulatory assessment and scientific studies on a myriad of spatial and temporal scales. To determine the accuracy of the simulations involving visibility and particulate matter, a preliminary evaluation of the aerosol component of CMAQ was performed (Mebust *et al.*, accepted for publication).

The visibility portion of the evaluation compared visibility observations in the eastern United States, for July 11–15, 1995, against the CMAQ simulations, using both the Mie efficiency theory approximation and the IMPROVE mass reconstruction technique (Eder *et al.*, 2000b). Comparison of model results with observed spatial and temporal patterns of visibility degradation during the specified time period reveals reasonable agreement, as CMAQ captured the main visibility gradients, maxima and minima. The Mie approximation and mass reconstruction methods for calculating deciviews generally underpredict visibility degradation by ~7 and ~10 dv, respectively. The correlation coefficient between the two methods, $r^2 = 0.97$, shows excellent agreement for the five-day simulation. However, only marginal agreement exists between each method and the observations; $r^2 = 0.32$ for the Mie theory approximation and $r^2 = 0.30$ for the mass reconstruction method.

The particulate matter evaluation, using observations of sulfate, nitrate, $PM_{2.5}$, PM_{10}, and organic carbon from 18 stations of the IMPROVE network for eight days in June 1995, reveals that, with the exception of sulfate, the model generally underpredicts aerosol concentrations (Eder *et al.*, 2001a). These underpredictions are consistent across the model domain throughout the simulation period. More specifically, good agreement was found between simulated and observed sulfate concentrations ($r^2 = 0.63$; median bias = 0.01), with both the simulated mean (4.98µg/m^3), and coefficient of variation (79.16%) closely matching those observed (4.83µg/m^3, 71.63%). Conversely, very poor agreement was found between simulated and observed nitrate concentrations. Although the simulated mean (0.21 µg/m^3) was relatively close to the observed mean (0.31 µg/m^3), the overall r^2 (0.005) and median bias (-0.88) were very low. Fair agreement occurred between simulated and observed $PM_{2.5}$ concentrations ($r^2 = 0.55$; median bias = -0.34). The simulated mean (9.06 µg/m^3) and coefficient of variation (62.06%) reasonably match those observed (12.96 µg/m^3, 55.39%). The level of agreement between simulated and observed PM_{10} concentrations was not as good as for $PM_{2.5}$. Although the simulated mean (13.74 µg/m^3) and coefficient of variation (73.74%) are reasonably close to those observed (19.40 µg/m^3, 50.26%), the overall r^2 (0.13) and median bias (-0.38) were low. The simulated mean (1.53 µg/m^3) and coefficient of variation (44.23%) reasonably match those observed (2.32 µg/m^3, 47.34%).

Potential sources of error in these model simulations, for both visibility degradation and speciated aerosol concentrations, include uncertain emission inventories, erroneous input meteorological data, and an incomplete understanding of aerosol dynamics in the CMAQ aerosol component. Inadequacies in evaluation data sets were identified. EPA recently implemented the National $PM_{2.5}$ Monitoring Network, consisting of mass monitoring (1100 sites), routine chemical speciation (300 sites), and supersite characterization. These network measurements will eventually produce a valuable database, allowing a more thorough evaluation of CMAQ.

2.2.1.10 Ozone Initial and Boundary Concentrations for Models-3/CMAQ From Ozone Climatology

The setting of initial and boundary concentration (IC/BC) of air species for the CMAQ system represents clean ambient conditions in the eastern-half of the United States. The first examination is on the sensitivity of the IC/BC for ozone. The study noted large differences in observed vertical and horizontal distributions of ozone compared to those distributions used as IC/BC in CMAQ. The magnitude of the difference is large at upper tropospheric levels. Because of stratosphere-troposphere exchange, the upper troposphere is characterized with high concentrations of ozone (hundreds of ppbv). However, the current IC/BC artificially sets the ozone level as 70 ppbv in the upper troposphere throughout the model domain. The large difference of the standard ozone IC/BC specification from a more realistic situation might limit the capability of the CMAQ system, and cause uncertainty in CMAQ's performance.

The purpose of this research was to improve the IC/BC setting for the Models-3/CMAQ modeling system, and to assess the influence of introducing stratospheric ozone into the troposphere on regional and urban air quality and on the tropospheric ozone budget. The simulation covered the entire United States with 108-km grid cell size from July 2–12, 1988. The domain was divided into 34 layers vertically up to 40 millibars. In addition to a base case with standard IC/BC, ozone initial and boundary concentrations were specified based on ozone climatology (Logan, 1999), which was derived from 15 years of surface, satellite, and ozonesonde data across the globe. The new IC/BC specification enabled the CMAQ model to study ozone cross-tropopause flux transporting to the lower troposphere, and to analyze the impact of intercontinental ozone transport. Potential vorticity, which is usually used as a dynamic tracer of ozone flux, was calculated in the model and its trend related to ozone variation. The tropospheric ozone residual (TOR) data derived from satellite observational results were used for comparison with the modeled tropospheric ozone budget.

Since ozone climatology was based on observations, the derived ozone IC/BCs were in better agreement with the real atmosphere than the standard IC/BC. While this project is still ongoing, CMAQ simulation with the new IC/BC demonstrated transport of ozone vertically through the 34 layer domain from the stratosphere and upper troposphere down to the surface. It was responsible for more than 15 ppbv ozone increase within the boundary layer after the first four days of simulation. The change of IC or BC alone could lead to significant ozone variation. Sensitivity studies showed that after four days of simulation, the initial concentrations could cause over 10 ppbv ozone difference at the ground, and high concentrations of ozone at the boundaries could cause strong horizontal advection (up to ~40 ppbv/hr increase) in the upper troposphere. The comparison with TOR data (Fishman and Balok, 1999) shows promising consistency. Studies to relate the relationship of ozone variation, potential vorticity, and TOR are underway. The influence of IC/BC on ozone and its precursors will be studied further. A recommendation was made to introduce improved IC/BC into CMAQ, with an initial methodology using ozone climatology from a global scale observations database.

2.2.2 Aerosol Research and Modeling

The next release of CMAQ in FY-2002 will incorporate a new mechanism for treating secondary organic aerosol (SOA). The new method is based upon Schell *et al.* (2001) and partitions the species that form SOA between the vapor and particle phases. The same precursors as in the earlier versions of CMAQ are considered. These are toluene, xylene, cresol, long chain alkanes, internal alkanes, and monoterpenes. The surrogate for internal alkanes was changed to cyclohexene. The monoterpenes are now lumped according to the contribution to the national biogenic emissions inventory. The solution for the system is an algebraic system of nonlinear quadratic equations solved by a Newton-Raphson technique. Schell *et al.* (2001) showed that this approach is efficient even in three-dimensional simulations. The advantage of this approach over the previous method of using fractional aerosol yields is the incorporation of recent laboratory results showing the dynamic nature of the partitioning mechanism.

2.2.3 Atmospheric Toxics Pollutant Research

Development of new atmospheric simulation modeling capabilities for toxic pollutants during FY-2001 focused on mercury and two semi-volatile substances, atrazine and dioxin. The latter focus is on researching modeling capacities for additional slow reacting and toxic pollutants. These modeling efforts involve the use of CMAQ as the basis for air toxics pollutant modeling, but the relevant scientific issues and modeling approaches for mercury differ somewhat from those for atrazine and dioxin. Each effort is discussed separately below.

Modeling of Mercury.

During FY-2001, ASMD personnel continued participation in the first phase of an intercomparison study of numerical models for long-range atmospheric transport of mercury sponsored by the European Monitoring and Evaluation Programme (EMEP) and organized by EMEP's Meteorological Synthesizing Center - East in Moscow, Russia. This first phase of the intercomparison involves the simulation of mercury chemistry in a closed cloud volume given a variety of initial conditions. Results obtained from the CMAQ mercury (CMAQ-Hg) model and the other participating models from Russia, Germany, Sweden, and the United States were compared to identify key scientific and modeling uncertainties, and a report was issued to the EMEP governing body (Ryaboshapko *et al.*, 2001). The second phase of intercomparison involves full-scale model simulations of the emission, transport, transformation, and deposition of mercury over Europe and comparison of the modeling results to field measurements of elemental mercury gas, reactive gaseous mercury, and particulate mercury in air.

During FY-2001, a number of modification were made to the CMAQ-Hg model. Based on information derived from the model intercomparison study described above, the mechanism for sorption of Hg^{2+} compounds to elemental carbon aerosol in aqueous suspension was modified to use sorption equilibrium constants based on Seigneur *et al.* (1998). Also, new rate constants for the gas-phase oxidation of Hg^0 by molecular chlorine and hydroxyl radical were incorporated into the CMAQ-Hg model (as determined by Calhoun and Prestbo, personal communication, 2001) and Sommar *et al.* (2001), respectively. Finally, the Fortran subroutine for the CMAQ aqueous chemistry mechanism was optimized to more efficiently calculate the mercury chemistry in concert with the standard CMAQ mechanism. Further modification of the CMAQ-Hg chemical mechanism for mercury is expected in FY-2002 as additional chemical reactions are identified and as new rate constants are determined.

During FY-2001, an evaluation of the CMAQ-Hg model against observations of wet deposition of mercury was conducted. Measurements of the wet deposition of mercury obtained from the Mercury Deposition Network (MDN) (Vermette *et al.*, 1995) at 11 locations in the central and eastern parts of the United States were compared to CMAQ-Hg model simulations during two four-week periods in 1995. The results showed relatively good agreement between modeled and observed wet deposition of mercury for the period from April 4 to May 2 for which a Pearson correlation coefficient of 0.657 was computed. However, for the period from June 20 to July 18, the Pearson correlation coefficient was only 0.329. The inferior performance during the summer period was found to be largely due to the inability of the meteorological driver, MM5, to accurately define small-scale convective precipitation elements at the 36-km grid cell size employed for the CMAQ-Hg evaluation. The results of the CMAQ-Hg evaluation were described in a journal article (Bullock and Brehme, accepted for publication). Further CMAQ-Hg model evaluation will be performed during FY-2002 against MDN data collected in 2000 as the necessary MM5-derived meteorological input data become available.

Modeling of Semi-Volatile Compounds.

During FY-2001, the research effort involving atrazine was largely completed. It adapted CMAQ to simulate atrazine concentrations in air and precipitation from April to July of 1995 over the eastern two-thirds of the United States. To accomplish the simulation, chemistry and deposition algorithms were modified, while a new algorithm for gas-to-particle partitioning was added to account for the semi-volatile nature of atrazine. An initial examinaton showed that predictions were roughly consistent to ranges of air and deposition observations. A more complete evaluation used studies along the Mississippi River (Foreman *et al.*, 2000; Majewski *et al.*, 2000) and Lake Michigan (Miller *et al.*, 2000). Regarding observations along the Mississippi River, the model underpredicted precipitation concentrations and overpredicted air concentrations summed over gas and particulate forms within a mean factor of two. In particular, the model severely overpredicted lower limits in gas-phase concentrations. These errors appear to stem from the precipitation and atrazine emissions data that supported the simulations. Further work regarding atrazine may be conducted to support the papers that presented this research (Cooter and Hutzell, accepted for publication; Cooter *et al.*, accepted for publication).

In addition, research was initiated to develop versions of CMAQ that simulate the fate of dioxins and such simple aromatic compounds as benzene. The dioxins version will treat 17 Polychlorinated Dibenzofuran and Dibenzodioxin congeners because of their significant toxicity. The model expands upon the atrazine research because such similar processes control atrazine and dioxins as gas to particle exchange, low reactivity, and insignificant cloud chemistry (Lohmann and Jones, 1998). The expansion refines the new algorithm for gas to particle exchange based on effects from aqueous and organic aerosol components. Emphasis was placed on improving dry deposition and simplifying chemical mechanisms. In CMAQ, algorithms for dry deposition do not include organic factors that contribute to the deposition of dioxins and other persistent organic pollutants (Lorber and Pinsky, 2000). Simplifying the chemistry considers the low reactivity of dioxins and reduces computational requirements without compromising accuracy. The second model adapts chemical mechanisms within CCTM that represent aromatics as aggregated species.

2.2.4 Meteorological Modeling Studies

The Fifth-Generation Pennsylvania State University/NCAR Mesoscale Model (MM5) is the primary tool for providing meteorological input for Models-3/CMAQ. MM5 is widely used to generate meteorological characterizations 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 simulation period. The output represents a dynamically consistent multiscale meteorology simulation for various horizontal grid spacings and from continental to urban areal coverage. The MM5 output is ultimately used in the CMAQ emissions and chemistry modules to describe the planetary boundary layer characteristics and the atmospheric state variables.

2.2.4.1 Meteorology Modeling for Models-3/CMAQ Applications

Several projects were underway during FY-2001 using MM5 to support Models-3/CMAQ applications. MM5 Version 3 Release 4 (MM5v3.4) was released by the National Center for Atmospheric Research (NCAR), Boulder, Colorado, in November 2000. MM5v3.4 included the first general release of the ASMD-developed Pleim-Xiu Land-Surface Model (Pleim and Xiu, 1995; Xiu and Pleim, 2001). During FY-2001, MM5v3.4 was tailored for air quality applications with some minor modifications, and it was used for internal projects.

During FY-2001, a research effort was initiated to use MM5 to drive CMAQ for episodic evaluation based on the photochemical field studies from the SOS in Nashville during the summer of 1999. Several aspects of the 1999 case studies differ from the 1995 case studies that dominated previous research. The first change was to use NOAA-generated archived Eta model analyses as first-guess fields for MM5. The archived Eta fields have considerably better horizontal (40 km, degraded from 32 km) and vertical (25 levels) resolutions than the global fields (2.5-degree latitude/longitude with 10 levels). As a result, the need for a large-scale (*e.g.*, 108 km) intermediate domain was eliminated. In addition, the nesting ratio was changed to 4:1 for one-way-nested simulations in an effort to better simulate the finest-scale runs. Based on experience with the 1995 NARSTO-NE case studies and published research, the new configurations were set up to better simulate resolved convection and neighborhood scale processes. The new grid configurations and input data resolutions require a new FDDA strategy, and research in this area is on-going. Addition research is planned for 1999 photochemical field studies in Atlanta and Philadelphia and the 2000 Texas Air Quality Study (TexAQS 2000) based on the same continental 32-km domain, but with finer-scale nests focused over each area.

A preliminary demonstration of anisotropic weighting functions in FDDA was reported by Otte *et al.* (2001). The research used an observing-system simulation experiment to illustrate that anisotropic weighting functions have subtle but important impacts in FDDA. An extension of this work to air quality modeling is planned for FY-2002.

2.2.4.2 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 new land-surface model, known as the PX-LSM (Pleim and Xiu, 1995; Xiu and Pleim, 2001), includes explicit soil moisture and vegetative evapotranspiration along with the ACM PBL scheme (Pleim and Chang, 1992). A key feature of the model is an indirect data assimilation scheme where soil moisture is nudged according to biases in surface air temperature and humidity as compared to gridded surface analyses. The data assimilation scheme helps overcome the difficulties in soil moisture initialization and model errors.

The PX LSM was first released in the NCAR-supported MM5v3.4 in the fall of 2000. An updated version was recently released in MM5v3.5. Instructions for use of the PX LSM can be found in the MM5 tutorial that is on the NCAR MM5 website at http://www.mmm.ucar.edu/mm5/mm5-home.html.

Evaluation and further improvement of the PX- LSM through comparison to field experiment data are continuing. In addition to previous studies comparing model runs to surface fluxes over corn, grass, and soybeans, case studies were made for a mixed deciduous-coniferous forest field study in the Adirondack area of New York in July 1998, and two sites, grass and soybeans, near Nashville, Tennessee, that were part of the SOS 1999 field study (Pleim *et al.*, 2001). These comparison studies included evaluation of such meteorological parameters as surface level temperature and humidity, and surface fluxes of heat, moisture, and net radiation as well as ozone dry deposition velocity from a dry deposition model (see Section 2.2.5.2) that couples to the PX- LSM. Such comparisons to field surface flux and meteorology measurements are extremely valuable for improvement of the model's ability to simulate a variety of vegetation types.

2.2.4.3 Urban Canopy Parameterization in MM5

During FY-2001, an urban canopy parameterization (UCP) was developed and implemented in MM5 for fine-scale (~1-km horizontal grid spacing) simulations (Otte and Lacser, 2001). The urban canopy is defined as the volume from the surface to the tops of the buildings within grid points that have an urban land-use classification. The UCP accounts for the drag exerted by urban structures, the increase in turbulent kinetic energy particularly near the tops of buildings, and the changes to the energy budget due to anthropogenic heating and absorption and emission of radiation within the urban canopy.

The UCP was implemented into MM5v3.4 via modifications to the Gayno-Seaman planetary boundary layer parameterization and the Rapid-Radiative Transfer Model radiation scheme. The UCP was initially evaluated in a 1.3-km domain using a case study from the NARSTO-NE photochemical field study in 1995 with a focus over Philadelphia. Since the UCP is applied to the urban canopy, the vertical resolution of the MM5 UCP simulations was increased from 30 to 40 levels with 10 layers within the lowest 100 meters and the lowest level at 2 meters AGL so that several levels are within the urban canopy. The UCP was implemented in stages to evaluate its behavior in MM5. Incremental improvements included the impact on the momentum and turbulent kinetic energy (TKE) equations, various changes to the energy budget at the surface and within the urban canopy, and a sub-categorization of the urban areas into various zones (*e.g.*, residential, industrial, high-rise) to allow for more appropriate application of the UCP within urban areas. Sensitivity tests involved the specification of the canopy area density function and settings of urban characteristics within the urban sub-categories.

Initial evaluation of the UCP in MM5 is promising, and evaluations will continue through FY-2002. Ultimately, the MM5 fields generated with the UCP will be used in CMAQ for neighborhood scale studies.

2.2.4.4 Linking Meteorology and Chemistry Models

The Meteorology-Chemistry Interface Processor (MCIP) is the key processor allowing the consistent off-line linkage between meteorological models and CMAQ. It is essential that MCIP be compatible with upgrades to MM5 to preserve numerical and physical consistency between the meteorology and chemistry models. During FY-2001, the MCIP software was completely revised and upgraded with additional scientific capability. The revision enabled dynamic allocation of computational grid space and improved the program for both developers and users. The scientific upgrades included pass-through capabilities for MM5-output planetary boundary layer and radiation fields that were formerly re-calculated in MCIP; this enabled closer coupling of MM5 with the CCTM. MCIP was configured to support both MM5v2- and MM5v3-formatted output fields. Special treatment of new fields generated by the Pleim-Xiu land-surface model in MM5 was also added to MCIP. In addition, the Models-3 dry deposition scheme (M3Dry) was implemented, and two new toxic dry deposition species were added. Several new output fields were created in MCIP, as well, to support more sophisticated cloud microphysics, the Pleim-Xiu land-surface model, modeling of air toxics, and biogenic emissions processing. The upgraded software program (MCIP Version 2) was released in late FY-2001 to 25 beta testers in the CMAQ community, and early feedback was very positive. MCIP Version 2 will be officially released to the CMAQ community in early FY-2002.

As other meteorological models are used within the CMAQ community, MCIP will also be modified to process data from those sources, notably from the next-generation meteorology model, the Weather Research and Forecast (WRF) model. MCIP development will continue through FY-2002 and beyond.

