NOAA Technical Memorandum OAR ARL-236

FISCAL YEAR 1999 SUMMARY REPORT OF THE NOAA ATMOSPHERIC SCIENCES MODELING DIVISION TO THE U.S. ENVIRONMENTAL PROTECTION AGENCY

E.M. Poole-Kober
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(Editors)

Air Resources Laboratory
Silver Spring, Maryland
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Atmospheric Sciences Modeling Division
Research Triangle Park, North Carolina

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PREFACE

This document summarizes the Fiscal Year 1999 research and operational activities of the Atmospheric Sciences Modeling Division (ASMD), Air Resources Laboratory (ARL), 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, air pollution control activities, and abatement and compliance programs.

Established in 1955, the Division serves as the vehicle for implementing the agreements with the EPA, which funds the Division's research efforts in air pollution meteorology. ASMD conducts research activities internally and through contract and cooperative agreements for the National Exposure Research Laboratory (NERL) and other EPA groups. With a staff consisting of NOAA, EPA, and Public Health Service Commissioned Corps personnel, ASMD also provides technical information 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 operational activities outlined in this report should be sent to the Director, Atmospheric Sciences Modeling Division (MD-80), Environmental Protection Agency, Research Triangle Park, NC 27711 or email: francis.schiermeier@noaa.gov.

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ABSTRACT. During Fiscal Year 1999, the Atmospheric Sciences Modeling Division provided meteorological and modeling assistance to the U.S. Environmental Protection Agency. This ranged from the conduct of research studies and model applications to the provision of advice and guidance. Research efforts emphasized the development and evaluation of air quality models using numerical and physical techniques supported by field studies. Among the significant research studies and results were the distribution of an updated version of Models-3/CMAQ, initiation of the Models-3/CMAQ Help Desk, continued evaluation, modification and application of RELMAP and Models-3/CMAQ for mercury and atrazine, continued improvement of emissions models, continued initial work on the Multimedia Integrated Modeling System (MIMS), continued study of dispersion in the convective boundary layer and in urban areas in the Fluid Modeling Facility, and continued development of a statistical method for evaluating model performance.

1. INTRODUCTION

In Fiscal Year 1999, the Atmospheric Sciences Modeling Division (ASMD) continued its commitment for providing goal-oriented, high-quality research and development, and operational support to the U.S. Environmental Protection Agency (EPA). Using an interdisciplinary approach emphasizing integration and close cooperation with the EPA and public and private research communities, the Division's primary efforts were studying processes affecting dispersion of atmospheric pollutants, modeling pollutant dispersion on all temporal and spatial scales, and developing multimedia model frameworks in a high performance computing and communications environment. The technology and research products developed by the Division are transferred to the public and private national and international user communities. Section 2.1 discusses Division participation in international activities, while Sections 2.2 through 2.4 outline the Division research activities in support of the short- and long-term needs of the EPA and 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.

2.1.1.1 International Technical Meetings

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

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

2.1.1.2 Regional/Transboundary Transport of Air Pollution

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

2.1.2 United States/Japan Environmental Agreement

The Division Director serves as the United States Co-Chairman of the Air Pollution Meteorology Panel under the United States/Japan Agreement on Cooperation in the Field of Environment. The purpose of this 1975 agreement is to facilitate, through mutual visits and reciprocal assignments of personnel, the exchange of scientific and regulatory research results pertaining to control of air pollution. In addition to a visit to the United States by a member of the Air Quality Bureau of the Japan Environment Agency, additional interactions were maintained through correspondence and exchange of research findings.

2.1.3 United States/Russia Joint Environmental Committee

The Division Director serves as the United States Co-Chairman of the United States/ Russia Working Group 02.01-10 on Air Pollution Modeling, Instrumentation, and Measurement Methodology, and as Co-Leader of the United States/Russia Project 02.01-11 on Air Pollution Modeling and Standard Setting. The purpose of the 1972 Nixon-Podgorny Agreement forming the US/USSR Joint Committee on Cooperation in the Field of Environmental Protection 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-1999. An annual Working Group meeting was held at ASMD in Research Triangle Park, North Carolina, during March

1999. The Director visited the Main Geophysical Observatory in St. Petersburg, Russia, during June1999 as the United States representative to participate in a jubilee, symposium, and conference in honor of the: 150th anniversary of the A.I. Voeikov Main Geophysical Observatory; 200th anniversary of the birthday of Academician A. Ya. Kupffer, the Founder and First Director of the Main Geophysical Observatory; and 165th anniversary of the establishment of the Russian Hydrometeorological Society.

During this visit and in honor of the 150th anniversary, President Yeltsin signed an edict decorating a group of Main Geophysical Observatory scientists for their achievements. All are collaborators under the United States/Russia Working Group. The award recipients were:

The Order of Honor: Prof. M.E. Berlyand and Dr. E.Yu. Bezuglaya
The Order of Friendship: Prof. V.D. Stepanenko and Prof. E.L. Genikhovich
Honored Meteorologist of the Russian Federation: Dr. S.S. Chicherin

2.1.4 Meteorological Coordinating Committees

2.1.4.1 Federal Meteorological Committee

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

2.1.4.2 Interdepartmental Meteorological Committee

The Division Director serves as the EPA 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, 1999).

The Division Director also serves on the ICMSSR Committee for Cooperative Research and on the ICMSSR Joint Action Group for High Performance Computing and Communications.

Other Division members serve on the ICMSSR Working Group for Atmospheric Transport and Diffusion and on the ICMSSR Working Group for Climate Services.

2.1.5 Board on Atmospheric Sciences and Climate

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

2.1.6 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.

2.1.7 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 are emerging interests 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.

2.1.8 Section 812 Assessment Work Group

A Division scientist is a member of the 812 Assessment Work Group, in coordination with the EPA Office of Program Assessment and Review and the EPA Office of Policy, Planning, and Evaluation, with responsibility for developing approaches to assess regional air quality and acidic deposition. The responsibilities of this working group are to produce a prospective assessment of the benefits and costs of the Clean Air Act Amendments (CAAA) of 1990. Model predictions for the assessment are for the years 2000 and 2010 assuming both full implementation and no implementation of the 1990 CAAA. Work in FY-1999 emphasized completion of the technical assessments and their review by EPA's Science Advisory Board during the spring and summer of 1999. A court-ordered deadline of November 15, 1999, for publication of the assessment was an important constraint on the last phase of work.

2.1.9 Chesapeake Bay Program Air Subcommittee and Chesapeake Bay Program Modeling Subcommittee

A Division scientist is a member of the Air Subcommittee, a working subcommittee of the Chesapeake Bay Program. Previously this Subcommittee was an advisory group to the Implementation Committee. The subcommittee has responsibility for advice and leadership on issues of atmospheric deposition to the watershed and the Bay, on overseeing application of the Regional Acid Deposition Model (RADM) to link atmospheric deposition with watershed models, and in dealing with the potential role of atmospheric deposition on Bay restoration efforts. The Air Subcommittee also works with other Chesapeake Bay committees to define the top priority air quality scenarios to be simulated by RADM. The Division scientist is also an ex officio member of the Modeling Subcommittee of the Implementation Committee. This Subcommittee has responsibility for overseeing the application of water quality models and coordinating the linkage of RADM with those models and the interpretation of the findings.