For on-line linkage of the meteorology and chemistry models, work is underway to implement the MCNC[4] MCPL©[5] (model couple) module in the CMAQ system. This will enable the meteorology model and CCTM to be run simultaneously (on-line) with data transfer at granularities as fine as either model's integration time step. Using MCPL in an on-line mode also facilitates feedback from CCTM back to the meteorology model during integration. MCPL also offers an off-line capability to mimic the functionality of the MCIP program.

2.2.5 Dry Deposition Studies

2.2.5.1 Dry Deposition Research

Models.

The initial development of the next generation deposition velocity model, which is called the Multi-Layer Bio-Chemical dry deposition model (MLBC) was completed, and a journal article describing the model was prepared. The model uses an improved Gaussian quadrature integration scheme, which reduces the number of layers needed in the integration and is more accurate; a significantly revised aerodynamic resistance model based on similarity theory; a simplified boundary layer resistance model; and a revised and enhanced short- and long-wave canopy radiation model. Rather than based on the typical Jarvis scheme, the stomatal resistance is based on a model of Farquhar *et al.* (1980), which calculates stomatal conductance by considering photosynthesis and respiration processes. This method provides more insights into the biochemical mechanisms governing photosynthesis and respiration, and how these are tied to stomatal conductance considering the direct and indirect effects of environmental factors.

MLBC also has a new cuticular resistance model. Plant cuticles are a lipophilic polymer membrane that consists of an insoluble bipolymer cutin and waxlike lipids. Diffusion across this layer can be either directly from the air to the layer, or from the air to a thin water film that usually exists on outdoor surfaces, and from the water layer to the cuticle. Diffusion equations for each of these pathways are developed that depend on the chemistry of the cuticle, water, and each pollutant. Tests of this model against data collected in the field studies show significant improvement over the present generation of models. After its completion, MLBC will be modified for use in Models-3/CMAQ, and combined with other improvements in deposition velocity modeling discussed below.

Model Evaluation.

A journal article has been prepared describing the results of the evaluation and sensitivity tests of the MLBC. Results show that the model accurately predicts fluxes of CO_2 and the

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[4]MCNC, Research Triangle Park, North Carolina

[5]Copyright 1997-2001 MCNC, Inc.

deposition velocity of O_3 and SO_2. Tests show improvements over previously used deposition velocity models. Differences of the model outputs between different sites with different plants are not large. Model sensitivity to the changes of input variables was also conducted. The model produces very reasonable response to the environmental conditions (air temperature, leaf temperature, pressure, humidity, wind speed, solar radiation, vertical temperature gradient, and CO_2 concentration etc.), indicating that the model has the application potential to a wide range of climate conditions, and can be used in the Clean Air Status And Trends Network (CASTNet). The model outputs depend on the accuracy and precision of input variables; therefore, a good quality assurance measurement program is required to get good performance of the model.

Statistical analyses suggest that the photosynthesis model works better for C_3 plants than for C_4 plants. The scheme for C_4 plant photosynthesis proposed by von Caemmerer and Furbank (1999) considers more variables, and may be worth testing in future studies. The model overestimated the amplitudes of both seasonal and diurnal cycles for SO_2 deposition velocity. The model also shows high sensitivity to changes in humidity. This could be due to the weight relative humidity was given in the function computing the water thickness on a leaf surface. Therefore, further testing should be performed on this empirical function, or it could be replaced with the method described by Xiao *et al.* (2000). Evaporation from wet leaves occurs in real situations, but is not considered in the model, resulting in underestimation in both the weekly daytime averages and hourly averages. This further suggests that the method developed by Xiao *et al.* (2000), or a similar method be used in the model. Analysis shows that stomata are the dominant control factor for CO_2, H_2O, and O_3 fluxes, while cuticle and aerodynamic resistance play important roles for SO_2 flux.

Field Measurements for Model Applications.

The atmospheric resistance term in the model, R_a, depends on onsite measurements of turbulence. The previous version of the model, the MLM (Multi-Layer inferential dry deposition Model), was designed to use a simple and robust measurement of turbulence, the standard deviation of the wind direction, σ_θ. The MLBC was designed to use either similarity theory, with the requirement to measure the difference of temperature with height, ΔT, or the simpler σ_θ method. Tests over both a soybean field and a forest show that the differences between the two methods are small, although the similarity theory method is slightly better.

Similarity Theory Evaluation.

Similarity theory is used extensively in both the dry deposition model and other parts of atmospheric dispersion models. The theory was evaluated extensively over ideal conditions, but very infrequently over the rough real world sites where it is usually used. The extensive set of meteorological measurements were recorded as part of the dry deposition field studies and used to evaluate similarity theory over agricultural fields and forests. More particularly, research focused on looking at the integral forms of the stability correction factors for temperature and momentum, Ψ_m and Ψ_T. Preliminary results show that similarity theory seems to do a good job, even over the forests. Existing models of Ψ_m and Ψ_T from Paulson (1970) and Byun (1990) do quite well in moderate stability, but less well in stronger stability. In some cases, the models do well for unstable conditions, but in others they overestimate the correction needed to the neutral case. The models seem to do their worst over corn fields, where roughness elements are less dense than the leaf canopy of a forest or soybean plants.

2.2.5.2 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, PX LSM, implemented in MM5. Since the PX-LSM has an explicit 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 new dry deposition model, M3Dry, was incorporated into the new version of the (MCIPv2).

The combined PX-LSM and M3Dry models were previously evaluated for ozone deposition by comparing model results with field measurements at Bondville, Illinois, and Keysburg, Kentucky (Pleim *et al.*, 1996; Pleim *et al.*, 1997). Further evaluation studies were performed for a 1998 mixed forest study in New York (Pleim *et al.*, 2001), and two sites, grass and soybeans, near Nashville, Tennessee, that were part of the SOS 1999 field study. Sensitivity of CMAQ to the new dry deposition scheme was studied for the NARSTO 1995 modeling study (Pleim and Byun, 2001). Further sensitivity experiments will be performed for the 1999 SOS/Nashville study.

2.2.6 Technical Support

2.2.6.1 North American Research Strategy for Tropospheric Ozone

NARSTO (formerly known as the North American Research Strategy for Tropospheric Ozone) 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, particulate matter, and other air quality problems. It includes a management function for performing this coordination across the public and private sector organizations sponsoring air quality 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-2001, the ongoing NARSTO science assessment of tropospheric ozone was completed, with the publication of a special NARSTO issue of *Atmospheric Environment* (2000). This Special Issue contains a set of critical review papers, commissioned specially for the ozone assessment that covers relevant areas including ambient measurements and networks, field studies, source emissions, atmospheric chemistry, and meteorological and air quality models. The second part of the ozone assessment, an Assessment Report (NARSTO Synthesis Team, 2000) relating the state-of-science to outstanding air quality management issues, was published in October 2001.

2.2.6.2 Western Regional Air Partnership Air Quality Technical Forums

The Western Regional Air Partnership (WRAP) is a broad-based regional air quality coordinating organization composed of States and Tribes in the western United States, U.S. Departments of Agriculture and Interior, EPA, and other affected stakeholders representing industry, environmental groups, and other interested parties. A Division scientist participated in the Air Quality Modeling Forum (AQMF) and Research and Development Forum (R&DF), which are two of several committees of WRAP formed to provide technical guidance. WRAP is a follow-on organization to the Grand Canyon Visibility Transport Commission, whose objective was to provide technical and policy input needed to regulate regional haze in the western United States. AQMF provides WRAP with technical analyses needed to meet practical, real-world objectives, especially as they relate to meeting the regulatory requirements of the EPA regional haze rule (RHR) published July 1, 1999 (Regional Haze Regulations, 1999). Specific AQMF modeling assessments on regional visibility include (1) relative incremental contribution of a given source or source control on visibility at one or more Class I areas; (2) cumulative impact of regional source growth or control on Class I areas throughout the region; (3) impact of regional sources during periods of high and low visibility conditions; and (4) evaluation of cost-effective alternatives for improving regional haze. Time frames required by RHR are (1) near-term (SO_2 regional emission trading program plan due October 1, 2000); (2) intermediate to long-term (additional requirements for regional visibility modeling due December 31, 2003); and (3) long-term (modeling to support State Implementation Plans due no later than December 31, 2008). WRAP AQMF is using Models-3/CMAQ for performing the intermediate- and long-term modeling for RHR.

The AQMF strategy is to facilitate the conducting of both the short term (RHR 109) and full implementation of the RHR Section 108 requirements. This approach involves setting up two teams, one to perform modeling startup of the CMAQ and other modeling systems for the short term tasks, and one to establish the WRAP regional modeling center run by the University of California at Riverside, to implement the various modeling requirements for the RHR Section 108. Efforts are underway to address the need to develop and implement an improved modeling methodology and parameterizations for fugitive dust emissions and for the modeling of smoke emissions from both wildland and prescribed-burn fires into the CMAQ modeling system.

2.2.6.3 Climatological and Regional Analyses of CASTNet Data from 1989-1999

The spatial and temporal variability of ambient air concentrations of SO_2, SO_4^{2-}, NO_3^-, HNO_3, NH_4^+ and O_3 obtained from the CASTNet was originally examined in 1998 using an objective, statistically based technique called rotated principal component analysis (Eder and Sickles, 1998). This initial analysis, which covered the period October 1989 through August

1995, allowed for the identification and subsequent characterization of homogeneous influence regimes associated with each of the six species. Depending on the species, either two (NO_3^-), three (SO_2, SO_4^{2-}, NH_4^+, O_3), or four (HNO_3) influence regimes were identified by the analysis. Examination of the temporal variability of these homogeneous influence regimes through time series and spectral analysis revealed various seasonal and annual cycles of differing strengths and timing.

This analysis provided evidence of, and considerable insight into the regional-scale behavior of these species' air concentrations, which suggested that exclusively local strategies to reduce their concentrations through reductions in emissions may be wholly inadequate without parallel management of regional emissions. Research using data from the period August 1995 through December 1999 will help characterize the impact (on various spatial and temporal scales) of the Clean Air Act Title IV's Phase I emission reductions that began in 1995 for SO_x and 1996 for NO_x.

2.2.6.4 Evaluation of the Use of NEXRAD Stage IV Data in the Multimedia Modeling of Pollutant Transport

The Multimedia Integrated Modeling System (MIMS) is being designed to model the cycling of pollutants and nutrients between the atmosphere and the earth's surface, including water bodies and groundwater. The ability to accurately model atmospheric, hydrological, and surface processes that transport chemicals is highly dependent on precipitation types, rates, and totals. Historically, the only data available for model input was from the National Weather Service rain gauge networks. More recently, however, a data set called NEXRAD Stage IV has become available that assimilates both rain gauge data and WSR-88D (Weather Surveillance Radar 1988 Doppler Version) into a comprehensive hourly, national data set with a 4-km^2 resolution.

Since these data are available on a much finer scale than that of the rain gauge network, it was assumed that they would be superior for input into atmospheric and hydrological models. The purpose of this research is to investigate this supposition, while identifying possible limitations of the NEXRAD Stage IV data through a comparison with ground truth data obtained from a small but very dense rain gauge network near Lizzie, North Carolina (Eder *et al.*, 2001b). This research, which has entered into its second year of data collection will use a variety of visualization and spatial statistical techniques. Accuracy, bias, and the confidence with which areal estimates on various scales can be made.

2.3 Modeling Systems Analysis Branch

The Modeling Systems Analysis Branch provides Information Technology (IT) and facilities infrastructure support to the Division, heads development of the Multimedia Integrated Modeling System (MIMS) framework, provides leadership to EPA's IT Research and

Development (formerly HPCC) program, and performs research on biogenic and anthropogenic emissions modeling.

2.3.1 Technology Support for the Models-3/CMAQ Modeling System

2.3.1.1 Models-3 Version 4

A new release of Models-3 (Version 4.1) was prepared and distributed during FY-2001. This release included the SMOKE© emissions model, an accompanying SMOKE© Tool, and a revised and improved File Converter tool. The File Converter is capable of converting files of known content between ASCII, SAS®[6], and the network Common Data Format (CDF) Input/Output Application Interface (I/O API) formats. The science algorithms, supporting processors, and tutorial input files were made available by anonymous ftp (ftp://ftp.epa.gov/amd).

The Models-3 framework Version 4.1 for an UNIX®[7] operating system, was developed on a Sun™[8] workstation with a Solaris 2.7 operating system™[9], and released in June 2001. Models-3 documentation was made available via the Web at http://www.epa.gov/asmdnerl/models3. The updated Models-3 framework was released for Sun™ workstations and Microsoft® Windows™ NT®[10] operating system. The framework has been encumbered with performance problems and licensing expenses of Orbix™[11], a commercial software component of the framework supporting distributed applications using object-oriented client-server technology. Further development of Models-3 framework is now directed away from the use of products that require licensing fees to the runtime user and version compatibility between the products. Specifically, during FY-2001, substantial progress was made on a Java-based modeling framework with a new operating paradigm supported under the MIMS development program, which is expected to replace the current framework during FY-2002.

2.3.1.2 Models-3/CMAQ Stand-Alone Version

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[6]SAS is a registered trademark of SAS Institute, Inc.

[7]UNIX is a trademark of AT and T.

[8]Sun is a trademark of Silicon Graphics, Inc.

[9]Solaris 2.7 operating system is a trademark of Sun Microsystems.

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

[11]Orbix is a registered trademark of IONA Technologies Ltd.

During the Fall 2000, a stand-alone version of the Models-3/CMAQ modeling system was released with numerous enhancements, including:

- Code needed to run the CMAQ initial conditions preprocessor (ICON), CMAQ emissions-chemistry interface preprocessor (ECIP), and CMAQ Chemistry-Transport (CTM) model on a parallel multi-processor platform like the CRAY® T3E™[12].

- CMAQ codes became Fortran 90 compliant, so that applications could be run on a parallel platform.

- Single-source codes that can be compiled on any platform, eliminating the need to maintain separate codes for different platforms.

- New aerosol module, which incorporated variable standard deviations into the modal approach using a new aerosol surface area species.

2.3.1.3 Models-3/CMAQ Reverse Gridding Utility

The spatial allocation of emission-related data to grid cells is computationally one of the most time-consuming aspects of processing emission data for air quality modeling. In the Models-3/CMAQ modeling framework, spatial allocation is accomplished with a Geographic Information System (GIS). Typically, when data are provided by such political units as state or county, the state and county identifier codes are removed as part of the gridding process. Normally, this is not a problem, because gridded emission and modeled air-quality concentration data are evaluated on the basis of the grid cells. However, until recently, it has been impossible to reverse allocate the data to geographic units without the use of GIS. To address this problem, a generic reverse-gridding utility was created for the Models-3 system. Although the utility was written in Fortran, it can be used either independently from or within the Models-3 system. The reverse gridding utility accepts gridded-emission data in the format used by the Models-3 system, and produces either ASCII or network CDF I/O API formatted files of emission data by state or county. This is accomplished by using the ASCII spatial surrogate files prepared as part of the emission data gridding. The reverse gridding utility may be extended for use with such other geographic areas as hydrological units (drainage basins), which could aid multi-media modeling applications of nutrient deposition. After additional testing, the reverse gridding utility was released via the Models-3 web page during the Fall 2001 as a patch to the Models-3 Version 4.1 release.

2.3.1.4 Models-3/CMAQ Support and Training

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[12]Cray is a registered trademark and Cray T3E is a trademark of Cray Research.

Community Modeling and Analysis System.

ASMD entered into a cooperative agreement for a four-year research grant to initiate the Community Modeling and Analysis System (CMAS) center for user support, maintenance, and improvements of Models-3. CMAS is intended to encourage membership and participation from the state and local governments, industry and academia, as well as federal agencies. The initial work of CMAS will be to provide direct user support and training to users of Models-3/CMAQ.

Models-3 Help Desk.

The EPA Help Desk continued support for Models-3/CMAQ. The Help Desk has a support structure consisting of a collection of individual scientists to answer user questions in specific areas. The telephone number for the Help Desk is 919-541-0157. The Models-3/CMAQ web site (http://www.epa.gov/asmdnerl/models3/) also provided user support for the stand-alone version, *i.e.,* without the Models-3 framework. These codes may be downloaded and adapted to execute on any computing platform. The downloaded files contain code programmed to ingest the data sets for a tutorial using the CB-IV chemical mechanism. The web site also contains *Model Change Bulletins* where known problems with the system are listed along with the instructions to solve the problem. Models-3 *Public Forum* area continued on the SCRAM (Support Center for Regulatory Air Models) web site (http://www.epa.gov/scram001). This area provides a central location for the discussion of issues related to the operation and use of Models-3. A mailing list was used to communicate with Models-3 users and others by sending messages to m3list@tempest.rtpnc.epa.gov. Registration of users on the mailing list is managed by the Models-3 Help Desk.

2.3.2 Support for Multimedia Modeling

2.3.2.1 Development of the Multimedia Integrated Modeling System

Successful modeling cross-media ecosystems entails solving such scientific and computational challenges as ensuring that consistent assumptions are used at the boundary of the media and managing the large number of models and data sets that are typically required. The Multimedia Integrated Modeling System (MIMS) project is conducting research and developing solutions for some of those challenges. The MIMS framework is addressing the computational and data management issues. The framework is a software infrastructure or environment that will support constructing, composing, executing, and evaluating complex modeling studies.

The MIMS development team started development of the MIMS framework during FY-2001. The focus of the effort was on developing software to support configuration and management of complex model executions. The team adopted Argonne National Laboratory's Dynamic Information Architecture System (DIAS) (Christiansen, 2000) as the central approach for specifying model interactions and coordinating execution. DIAS organizes concepts to be modeled as domain objects such as the atmosphere, a group of people, and a chemical. Each domain object has a well defined set of parameters that describes its state and processes that changes its state. Models implement domain objects' processes and use the domain objects' parameters as inputs and outputs. Writing or wrapping models to work with domain objects eliminates direct dependencies between models. To support this paradigm, Argonne has developed a software library that provides discrete event-based coordination of models.

The MIMS framework layers on top of the DIAS library a number of capabilities to assist modelers when they configure and execute their models. The framework's graphical user interface provides a visual representation of the models' configurations, interconnections, and execution statuses. The configuration is represented by an extensible set of parameters that correspond to model inputs and outputs. Types of parameters range from integers and strings to such complex concepts as a regular grid on the earth's surface or a set of chemical reactions. New types of parameters and models can easily be supported, which allows basic graphical user interfaces for models to be developed more quickly in MIMS than would be possible with a custom user interface.

The framework also includes support for the repeated execution of models. This is commonly used in evaluations of alternative management approaches, sensitivity and uncertainty studies, and optimization and calibration runs. The framework includes a foundation to support these various types of repeated execution and a full implementation for stepping forward through time. Several prototype versions of the framework have been provided to interested parties within EPA to prompt feedback on how to better meet their needs. The first public release of the MIMS framework is planned for Spring 2002 to support Models-3/CMAQ.

2.3.2.2 Rain Gauge Network

A network of 10 rain gauges was established within a small watershed near the Neuse River in eastern North Carolina. This region is being scrutinized by environmental scientists because of the region's explosive growth of animal husbandry and concerns about estuary eutrophication and nitrogen deposition. This rural area consists of a mixture of farmlands, swine facilities, and densely-wooded snake-invested bottomlands. Precipitation data from this network will complement other surface hydrology, water quality, and ground water measurements that are being collected by scientists from U.S. Geological Survey (USGS) and the NERL/Athens Division to support modeling studies of the watershed. Precipitation data from the gauges will also be useful for evaluating daily NEXRAD data.