Work in FY-1999 focused on creation and development of the Extended RADM that incorporated the full dynamics of secondary inorganic fine particle formation to study ammonia deposition. Using the newly developed Extended RADM, NAPAP (National Acid Precipitation Assessment Program) ammonia emissions were adjusted through a primitive model inversion. A preliminary study of ammonia deposition was prepared for FY-2000 work on the definition of a reduced nitrogen airshed for the Chesapeake Bay watershed. The FY-1999 work also involved a redefinition of the oxidized nitrogen airshed for the watershed in continued support of the 1997 Chesapeake Bay Agreement Re-evaluation.

2.1.10 Megacity Impact on Regional and Global Environments

A Division scientist was asked to serve as a member of the External Advisory Panel on the Megacity Impact on Regional and Global Environments (MIRAGE) project at the National

Center for Atmospheric Research (NCAR), Boulder, Colorado. The MIRAGE project has become an official NCAR program jointly directed by the NCAR Research Aviation Facility and the Atmospheric Chemistry Division. The advisory panel is composed of 11 scientists from academia and federal agencies, who are presently involved in urban environmental research. The panel is expected to review the overall program inception, review progress of various studies, and participate in the planning of field experiments. The objective of the project is to study how megacities affect the environment on local, regional, and global scales. The study will be carried out through field study data collection to better understand the physical processes and use of models to help diagnose how human activities in megacities produce their impacts. The initial focus will be on two megacities: Mexico City, Mexico, and Beijing, People's Republic of China. In FY-1999, a proposal to the National Science Foundation (NSF) was developed for a first phase umbrella project relating to Mexico City under which universities could send collaborative proposals. Measurement campaigns in Mexico City are envisioned for the wet and dry season. Dates are uncertain at this time.

2.1.11 North American Research Strategy for Tropospheric Ozone

The North American Research Strategy for Tropospheric Ozone (NARSTO) program was established in FY-1995 to address ozone research and coordinate collaborative research among all North American organizations performing and sponsoring tropospheric ozone studies. Sponsors include the private sector and State, Provincial and Federal governments of the United States, Canada, and Mexico. The coordination of NARSTO Federal research activities is facilitated by the Subcommittee on Air Quality Research of the Committee on Environment and Natural Resources within the National Science and Technology Council. Four technical teams were established: Analysis and Assessment; Observations; Modeling and Chemistry; and Emissions. A major goal of NARSTO is to produce a scientific assessment of the state of tropospheric ozone science. A draft of the 1999 NARSTO scientific assessment was written and is under review by the National Academy of Science. A Division scientist was chosen to co-author one of the 24 critical review papers that were commissioned to provide technical background to the NARSTO assessment group. During FY-1999, the critical review paper on modeling and evaluation of advanced models went through the journal review process and was accepted for publication (Russell and Dennis, in press). A total of 17 of the 24 critical review papers were accepted for publication.

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

2.1.12 International Task Force on Forecasting Environmental Change

A Division scientist is a member of the International Task Force on Forecasting Environmental Change that addresses the methodological and philosophical problems of forecasting under the expectation of significant structural changes in the behavior of physical, chemical or biological systems. Three planned workshops were held at the International Institute for Applied Systems Analysis in Laxenburg, Austria. Internal reviews were completed, and a draft monograph of the workshop discussions was finished in FY-1999.

2.1.13 Regional Acid Deposition Model Application Studies

Efforts during FY-1999 concentrated on completion of the Extended RADM, its initial testing, and conversion of its code to operate on the Cray T3D™[1] massively parallel computer for application studies. The Extended RADM incorporates the full dynamics of secondary inorganic fine particle formation to be able to simulate ammonia (reduced nitrogen) deposition in addition to oxidized nitrogen deposition. The full coupling is required to account for ammonia deposition and partitioning of total ammonia into gaseous ammonia and particulate ammonium. 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. The new model will allow the extension of the estimation of airsheds to ammonia. As part of the preparation of the model for applications, the primitive model inversion done with RADM/RPM to adjust the NAPAP ammonia emissions to more realistic values was redone with the Extended RADM, taking advantage of full dynamics in the model. The Extended RADM represents a step in the transition to Models-3/CMAQ for application simulations.

In FY-1999, a RADM study was completed to more accurately estimate source region responsibility for the nitrogen deposition to the different water basins of the Bay from within the Bay airshed. These results are input to a cost analysis study by Resources for the Future (RFF) of different types of air controls relative to their ability to reduce the nitrogen load to the Bay and relative to water controls (http://www.rff.org/environment/water.htm). A draft report was completed by RFF.

In FY-1999, RADM/RPM was used to complete an analysis of a Congressional proposal that included emission reductions related to acid rain that were beyond those called for in the 1990 CAAA. The analysis examined reductions in sulfur and nitrogen deposition and concurrently reductions or changes in ambient levels of sulfate and nitrate particles and gaseous ozone. This work was carried out in coordination with the EPA Office of Air and Radiation, Acid Rain Division, Washington, DC.

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[1]Cray T3D is a trademark of Cray Research, L.L.C., a wholly owned subsidiary of Silicon Graphics, Inc.

In FY-1999, oxidized nitrogen range of influence mapping was completed for more than 100 emission source subregions to support the development of airshed estimates for coastal estuaries. RADM runs for these mappings were completed during FY-1998 and FY-1999, requiring more than 6,000 Cray-C90™[2] computer hours. Using the procedure developed for the Chesapeake Bay and outlined in Dennis (1997), airsheds for 19 coastal watersheds along the East and Gulf Coasts were defined. Descriptions of these airsheds are expected to be available on the Division's multi-media web site in FY-2000. This work is coordinated with the NOAA assessment of atmospheric deposition to coastal estuaries now underway.

2.1.14 Atmospheric Sciences Modeling Division Library Home Page

The ASMD Library maintains a world-wide web (WWW) home page (http://www.epa.gov/asmdnerl/library/library.htm), which provides a brief overview of the Library's history and location. The purpose of the home page is to make accessible information about the Library's collection, policies, and services to the Division staff and other users in Research Triangle Park, North Carolina, and other locations. The home page provides WWW interface connections to the EPA and NOAA on-line catalogs in which the Library's book and journal collections are cataloged. In addition, the page provides links to other information resources through the agencies' home pages and to other WWW resources that reflect the Library's collection and staff needs. Division library staff provided HTML (HyperText Markup Language) documents of the FY-1998 annual report and 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/).