2.3.3 Research on Emissions Modeling

2.3.3.1 Anthropogenic Emissions

During FY-2001, the Sparse Matrix Operator Kernel Emissions (SMOKE)© system was introduced as an integral part of the Models-3 air quality modeling system, replacing the

Models-3 Emission Processing and Projection System (MEPPS). SMOKE© was originally developed as a prototype for the Models-3 system by the MCNC-North Carolina Supercomputing Center in cooperation with the Division (Houyoux and Vukovich, 1999). The sparse matrix approach to repetitive computations with large emission databases decreases processing time by at least an order of magnitude (hours to minutes). In addition to being modified to run with the current Models-3 framework, SMOKE© was enhanced to allow user-defined specification of such major elevated point-source emissions (MEPSE) as large electric utility stacks. The user may define MEPSEs by the mass of daily emissions for different pollutants and/or by physical stack parameters (height, diameter, temperature, flow). Enhancement to allow use of hourly continuing emission monitoring data from electric utilities was initiated in FY-2001. ASMD provided source category-specific emission-species data that allow SMOKE© to produce particulate matter species from reported $PM_{2.5}$ emissions for use in CMAQ.

During FY-2001, the SMOKE© Tool was developed and released as part of the Models-3 system as a utility to provide input files and quality control functions for SMOKE©. The SMOKE© Tool is derived from MEPPS, and consequently remains based on the SAS® software system. The SMOKE© Tool includes the ability to import and quality assure emission-related data, tools to analyze and visualize the emission data using the ARC/Info™[13] geographic information system (also required to use SMOKE© Tool), and the ability to output a user defined modeling grid and gridded spatial surrogate data files required by SMOKE©. Reducing licensing costs and eliminating dependencies on third-party software are key goals of future Models-3 development. SMOKE© Tool can be used either within the current Models-3 framework or independently without the framework. A separate Spatial Tool to define grids and grid spatial surrogate data (coded in C) is under development. SMOKE© will be used in the new Java-based Models-3 framework based on the MIMS framework planned for release in FY-2002. SMOKE© Tool will not be in the new framework. However, its functions will gradually be replaced by new tools not dependent on ARC/Info® or SAS®, which may be used independently or in the new Models-3 framework.

2.3.3.2 Biogenic Emissions

ASMD continued to develop and test algorithms for simulating airborne emissions from natural and biogenic sources. These sources include hydrocarbons from vegetation, nitric oxide and ammonia from soils, nitric oxide from lightning, and ammonia from livestock operations. The algorithms were integrated into the Biogenic Emissions Inventory System (BEIS), the third generation of which was incorporated into the FY-2001 release of SMOKE©. A Division web site was created to provide additional information on the Division's biogenic emissions research, slides of presentations, and access to data and computer algorithms. The web address is http://www.epa.gov/asmdnerl/biogen.html.

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[13]ARC/Info is a trademark of ESRI.

Regional air quality models need accurate characterization of vegetation cover to estimate biogenic emissions and dry deposition. However, most satellite-derived data sets, while providing good spatial resolution, do not resolve vegetation species and crop types. Isoprene emissions vary among tree species, with extremely high emissions from oaks, but negligible emissions from maples. Division scientists have constructed a 1-km vegetation database for North America, called the Biogenic Emissions Land use Database (BELD3). The USGS1-km land-use/land-cover (LULC) data set derived from the NOAA Advanced Very High Resolution Radiometer (AVHRR) satellite imagery was coupled with forest inventory data from the U.S. Forest Service and the 1992 Agricultural Census. The 1990 Census was used to denote urbanized regions. Each 1-km pixel includes percent forest cover, percent crop cover, Federal Information Processing Standard code, and the USGS LULC class. In the United States, each pixel is further divided into tree species and crop types. This data set provides much greater spatial resolution than earlier county-based land-use data sets developed for biogenic emission calculations. It should provide a more accurate basis for vegetation-sensitive calculations for such regional air quality models as CMAQ. The data set can be accessed at http://www.epa.gov/asmdnerl/biogen.html.

2.3.3.3 Inverse Modeling of Ammonia Emissions

Approximately 85% of NH_3 emissions are estimated to come from agricultural non-point sources, with a suspected strong seasonal pattern in these NH_3 emissions. However, current NH_3 emission inventories' lack intra-annual variability. The Branch is applying the adaptive-iterative Discrete Kalman Filter inverse modeling technique (Gilliland and Abbitt, 2001; Haas-Laursen *et al.*, 1996) to estimate seasonally varying NH_3 emission for the eastern United States. The Branch used the CMAQ modeling and ammonium (NH_4^+) wet concentration data from the National Atmospheric Deposition Program network for this application. The inverse modeling technique estimates the emission adjustments that provide optimal modeled results with respect to wet [NH_4^+], observational data error, and emission uncertainty. Final products of this research will include monthly emission estimates from each season of 1990. Results for January, April, and June 1990 are currently available. The results confirm that annual average NH_3 emission estimates can introduce substantial errors into air quality modeling results. Based on the inverse modeling method, the annual emission values should be decreased by 64% for January 1990, 26% for April 1990, and increased by 25% for June 1990. More details from these results can be found in Gilliland *et al.* (in press).

Simulations are currently underway to develop emission adjustments for October 1990, which along with results from January, April, and June will provide a first estimate of the seasonal variation in NH_3 emissions. The next step in this research will be to expand to more recent years to provide information about the interannual variability, as well as the seasonality, in NH_3 emissions. Additionally, the inverse modeling method will be modified and tested to address spatial variability in the emissions by considering individual source types and their spatial distribution.

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 on exchange of air pollutants with other media. Branch scientists also conduct 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.

2.4.1 Compartmental Multimedia Modeling

The transport and environmental fate of toxic pollutants is an inherently multimedia chain of events. One key area of uncertainty in current spatial, multimedia models is the lack of proper characterization of intermedia fate and transport elements. This is a principle strength of fully coupled hybrid compartmental (FCCM) models. FCCM models include both well-mixed or uniform as well as non-uniform media descriptions that are tightly integrated through well-posed intermedia physical boundary conditions. Simultaneous solution of the media expressions imposes a chemical mass balance across the entire multimedia system. Recent implementations of this modeling approach include the mechanistic descriptions of intermedia transport parameters, the accounting for time-dependent parameter variability, and the inclusion of vegetation and aquatic biota compartments. These models are most appropriate for the study of widely distributed (*i.e.*, non-point source), relatively non-reactive organic chemicals at scales ranging from a small watershed up to 10^3 km^2. An internal EPA Grant was awarded in 1999 to support research regarding the development of a "next generation" of these models, using the FCCM model MEND-TOX, as a point of departure.

Several case studies using MEND-TOX were completed that explore various aspects of FCCM model behavior. During FY-2001, a manuscript was accepted for publication that describes the linkage of MEND-TOX and ongoing Division research regarding the development of enhanced algorithms describing gas-phase dry deposition to vegetated surfaces (Cooter and Cohen, accepted for publication). Subsequently, this work was combined with previous MEND-TOX applications to produce two manuscripts— a description of the FCCM approach, and a summary of case study results— for publication (Cohen and Cooter, accepted for publication; Cohen and Cooter, accepted for publication). Internal reports summarizing the potential implementation and advancement of FCCM concepts under Multimedia Integrated Modeling System (MIMS) framework were assembled during FY-2001. Critical design and implementation issues were highlighted and will be explored during FY-2002 through a limited series of evolving pilot models. The first such pilot, in which all media are assumed to be homogeneous, is illustrated in Figure 5.

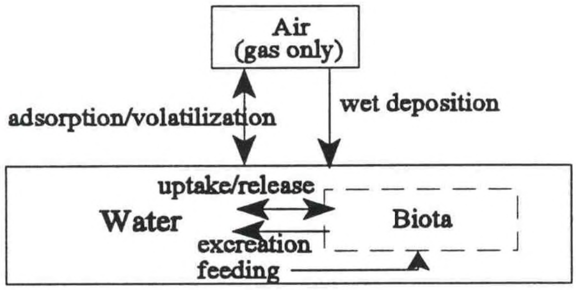


Figure 5. The three compartment FCCM phase I pilot model.

Specific MIMS framework issues exclusive to the Phase I compartmental model study include using the framework to build and define a set of model equations from individual objects or components, use of interchangeable model components for re-specification of the model equations, input from several information sources spanning a wide range of time scales, implementation of a numerical solver suitable for systems of stiff ordinary differential equations, and the iterative solution of the equation system that defines our multimedia environment. During FY-2002, the results of the Phase I pilot will be evaluated. Based on the results of the evaluation, the pilot could be expanded to address a variety of such other design issues as the inclusion of non-homogeneous media (described *via* partial differential equations), additional mechanistic transfer processes, additional media, and linkages with other Division model implementations under the MIMS framework.

2.4.2 Application of the Concept of Saltation-Driven Resuspension of PM_{10}

A method for estimating the vertical flux of resuspension particles smaller than 10 micrometers (PM_{10}) emitted during wind erosion was developed for Owens Lake, a large dust-source area in California. Owing to the size of the potentially dust-emitting dry lake bed (about 130 km^2) and the large effort and expense to rigorously measure vertical mass fluxes using micometeorological methods, an alternate method using cheaper and more easily accomplished measurements was developed. The method assumed that the emission mechanism for vertical flux of PM_{10} is dominated by sandblasting by hopping (saltating) sand particles. Sand grains absorb momentum from the wind and deliver it to the surface. When the kinetic energy of the impaction of sand grain overcomes the binding energy holding particles $d<10\mu m$ in place, resuspension occurs.

Using the assumption that sandblasting dominates PM_{10} emissions, the model of PM_{10} dust emissions used measurements of sand mass flux on the surface of the lake bed, a model of dust transport, and high quality measurements of PM_{10} at several locations near the shoreline of Owens Lake. The method allowed the estimation of mass fluxes for the most active areas of dust emissions at Owens Lake as follows:

- Sand fluxes are presently being measured in a 1 km by 1 km grid of 130 sand flux samplers.
- The concentration of PM_{10} (particle mass for particle size smaller than 10 μm) is measured at several locations along the shoreline of Owens Lake using continuous measuring TEOM (Tapered-Element Oscillating Microbalance) instruments.
- The concentrations are modeled using CALPUFF. Initially, a first guess value for the ratio of vertical mass flux of PM_{10} to horizontal sand mass flux (F_a/q) is used with the 130 q values to give the F_a (vertical fluxes of PM_{10}) for each 1 km^2 area of Owens Lake. These F_a values are used in the model and the concentration field is calculated.
- The ratios of the calculated concentrations at the locations of the TEOM instruments to the actual concentrations are found. Using the mean of these ratios the first guess F_a/q value is adjusted so that the predicted and measured concentrations agree.
- One F_a/q value is found for each hour of a dust storm.
- An example of a dust storm that took place on May 2–3, 2001, is shown in Figure 6. Owens Lake is shown having a grid work with a sand motion detector at the center of each grid square. The number appearing in each square is the total mass flux of sand for the entire storm. Superimposed are boundary observations of the dust plumes taken for each hour of the storm from three mountain locations surrounding the lake. TEOM PM_{10} instruments are shown on the map at Olancha, Dirty Socks, Shell Cut, Flat Rock, Keeler, and Lone Pine.

- All dust storms are analyzed. Owens Lake is divided into three areas having distinct surface characteristics. Because these areas are the dominant source areas for given TEOM receptors, during defined wind direction ranges, the times are restricted to those hours when winds were within the wind direction range. One-hour F_a /q values that apply to the three distinct source areas of the lake were calculated.

- Micrometeorologically and wind-tunnel determined F_a/q values for small areas of the lake were found and were compared to the large-scale F_a/q values. Agreement was satisfactory.

- Using this method, areas of the strongest emissions of Owens Lake were identified and estimates of the total production of PM_{10} dust were calculated.

2.4.3 Comparison of Wind-Tunnel Measurements of the Flow and Turbulence Fields in Arrays of Two- and Three-Dimensional Buildings

A laboratory study of the complex flow patterns within arrays of two-dimensional and three-dimensional buildings to simulate the types of flow fields that might be found in urban street canyons was conducted in the meteorological wind tunnel at the Fluid Modeling Facility (FMF). This study is an integral component of the Division's modeling of particulates and air toxics at neighborhood scales (Poole-Kober and Viebrock, 2000), a project to develop linkages between Eulerian grid-based air quality models and human exposure at finer scales. Additionally, the FMF staff have been collaborating with Los Alamos National Laboratory and Lawrence Livermore National Laboratory to utilize the study data for improving computational fluid dynamics models of flow and dispersion in urban and industrial areas. Previous annual report entries (Poole-Kober and Viebrock, 1999; 2000) describing this long-term project have discussed a series of flow visualizations and surface pressure measurements on the buildings and the mean flow and turbulence in the array of two-dimensional buildings. Here, the focus is on a comparison of the flow and turbulence fields for arrays of two- and three-dimensional buildings.

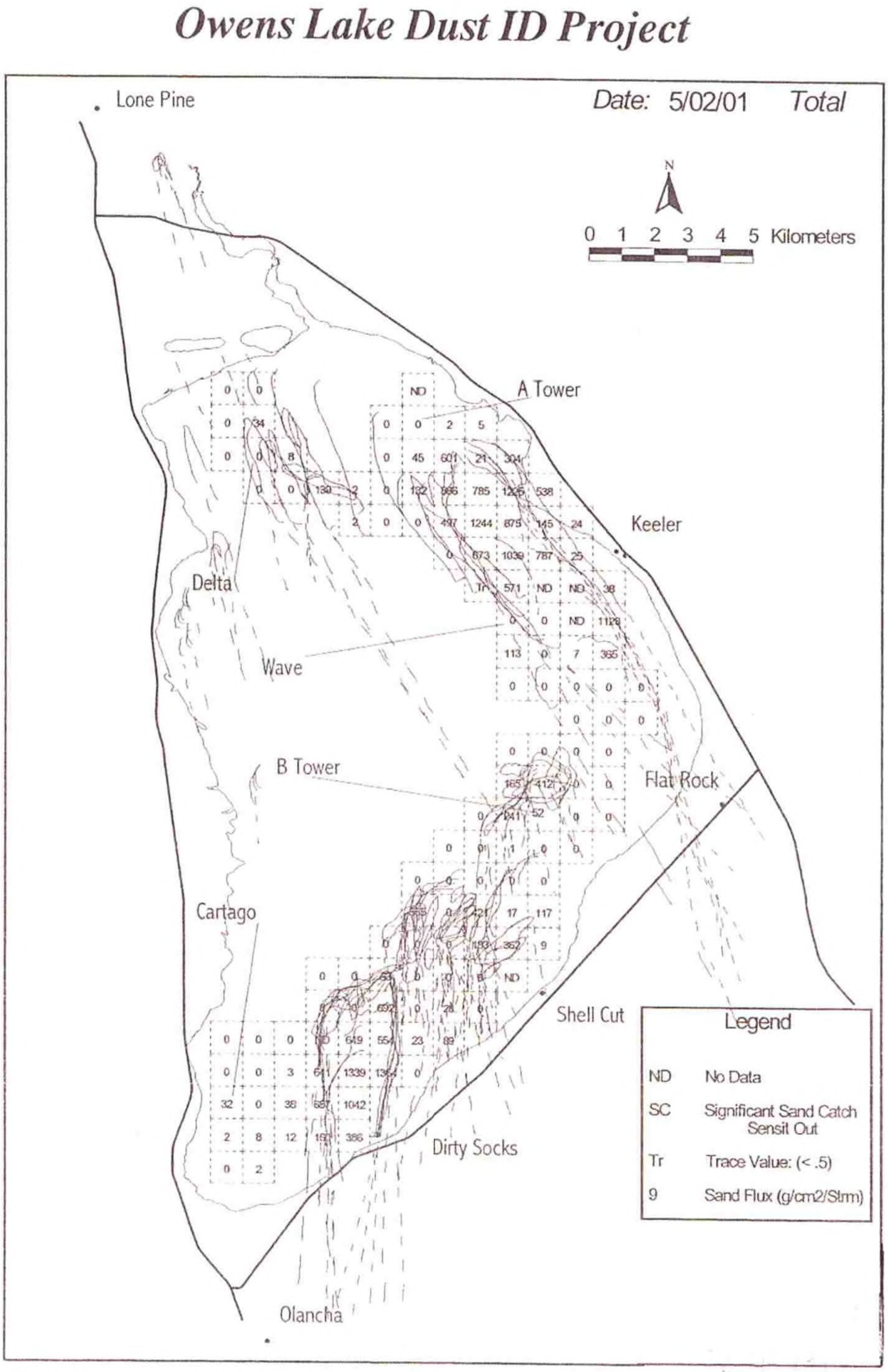


Figure 6. An example of a dust storm during May 2–3, 2001.

For the 2D array in the wind tunnel, seven rectangular buildings, each the width of the tunnel and height and downwind dimension equal to 15 cm, were placed with an alongwind separation of 15 cm (Figure 7a). The 3D array consisted of seven rows of eleven cubical buildings where each cube had a height of 15 cm (Figure 7b). High resolution measurements of the three components of mean and turbulent velocities were obtained around and above the buildings. The approach flow to the building array was a simulated neutral atmospheric boundary layer with a depth of approximately 12 building height. There was sufficient upwind fetch for the boundary layer to grow to equilibrium before reaching the upwind edge of the buildings. The approach flow at z = building height (H) was 3m/s, ensuring that Reynolds number independence was satisfied. Measurements of the three components of velocity and the turbulence intensities were obtained with pulsed-wire anemometry (Bradbury and Castro, 1971). Measurements (on the longitudinal centerline of the building array) were collected from 3.5 H upstream to 7.5 H downstream of the building arrays and up to 3 H in the vertical. Figure 8 shows a cross section of the mean wind and the turbulent kinetic energy (TKE) fields around and upstream of the first three buildings in the 2D array and the first three rows of cubical buildings in the 3D array. The cross sections are along the centerline of the tunnel, which in the 3D array is centered on buildings (not in a street canyon).

There are several noticeable differences in the flow fields of the 2D and 3D cases. At the leading edge and immediately above the rooftop of the first building row, the TKE is much larger in the 2D case. The presence of the wide buildings requires the air to move more forcibly over the obstruction resulting in stronger jetting action and associated shear induced turbulence beyond the leading top edge. This region of high turbulent energy is advected downwind over several more buildings (rows). The strong recirculation just upwind of the first 2D building, again as the result of the blockage by the wide buildings, appears both in the flow vectors and in high turbulence levels. Also, in the flow for the 2D buildings there is significant vertical motion for up to several building heights above the first row whereas the flow becomes nearly horizontal just a short distance above the buildings in the 3D case. The primary reason for these various differences is that the recirculation, jetting and vertical motions are much less pronounced because the air stream can flow between as well as over the buildings in the 3D arrangement.

Finally, distinct differences appear in the regions of circulation within the street canyons. Between the 2D buildings the vortex is symmetric and is centered in the canyon. With the 3D building array, the vortex is clearly asymmetric with the center shifted toward the upwind building face leaving a broad area of downward motion. This asymmetry is likely due to the lateral (cross-stream) canyon motions that result from the edge effects as the flow moves around the sides of the cubical buildings.

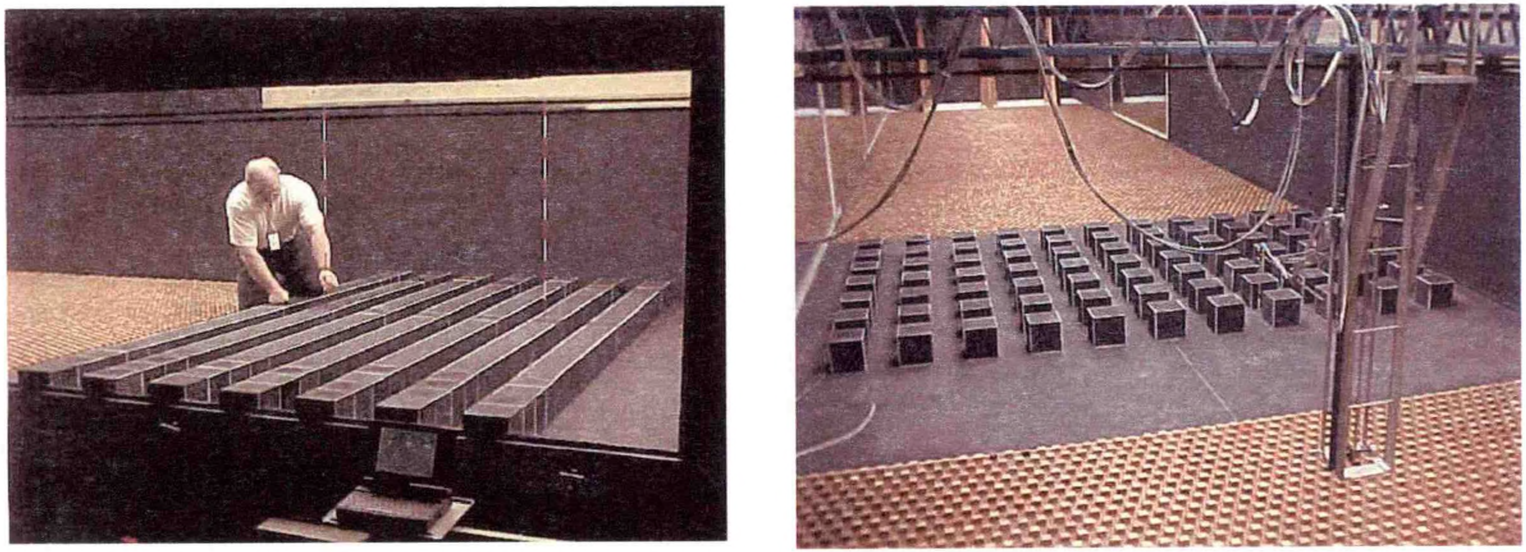


Figure 7. Building arrays in the wind tunnel: a) two-dimensional buildings, flow left to right; b) three-dimensional buildings, looking into the flow.

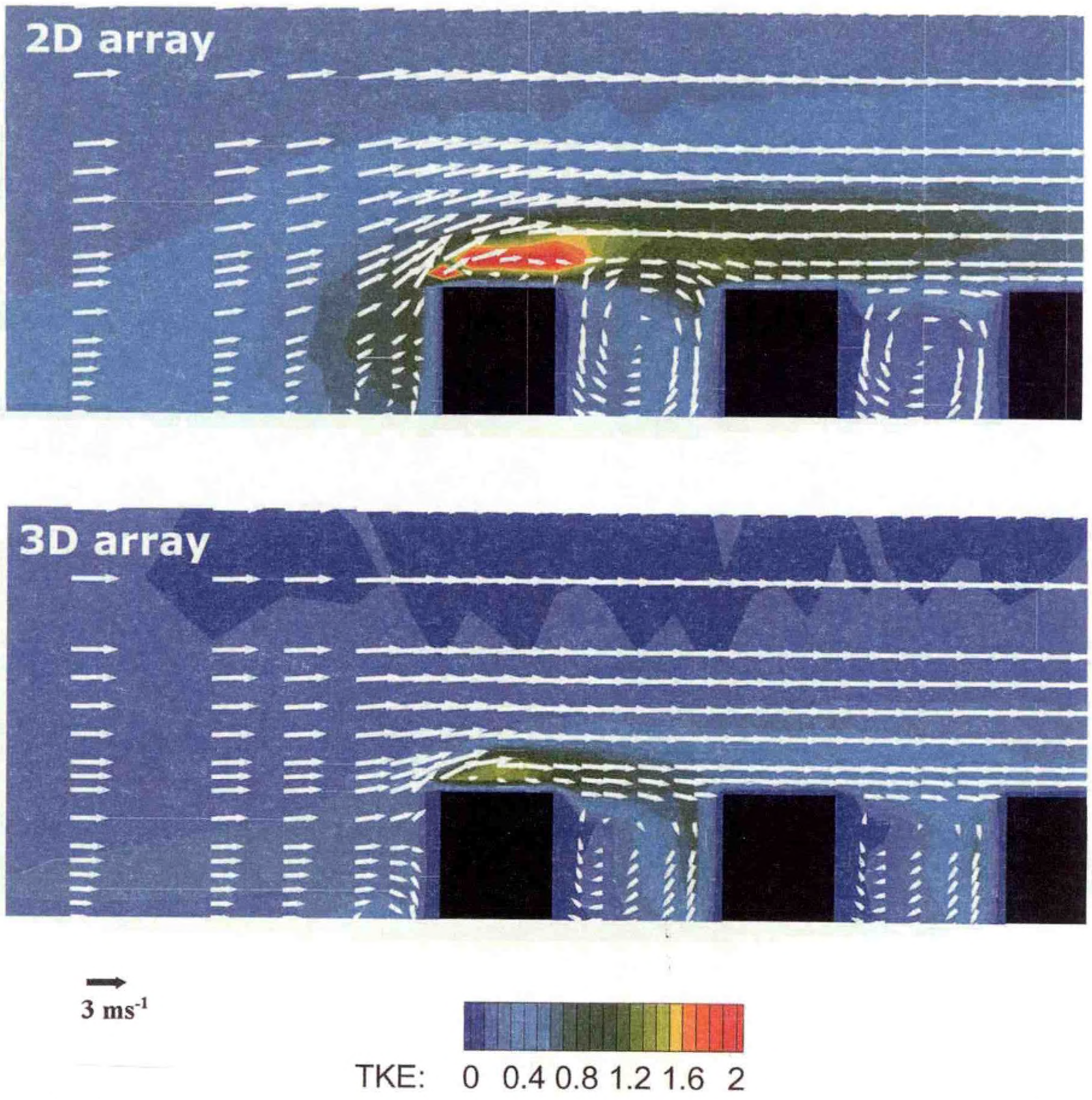


Figure 8. Mean velocity vectors and turbulent kinetic energy (m^2s^{-2}) in the centerplane of the wind tunnel for the area surrounding the first three rows of buildings.

2.4.4 Atmospheric Correction / Image Processing

One of the physical *state* variables characterizing a landscape is its spectral albedo, or reflectance, function. During June 1999, spectral upwelling radiance was measured for a 10 km x 60 km swath of the lower Neuse River Basin by NASA/Dryden field operations. The detector— Airborne Visible and Infrared Imaging Spectrometer (AVIRIS)—is a nadir-looking spectral radiometer that collects radiance data [W/m2/sr/nm] in 224 bands (10 nm bandwidth) from 380 nm to 2510 nm, with a spacial resolution of 20 m. Processing of AVIRIS data to derive surface reflectance requires compensation for atmospheric effects, including backscatter and absorption. The MODTRAN radiative transfer model was used to create data for a look-up table interpolation approach (inverting radiance to determine reflectance has no closed form since reflectance-to-radiance is strongly non-linear). Using MODTRAN, upwelling radiance was calculated for atmospheric conditions and geodesic configuration prevailing at the time of overflight. *Pixel-wise* correction for water vapor is necessary due to its great spacial variability. *Scene-wise* correction was adequate for other gasses and aerosols having negligible spacial variability within the scene. One unexpected discovery of this work is the difference in detectable precipitable column water vapor over agricultural fields vs. forest canopies (Figure 9). This could lead to an automated classification scheme. Automated image classification will be validated by field reference data.

Figure 9. Water vapor highlighted scene, with river, lakes, and clouds in black.

2.4.5 Local Scale Modeling of Human Exposure Microenvironments

A project to specifically improve the methodology for real-time site specific modeling of human exposures to motor vehicle emissions is ongoing. This project is being pursued in collaboration with other projects. The goal is to develop improved methods for modeling air pollution from the source through the air pathway to human exposure in significant microenvironments. Local-scale modeling refers to spatial scales from the size of an individual vehicle to the order of 1 km. A complete modeling framework from source-to-exposure, together with some measurements, is principally being set up in the Research Triangle Park area of North Carolina and in New York City, which can be transferred to other locations. Human exposure models use simplified assumptions based on a few fixed air monitoring stations or modeled concentrations from regional-scale motor vehicle emission/transport models resulting in great uncertainty in their estimations. The refined modeling will be used to provide improved linkage between source emissions and human exposures to provide refined exposure factors for significant microenvironments.

Real-time site-specific motor vehicle emission models capable of capturing real-world emissions are needed to support human exposure modeling. Development of a real-time **Micro**scale automobile emission **Fac**tor model for **P**articulate **M**atter (MicroFacPM) was completed and supporting papers should be published during FY-2002. Now MicroFacPM along with the **Micro**scale automobile emission **Fac**tor model for **C**arbon **M**onoxide (MicroFacCO) will be applied to roadway dispersion models to evaluate there performance. These models can be used to demonstrate the sensitivity of emission estimates to real-time input parameters for vehicle fleet composition, vehicle speed, and meteorological conditions.

Refined modeling using computational fluid dynamics (CFD) simulations and measurements are being applied to develop refined air dispersion models for linkage to human exposure microenvironmental models. This modeling framework will help to establish the direct relationships between source-to-exposure concentrations specific to the particular exposure microenvironment. Output from this deterministic modeling of microenvironmental concentrations and measured microenvironmental concentrations for a range of scenarios will be used to develop distributions of potential exposure that is probabilistically-based to support population-based human exposure modeling. Figures 10, 11, and 12 provide examples of CFD simulation models for a multi-block area in New York City that were set up for evaluation. CFD simulations provide opportunities for expanding and improving capabilities for modeling exposures to environmental pollutants. A cooperative research project with Fluent, Inc., is examining and evaluating the application of CFD models for simulating air pollution along the pathway from source to human exposures. While the goal ultimately is to model a large urban neighborhood, there is first a need to examine the simulation of an atmospheric boundary layer and pollutant dispersion in absence of urban obstacles. The detailed spatial resolution of environmental pollution concentrations that is possible from CFD simulations can provide important information that is not available from a single-point measurement. Output of CFD simulations can be used to develop better simplified modeling methods in the same way as field and wind tunnel study measurements are used. Through further research, validation and testing, CFD modeling has the potential to become a reliable tool for estimating pollutant concentrations for situations that today have no reliable modeling method.

Example Wind Profiles through the Domain

***Upstream Boundary Condition: U(10m)=5m/s, 1/7th Power Law**

***10 meter increments (0-250 m altitude)**

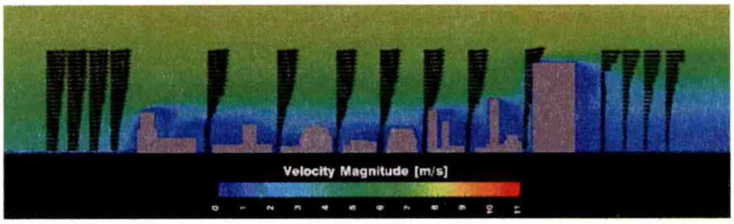


Figure 10. Example effect of urban buildings on wind profiles.

CFD Example: 3-D Wind
(NYC near 59th St;

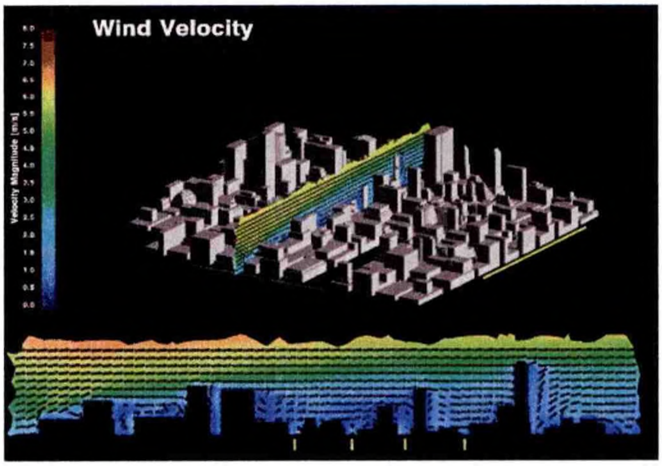


Figure 11. Example vertical slice of full 3-D solution for wind.

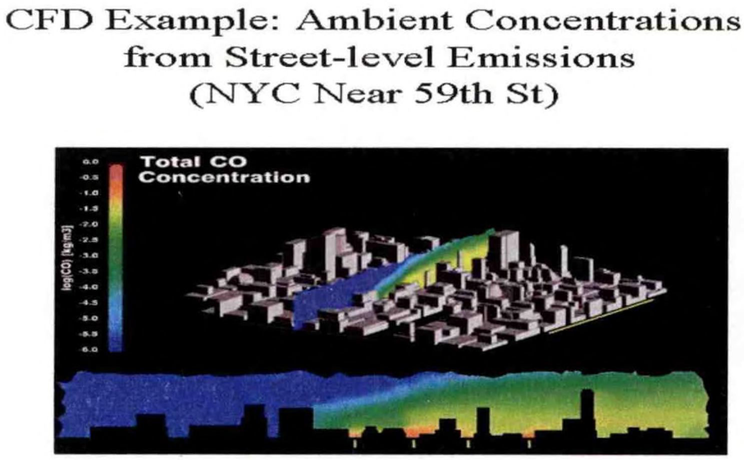


Figure 12. Example vertical slice of full 3-D solution for concentration.

2.5 Air Policy Support Branch

The Air Policy Support Branch supports the 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 simulations 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; and providing meteorological assistance and consultation to support OAQPS in developing and enforcing Federal regulations and standards and assisting EPA Regional Offices.

2.5.1 Modeling Studies

2.5.1.1 CMAQ Proof of Concept: Continental United States Application

As part of a proof-of-concept effort designed to more fully understand the details of the Models-3/CMAQ modeling system and lay the groundwork for using CMAQ in regulatory support modeling exercises, Models-3/CMAQ was configured and successfully applied for the entire year of 1996 over the continental United States. The simulations were completed for a 36-km grid with eight vertical layers. The meteorological input fields were developed using MM5 and the emissions were based on a version of the National Emissions Trend inventory.

A base case simulation using the May 2000 release of CMAQ was completed and evaluated against a limited ambient database. Generally, comparisons between model predictions and ambient data for particulate matter (PM) smaller than 2.5 microns ($PM_{2.5}$)—paired in space and time—showed good agreement as shown in Figure 13.

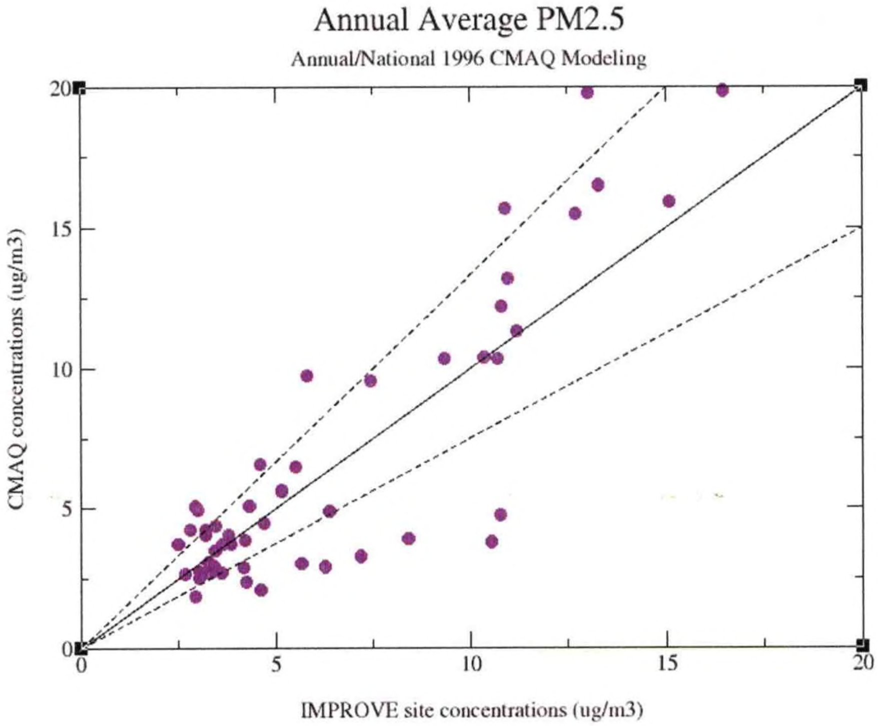


Figure 13. Comparison of annual average IMPROVE site concentrations and model concentrations of $PM_{2.5}$ (paired in space and time) for the 1996 national CMAQ application. Dashed lines indicate 25% error.

However, based on this particular CMAQ application, there appear to be some fine particulate performance issues that still need to be resolved. This may not necessarily be indicative of a problem with the air quality model itself, as some combination of meteorological and emission inputs could also be responsible. It should also be noted that most other existing PM models are subject to the same $PM_{2.5}$ performance questions. The considerable overestimation (factor of 5) of particulate nitrates in the model, especially in the winter (Figure 14), is of particular concern. Several diagnostic tests are planned to better determine the causes of these over predictions.

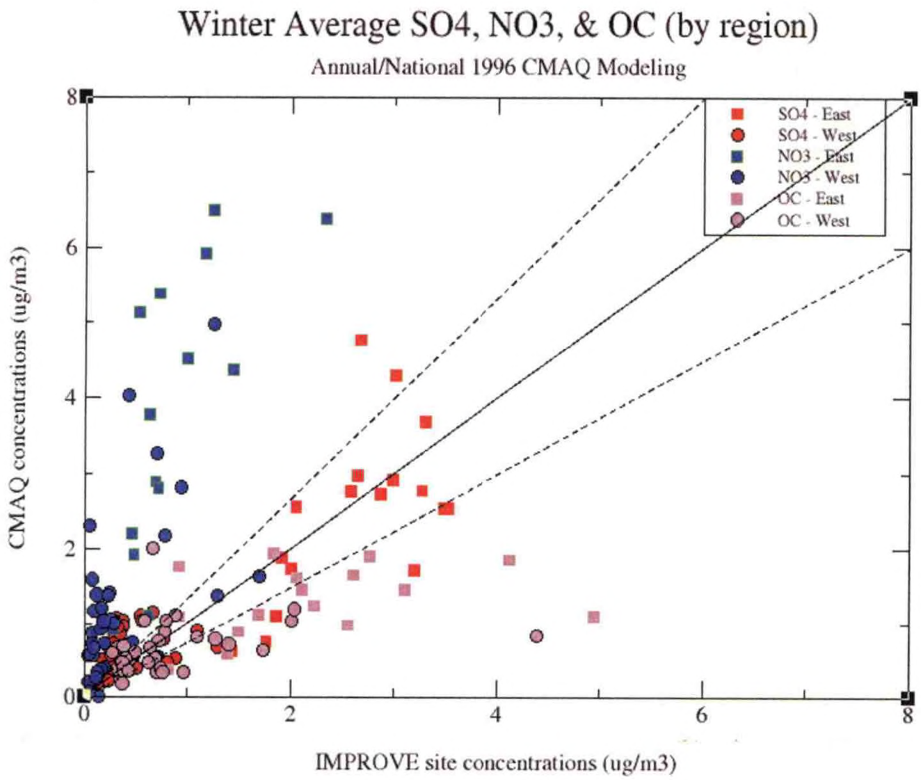


Figure 14. Comparison of winter average (December-February) Interagency Monitoring of PROtected Visual Environments (IMPROVE) site concentrations and model concentrations of sulfate ion, nitrate ion, and organic carbons by region for the 1996 national CMAQ application.