2.2 Atmospheric Model Development Branch

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

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

2.2.1 Models-3 Community Multiscale Air Quality Modeling

2.2.1.1 Introduction

The U.S. Environmental Protection Agency released a new air quality modeling system, Models-3 Community Multiscale Air Quality (CMAQ), in June 1998 and a revision in 1999. Models-3/CMAQ is a computer-based system that can simultaneously simulate the transport, physical transformation, and chemical reactions of multiple pollutants across large geographic regions. The modeling system is useful to states and other government agencies for making regulatory decisions on air quality, as well as to research scientists for performing atmospheric research. It is a combination of Models-3, a flexible software framework, and the CMAQ modeling system for supporting air quality applications ranging from regulatory issues to scientific research on atmospheric processes. The CMAQ models also can be used independently of the Models-3 system framework, providing more flexibility for advanced research and applications. The first released version of Models-3/CMAQ was tested against a photochemical ozone episode in the northeastern United States for the period July 12–15, 1995. The initial test results were very promising when compared with observed surface ozone concentrations. A rigorous evaluation effort is continuing through FY-2000.

The EPA document, *Science algorithms of the EPA Models-3 Community Multiscale Air Quality (CMAQ) modeling system*, was released in FY-1999 (U.S. Environmental Protection Agency, 1999c). The document's 18 chapters describe all the key state-of-science atmospheric science features and options that are embodied in the CMAQ system. Collectively, it provides the scientific basis and point of reference for the state of the science captured in the July 1998 initial, and to a large extent the subsequent June 1999, release of CMAQ. The document is available at http://www.epa.gov/asmdnerl/models3/CMAQ/index.html. As a living document, with advancements made in the state-of-science in air quality modeling, the CMAQ science documentation will be updated periodically.

2.2.1.2 Development of the Community Multiscale Air Quality Modeling System

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

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

Science submodels in the CMAQ system are the Mesoscale Model Version 5 (MM5), Models-3 Emissions Processing and Projection System (MEPPS), and the CMAQ Chemical-Transport Model (CCTM). There are several interface processors that link other model input data to the CCTM. The Meteorology-Chemistry Interface Processor (MCIP) processes MM5 output to provide a complete set of meteorological data needed for CCTM. MCIP is designed in such a way that other meteorological models can be linked with minimal effort. Initial and boundary conditions are processed with the processors, ICON and BCON, respectively, and the Emissions-Chemistry Interface Processor (ECIP) combines area- and point-source emissions to generate three-dimensional gridded emission data for CCTM. A photolytic rate constant processor, which is based on RADM's JPROC, computes species-specific photolysis rates for a set of predefined zenith angles and altitudes. An alternative detailed-science version adopts state-of-the-science radiative transfer models with a possibility of taking into account the total ozone column (from TOMS satellite data) and turbidity. In addition, a Plume Dynamics Model (PDM) is used to provide major elevated point-source plume dispersion characteristics for driving the plume-in-grid processing within CMAQ.

The second public release of the CMAQ modeling system occurred in June 1999. There were few science changes to CMAQ although significant changes were made in the emissions data and the physics options used with MM5. As in 1998, a specific configuration of the CMAQ system was used for testing against data from a July 1995 ozone episode during the North American Research Strategy for Tropospheric Ozone – NorthEast (NARSTO-NE) field study in the northeastern United States. This version of the model is known as the Air Management Version (AMV) and was configured for use by the EPA Office of Air Quality Planning and Standards (OAQPS) and other groups involved in policy and regulatory analyses for air quality management. CMAQ was configured with the Carbon Bond-IV (CB-IV) chemical mechanism for these tests, the same mechanism used in other ozone air quality models for regulatory purposes. Model testing will continue in FY-2000, and will include examining the impacts of decreasing the vertical resolution on simulation results.

2.2.1.3 Transport Processes within the Community Multiscale Air Quality System

Governing set of equations in generalized coordinates.

CMAQ's dynamic processes are expressed with a set of governing equations capable of handling the fully-compressible atmosphere (Byun, 1999a). Together with the generalized coordinates, they facilitate linkage of the CCTM to many different types of meteorological models (Byun, 1999b). The generalized CCTM can deal with several different conformal map projections as horizontal coordinates, and many popular vertical coordinates used for atmospheric modeling studies. Conformal maps supported are Mercator, Lambert, and Polar Stereographic projections. Vertical coordinates supported are height and pressure coordinates and terrain-following coordinates, such as time-dependent hydrostatic pressure (Sigma-p), time-independent reference hydrostatic pressure (Sigma-p_o), and time-independent scale height (Sigma-z) coordinates. The CMAQ system was tested and released using data from MM5. CMAQ was externally linked with meteorology data from RAMS (Regional Atmospheric Modeling System) meteorology output by the National Institute of Environmental Science in Japan in collaboration with Kyushu University, and URMM (Urban-Regional Multiscale Model) diagnostically analyzed meteorology data at the Georgia Institute of Technology.

Advection and mixing algorithms.

The transport process, in principle, consists of advection and diffusion that cause the movement and dispersion of pollutants in space and with time. It is assumed that the transport of pollutants in the atmospheric turbulent flow field can be described by means of differential equations and appropriate initial and boundary conditions. Numerical schemes for solving the transport equation must meet a convergence condition and correctly model the conservative, dissipative, and dispersive properties of the governing equation. Numerical algorithms for the advection and diffusion processes implemented in CMAQ satisfy these properties. In CMAQ CCTM, advection is represented in flux form. Advection algorithms implemented are the Bott scheme based on a polynomial description of subgrid concentration, Yamartino-Blackman cubic scheme, and a piecewise parabolic method. Atmospheric mixing processes are represented in Reynolds flux terms. Simple local and non-local vertical mixing schemes are available in CCTM. Local eddy diffusion (K-Theory) can be used for vertical mixing in all stability conditions. Alternatively, a simple non-local scheme for transport during convective conditions in the boundary layer, known as the Asymmetric Convective Model (ACM) (Pleim and Chang, 1992), was added to CCTM and will be available in the June 2000 release. Other algorithms under study include turbulent kinetic energy methods, and transilient turbulence methods. The deposition flux is represented as the bottom boundary condition in the vertical mixing algorithms. An eddy diffusion algorithm is used for the horizontal diffusion process in CCTM. Research was on-going during FY-1999 on the characterization of the advection and diffusion processes in CMAQ.

2.2.1.4 Aerosol and Visibility Module

Major improvements are being made to the aerosol module. The version has a fixed geometric standard deviation in all three log-normal modes (Aitken, accumulation, and coarse). This involves predicting two characteristics of the modes, the total mass (as the sum of the constituent species) and the total number. Each constituent mass is converted to a constituent volume by dividing by a standard density. Dividing the sum of the constituent volumes by $\pi/6$ yields the third moment of the number distribution. Using these two characteristics, the geometric mean diameter is calculated. This, along with the modal rates of growth, coagulation, and new particle production, allows new values for the mass and number to be predicted. The use of a fixed geometric standard deviation is a limitation that was removed.

A box model with variable geometric standard deviations in the Aitken and accumulation modes was completed. In addition to the total number and mass in each mode, the total surface area of each mode is a predicted variable. A simple analytical formula computes the geometric standard deviation from the number and the second and third moments. The second moment is obtained from the surface area by division by π. Work is underway to integrate the box model enhancements into the three-dimensional CMAQ code. Preliminary results using the new aerosol code in the United States and in Europe were reported at the European Aerosol Conference in Prague, Czech Republic.

2.2.1.5 Photolysis Rates

Photolysis rates for the Models-3/CMAQ are computed using a table-interpolation method (Roselle *et al.*, 1999). A table was prepared of photolysis rates for different times of day, latitudes, and heights. Photolysis rates for individual grid cells of CMAQ were then computed by interpolating values from the table. Development of the photolysis rate model continued during FY-1999. A new cloud attenuation scheme was developed and tested through collaboration with MCNC[3] that couples clouds used in the photolysis rate model with those in the cloud chemistry model. Also, a method was developed to couple aerosol and gas-phase chemistry to include the effects of aerosols on photolysis rate calculations. Testing and evaluation will continue in FY-2000.

2.2.1.6 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 (Roselle and Binkowski, 1999). The sub-grid cloud model, which is based on the RADM cloud module (Walcek and Taylor, 1986; Chang *et al.*, 1990; Dennis *et al.*, 1993), simulates

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[3]A company located in Research Triangle Park, North Carolina.

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. During FY-1999, the cloud model was updated with the new aerosol model. Work was initiated to incorporate an alternative cloud module, the MCNC cloud module, into CMAQ. The implementation of the cloud model in CMAQ will be evaluated in FY-2000 using available wet deposition data sets.

During FY-1999, a detailed grid-resolved cloud model was developed. This model includes a microphysical submodel for following the evolution of the cloud. It will also consider cloud lifetimes that extend beyond the CMAQ synchronization timestep, thus maintaining the partition between gas and aqueous-phase pollutants during the gas-phase chemistry calculations. Testing and evaluation of this model will continue in FY-2000.

2.2.1.7 Subgrid Scale Plume-in-Grid Modeling in the CMAQ System

A plume-in-grid (PinG) technique was developed for the CMAQ modeling system to provide a more realistic scientific treatment of the physical and chemical processes affecting pollutant species contained in subgrid scale point source plumes. In contrast to the traditional Eulerian grid modeling method of instantly diluting point source emissions into entire grid cell volumes, the PinG algorithms simulate the gradual growth of subgrid scale plumes and more properly treat the temporal evolution of photochemistry in individual plume cells during the subgrid scale phase. The PinG algorithms were successfully implemented and tested in the Models3/CMAQ modeling system and were made available in the June 1999 public release of the science algorithms. The plume-in-grid modeling features and numerical techniques were described in Gillani and Godowitch (1999).

The key modeling components developed to simulate the relevant processes at the proper spatial and temporal scales for pollutant plumes include a plume dynamics model (PDM) processor and a Lagrangian reactive plume model (PinG module). PDM determines the position and physical dimensions of individual plume sections by simulating plume rise, vertical and horizontal plume growth, and plume transport (Godowitch *et al.*, 1995). The PinG model simulates the relevant plume processes by a moving array of attached cells representing a plume vertical cross-section (Godowitch *et al.*, 1999). PinG is capable of simulating a single plume or multiple point-source plumes from continuous hourly emission releases. The PinG module was integrated into CCTM. It is exercised simultaneously during a CCTM simulation to utilize grid concentrations as boundary conditions. An important feedback occurs when a plume section reaches grid cell size as the subgrid plume treatment ceases and plume concentrations are included in the Eulerian grid.

Model simulations were successfully performed with the RADM2 and CB-IV gas-phase chemical mechanisms, the same chemistry mechanisms employed in the parent grid model. Selected model test run results for a single major point source with high NO_x emissions, which were treated by PinG and without PinG, were presented in Godowitch *et al.* (1999). Qualitatively, the results at various downwind distances were encouraging with the modeled plume ozone and other photochemical species exhibiting the same evolutionary pattern found in real-world plume measurements. A quantitative evaluation of PinG simulation results is planned in conjunction with an upcoming CCTM evaluation using plume data obtained during the Southern Oxidants Study's summer 1995 field experiment in the greater Nashville region. Additional work to extend the PinG model to treat aerosol species is anticipated during the upcoming year.

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

With interest in fine particles and toxic pollutants, there is an opportunity to extend air quality models by adding the capability for improving exposure assessments. An analysis to rationally link emissions-based modeling with ambient and exposure monitors to provide concentration fields as critical inputs to models of human exposure and epidemiological studies was initiated. Mechanisms under investigation for adverse health impacts consist of numerous causal hypotheses, including concentration loading of pollutants and their chemical constituents and physical properties. However, the distribution of pollutant concentration fields for different causal pollutants may be highly complex at neighborhood scales. The location and temporal sampling of typical networks in urban areas are sparse, and the resulting concentration fields are poorly resolved. Emissions-based modeling systems capable of modeling $PM_{2.5}$ and PM_{10} from horizontal resolutions ranging from regional (~36 km) to urban scales (4 km) are being tested and evaluated. Since urban areas introduce fresh sources of pollutants into a regional background, significant subgrid spatial variability of the concentration fields with corresponding impact on exposure levels is anticipated. Stationary monitors used to drive human exposure models are limited in their ability to characterize this variability.

A modeling project was begun to resolve air quality fields at neighborhood scales and develop methods to serve as a bridge between these modeling and monitoring approaches to determine concentration variations arising from the juxtaposition of regional and urban sources. The overall effort will involve modeling air quality at fine scales complemented with flow visualization techniques and computational fluid dynamics modeling, and developing functional linkages with ambient fixed site and personal exposure monitoring data.

2.2.1.9 Aggregation Research for Models-3/CMAQ

In support of studies mandated by the 1990 CAAA, the Models-3/CMAQ is planned to be used by 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.

Unfortunately, it is not financially feasible to execute CMAQ over such extended time periods. Therefore, in practice, CMAQ must be executed for a finite number of episodes or events, which are selected to represent a variety of meteorological classes. A statistical procedure called aggregation must then be applied to the outputs from CMAQ to derive the required seasonal and annual estimates.

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

The stratified sample was then evaluated through a comparison of aggregated estimates of the mean extinction coefficients (b_{ext}) to the actual mean b_{ext} observed at 201 stations nationwide. The b_{ext} was selected as a surrogate for $PM_{2.5}$ because it had been used successfully in a similar study involving RADM (Eder and LeDuc, 1996a; 1996b). Results from the evaluation revealed a high level of agreement with mean aggregated estimates of b_{ext} generally falling within ± 10 percent of the observed mean for the time period 1984-1992, indicating that the aggregation and episode selection scheme was indeed representative (Cohn *et al.*, 1999; accepted for publication).