Several diagnostic simulations were completed investigating the effects of certain model inputs and physiochemical options. The first set of tests quantified the impacts of employing the RADM2 chemical mechanism as opposed to the CB-IV mechanism, which was used in the base case. For the most part, the simulated particulate concentrations were not greatly affected. The second set of tests looked at the impacts of reducing the highly uncertain ammonia emissions inventory by 50% for January 1996. While this improved the model nitrate predictions considerably, additional emissions development research is required before such a change can be justified. The third set of tests looked at the impacts of varying boundary conditions on CMAQ model predictions. A qualitative assessment determined that model performance for ozone could be improved by using climatological average inputs as opposed to the default concentrations that are built into CMAQ. These runs also highlighted the potential impacts of intercontinental transport on air quality in the western United States.

2.5.1.2 The National-Scale Air Toxics Assessment

Under the CAAA of 1990, EPA is required to regulate emissions of 188 listed air toxic pollutants. The EPA National-Scale Air Toxics Assessment includes 33 air toxics that present the greatest threat to public health in the largest number of urban areas. These 33 air toxics include 32 hazardous air pollutants (HAPs) and diesel particulate matter. The goal of the national-scale assessment is to characterize risks and health effects of these air toxics on a broad scale to identify pollutants of greatest concern to the greatest number of people. The results will be used to identify pollutants and areas of the country requiring additional investigation.

The Assessment System for Population Exposure Nationwide (ASPEN) model was used to estimate the 1996 ambient concentrations based on the1996 emissions (U.S. Environmental Protection Agency, 2000). This model is based on the Industrial Source Complex Long-Term model (ISCLT), which simulates the behavior of the pollutants after they are emitted into the atmosphere. ASPEN uses estimates of toxic air pollutant emissions and meteorological data from more than 350 National Weather Service Stations to estimate air toxics concentrations nationwide. The ASPEN model takes into account such important determinants of pollutant concentrations as rate of release, location of release, the height of release, wind speed and direction from the meteorological stations nearest to the release, breakdown of the pollutants in the atmosphere after being released (*i.e.*, reactive decay), settling of pollutants out of the atmosphere (*i.e.*, deposition), and transformation of one pollutant into another (*i.e.*, secondary formation). The model estimates toxic air pollutant concentrations for every census tract in the continental United States, Puerto Rico, and the Virgin Islands. Census tracts are land areas defined by the U.S. Bureau of the Census and typically contain about 4,000 residents each. Census tracts are usually smaller than 2 square miles in size in cities, but much larger in rural areas.

Modeled ambient concentration maps allow states to view 1996 ambient concentration estimates (in micrograms per cubic meter) based on the median concentration in each county. The maps are color-coded (by percentile breakdown relative to the rest of the country) to show how each county's median concentration compares to the rest of the United States. The median concentration is the value for which 50% of the census tracts in the county have ambient concentrations less than the median, and 50% of the census tracts in the county have ambient concentrations greater than the median. Lists of the modeled ambient concentrations for benzene for each state is available at http://www.epa.gov/ttn/atw/nata/. Several conclusions can be reached from the results of this study:

- Concentration estimates are a complex function of a number of factors, including emissions density (number of sources in a particular area), meteorology, and source characteristics, rather than just related to total emissions. Both emissions and estimated concentrations of the 32 HAPs available to date are generally higher in urban than in rural areas.

- Some pollutants are more evenly distributed around the country (*e.g.*, benzene, which is present in gasoline), while others are linked to areas of industrial activity (*e.g.*,vinyl chloride).

- There is considerable variability between the national, state, and the county level in terms of contributions by source type.

- The highest ambient average concentration of the individual pollutants occurs in different States (i.e., no one State has the highest concentrations of all the pollutants), because different types of sources are contributing to emissions in different areas of the country.

- Of the four main source types (area and other, major, on-road, non road), no one type is a main contributor to the estimated concentrations of the 32 HAPs available to date. The results show that, on a national level, about half of the pollutants have area and other sources as the dominant contributing source type. Source type contributions for benzene concentration in each state is available at http://www.epa.gov/ttn/atw/nata/.

2.5.1.3 Statistical Evaluation of Model Performance

Within the American Society for Testing and Materials (ASTM) work continues on the development of an ASTM Standard Guide that would provide guidance on the construction of objective statistical procedures for comparing air quality simulation modeling results with tracer field data. Thus far, those most involved in the development of this ASTM Guide have been scientists within the European community, where there is still strong interest in short-range plume and puff dispersion models. In December 2000, the guide was finalized and published by ASTM with the designation number of D-6589-00, and entitled, *Standard Guide for Statistical Evaluation of Atmospheric Dispersion Model Performance* (available from the ASTM web site, http://www.astm.org/). The publication of this guide is an important step towards developing statistical evaluation procedures for use in selecting and recommending preferred air quality simulation models for use in routine regulatory assessments.

Work will now be directed toward establishing test methods for use in evaluating plume dispersion models. In finalizing the guide, a series of investigations were completed to refine and test a draft evaluation procedure that is described within D-6589 (Irwin, 2001). During the Fall 2001, work was completed on revising Fortran software and databases that implement a draft evaluation procedure described in the annex of D-6589, for public use and evaluation. This procedure measures how well short-range dispersion models characterize the variation of the centerline maximum concentration at the surface as a function of transport distance and stability. To demonstrate this procedure, work is underway to evaluate several modern plume dispersion models using tracer field data from three extensive field experiments. If these results prove successful, work will be initiated to convert the D-6589 annex into a formal ASTM Standard Procedure, which can then be formally recommended for use.

2.5.1.4 The Krakow Urban Air Pollution Project

The former Polish capitol, Krakow, is located in the Vistula River Valley and frequently experiences extended periods of stagnation, especially in wintertime. With emissions from such old technologies as factories, steelworks, and small family manufacturing sites, Krakow frequently experiences air pollution problems. In recent years, Krakow has seen a rapid increase in the numbers of cars and associated traffic congestion resulting from a lack of bypasses surrounding the city, which is anticipated to add to existing air pollution impacts. Starting in 1991 with support from the EPA Office of International Activities, a pilot program for Poland was initiated to develop a formal air pollution abatement program. A seven-station automated air-monitoring network was installed in Krakow and training was initiated in the collection and analysis of air monitoring data. In December 1998, the pilot program was extended to include training in the application of air dispersion modeling, for the ultimate purpose of investigating the benefits of alternative control abatement strategies. The CALMET/CALPUFF (Scire *et al.*, 2000a; 2000b) modeling system was selected to provide a flexible system that would prove useful throughout Poland. In the Spring 2001, the comparisons of simulation results for sulfur-oxide (SO_2)with monitoring data for seven sites in Krakow for 1998 were completed (Irwin *et al.*, 2001a).

The comparison of annual and monthly concentration values is shown in Figure 15. The larger variance in the estimates versus observed, may signal a need for local emission inventory adjustments. For instance, the bias to overestimate concentration at Site 3, Figure 15(A), is seen in Figure 15(B) to relate to overestimation of the winter month concentration values (solid red circles). The bias to underestimate at Site 4, Figure 15(A), is seen in Figure 15(B) to relate to underestimation of the winter month concentration values (solid blue circles).

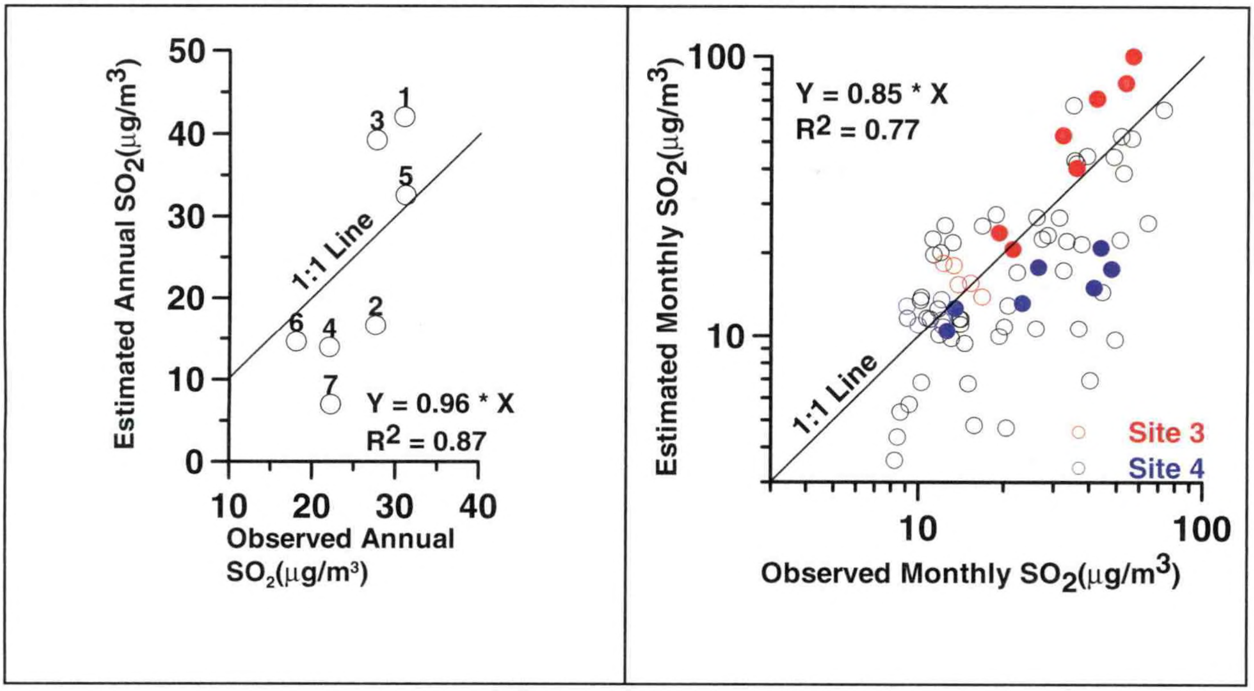
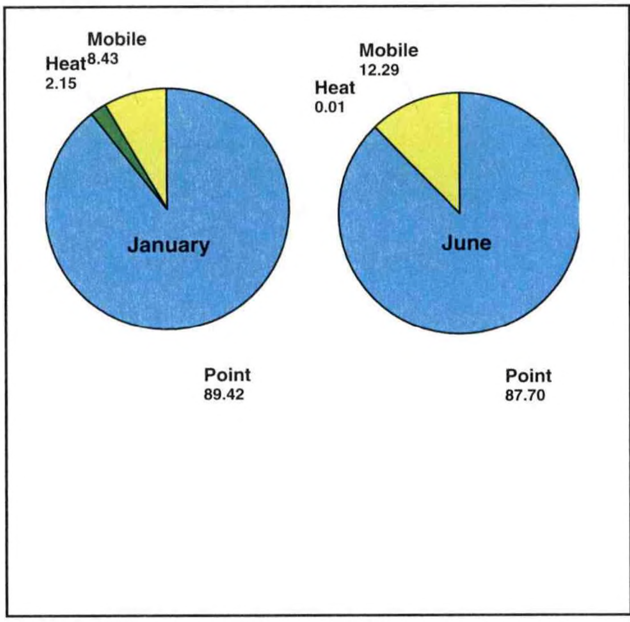


Figure 15. Comparison of observed and estimated A) annual average and B) monthly average SO2 concentration values. Linear regression results (with zero intercept) and site locations are annotated within the figures.

Figure 16 illustrates the estimated relative emissions for January and June 1998. Figure 15 illustrates the contribution to the total SO_2 concentration estimated for Site 5 from each of the three emission inventories. Only results for Site 5 are shown in Figure 17 since the contribution from the three emission inventories (point, heat, mobile) to the total SO_2 concentration estimated at each site is fairly consistent across all sites. Figure 17 shows the definite seasonal variation in the relative impact from the three source types, and the relative importance during the heating season of the heat production emissions. These results shown in Figures 16 and 17 illustrate that although the emissions from tall stacks can be considerably larger than from low level releases, the local impact from these emissions is limited to periods of the day and seasons of the year when these emissions reach the surface.



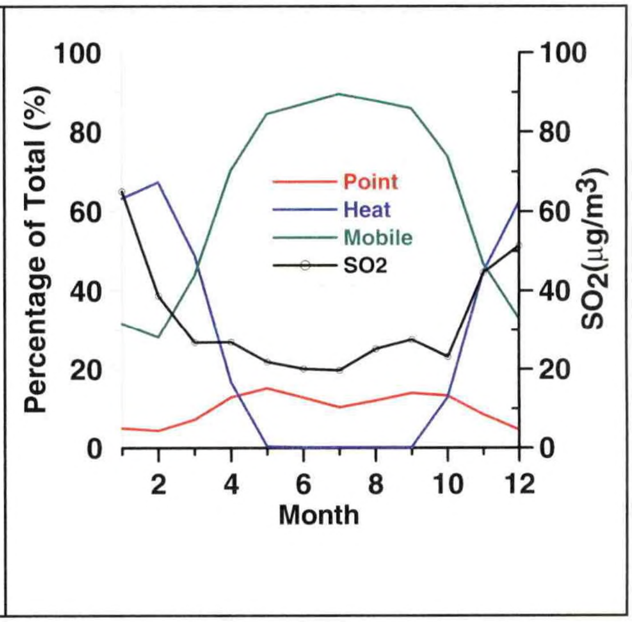


Figure 16. Relative emissions (percent) for January and June 1998 from the three source inventories

Figure 17. The percentage contribution to the total SO_2 concentration estimated for Site 5 from each of the three emission inventories. Black line is simulated total SO_2.

The basis for sponsorship by the U.S. Agency for International Development for the Krakow Urban Air Pollution Project was removed with the acceptance of Poland into the North Atlantic Treaty Organization Alliance. The project successfully trained the staff in the operation of the CALPUFF modeling system, and provided a basis for investigating the benefits of alternative control abatement strategies in future years.

2.5.1.5 Estimating Background Concentration for Diesel PM

Background concentrations are an essential part of the total air quality concentration to be considered in determining source impacts. Background air quality includes pollutant concentrations due to natural sources, nearby sources that are unidentified in the inventory, and long-range transport into the modeling domain. Typically, monitored air quality data should be used to establish background concentrations.

The ASPEN model is based on ISCLT Version 2.0 Gaussian plume model. The ASPEN model calculates concentrations at receptors in a concentric grid of 12 rings and 16 radial distances with a maximum distance of 50 km. However, sources at distances more than 50 km from the receptor contribute to the total concentration at the receptor location.

For diesel PM, a modeling based approach was developed to provide a rough approximation of concentrations due to transport from sources located between 50 km and 300 km from the receptor. A schematic plot showing the relationship between the census tract centroids at a distance 50 km – 300 km and modeling receptors allocated at census tract centroids is shown in Figure 18. In this figure, the receptor is shown as a blue star and a contribution from emission sources within a ring of 50 km – 300 km (shown in red) is considered. The background concentration at each receptor is the sum of concentrations resulting from all sources within the 50 km – 300 km radius.

This approximation was based on results from existing CALPUFF simulations from an elevated source (35 m) and a surface release (2 m) for three geographical areas: Boise, Idaho, Medford, Oregon, and Pittsburgh, Pennsylvania. These simulations were made as part of a series of simulations to compare ISCLT results with CALPUFF results (U.S. Environmental Protection Agency, 1993). CALPUFF is a Lagrangian puff model, which was originally designed for mesoscale applications, and it can operate in a range of 0 – 300 km from the source (Scire *et al., 2000b*). For these CALPUFF simulations, CALPUFF was run using ISC meteorology. Therefore, these CALPUFF results are not the result of a full-scale refined analysis, in which the meteorological conditions are allowed to vary in space and time.

The approach has several limitations. The estimates assume a complete and accurate inventory. Use of the ISCLT meteorology in CALPUFF does not account for wind flow in rivers and valleys as in mountainous terrain. The local wind flow patterns could cause concentrations to be significantly different at specific locations. Using three specific locations to obtain a national average parameterization is simplistic. Finally, using CALPUFF with site specific information on emission release height, stack parameters, wet and dry deposition, meteorological wind field, etc., would give different estimates. Thus, these estimates of the impact of emissions located greater than 50 km but less than 300 km are considered as an approximation of background concentration until more reliable estimates can be obtained from monitoring data or when improved modeling techniques are developed.

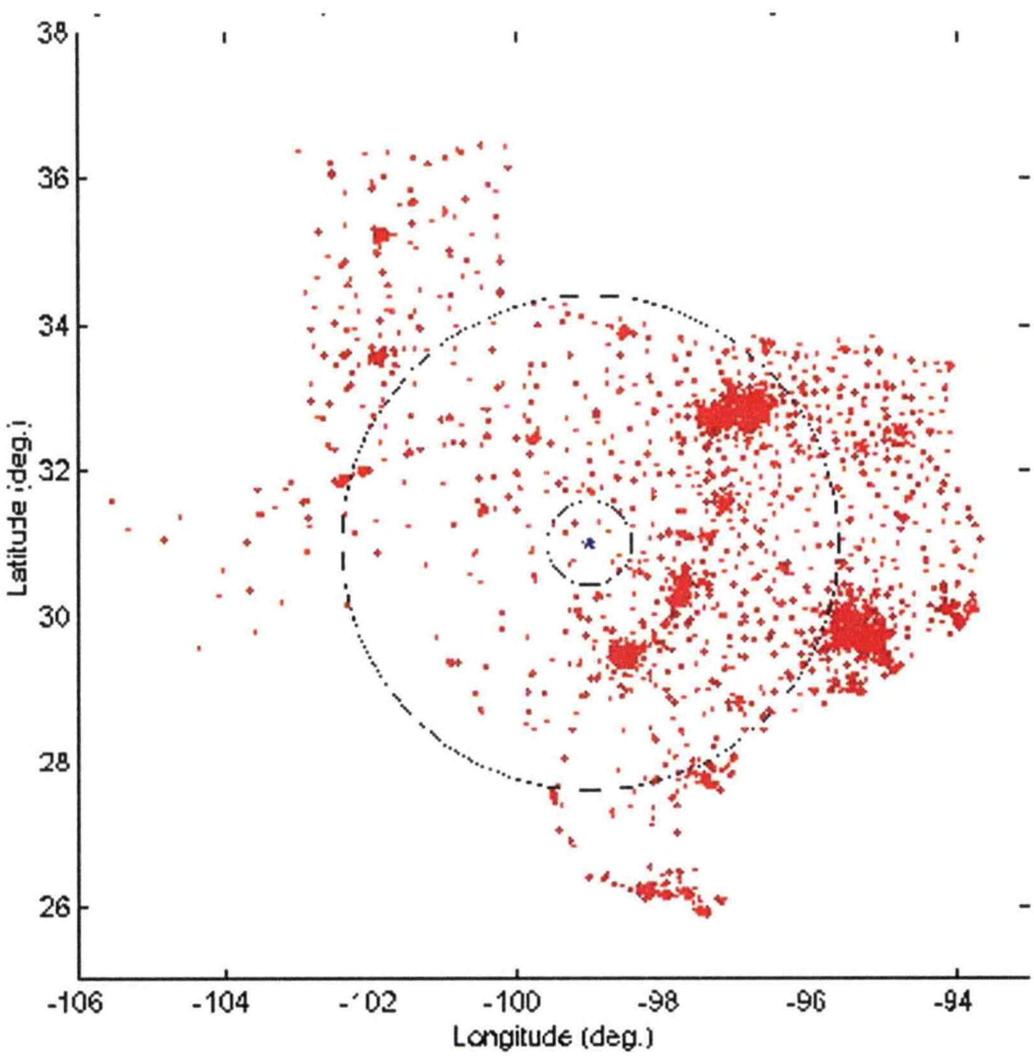


Figure 18. Schematic map of census tract centroids and rings of radius 50 km, 300, km.

2.5.1.6 A Simplified Approach for Estimating Secondary Production of Hazardous Air Pollutants Using the OZIPR Model

Title III of the CAAA regulates chemicals classified as hazardous air pollutants (HAPs). These are substances that are either known to cause, or are suspected of causing, a threat of adverse human health effects. These compounds are found in the atmosphere as a result of primary emissions or from the transformation of organic compounds emitted by stationary or area sources. Carbonyl compounds represent an important class of organic compounds found on the list of HAPs. This study examines three of these compounds, formaldehyde, acetaldehyde, and acrolein, to determine the relative importance of their formation through primary and secondary processes.

Several complex models exist that include both dispersion and atmospheric chemistry to yield HAPs concentration estimates. However, these models are very expensive to execute, often requiring the use of supercomputers. The goal of this study was to explore whether a simplified approach could provide useful estimates of total HAPs concentrations. The approach taken was to estimate secondary HAPs production with a stand-alone model run in a personal computing environment that incorporated only nondispersive processes such as photochemistry. Results from this model would then be coupled to those from a relatively simple dispersion model to estimate total ground-level HAPs concentrations. The study results indicate that such a process is possible and yields reasonable estimates.

The photochemical modeling used the OZIPR (OZone Isopleth Plotting program, Research version one) model, a one-dimensional box model with a time-varying box height. Emissions were added to the box by time of day; such factors as temperature, relative humidity, atmospheric pressure, solar radiation, and deposition were used to determine chemical reaction rates. The reaction mechanism used in the study is based on the widely used SAPRC97 mechanism. The model produces chemical concentration estimates as a function of time. These estimates can then be used in conjunction with output from other models that account for dispersion, but not for chemical transformations. The output data from the OZIPR model are presented in several ways (*e.g.*, annual and seasonal averages, time series profiles) to facilitate their use with dispersion models.

Ten study areas were selected for this project: Atlanta, Boston, Chicago, Denver, Houston, Los Angeles, Phoenix, Pittsburgh, Seattle, and Washington DC. In each study area, urban and rural counties were chosen. The urban counties are centered on the cities in question; the rural counties are near enough to the urban areas to have similar meteorological patterns, but different emissions based on their lower population and distinct land use patterns. As many as 48 model runs were needed to adequately characterize each city.

The results show that secondary formation generally accounted for approximately 90% of the ambient formaldehyde and acetaldehyde, and approximately 85% of acrolein; these percentages varied only slightly between cities (U.S. Environmental Protection Agency, 1999a). Annual averages for the urban secondary formation of formaldehyde ranged from 3.0 $\mu g\ m^{-3}$ for Seattle to 13.4 $\mu g\ m^{-3}$ for Los Angeles. For acetaldehyde, the corresponding numbers are 5.0 $\mu g\ m^{-3}$ for Phoenix to 18.0 $\mu g\ m^{-3}$ for Los Angeles; for acrolein, the values are 0.2 $\mu g\ m^{-3}$ (five cities) to 0.7 $\mu g\ m^{-3}$ for Los Angeles. Generally, the rural values for each of the three HAPs ranged between 30% and 50% less than the urban values. The ambient formaldehyde concentrations were usually greater for southern cities.

The user can use results of this study in a number of ways that are fully described in the report (U.S. Environmental Protection Agency, 1999b). The most elaborate information can be obtained from running OZIPR using city-specific parameters. If that is not feasible, tables in the report can be used in conjunction with a dispersion model to provide seasonal and hourly adjustments to account for secondary production of HAPs. Finally, when the location of interest is dissimilar from those studied here and the OZIPR model cannot be run, the report provides guidance on adjusting estimates of aldehyde and the other pollutants to account for secondary HAPs production.

2.5.1.7 Long Range Transport Screening Calculations Using CALPUFF

During the New Source Review (NSR) process, there are occasions when it becomes necessary to assess impacts to Class I areas at distances beyond 50 kilometers (km) from the proposed source. Because EPA determined that steady-state plume dispersion models are not appropriate beyond 50 km, the agency proposed in 1998 to adopt the CALPUFF/CALMET modeling system for distances beyond 50 km. EPA and the Federal Land Managers (FLMs) developed a CALPUFF screening method to expedite the NSR process. The screening method provides permit applicants, permitting authorities, and the FLMs with a quick and easy method to estimate concentration values and impacts to such Air Quality Related Values (AQRVs) as visibility, and deposition of sulfur and nitrogen to soils and vegetation. To illustrate the capabilities of the CALPUFF screening technique, a series of investigations were summarized and presented at a conference (Irwin and Notar, 2001). The investigation focused on the extent of the receptor ring needed for the screening analysis in the context of simulating the impact of primary emissions of SO_2. Results for the two investigations revealed that year-to-year variations occur in the screening results on the order of 25-30%, which confirmed previous conclusions (U.S. Environmental Protection Agency, 1998). Results for Mammoth Cave National Park confirmed previous conclusions (U.S. Environmental Protection Agency, 1998) that the screening procedure may not always provide results higher than would be generated by a refined analysis. The screening results for the 3-hr averaging time were of the right order of magnitude, but were over 20% lower than that determined by the refined analysis. Using receptor arcs that extend 90 degrees to either side of the extent of the Class I area(s) of concern seems to be sufficient. This was a tentative conclusion, which needs to be confirmed in more situations. Herb, this paragraph was different from the one I used.

2.5.1.8 Uncertainty Characterization in Air Quality Modeling

The characterization of uncertainty in the air quality modeling results is often called upon in formal risk assessments. Air quality modeling involves a series of linked models, from the characterization of the emissions, to the characterization of the meteorological conditions, to the transport and fate of the emissions, each of which has its own uncertainties. To stimulate discussion, a review of concerns was prepared and presented at a conference (Irwin *et al.*, 2001b) and a workshop. This discussion reviews some of the issues involved in summarizing not only the combined uncertainty of risk estimates, but also methods for apportioning the uncertainty to the various models (emissions, transport, transformation, removal, exposure, and risk). The goal of the discussion was to make the environmental modeling community aware that there is interest in developing a consensus on technical procedures and methods for use in characterizing uncertainty in modeling. If there is sufficient interest and in the spirit of the National Transfer and Advancement Act of 1995 (Section 12(d) of Public Law 104-113), it was proposed that a community of participants be formed, where ideas can be openly debated, collaboration stimulated, and consensus promoted for general usage. Two alternatives were considered: form an ad hoc workgroup, or join an existing group whose purpose is to stimulate collaboration and development of consensus guidance. In this regard, the American Society for Testing and Materials provides an open, consensus development process. Committee D-22 on Sampling and Analysis of Atmospheres has experts whose interest are ambient air, workplace atmosphere, source emissions, indoor air, acidic deposition, meteorological conditions, sampling strategies, calibration procedures, quality assurance practices, and development of international standards in these fields.

2.5.1.9 Trajectory Analyses for $PM_{2.5}$

The Hybrid Single-Particle Lagrangian Trajectory (HYSPLIT) model is being run for a selected number of sites for specific time periods in 2000. It was concluded that a back trajectory database would be helpful to determine potential source origins of elevated ambient air concentrations of $PM_{2.5}$. The trajectory database can be used as input to residence time analyses, and can be used in combination with wind data to help locate the probable sources for the high $PM_{2.5}$ values that were measured during the year 2000. The procedure for executing the HYSPLIT model consisted of running it for five levels, four times per 24-hour period and for five days in length backwards in time. The Eta Data Assimilation System (EDAS), which covers the United States, was the input meteorological data set chosen for the trajectories. The archived data set has a horizontal grid size of 80 km.

2.5.1.10 Enhancements to AERMET

AERMET, the meteorological preprocessor for EPA's new state-of-the-science regulatory air quality dispersion model, was upgraded and released for beta testing. AERMET processing is solidly based on the planetary boundary layer (PBL) theory; important divisions within the PBL (*e.g.*, the surface layer and the mixed layer) are modeled separately. Similarity theory is used to model the surface layer. AERMET algorithms provide hourly estimates of the following surface and mixed layer parameters: Monin-Obukhov length, friction velocity, surface heat flux, and convective scaling velocity. Hourly estimates of convective and mechanical mixing heights are also provided.

To make these estimates, AERMET uses a variety of data sources including National Weather Service surface and upper-air data, and where available, data from an on-site meteorological monitoring program (*e.g.*, data from a meteorological tower). These data are processed in three stages. In the first stage, data are extracted from one or more archives and subjected to various quality assessment checks. In the second stage, data from the surface, upper-air, and on-site archives are merged and written to a merge file in 24-hour blocks. In the third stage, data are processed to provide hourly PBL estimates.

Enhancements in this upgrade to AERMET include the addition of code for extracting and processing data from National Climatic Data Center (NCDC) archives for surface- and upper-air data. This will facilitate the use of meteorological data as it becomes available from NCDC. The upgrade also includes the addition of a bulk Richardson algorithm for processing the stable boundary layer, improvements to make it user friendly, improvements in error reporting, and numerous debugging.

2.5.2 Modeling Guidance

2.5.2.1 Support Center for Regulatory Air Models

During FY-2001, a restructured SCRAM (Support Center for Regulatory Air Models) website was released to the general public. The new website re-packages the models with descriptions and their component files: model executable, source code, users guide, test cases, and other relevant files. The restructuring process was modeled after the Code of Federal Regulations (CFR) area that provides classification of models and recommendations for specific model use (40CFR Part 51, Appendix W). The SCRAM reorganization was accomplished at the request of the modeling community to provide a concise organization of modeling information.

A SCRAM presentation was made to the Atmospheric Science Librarians International conference at the 81st American Meteorological Society Annual Meeting in Albuquerque, New Mexico, held on January 14–18, 2001. The presentation, *Air Dispersion Models at the U.S. EPA*, provided an overview of the different classifications of models and their uses. In addition, an on-line demonstration of SCRAM, its models, and other utilities was provided.

2.5.2.2 Models-3 Help Desk

Models-3/CMAQ is a multiscale air quality model, which provides modeling in a one atmosphere environment using a graphical user interface-based framework, accounting for such processes as chemistry and aerosol interactions, and providing graphical and tabular output. The Models-3 Help Desk is an OAQPS initiative to provide full-time assistance to Models-3/CMAQ users, during both the installation and model application. A formal support network comprises the Help Desk with capable and accessible technical experts who are knowledgeable in the different modules and scientific processes that are performed within the model. During FY-2001, the Models-3 Help Desk responded to various users including Regional and State EPA offices, and international users in Canada and Great Britain. The new release of Models-3 (version 4.1) was distributed by the Help Desk via digital linear tapes (DLT). Nineteen users received DLT tapes. In addition, a Models-3 version compatible with the Windows NT® operating system was prepared on CD-ROM and sent to the National Technical Information Service for distribution. Proprietary software needed to run Models-3 is also provided with the CDs.

2.5.2.3 Ad Hoc Meteorological Modeling Workgroup

The Branch hosted a gathering of over 30 members of the meteorological modeling community in August 2001 as part of the 2nd annual meeting of the Ad Hoc Meteorological Modeling Workgroup. The purpose of the meeting was to foster a community exchange of information related to numerical meteorological modeling for eventual air quality purposes. There were 16 individual presentations summarizing current MM5 and Regional Atmospheric Modeling System (RAMS) meteorological modeling activities and several roundtable discussions of issues related to best practices in using simulated meteorological data for air quality modeling. Among the issues discussed were model performance evaluations, computing platforms, analysis software, MM5 physics options, and the status of the RAMS model. Participants included staff from State governmental air management agencies, modelers from regional planning organizations, meteorological modeling consultants, industry representatives, university researchers, as well as staff from other Federal government agencies.

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APPENDIX A: ACRONYMS, ABBREVIATIONS, AND DEFINITIONS

ACM	Asymmetric Convective Model
AERMET	Meteorological preprocessor
AIRS	Aerometric Information Retrieval System
AQMF	Air Quality Modeling Forum
AQRV	Air Quality Related Values
ARL	Air Resources Laboratory, NOAA
ASLI	Atmospheric Science Librarians International
ASMD	Atmospheric Sciences Modeling Division
ASPEN	Assessment System for Population Exposure Nationwide
ASTM	American Society for Testing and Materials
AVHRR	Advanced Very High Resolution Radiometer
AVIRIS	Airborne Visible and Infrared Imaging Spectrometer
BASC	Board on Atmospheric Sciences and Climate (NRC/NAS)
BCON	Boundary CONditions processor
BEIS	Biogenic Emissions Inventory System
BELD3	Biogenic Emissions Land use Database
CAAA	Clean Air Act Amendments of 1990
CALMET	A diagnostic meteorological model
CALPUFF	CALifornia PUFF (transport and dispersion) model
CAPITA	Center for Air Pollution Impacts and Trends Analysis
CASTNet	Clean Air Status and Trends Network
CB-IV	Carbon Bond-IV
CCMS	Committee on the Challenges of Modern Society
CCTM	CMAQ Chemistry-Transport Model
CDF	Common Data Format
CD-ROM	Compact Disk - Read Only Memory
CFD	Computational Fluid Dynamics
CFR	Code of Federal Rgulations
CIRA	Cooperative Institute for Research in the Atmosphere
CMAQ	Community Multiscale Air Quality modeling system
CMAQ-Hg	CMAQ mercury model
CMAS	Community Modeling and Analysis System
CTM	Chemistry-Transport Model
DIAS	Dynamic Information Architecture System
DLT	Digital Linear Tape
ECIP	Emissions-Chemistry Interface Processor
EDAS	Eta Data Assimilation System
EMEP	European Monitoring and Evaluation Programme
EPA	Environmental Protection Agency
Extended RADM	Regional Acid Deposition Model with full dynamics of secondary inorganic fine particle formation taken from the RPM
FCCM	Fully Coupled hybrid Compartmental Model

FCMSSR	Federal Committee for Meteorological Services and Supporting Research
FDDA	Four-Dimensional Data Assimilation
FLMs	Federal Land Managers
FMF	Fluid Modeling Facility (EPA)
FTP	File Transfer Protocol
FY	Fiscal Year
GIS	Geographic Information System
HAP	Hazardous Air Pollutant
HPCC	High Performance Computing and Communications
HTML	HyperText Markup Language
HYSPLIT	Hybrid Single-Particle Lagrangian Trajectory model
IAMSLIC	International Association of Aquatic and Marine Science Libraries and Information Centers
ICMSSR	Interdepartmental Committee for Meteorological Services and Supporting Research
IC/BC	Initial and boundary conditions
ICON	Initial CONditions processor
IMPROVE	Interagency Monitoring of PROtected Visual Environments
I/O	Input/Output
ISCLT	Industrial Source Complex model - Long Term
ITMs	International Technical Meetings
JPROC	Photolysis rate processor
LULC	Land Use/Land Cover
LES	Large-eddy simulation
M3Dry	Models-3 dry deposition scheme
MCIP	Meteorology-Chemistry Interface Processor
MCPL	Model couple module in the CMAQ system
MDN	Mercury Deposition Network
MEND-TOX	Multimedia ENvironmental Distribution of TOXics
MEPPS	Models-3 Emission Processing and Projection System
MEPSE	Major Elevated Point-Source Emissions
MicroFacCO	Microscale automobile emission Factor model for Carbon Monoxide
MicroFacPM	Microscale automobile emission Factor model for Particulate Matter
MIMS	Multimedia Integrated Modeling System
MLBC	Multi-Layer Bio-Chemical dry deposition model
MLM	Multi-Layer inferential dry deposition Model
MM5	Mesoscale Model - Version 5
Models-3	Third generation air quality modeling system
MODTRAN	MODerate resolution TRANSmittance
NARSTO	Formerly North American Research Strategy for Tropospheric Ozone
NARSTO-NE	NARSTO-NorthEast
NASA	National Aeronautics and Space Administration
NATO	North Atlantic Treaty Organization

NATO/CCMS	North Atlantic Treaty Organization Committee on Challenges of Model Society
NCAR	National Center for Atmospheric Research
NCDC	National Climatic Data Center
NERL	National Exposure Research Laboratory
NESC	National Environmental Supercomputing Center (EPA)
NEXRAD	NEXt generation RADar
NOAA	National Oceanic and Atmospheric Administration
NSR	New Source Review
NWS	National Weather Service
OAQPS	Office of Air Quality Planning and Standards (EPA)
OCLC	Online Computer Library Center
OMB	Office of Management and Budget
OZIPR	OZone Isopleth Plotting program, Research version
PBL	Planetary Boundary Layer
PDF	Probability Density Function
PDM	Plume Dynamics Model
PinG	Plume-in-Grid algorithm
PM	Particulate Matter
$PM_{2.5}$	Particulate matter smaller than 2.5 microns
PM_{10}	Particulate matter up to 10 micrometers in size
PX LSM	Pliem-Xiu Land-Surface Model
QA/QC	Quality Assurance/Quality Control
RADM	Regional Acid Deposition Model
RAMS	Regional Atmospheric Modeling System
R&DF	Research and Development Forum
RHR	Regional Haze Rule
RPM	Regional Particulate Model
RPO	Regional Planning Organization
RRWG	Reactivity Research Work Group
SAIL	Southeast Affiliate of IAMSLIC Librarians
SAPRC99	Chemical mechanism
SASWG	Standing Air Simulation Work Group
SBL	Stable Boundary Layer
SCRAM	Support Center for Regulatory Air Models
SHEDS	Stochastic Human Exposure and Dose Simulation
SIP	State Implementation Plan
SMOKE	Sparse Matrix Operator Kernel Emissions
SO_2	Sulfur Dioxide
SOA	Secondary organic aerosol
SOS	Southern Oxidants Study
TEOM	Tapered-Element Oscillating Microbalance instruments
TexAQS 2000	2000 Texas Air Quality Study
TKE	Turbulent Kinetic Energy

TOR	Tropospheric ozone residual
UCP	Urban canopy parameterization
USGS	U.S. Geological Survey
US/USSR	United States/Union of Soviet Socialist Republics
UV	Ultraviolet
VOC	Volatile organic compounds
WRF	Weather Research Forecasting
WRAP	Western Regional Air Partnership
WSR-88D	Weather Surveillance Radar 1988 Doppler Version
WWW	World-Wide Web

APPENDIX B: PUBLICATIONS

Air Pollution Modeling and Its Application XIV. Gryning, S.-E., and F.A. Schiermeier (Eds.). Proceedings of the Twenty-Fourth NATO-CCMS International Technical Meeting on Air Pollution Modeling and Its Application, May 15–19, 2000, Boulder, Colorado. Kluwer Academic/Plenum Publishers, New York, NY, 834 pp. (2000).