2.2.1.10 Collaborative Model Evaluation Studies for Particulate Matter

A project to develop a Models3/CMAQ capability to serve current and future needs of the Southern Oxidants Study (SOS) community was initiated with a modeling center at the University of Alabama-Huntsville, Huntsville, Alabama. After establishment of this Center for Models-3/CMAQ, performance evaluation will be conducted for specific episode simulations. The model-data intercomparisons will be made for selected case studies using targeted data from aircraft, meteorological observations, and surface chemistry sites for selected periods from the 1999 SOS-Nashville field experiment, focusing on speciated- and size-resolved particulate matter.

A research collaboration between the Washington University Center for Air Pollution Impacts and Trend Analysis (CAPITA) in St. Louis, Missouri, and the Division was initiated to (1) evaluate the performance of Models-3/CMAQ and (2) assess 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 would utilize CAPITA's consolidated database of PM data sets. This project serves to facilitate the use of Models-3/CMAQ by an extended community. This aids in its evaluation and utility to address major and pertinent issues of developing science-based strategic plans for dealing with NAAQS issues, including $PM_{2.5}$, PM_{10}, and ozone. This research provides and utilizes methods to perform essential scientific evaluation of the performance of CMAQ in modeling fine particles. Modeling of $PM_{2.5}$ is needed for performing environmental assessments and for implementing the requirements of the $PM_{2.5}$ NAAQS State Implementation Plans (SIPS) and Regional Haze Rule (RHR).

An Interagency Agreement with the National Park Service (NPS) was initiated to develop, implement, and utilize 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. NPS, in collaboration with the Cooperative Institute for Research in the Atmosphere at the Colorado State University, Fort Collins, Colorado, will implement, test, and evaluate the performance of Models-3/CMAQ against observed pollutant fields in the West. Then the focus will be on incorporating advanced smoke emission from fires (prescribed, agricultural, and natural) into the Models-3/CMAQ. This project will 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.

2.2.2 Aerosol Research and Modeling

As noted in Section 2.2.1.4, a variable geometric standard deviation is now used in the aerosol module of CMAQ. This work resulted from a comparison of aerosol modules funded by the Coordinating Research Council in Atlanta, Georgia (*Fiscal year 1998 summary report,* 1999). The comparison of the CMAQ thermodynamics codes with others will be published (Zhang *et al.*, accepted for publication). The comparison of the aerosol dynamics codes showed that the CMAQ version with a fixed geometric standard deviation was inadequate and resulted in the development of the new version described in Section 2.2.1.4. A report will be published (Zhang *et al.*, in press).

The new version is able to reproduce the Hazy case of Seigneur *et al.* (1986) to a higher degree of fidelity than any of the sectional models described in the report comparing the CMAQ aerosol dynamics module and sectional models. An independent study by Fernandez *et al.* (1998) of the same difficult case required many more sections than used by the sectional models in the comparison study to yield an acceptable degree of fidelity. The Fernandez *et al.* (1998) study and the comparison of the new CMAQ aerosol module with the test case showed that a very large number of sections is necessary to achieve sufficient fidelity. The results of Russell and Seinfeld (1998) support the view that accounting for both particle number and mass in a sectional model is necessary to model particle behavior accurately. This is not common practice with existing sectional models. Note that CMAQ does predict consistent behavior of the number and mass. The new version adds surface area to allow both a geometric mean diameter and geometric standard deviation to vary, thus capturing the variation of the size distribution with changes in ambient conditions.

Work is also underway to improve the representation of both biogenic and anthropogenic organic material in the particles. There is an ongoing effort to improve the representation of primary particle emissions. Finally, given the increasing availability of observations, a preliminary evaluation against species mass and visual range is planned.

2.2.3 Atmospheric Toxic Pollutant Research

2.2.3.1 Atmospheric Toxic Pollutant Modeling

During FY-1999, modeling studies were conducted using previously developed simulation capabilities for atmospheric mercury based on the REgional Lagrangian Model of Air Pollution (RELMAP) (Eder *et al.*, 1986) in response to scientific critiques of model results presented at various conferences and workshops, organized peer reviews of journal articles submitted for publication, and specifically to the incremental effects of mercury air emissions from Canada on the magnitude and pattern of mercury deposition across the United States. Development of new atmospheric simulation modeling capabilities for toxic pollutants during FY-1999 focused on two separate pollutants of interest: mercury and semi-volatile organic compounds. Both modeling efforts involve the use of CMAQ as the basis for air toxic pollutant modeling, but their relevant scientific issues and modeling approaches differ somewhat. Each effort is discussed separately below.

Mercury Modeling.

The RELMAP mercury model was developed to simulate the emission, transport, dispersion, atmospheric chemistry, and deposition of mercury across the continental United States (Bullock *et al.*, 1997). Its atmospheric chemistry algorithm, based on formulations of Petersen *et al.* (1995), considers the aqueous reaction of elemental mercury with ozone to produce inorganic mercury in precipitation. This mercury wet deposition is augmented by adsorption of inorganic mercury to carbon soot particles in cloud water and is moderated by the catalytic reduction of inorganic mercury to elemental mercury by ubiquitous sulfite ions also in cloud water. This model was used in the development of the *Mercury Study Report to Congress* (U.S. Environmental Protection Agency, 1997) to estimate the magnitude and pattern of mercury deposition throughout the United States from domestic emissions and from the global average concentration of elemental mercury from sources all around the world. During FY-1999, an inventory of Canadian air emissions of mercury was made available from Environment Canada, and was used to revise previous mercury deposition estimates. By simulating these Canadian mercury emissions in the same manner as previously done for United States emissions, an assessment of the incremental effect of Canadian sources on the total mercury deposition pattern across the United States was obtained. These results suggest that Canadian sources account for no more than 20 percent of mercury deposition to all U.S. locations, with the exception of the extreme northern section of the Rocky Mountain region near the Canadian border. These results were presented at the *5th International Conference on Mercury as a Global Pollutant* in Rio de Janeiro, Brazil, and are due to be published in the peer reviewed scientific literature within the next year.

Recent laboratory studies of chemical reactions of mercury and its compounds in air and in water (Lin and Pehkonen, 1999) suggest that the chemistry mechanism of the RELMAP mercury model may not accurately reflect the complex nature of mercury chemistry, especially in cloud water. In response, work was begun to modify CMAQ to include mercury and various mercury compounds as modeled pollutant species. The CMAQ existing gas- and aqueous-phase chemistry mechanisms for tropospheric ozone and acid deposition simulation provide a convenient basis for the simulation of complex mercury chemistry. During FY-1999, gas-phase reactions of elemental mercury with ozone and chlorine were added to CMAQ, and some preliminary model testing was performed. Work on expanding the CMAQ aqueous chemistry mechanism was started also. However, there remains serious uncertainty about variations in the concentration of chloride ions in cloud water from marine to continental locations. Work on the aqueous chemistry mechanism for mercury will continue through FY-2000. This work will involve collaboration with other modelers in academia and at other government agencies.