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Vukovich, F., A. Gilliland, A. Venkatram, and J. Sherwell. On performing long-term predictions of ozone using the SOMS model. *Atmospheric Environment* 35:569–578, 2001.

Walsh, K., and A. Gilliland. Regional variations in sulfate and nitrate on annual, seasonal, and synoptic time scales. *Journal of Air & Waste Management Assocociation* 51:174–185 (2001).

Weil, J.C., W.H. Snyder, R.E. Lawson, Jr., and M.S. Shipman. New developments in dispersion experiments and models for the convective boundary layer. In *Air Pollution Modeling and Its Applications XIV.* Volume 24. Gryning, S-E., and F.A. Schiermeier (Eds.). Kluwer Academic/Plenum Publishers, New York, 445–454 (2001).

Xiu, A., and J.E. Pleim. Development of a land surface model. Part I: Application in a Mesoscale Meteorological Model. *Journal of Applied Meteorology* 40:192–209 (2001).

APPENDIX C: PRESENTATIONS

Benjey, W.G., and S.K. LeDuc. Status and implications of Models-3. Presentation at the Fall 2000 Meeting of the Standing Air Emissions Working Group, Washington, DC, October 20, 2000.

Benjey, W.G. Emission modeling procedures. Presentation to the Neighborhood Modeling Team of the Atmospheric Sciences Modeling Division, Research Triangle Park, NC, March 29, 2001.

Benjey, W.G. The status of smoke and reactivity capabilities. Presentation to the Joint Industry Committee on Atmospheric Reactivity, Research Triangle Park, NC, April 16, 2001.

Benjey, W.G. Anthropogenic emissions and SMOKE in MIMS. Presentation at the Multimedia Integrated Modeling Systems Peer Review, Research Triangle Park, NC, April 4, 2001.

Benjey, W.G. Emission Modeling: Status and Future . Presentation to the International Transport of Air Pollution Committee, Washington, D.C., August 28, 2001.

Benjey, W.G. Models-3/CMAQ and forestry SMOKE emissions. Presentation to the U.S. Forest Service Regional Modeling Center managers, Athens, GA, August 23, 2001.

Bullock, O.R., Jr. The importance of emission speciation to the atmospheric transport and deposition of mercury. Presentation at the Conference on Assessing and Managing Mercury from Historic and Current Mining Activities, San Francisco, CA, November 29, 2000.

Bullock, O.R., Jr. Modeling and monitoring of atmospheric mercury. Presentation at the U.S. EPA Region 5 Office, Chicago, IL, January 18, 2001.

Ching, J.K.S. Air quality modeling of PM and air toxics at neighborhood scales to improve human exposure assessments. Presentation at the International Society of Exposure Analysis 10th Annual Conference, Monterey Peninsula, CA, October 25, 2000.

Ching, J.K.S. Modeling PM and air toxics at neighborhood scales and their linkages to human population and personal exposure models. Presentation at the 7th International Conference on Atmospheric Sciences and Applications to Air Quality Modeling Challenges, Taipei, Taiwan, November 2, 2000.

Ching, J.K.S. Neighborhood scale modeling to support exposure modeling. Presentation at the Human Health, Remote Sensing and Urbanization Meeting, Atlanta, GA, April 10, 2001.

Ching, J.K.S. Air quality modeling—Models-3/CMAQ. Presentation at the SIAM Conference, University of Houston, TX, April 27, 2001.

Ching, J.K.S. Status of neighborhood scale modeling project. Briefing to the Director of the National Exposure Research Laboratory and staff, Research Triangle Park, NC, July 3, 2001.

Ching, J.K.S. Neighborhood scale modeling. Presentation at the NERL/NHEERL Exposure to Dose Modeling Workshop, Research Triangle Park, NC, July11, 2001.

Ching, J.K.S. Modeling gridded PM and air toxics concentrations and their sub-grid concentration distributions for use in exposure modeling. Presentation at the Third Annual Meeting of the NERL/ORD University Partnership Agreements for Conducting Research on Source-to-Dose Human Exposure Modeling, Research Triangle Park, NC, August 28, 2001.

Cooter, E.J. Regional modeling of the atmospheric transport and deposition of atrazine. Presentation at the Society of Environmental Toxicology and Chemistry 21st Annual Meeting, Nashville, TN, November 14, 2000.

Cooter, E.J. Next generation compartmental modeling. Presentation at the Multimedia Integrated Modeling Systems Peer Review, Research Triangle Park, NC, April 3, 2001.

Dennis, R.L. Atmospheric deposition and airsheds. Seminar at the U.S. Environmental Protection Agency, Region 2 Office, New York City, NY, October 5, 2000.

Dennis, R.L. Operational evaluation of CMAQ for ozone. Presentation at the SASWG Meeting (by phone), Washington, DC, October 20, 2000.

Dennis, R.L. A modeling study of the effect of acid rain controls on fine particle concentrations of sulfate in eastern North America. Presentation at NARSTO Symposium — Tropospheric Aerosols: Science and Decisions in an International Community, Queretaro, Mexico, October 25, 2000.

Dennis, R.L. Determination of the airshed domains for modeling atmospheric deposition of oxidized and reduced nitrogen to the Neuse River Basin. Presentation at the American Institute of Hydrology on Atmospheric, Surface, and Subsurface Hydrology and Interactions, Research Triangle Park, NC, November 7, 2000.

Dennis, R.L. Atmospheric transport and deposition. Presentation at the Chesapeake Bay Shared Resources Workshop, Dewey Beach, DE, November 15, 2000.

Dennis, R.L. Atmospheric transport and deposition of nitrogen to coastal estuaries. Seminar at the Duke Nicholas School of the Environment, Durham, NC, November 27, 2000.

Dennis, R.L. Issues related to nitrogen meteorology and atmospheric chemistry. Presentation at the North Carolina State Workshop on Future Directions in Air Quality Research: Ecological, Atmospheric, Regulatory/ Policy/ Economic and Educational Issues, Research Triangle Park, NC, February 14, 2001.

Dennis, R.L. Atmospheric exchange and deposition. Presentation at the Multimedia Integrated Modeling Systems Peer Review, Research Triangle Park, NC, April 4, 2001.

Dennis, R.L. Coastal studies — Nitrate and ammonia. Presentation to the Air Resources Laboratory program review, Research Triangle Park, NC, May 9, 2001.

Dennis, R.L. Sulfate nonlinear response to SO_2 emissions reduction. Presentation to the OAQPS Modelers Meeting, Research Triangle Park, NC, May 11, 2001.

Dennis, R.L. Science questions. Presentation at the EMEP/EPA Workshop on Photo-oxidants, Fine Particles, and Haze Across the Arctic and North Atlantic: Transport Observations and Models, Columbia University Lamont-Doherty Earth Observatory, Palisades, NY, June 12, 2001.

Dolwick, P.D. CMAQ proof of concept: Western United States ozone modeling. Presentation at the LADCO Models-3/CMAQ training session, Research Triangle Park, NC, January 31, 2001.

Dolwick, P.D. The Models-3/Community Multiscale Air Quality modeling system: Introduction and preliminary results. Presentation to the EPA Deputy Assistant Administrator, Research Triangle Park, NC, April 17, 2001.

Dolwick, P.D. CMAQ proof of concept modeling. Presentation at the April 2001 SASWG Meeting (by phone), Chicago, IL, April 20, 2001.

Dolwick, P.D. OAQPS proof of concept CMAQ modeling. Presentation at the Ad Hoc Air Quality Group, Research Triangle Park, NC, May 10, 2001.

Dolwick, P.D. Numerical air quality forecasting: Description of planned projects and preliminary recommendations for U.S. EPA involvement. Presentation to the Air Quality Index—Long Range Planning Team, Durham, NC, May 16, 2001.

Dolwick, P.D. Plans for BEIS-3 sensitivity modeling within U.S. EPA/OAQPS, Des Plaines, IL, May 22, 2001.

Dolwick, P.D. Background and goals of the Ad Hoc Meteorological Modeling Workgroup, Research Triangle Park, NC, August 23, 2001.

Eder, B.K. Preliminary evaluation of CMAQ using visibility parameters. Briefing for the OAQPS, Emissions, Monitoring and Analysis Division Director, Research Triangle Park, NC, October 17, 2000.

Eder, B.K. Preliminary evaluation of CMAQ using visibility parameters. Presentation at SASWG Meeting (by phone) in Washington, DC, October 20, 2000.

Eder, B.K. On the use of NEXRAD Stage IV data in the multimedia modeling of pollutant transport. Presentation at the Multimedia Integrated Modeling Systems Peer Review, Research Triangle Park, NC, April 3, 2001.

Eder, B.K. A preliminary evaluation of Models-3/CMAQ using visibility and aerosol data. Presentation at the Ad-Hoc Air Quality Group, Research Triangle Park, NC, May 11, 2001.

Eder, B.K. A preliminary evaluation of Models-3/CMAQ using visibility and aerosol data. Invited speaker, North Carolina State University, Department of Marine Environmental Atmospheric Science Seminar Series, Raleigh, NC, September 10, 2001.

Eder, B.K. A preliminary evaluation of Models-3/CMAQ using aerosol data. Presentation at the BOSC Meeting, Research Triangle Park, NC, September 19, 2001.

Eder, B.K. Presentation on the dangers of lightning, Kingswood Elementary, Raleigh, NC, September 28, 2001.

Gillette, D.A. The concept of vegetation "streets" in dust emission modeling. Seminar presented at the University of Paris 12 (Creteil cedex), France, October 13, 2000.

Gilliland, A.B. Seasonal estimates of ammonia using inverse modeling techniques. Poster presentation at the Shared Resources Workshop, Dewey Beach, DE, November 16,2000.

Gilliland, A.B. Multimedia Integrated Modeling System (MIMS) development and challenges for multimedia modeling. Presentation at the Multimedia Integrated Modeling Systems Peer Review, Research Triangle Park, NC, April 3, 2001.

Gilliland, A.B. Seasonal estimates of ammonia using inverse modeling techniques. Poster presentation at the Multimedia Integrated Modeling Systems Peer Review, Research Triangle Park, NC, April 3, 2001.

Gilliland, A.B. Overview of multimedia integrated modeling activities. Presentation at the NOAA ARL peer review, Research Triangle Park, NC, May 9, 2001.

Gilliland, A.B. Seasonal estimates of ammonia using inverse modeling techniques. Poster presentation at the ARL peer review, Research Triangle Park, NC, May 9, 2001.

Huber, A.H. Advances in human exposure modeling. Presentation at the EMPACT National Meeting (by phone), Philadelphia, PA, January 25, 2001.

Irwin, J.S., K. Steinberg, C. Hakkarinen, and H. Feldman. Uncertainty in air quality modeling for risk calculations. Fifth Annual George Mason University Transport and Dispersion Modeling Workshop, Fairfax, VA. July 18, 2001.

Lacser, A., and T.L. Otte. Implementation of an urban canopy parameterization in a mesoscale model. Fifth Annual George Mason University Transport and Dispersion Modeling Workshop, Fairfax, VA. July 18, 2001.

Leduc, S.K. Floods. Presentation to three fifth-grade classes at Lincoln Trail Elementary School, Mahomet, IL, November 8, 2000.

Leduc, S.K. Floods. Presentation to three first-grade classes at Sangamon Elementary School, Mahomet, IL, November 8, 2000.

Leduc, S.K. Floods. Presentation to three first-grade classes at Memorial Elementary School, Paris, IL, November 9, 2000.

Leduc, S.K. Modeling air quality. Presentation at an honors colloquium at Meredith College, Raleigh, NC, November 29, 2000.

Leduc, S.K. Supporting the data needs of the coastal community II: Hurricane Floyd post-event. Oral and Poster presentation at the AMS 17th International Conference on Interactive Information Processing Systems for Meteorology, Oceanography, and Hydrology, Albuquerque, NM, January 14, 2001.

Otte, T.L. Weather basics: Evaporation and condensation. Presentation to 2nd grade (two sessions), Fuquay-Varina Elementary School, Fuquay-Varina, NC, December 12, 2000.

Otte, T.L. Weather basics: Evaporation and condensation. Presentation to 2nd grade (five sessions), Dillard Drive Elementary School, Raleigh, NC, December 15, 2000.

Otte, T.L. Weather maps and forecasting. Presentation to 5th grade (four sessions), Swift Creek Elementary School, Raleigh, NC, January 9, 2001.

Otte, T.L. MM5 overview. Presentation at the Neighborhood Scale Modeling Group, Research Triangle Park, NC, January 23, 2001.

Otte, T.L. Weather basics: Evaporation and condensation. Presentation to 2nd grade (2 sessions), Olive Chapel Elementary School, Apex, NC, March 9, 2001.

Otte, T.L., and S.K. LeDuc. Weather Jeopardy. (2 sessions). Presentation at 9th Expanding Your Horizons Workshop, North Carolina State University, Raleigh, NC, March 13, 2001.

Otte, T.L. Some modeling activities at ASMD. Presentation at NARSTO-NE-OPS Workshop, University of Maryland, College Park, MD, March 23, 2001.

Otte, T.L. Weather basics: Evaporation and condensation. Presentation to 2nd grade (four sessions), Swift Creek Elementary School, Raleigh, NC, March 30, 2001.

Otte, T.L. Weather Jeopardy. Presentation at the *Science Day* (four sessions), St. Mary Magdalene School, Apex, NC, June 6, 2001.

Otte, T.L. EPA/ORD meteorological modeling activities. Presentation at the Ad Hoc Meteorological Modeling Workgroup, Research Triangle Park, NC, August 23, 2001.

Otte, T.L. MCIP Version 2. Atmospheric Model Development Branch Seminar, Research Triangle Park, NC, August 27, 2001.

Pierce, T.E. Guidance on biogenic emission inventory preparation. Presentation at the Emissions Inventory Improvement Plan Workshop, Raleigh, NC, October 10, 2000.

Pierce, T.E. Development of biogenic emission inventories and improved vegetation databases. Presentation at the Multimedia Integrated Modeling Systems Peer Review, Research Triangle Park, NC, April 3, 2001.

Pierce, T.E. Development of the third generation of the Biogenic Emissions Inventory System (BEIS). Presentation at the NOAA ARL peer review, Research Triangle Park, NC, May 9, 2001.

Pierce, T.E. Recommendations for biogenic emissions modeling to support regional air quality models. Presentation at a Biogenic Emissions Workshop sponsored by the Lake Michigan Air Directors for the Regional Planning Offices, Chicago, IL, May 22, 2001.

Pierce, T.E. Meteorology can be exciting. Presentation to two first-grade classes, Morrisville Elementary School, Morrisville, NC, August 31, 2001.

Pleim, J.E. Evaluation of a coupled land-surface and dry deposition model. Invited presentation at the American Geophysical Union Fall 2000 Meeting, San Francisco, CA, December 17, 2000.

Pleim, J.E. A new land surface model in MM5. Invited presentation at the WRF Land-Surface Modeling Workshop, NCEP/EMC, Camp Springs, MD, October 23, 2000.

Pleim, J.E. U.S. EPA's Models-3/Community Multiscale Air Quality Model (CMAQ). Invited presentation at the DOE Atmospheric Programs Annual Meeting, Raleigh, NC, February 22, 2001.

Poole-Kober, E.M. Atmospheric Science Librarians International. Poster presentation at the 26th IAMSLIC Annual Conference, Victoria, British Columbia, Canada, October 3, 2000.

Roselle, S.J. U.S. EPA's multi-pollutant Models-3/Community Multiscale Air Quality model. Presentation at NARSTO Symposium — Tropospheric Aerosols: Science and Decisions in an International Community, Queretaro, Mexico, October 25, 2000.

Roselle, S.J. CMAQ Sulfate Tracking Model. Presentation at Ad Hoc Air Quality Group, Research Triangle Park, NC, May 11, 2001.

Schiermeier, F.A. Demonstration of the Supercomputing Center and Scientific Visualization Laboratory. Presentation for the U.S. Department of Defense Officials, Research Triangle Park, NC, October 16, 2000.

Schiermeier, F.A. Atmospheric Sciences Modeling Division regional deposition modeling applications. Presentation at the Standing Air Simulation Work Group Meeting, Washington, DC, October 21, 2000.

Schiermeier, F.A. Computer demonstration of Models-3/CMAQ control scenario applications. Presentation at the Twenty-Second United States/Russia Working Group Meeting on Air Pollution Modeling, Instrumentation, and Measurement Methodology, Main Geophysical Observatory, St. Petersburg, Russia, November 8, 2000.

Schiermeier, F.A. Interim summary of EPA involvement in the Committee for Agency Cooperative Research. Presentation for the ICMSSR Committee for Agency Cooperative Research, Washington, DC, December 14, 2000.

Schere, K.L. Uncertainty in applying and evaluating air quality models. Presentation at the U.S. EPA Models Evaluation and Peer Review Workshop, Alexandria, VA, November 29, 2000.

Schere, K.L. Status of U.S. EPA's Models-3/CMAQ. Presentation at the PM Supersites Workshop, U.S. Environmental Protection Agency, Research Triangle Park, NC, March 21, 2001.

Schere, K.L. Status of Models-3 and CMAQ. Presentation at the EPA/OAQPS — Briefing for the Director, Office of Air Quality Planning and Standards, and staff, Research Triangle Park, NC, April 5, 2001.

Schere, K.L. Models-3/CMAQ: Community Multiscale Air Quality modeling. Presentation at the NOAA ARL Peer Review, Research Triangle Park, NC, May 9, 2001.

Schere, K.L. The NARSTO ozone assessment and long-range transport. Presentation at the MIT Symposium on Exporting and Importing Air Pollution, Regional and Global Transport, Dedham, MA, July 11, 2001.

Schere, K.L. WRF model development and status. Presentation at the Ad-Hoc Meteorological Modeling Workgroup, Research Triangle Park, NC, August 24, 2001.

Streicher, J.J. Computer simulation graphics as an exposure analysis tool: Applications in solar UV exposure. Presentation at the RACHET seminar, Research Triangle Park, NC, December 7, 2000.

Streicher, J.J. Use of surface reflectance for ecological monitoring and change detection in the Lower Neuse River Basin, NC, at the Tenth NASA/JPL Airborne Earth Sciences Workshop, Pasadena, CA, February 28, 2001.

Streicher, J.J. Modeling continuous exposure to solar radiation. Presentation at the 29th meeting of the American Society for Photobiology, Chicago, IL, July 10, 2001.

Streicher, J.J. Advances in photobiology using computer graphical analysis. Presentation at the EMPACT National Meeting, Philadelphia, PA, August 7, 2001.

West, J.L. Air quality research: Future directions. Poster presentation the NARSTO Meeting, Research Triangle Park, NC, February 12, 2001.

West, J.L. Quality systems science center activities and future directions. Presentation at the NARSTO Annual Executive Assembly Meeting, March 6, 2001.

APPENDIX D: WORKSHOPS AND MEETINGS

NARSTO-NE Ozone and Particle Study Workshop, Albany, NY, October 2–4, 2000.