Transport and Deposition of Semi-Volatile Compounds.

To simulate the fate of compounds that are considered semi-volatile and toxic, CMAQ was modified to introduce a semi-volatile compound into the atmosphere as gaseous emissions from an area source. Once emitted, the gas can transform via OH addition or partition onto ambient particulate matter as a trace species. The partitioning assumes equilibrium between the gas and particulate phases based on empirical and theoretical work (Pankow, 1987; 1994). Concentrations in each phase then depend on the total ambient concentration and partitioning ratios. Besides these chemical and physical processes, the compound undergoes advection, diffusion, and deposition.

CMAQ was selected to address this issue based on how the model estimates particulate matter in the lower troposphere. The estimate uses a tri-modal distribution and internal mixture of inorganic and organic species to describe particulate matter. The inorganic species divide into two components: aqueous and dry. These aspects permit studying how a semi-volatile compound partitions onto particulate matter in different ways. The compound adsorbs onto surface areas from a combination of inorganic species within particulate matter. In addition, the semi-volatile compound absorbs into either the organic species or aqueous component within particulate matter. CMAQ then is able to help assess how meteorology and gas to particle partitioning combine to control the fate of semi-volatile compounds over regional and local scales.

The modified model is being tested with a herbicide called atrazine. The effort uses atrazine emissions predicated on its usage, and a soil model under energy balance conditions. The model domain covers the eastern United States and the simulation spans several days in early July of 1995. Results include atmospheric concentrations and deposition rates. Exploration produced some interesting results, including the areas where degradation of atrazine becomes significant, and the controlling species and processes that dominate deposition as a function of location. An unexpected result stems from the approach to gas to particle partitioning. The approach allows atmospheric humidity and the aqueous component to vary partitioning by a factor of ten. The result may explain observations that contradict predictions from theory (Hillery *et al.,* 1997).

Research and development will continue in FY-2000 and will include comparing modeling results and observations to assist in the development of a special version of CMAQ that can be released to the public. The special version will specifically model atrazine as semi-volatile and handle other semi-volatile compounds as well.

2.2.3.2 Atmospheric Mercury Field Research

The Florida Atmospheric Mercury Study (FAMS) was conducted to characterize the atmospheric loadings of mercury to Florida (Guentzel, 1997). This study developed a simple box model that suggested the dominant source of mercury in rainfall to south Florida was from trade wind (long-range) transport from the Atlantic Ocean. The South Florida Atmospheric Mercury Monitoring Study (SoFAMMS) was conducted to investigate potential source-receptor relationships between anthropogenic point-source emissions in southeast Florida and atmospheric wet deposition of mercury (Dvonch *et al.*, 1998). This study used a multi-variate source apportionment approach and concluded that approximately 70 percent of the mercury in rainfall to southeast Florida was from waste incineration and oil combustion sources. The FAMS and SoFAMMS studies both identified atmospheric wet deposition as the dominant pathway for mercury into the Florida Everglades. The magnitude of local anthropogenic source contributions, however, remains a subject of contentious debate. Both studies highlighted the importance of reactive gaseous mercury (RGM) and meteorological transport in explaining the transport and deposition of mercury to south Florida. No reliable ambient RGM measurement technologies were available during either the FAMS or SoFAMMS studies.

Reliable methods for discriminative measurement of ambient RGM and Hg^0 were developed using annular denuder technology (*e.g.*, http://www.tekran.com/access/1130.html). The new instrumentation under evaluation provides a unique opportunity to evaluate, via aircraft measurements, the FAMS study hypothesis of long-range transport of RGM to Florida in the marine free troposphere. During FY-1999, an interagency agreement was developed to use the NOAA DeHavilland Twin Otter (DHC-6-300) aircraft to obtain measurements of RGM, Hg^0, and other ancillary measurements, in upwind air off the coast of Florida during February and June of 2000. Ancillary measurements of ozone (O_3), carbon monoxide (CO), sulfur dioxide (SO_2), nitrogen oxides (NO, NO_X, NO_Y), condensation nuclei (CN), and various trace elements in aerosol form will be used to identify sources of observed RGM.

2.2.4 Meteorological Modeling Studies

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

2.2.4.1 Meteorology Modeling for Models-3/CMAQ Applications

Several projects were underway during FY-1999 using MM5 to support Models-3/CMAQ applications. MM5 Version 2 Release 10 (MM5v2.10) was used, and was tailored for air-quality applications with some minor modifications. The significant changes included standardizing the radius of the earth in the emissions and chemistry modules, enabling analysis nudging FDDA, and initialization from one-way nesting to occur in the same simulation.

MM5 was run for July 1–22, 1995, for the Models-3/CMAQ evaluation and the NARSTO Meteorology Model Intercomparison Study. MM5 was configured with a series of four one-way nested domains. The 108-km domain was nearly continental, and the 36-km domain included most of the United States east of the Rocky Mountains. There were two sets of 12-km and 4-km domains, one for each region of interest that corresponded with two intensive field studies, NARSTO-NE and SOS-Nashville, during the period. There were five overlapping simulations that provided four days each for chemistry and emissions simulations with 12 h for model spin-up. The MM5 physics options were upgraded from the Models-3/CMAQ demonstration in FY-1998, and the land-use representation near coastlines was refined in MM5 to be more consistent with the emissions and chemistry models. Comparison of the MM5 simulations with satellite, radar, and conventional observations showed promising results. In areas where MM5 did not generate favorable results, further work will be done in FY-2000 to understand and improve the simulations. Improved MM5 simulations will be included as part of the model evaluation in FY-2000 as sensitivity experiments.

A major research effort with MM5 involved the addition of the observation nudging FDDA to air-quality simulations for Models-3/CMAQ. A major data pre-processing phase was completed, and several observation nudging experiments were conducted for the July 1995 cases. Sensitivities to time range of influence, radius of influence, type of observation, and region of influence function were evaluated. Preliminary research indicates that observation nudging improves the meteorology simulations at fine resolutions. Additional work will continue during

FY-2000 to refine the nudging strategy and extend the technique to additional case studies, ensuring that MM5 is not specifically tuned for July 1995.

For the June 1999 Models-3/CMAQ public release, a version of MM5v2.10 with air-quality enhancements was configured and run on a Sun™[3] workstation since other components of Models-3/CMAQ were designed and released for that system. Several modifications were required to the official NCAR version of MM5 to enable it to run on the Sun™ workstation. This workstation was made available with the Models-3/CMAQ release. As part of the release, two documents were written. The first document (Otte, 1999a) discusses the standard MM5v2 physics options and how they relate to Models-3/CMAQ. The second document (Otte, 1999b) is a user's guide and tutorial for MM5 users who plan to apply their output to CMAQ. Two overview classes relating MM5 to CMAQ were taught in conjunction with Models-3/CMAQ training during FY-1999.

Preliminary work was completed on the transition to MM5 Version 3, released by NCAR in July 1999. There are several significant changes in MM5v3. Some of the highlights of those changes include a new output format, Year-2000 compliance, a new land-surface model, restructuring of the pre- and post-processing programs in Fortran 90, elimination of the hydrostatic dynamics option, addition of new physics options, and support for additional input background fields. Initial testing with MM5v3 revealed several minor bugs that were reported back to NCAR for including in the updates to the official release. It is anticipated that the Division will fully transition to MM5v3 in FY-2000.

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 modified version of MM5 is called MM5PX (Pleim and Xiu, 1995) in which a new land-surface model, including explicit representation of soil moisture and vegetative evapotranspiration, along with the Asymmetric Convective Model (ACM) replaces the standard surface and PBL schemes available in the MM5 system. FY-1999 efforts included applications of MM5PX to air quality modeling, further testing and evaluation, and system development for transfer to the MM5 community modeling group at NCAR.

The MM5PX model and its preprocessing programs were upgraded to be portable, user-friendly, and easily integrated into the community modeling system. The operational system is based on MM5 v2.10 with the terrain processor from version 2.12, which can process the 1-km resolution U.S. Geological Survey (USGS) land-use data and the soil-texture data needed by the PX model. In addition to the standard MM5 preprocessors, the PX system also includes two

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[3]Sun is a trademark of Sun Microsystems.

additional preprocessors: *Vegeland* for processing of vegetation and soil data, and *InitPX* for processing initial fields of soil moisture and soil temperature. MM5PX is being updated to MM5 v3. This version will then be incorporated into the NCAR community modeling system.

The MM5PX is being used to provide meteorology and soil moisture conditions to the Lake Michigan Mass Balance project for simulation of atrazine emissions, transport, and deposition. The MM5PX was run for the entire spring and early summer of 1995 at 36-km and 12-km grid resolution centered on the Lake Michigan region. These runs will also be used to evaluate the long-term capabilities of MM5PX to track seasonal changes in vegetation and soil moisture conditions. Model simulations will be compared to two surface flux field experiments conducted in Alabama and Kentucky. This study will be particularly valuable for evaluating the seasonal vegetation growth algorithms and the indirect soil moisture nudging scheme.

2.2.5 Dry Deposition Studies

2.2.5.1 Dry Deposition Research

The dry deposition field campaign was completed in the fall of 1998. While the field programs ran, an extensive and unique database of pollutant deposition velocity and boundary layer meteorology was compiled. Studies were completed over a variety of ecosystems, in various geographical and climatological regions of the country and are summarized in Table 1.

Table 1. Summary of deposition research field programs

Location	Vegetative Land Use	Dates
Beaufort, NC	Pasture	06/10/94 - 07/26/94
Bondville IL	Corn	08/18/94 - 10/22/94
Sand Mountain, AL	Pasture	04/14/95 - 06/13/95
Keysburg, KY	Soybean	06/22/95 - 10/11/95
Durham, NC	Pine Forest	04/14/96 - 05/14/96
Plymouth, NC[4]	Soybean	07/17/96 - 08/15/96
Tuckerton, NJ	Salt Water Estuary	08/27/96 - 10/15/96
Kane, PA	Deciduous Forest	04/27/97 - 10/24/97
Boonville, NY	Mixed Forest	05/12/98 - 10/20/98

[4]Joint with Project NOVA, an EPA sponsored NO_x emissions study.

With the completion of the field programs, attention turned to data analysis and model development. Edited data sets were developed for most of the sites. The present generation of site-specific deposition velocity models was evaluated at all sites. A paper presenting a summary of the data and model evaluation from the agricultural sites was published (Meyers *et al*., 1998). A similar paper with data and model evaluation from the forest sites will be published. Focus is now on improving the deposition velocity models. Inclusion of a photosynthetic model for stomatal control and updated aerodynamic and boundary layer models promise to make better estimates of deposition velocity. If these models show improvement they will be turned over to the CASTNet (Clean Air Status and Trends Network) program for use. The science in the models will then be incorporated into Models-3 and future multi-media modeling programs.

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 implemented in MM5PX. Since MM5PX has a parameterization for evapotranspiration, the same stomatal and canopy conductances can be used to compute dry deposition velocities of gaseous species. This technique has the advantage of using more realistic conductance estimates resulting from the integrated surface energy calculation where the soil moisture is continually adjusted to minimize model errors of temperature and humidity. The dry deposition model was evaluated for ozone deposition by comparing model results with field measurements at Bondville, Illinois, and Keysburg, Kentucky (Pleim *et al.,* 1996; 1997). Further evaluation studies are underway that involve longer comparisons to field measurements in Alabama and Kentucky. The impact of the new dry deposition model and MM5PX on the simulation of air chemistry by CMAQ is being tested as part of the NARSTO-NE evaluation studies.

In addition to dry deposition model development for Models-3/CMAQ, a new technique for estimating dry deposition velocities directly from field measurements of meteorological parameters was developed. Bulk stomatal resistance is estimated based on similarity with latent heat flux. The technique is tested using the comprehensive field measurements made at Keysburg, Kentucky, in 1995 (Pleim *et al*., 1999). Potentially, this scheme could be used to estimate very accurate values for dry deposition velocity of ozone, and perhaps other gaseous species such as SO_2 or CO_2, from relatively inexpensive field networks without the need for direct chemical eddy correlation measurements.

2.2.6 Technical Support

2.2.6.1 North American Research Strategy for Tropospheric Ozone

The North American Research Strategy for Tropospheric Ozone (NARSTO) formally decided in 1999 to extend their scope beyond ozone to also include fine particles. (One consequence of this was a name change to NARSTO, dropping the words associated with the acronym). NARSTO is a coordinated 10-year research strategy to pursue the science-based issues that will lead to better management of the North American tropospheric ozone and other air quality problems. It includes a management plan for performing this coordination across the public and private sector organizations sponsoring ozone research, as well as those groups performing the research, including the university community. Canada and Mexico are also participating in the continental NARSTO program. During FY-1999, two Division representatives were involved in co-chairing key teams for the continental NARSTO program: the Modeling Team, and the Analysis and Assessment Team. Also, the first NARSTO-sponsored state-of-science assessment for tropospheric ozone neared completion. It is composed of a series of critical review papers on particular areas of the science, as well as an assessment report that indicates how the science can address outstanding policy issues in tropospheric ozone. The critical review papers are to be published in a Special Issue of *Atmospheric Environment* during early 2000. The second draft of the assessment report was in review by the National Research Council at the end of 1999, with publication anticipated in mid-2000. Several Division members are participating in the assessment as co-authors of certain critical review papers and the assessment report.