K.L. Schere

EPA Region 2 Office Meeting on Air and Water, New York City, NY, October 5, 2000.

R.L. Dennis

Workshop on the Role of Mineral Aerosols in Quaternary Climate Cycles: Models and Data, Max Planck Institute, Jena, Germany, October 8–10, 2000.

D.A. Gillette

SASWG Meeting, Washington, DC, October 20, 2000.

R.L. Dennis

Fall 2000 Standing Emissions Air Working Group, Washington, DC, October 20–21, 2000.

W.G. Benjey

WRF Land-Surface Modeling Workshop, National Center for Environmental Prediction/Environmental Modeling Center, Camp Springs, MD, October 23–24, 2000.

J.E. Pleim

NARSTO—Tropospheric Aerosols: Science and Decisions in an International Community. A Technical Symposium on Aerosol Science, Querétaro, Mexico, October 23–26, 2000.

R.L. Dennis
S.J. Roselle
K.L. Schere

Committee on Climate Services, Washington, DC, October 24, 2000.

S.K. Leduc

Workshop on Air Quality Modeling Challenges, Taipei, Taiwan, November 3, 2000.

J.K.S. Ching

2000 Annual Meeting of the American Institute of Hydrology on Atmospheric, Surface, and Subsurface Hydrology and Interactions, Research Triangle Park, NC, November 5–8, 2000.

A.B. Gilliland (Session chair: Integrated Multimedia Modeling)
R.L. Dennis

Chesapeake Bay Shared Resources Conference on Ammonia, Dewey Beach, DE, November 14–16, 2000.

R.L. Dennis
A. B. Gilliland
T. E. Pierce

U.S. EPA Models Evaluation and Peer Review Workshop, Alexandria, VA, November 28–30, 2000.

E.J. Cooter
K.L. Schere

Western Governors Association, Western Regional Air Partnership Research and Development Forum, Windblown and Mechanically Entrained Road Dust Workshop, Las Vegas, NV, December 14, 2000.

D.A. Gillette

Workshop on Biogenic Emissions Research, California Air Resources Board, Sacramento, CA, December 12–14, 2000.

T.E. Pierce

Electric Utilities Environmental Conference, Tucson, AZ, January 8–9, 2001.

J.L. West

AMS 17th International Conference on Interactive Information Processing Systems for Meteorology, Oceanography, and Hydrology, Albuquerque, NM, January 14–19, 2001.

S. K. Leduc

Integrated Mercury Monitoring Network Workshop, Chicago, IL, January 18, 2001.

O.R. Bullock, Jr.

The 84th Annual Meeting of the American Meteorological Society, January 13–17, 2001.

E.M. Poole-Kober

The Fifth Annual Meeting of Atmospheric Science Librarians International, Orlando, FL, January 16–18, 2001.

E.M. Poole-Kober

NARSTO Reactivity Research Work Group, Research Triangle Park, NC, January 17–18, 2001.

J.L. West

Southern Oxidant Study Review Meeting, Research Triangle Park, NC, January 29–31, 2001.

R.L. Dennis

Southern Oxidant Study Workshop, Research Triangle Park, NC, January 30, 2001.

B.K. Eder
T.L. Otte

Fifth Annual NERL Planning Meeting, Las Vegas, NV, January 30–February 1, 2001.

K.L. Schere

MIMS Neuse River Meeting, Research Triangle Park, NC, January 31, 2001.

R.L. Dennis

Conference on Future Directions in Air Quality Research, Research Triangle Park, NC, February 12–15, 2001.

S.K. Leduc (Conference organizer; Session chair: Carbon Dioxide)
R.L. Dennis
J.L West

International Atmospheric Mercury Model Intercomparison, Moscow, Russia, February 14–15, 2001.

O.R. Bullock, Jr.

Meeting of the Office of the Federal Coordinator for Meteorology Committee on Climate and Monitoring, Washington, DC, February 26, 2001.

S.K. Leduc

Implementation of Canada-Wide Standards Conference, Toronto, Canada, March 7–8, 2001.

J.L. West

Ninth Expanding Your Horizons Workshop, North Carolina State University, Raleigh, NC, March 13, 2001.

S.K. LeDuc
T.L. Otte

PM Supersites Workshop, U.S. EPA, Research Triangle Park, NC, March 21–21, 2001.

R.L. Dennis
B.K. Eder
K.L. Schere

Workshop on the Revised Protocol for Identification of Dust Producing Areas on Owens Lake, at Great Basin Unified Air Pollution Control District, Bishop, CA, March 21–23, 2001.

D.A. Gillette

NARSTO-NE-OPS Workshop, University of Maryland, College Park, MD, March 22–23, 2001.

T.L. Otte

Federal Information Technology Research and Development Meeting, Washington, DC, March 26, 2001.

S.S. Fine

Annual ASTM D22 Committee and Subcommittee Meetings, Phoenix, AZ, April 2–5, 2001.

J.S. Irwin

MIMS Program Review, Research Triangle Park, NC, April 3–5, 2001.

R.L. Dennis

NARSTO Reactivity Research Work Group, Research Triangle Park, NC, April 11–12, 2001.

J.L. West

NARSTO Executive Assembly Meeting, Toronto, Canada, April 17–18, 2001.

R.L. Dennis
J.L. West

Workshop: New Visions on Software Design, Washington, DC, April 17–19, 2001.

S.S. Fine

Human Exposure Program Review, U.S. EPA, Research Triangle Park, NC, April 18, 2001.

J.K.S. Ching

NOAA 2001 Constituent Workshop, Washington, DC, April 18, 2001.

S.K. Leduc

Spring 2001 Standing Emissions Air Working Group, Chicago, IL, April 20–21, 2001.

W.G. Benjey

EPA Emissions Inventory Conference, Denver, CO, April 30–May 3, 2001.

T.E. Pierce (Session chair: Ammonia Emissions)

High Performing Organization Workshop, Chapel Hill, NC, May 1–3, 2001.

W.G. Benjey

Air Resources Laboratory Program Review, Research Triangle Park, NC, May 9–10, 2001.

R.L. Dennis

Ad Hoc Air Quality Group, Research Triangle Park, NC, May 10–11, 2001.

R.L. Dennis
P.D. Dolwick
B.K. Eder
M.L. Evangelista
B.L. Orndorff
S.J. Roselle

Weather Research and Forecasting Model-Chemistry Working Group, NCAR, Boulder, CO, May 22–23, 2001.

K.L. Schere

LADCO Biogenics Modeling Meeting, Chicago, IL, May 22–23, 2001.

P. D. Dolwick

Persistant Bioaccumulative Toxin (PBT) Monitoring Strategy Development, Silver Spring, MD, May 22–23, 2001.

O.R. Bullock, Jr.

Institutional Ecological Economics Modeling Meeting, Solomons, MD, May 28–29, 2001.

S.S. Fine

American Geophysical Union Spring 2001 Conference, Boston, MA, May 29-31, 2001.

A.B. Gilliland (Session chair: Watershed-Ecosystem Coupling)

SEDRIS Technology Conference 2001, Lake Tahoe, NV, June 5–8, 2001.

S.K. Leduc

EMEP/EPA Workshop on Photo-Oxidants, Fine Particles, and Haze Across the Arctic and North Atlantic: Transport Observations and Models, Palisades, NY, June 12–15, 2001.

R.L. Dennis
P. D. Dolwick

Committee on Climate Services, Washington, DC, June 15, 2001.

S.K. Leduc

Federal Interagency Ecosystem Modeling Meeting, Rockville, MD, June 17–19, 2001.

S.S. Fine

Shenandoah Assessment Workshop, Shenandoah National Park, VA, June 19–21, 2001.

R.L. Dennis

Eleventh PSU/NCAR Mesoscale Model Users' Workshop, Boulder, CO, June 25–27, 2001.

T.L. Otte
J.E. Pleim

MIT Symposium on Exporting and Importing Air Pollution, Regional and Global Transport, Dedham, MA, July 10–12, 2001.

K.L. Schere

NARSTO NE-OPS Meeting, Philadelphia, PA, July 26–27, 2001.

J.L. West

AMS 9th Conference on Mesoscale Processes, 18th Conference on Weather Analysis and Forecasting, and 14th Conference on Numerical Weather Prediction, Ft. Lauderdale, FL, July 30–August 3, 2001.

T.L. Otte

Air Quality Index Meetings with the Puget Sound Clean Air Agency, Seattle, WA, August 6–8, 2001.

P. D. Dolwick

Texas Air Quality Study (TexAQS2000) Workshop, Austin, Texas, August 7–10, 2001.

R.L. Dennis
B.K. Eder
T.L. Otte
K.L. Schere
J.L. West

August 2001 Technical Meeting of the Regional Planning Organizations, St. Louis, MO, August 14–16, 2001.

P. D. Dolwick
M. Evangelista

CASES-99 Workshop II, Research Triangle Park, NC, August 20–22, 2001.

J.K.S. Ching

Ad Hoc Meteorological Modeling Workgroup, Research Triangle Park, NC, August 23–24, 2001.

P. D. Dolwick
M.L. Evangelista
B.L. Orndorff
T.L. Otte

EMEP Steering Body Meeting, Geneva, Switzerland, September 3–5, 2001.

R.L. Dennis

High-Performing Organization Training, Research Triangle Park, NC, September 4–6, 2001.

W.G. Benjey
F.S. Binkowski
S.A. Brown
O.R. Bullock, Jr.
J.K.S. Ching
E.J. Cooter
R.L. Dennis
B.K. Eder
S.S. Fine
P.L. Finkelstein
A.G. Gilliland
J.M. Godowitch
S.C. Howard
T.L. McDuffie
T.L. Otte
S.G. Perry
T.E. Pierce
J.E. Pleim
E.M. Poole-Kober
S.T. Rao
S.J. Roselle
J.H. Rudisill, III
K.L. Schere
D.B. Schwede
J.J. Streicher
R.S. Thompson
A.R. Torian
H.J. Viebrock
J.O. Young

National Institute of Standards Workshop, Gaithersburg, MD, September 6–7, 2001.

J.L. West

State and Regional Representatives Emissions Modeling Meeting, Chicago, IL, September 20–21, 2001.

W.G. Benjey

APPENDIX E: VISITING SCIENTISTS

1. Dr. Kiran Alapaty
   MCNC
   Research Triangle Park, NC

Dr. Alapaty visited the Division on January 9, 2001, to present a seminar on *Techniques to Improve Boundary Layer Simulations for Air Quality Applications.*

2. Yoram Cohen, Professor
   UCLA Department of Chemical Engineering
   University of California
   Los Angeles, CA

Professor Cohen visited the Division on February 27, 2001, to present a seminar on *Multimedia Modeling.*

3. Dr. Douglas Fox
   CIRA
   Fort Collins, CO

   Mr. John Vimont
   National Park Service
   Oak Ridge, TN

   Mr. Al Riebau
   US Forest Service
   Washington, DC

Dr. Fox, and Messr. Vimont and Riebau visited the Division during May 8–9, 2001, to discuss the IAG Project Review on fire emissions modeling for the CMAQ model.

4. Drs. Noor Gillani, Richard McNider, and Arastoo Biazar
   University of Alabama-Huntsville
   Huntsville, AL

Drs. Gillani, McNider, and Biazar visited the Division during April 4–5, 2001, to discuss the Cooperative Agreement Project Review on the CMAQ modeling center at the University of Alabama-Huntsville, Huntsville, AL.

5. Emily L. Harris, M.P.H.
   Senior Epidemiologist
   Arkansas Department of Environmental Quality
   Little Rock, AR

Ms. Harris visited the Division on April 29, 2001, to discuss advanced procedures on performing biogenic emission calculations for the State of Arkansas as part of a State Implementation Plan.

6. Dr. Avraham Lacser
Israel Institute for Biological Research
Ness Ziona, Israel

Dr. Lacser, on a two-year sabbatical from his home institute, is working with Division scientists on neighborhood-scale modeling issues with the MM5 and CMAQ models.

7. Dr. Alberto Martilli
Laboratory of Air and Soil Pollution
Swiss Federal Institute of Technology
Lausanne, Switzerland

Dr. Martilli visited the Division during September 26–29, 2001, to present a seminar on the development and evaluation of an urban surface exchange parameterization for mesoscale models, and to discuss the topic with Division staff.

8. Drs. S.T. Rao, Christian Hogrefe, and Michael Ku
New York State Department of Environmental Conservation
Albany, NY

Drs. Rao, Hogrefe, and Ku visited the Division on June 20, 2001, to discuss CMAQ modeling.

9. Drs. A. Russell, and T. Odman
Georgia Institute of Technology
Atlanta, GA

Messrs. T. Tomiyama, and A. Hayashi
Drs. S. Kobayashi, H. Kunimi, and S. Yamazaki
Petroleum Energy Center
Tokyo, Japan

Drs. Russell, Odman, Kobayashi, Kunimi, and Yamazaki, and Messr. Tomiyama, and Hayashi visited the Division during July 16–17, 2001, to discuss collaboration on street-corner scale modeling with the U.S. Environmental Protection Agency, Office of Research and Development, Japan Clean Air Program, and Georgia Institute of Technology.

10. Dr. Fred Vukovich
Science Applications International Corporation
Raleigh, NC

Dr. Vukovich visited the Division on October 18, 2000, to present a seminar on remote sensing databases for providing IC/BC inputs to CMAQ.

11. Drs. Vikram Vyas, Qing Sun, Sheng-Wei Wang, and Arunundram Chandrasekar,
Environmental Occupational Science Health Institute (EOSHI)
Rutgers University
Rutgers, NJ

Drs. Vyas, Sun, Wang, and Chandrasekar visited the Division during November 14–15, 2000, to discuss collaboration on air quality modeling at neighborhood scales.

12. Dr. Satoshi Yamazaki
Toyota Research
Tokyo, Japan

Dr. Akira Hayashi
Petroleum Energy Center
Tokyo, Japan

Dr. Kazuhiko Suzuki
Idemitsu Kosan Company
Tokyo, Japan

Dr. Shiunji Kobayashi
NIES and Petroleum Energy Center
Tokyo, Japan

Drs. Yamazaki, Hayashi, Suzuki, and Kobayashi, a group representing the Japan Clean Air Program, visited the Division on February 15, 2001, to discuss collaborating on CMAQ model development studies, especially on fine particulate matter and microscale modeling.

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

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

Dr. Arnold, a postdoctoral researcher, is in his third year with the 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 to make weight-of-evidence approaches objective.

2. Ms. Megin Chapman
   606 Oak Avenue
   Hamlet, NC

Ms. Chapman, a student in the School of Information and Library Science, North Carolina Central University (NCCU), Durham, North Carolina, worked in the library from May through July 2001. Ms. Chapman did this through NCCU as a practicum and earned three credit hours. She participated in handling library services during that period to gain experience in interlibrary loans, reference, and cataloging.

3. Dr. Shan He
   University Corporation for Atmospheric Research
   Boulder, CO

Dr. He, a post-doctoral researcher, is working with the Division on air quality model evaluation for particulate matter. He began a two-year visit with the Division on August 21, 2000.

4. Ms. Cassandra L. Hunsucker
   1713 Carolina Street
   High Point, NC

Ms. Hunsucker, a student in the School of Information and Library Science, University of North Carolina at Greensboro, spent April 14, 2001, in the library observing the activities and services provided and interviewing the Librarian as a class assignment. Ms. Hunsucker also visited with some of the research scientists, asking them questions about the benefits of having the library within the Division.

5. Rokjin Park
Department of Meteorology
University of Maryland
College Park, MD

Mr. Park, a graduate student, is working with the Division to develop a method for adjusting photolysis rates for the presence of aerosols.

6. Mr. Jason Smith
University of North Carolina at Chapel Hill
Chapel Hill, NC

Mr. Smith, a research assistant, assisted in the software framework design of the Multimedia Intergrated Modeling System.

7. Dr. Gail S. Tonnesen
University Corporation for Atmospheric Research
Boulder, Colorado

Dr. Tonnesen, a postdoctoral researcher, completed her third year with the 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 AND AWARDS

All personnel are assigned to the U.S. Environmental Protection Agency from the National Oceanic and Atmospheric Administration, except for those designated EPA, who are employees of the EPA, or SEEP, who are part of the EPA Senior Environmental Employment Program.

Office of the Director

Francis A. Schiermeier, Supervisory Meteorologist, Director (Until February 2001)
William B. Petersen, Supervisory Physical Scientists, Acting Director (Since February 2001)
Herbert J. Viebrock, Meteorologist, Assistant to the Director
Dr. Robin L. Dennis, Physical Scientist
Dr. Peter L. Finkelstein, Physical Scientist
Bruce W. Gay, Jr. (EPA), Program Manager
Evelyn M. Poole-Kober, Librarian
Jeffrey L. West, Physical Science Administrator
Dr. Basil Dimitriades (SEEP), Physical Scientist
Barbara R. Hinton (EPA), 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 (Until May 2001)
Dr. Jason K.S. Ching, Meteorologist
Dr. Brian K. Eder, Meteorologist
Gerald L. Gipson (EPA), Physical Scientist
James M. Godowitch, Meteorologist
Dr. William T. Hutzell (EPA), Physical Scientist
Dr. Michelle R. Mebust (EPA), Physical Scientist
Tanya L. Otte, Meteorologist
Dr. Jonathan E. Pleim, Physical Scientist
Shawn J. Roselle, Meteorologist
Tanya L. McDuffie, Secretary

Modeling Systems Analysis Branch

Thomas E. Pierce, Supervisory Physical Scientist, Chief (Since August 2001)
Dr. William G. Benjey, Physical Scientist
Dr. Steven S. Fine, Computer Specialist
Dr. Alice B. Gilliland, Physical Science Administrator
Steven C. Howard, Computer Specialist
Dr. Sharon K. LeDuc, Physical Scientist (Until October 2001)
John H. Rudisill, III, Equipment Specialist
Alfreida R. Torian, Computer Specialist
Gary L. Walter, Computer Scientist
Dr. Jeffrey O. Young, Mathematician
Ruby S. Borden (SEEP), Secretary

Applied Modeling Research Branch

William B. Petersen, Supervisory Physical Scientist, Chief (Until February 2001)
Dr. Ellen J. Cooter, Supervisory Meteorologist, Acting Chief (Since February 2001)
Dr. Dale A. Gillette, Physical Scientist
Dr. Alan H. Huber, Physical Scientist
Dr. Steven G. Perry, Meteorologist
Donna B. Schwede, Physical Scientist
John J. Streicher, Physical Scientist
Roger S. Thompson, Physical Scientist
Lawrence E. Truppi, Meteorologist
Ashok Patel (SEEP), Engineer
John Rose (SEEP), Machinist/Model Maker
Bruce Pagnani (SEEP), Computer Programmer
Sherry A. Brown, Secretary

Air Policy Support Branch

Mark L. Evangelista, Supervisory Meteorologist, Chief
Dennis A. Atkinson, Meteorologist
Dr. Desmond T. Bailey, Meteorologist
Patrick D. Dolwick, Physical Scientist
John S. Irwin, Meteorologist
Brian L. Orndorff, Meteorologist
Jawad S. Touma, Meteorologist

Thomas E. Pierce, Supervisory Physical Scientist, Chief, MSAB, received the EPA Bronze Medal —"For outstanding efforts in coordinating with State and local agency staff and industries to develop consensus approaches for generating emission inventory guidance under the Emission Inventory Improvement Program"