2.2.6.2 Southern Oxidants Study

FY-1999 was the ninth year of the multi-year Southern Oxidants Study (SOS), a major field and modeling project concerned with the generation and control of ozone, fine particles, and photochemical processes in the southern United States. A consortium of southeastern universities is coordinating the study. Division personnel are involved in providing technical leadership on aspects of air quality simulation modeling and aerometric data archiving. The last major SOS field study occurred in the Nashville/middle Tennessee region during the summer of 1999, following the Nashville studies in 1994 and 1995. During FY-1999, a major activity within the Division was obtaining and setting up data sets from the 1995 study, and configuring Models-3/CMAQ in a nested grid configuration on this area for model application and evaluation. CMAQ simulations for Nashville will begin in early FY-2000. Also, in April 1999, the Division hosted a Modeling Workshop of the Southern Oxidants Study in Research Triangle Park, North Carolina.

2.2.6.3 Western Regional Air Partnership Air Quality Modeling Forum

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, and the EPA, and others from industry, environmental groups, and other interested parties. The Air Quality Modeling Forum (AQMF) is one 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 is to provide technical and policy input needed to regulate regional haze in the western United States. AQMF is to provide

WRAP with technical analyses needed to meet the practical, real-world objectives, especially as they relate to meeting the regulatory requirements of the EPA regional haze rule (RHR) published July 1, 1999. Specific objectives of modeling regional visibility are (1) to assess the relative incremental contribution of a given source or source control on visibility at one or more Class I areas; (2) to assess the cumulative impact of regional source growth or control on Class I areas throughout the region; (3) to assess the impact of regional sources during periods of high and low visibility conditions; and (4) to evaluate the most 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 by December 31, 2003; and (3) long-term (modeling to support SIPs due no later than December 31, 2008. WRAP AQMF is investigating the utility of Models-3/CMAQ for performing the intermediate- and long-term modeling for RHR. One member of the Division actively participates in AQMF.

2.2.6.4 Multimedia Integrated Modeling System Meteorological Team

Accurate characterization of the atmosphere is an essential part of any environmental modeling endeavor. During the development of the Multimedia Integrated Modeling System (MIMS), research will be ongoing in ways designed to improve this characterization and its seamless integration into MIMS. MM5 v2 is used to generate meteorological data for CMAQ; however, additional models will be considered in the future. Two problems common to each of the meteorological models is that they are computationally intensive because of their complexity, and that they generate tremendous amounts of data. As a result, it is not feasible to execute MM5 or CMAQ over extended time periods (such as a full year). These constraints are exacerbated with MIMS, because unlike episodic air quality studies that typically simulate 10-day periods, MIMS will be required to perform much longer simulations to study the impact of nitrogen loading to the watershed. As a result, such statistical approaches as aggregation may be required. Such a procedure was applied successfully to air quality studies in the past including RADM simulations (Eder and LeDuc, 1996a; 1996b) and more recently CMAQ simulations (Cohn *et al.*, 1999). With aggregation, a limited set of meteorologically representative time periods are used to derive the required seasonal and annual estimates. Therefore, in practice, MM5 and MIMS may have to be executed for finite episodes or events, the results of which would be aggregated to achieve the requisite seasonal or annual results.

2.2.6.5 Climatological and Regional Analyses of CASTNet Data

In response to CAAA of 1990, the Clean Air Status and Trends Network (CASTNet) was created to establish an effective, rural monitoring and assessment network. The network's primary purpose is to identify and characterize broad-scale spatial and temporal trends of various air pollutants and their environmental effects in rural areas encompassing aquatic and terrestrial ecosystems. The purpose of this research is to facilitate such identification and characterization across a variety of spatial and temporal scales, focusing on the ambient air concentration patterns of SO_2, SO_4^{2-}, HNO_3, NO_3^-, NH_4^+, and O_3. This is achieved through the application of a multivariate statistical technique, rotated principal component analysis, to the weekly air concentration data from CASTNet for the period October 24, 1989, through August 15, 1995. Such analysis allows for the segregation of CASTNet stations into species-specific influence regimes or subregions whose ambient air concentrations exhibit statistically unique and homogeneous characteristics, presumably in response to a commonality of forcing factors (*i.e.*, meteorology, emissions, geography). An examination of the time series of these homogeneous characteristics will then be performed, using spectral density analysis that will facilitate understanding of the forcing factors responsible for the influence regimes.

This approach, which was used in the examination of other aerometric data, including SO_4^{2-} concentrations in precipitation (Eder, 1989), ambient air concentrations of O_3 (Eder *et al.*, 1993), as well as total column O_3 measurements (Eder *et al.*, 1999), has many advantages. First, it allows for comparison of ambient air concentrations between regions whose segregation is statistically and physically based; second, since stations within subregions exhibit homogeneous characteristics, this approach allows us to develop region-wide indicators that should provide meaningful insight into the variability of air concentrations within these subregions; and finally, the analysis of air concentration characteristics and trends will be based on an aggregation of data from many stations, as opposed to individual stations, thereby minimizing the effects of anomalous or even erroneous data often associated with a particular station. Such analysis is useful in that it provides weight of evidence concerning the regional nature of such species; facilitates understanding of the probable mechanisms responsible for their unique behavior among subregions; and identifies stations that exhibit either redundant (*i.e.*, highly correlated with other stations) or unique (not correlated with other stations) behavior, allowing network designers to reduce or augment the network, thereby increasing its efficiency.

2.2.6.6 Utilization of NEXRAD Data for Input into MIMS and Evaluation of MM5

The ability to accurately model both atmospheric and surface processes involving chemicals is highly dependent on precipitation types, rates and totals. In addition to controlling the wet deposition of such chemicals, precipitation plays a major role in the hydrological cycles of both the atmosphere and ground. Unfortunately, uncertainties exist in modeling precipitation. To quantify these uncertainties and to improve the quality of these data, precipitation analysis fields obtained from the NWS Stage IV NEXRAD (NEXt generation RADar) will be incorporated into two studies. The first study will use NEXRAD data to evaluate precipitation estimates from the Penn State/NCAR MM5 being used by the Models-3 CMAQ modeling community. The second application will involve assimilation of NEXRAD precipitation data into the surface models associated with MIMS. The Stage IV NEXRAD data set consists of precipitation data fields that have assimilated both rain gauge data and WSR-88D data into a comprehensive hourly, national data set. Visualization and statistical tools will be utilized to judge the quality of the NEXRAD data set. If it is deemed to be acceptable, the data set will then be used to evaluate the precipitation fields of MM5, and it will be assimilated into the MIMS surface models.

2.3 Modeling Systems Analysis Branch

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

2.3.1 Emission Modeling

The emission processing capability of Models-3 was improved during FY-1999 by (1) enhancing and stabilizing the Models-3 Emission Processing and Projection System (MEPPS) for release of Models-3 Version 3.0, and (2) continuing work on a fundamentally different emission processing system, the Sparse Matrix Operator Kernel Emission (SMOKE©)[5] system. MEPPS was used to process emission data for planned evaluation runs of Models-3/ CMAQ. Specifically:

- The Models-3 Version 3.0 release incorporated the results of substantial testing and a series of bug fixes for MEPPS and its companion data input processor, the Inventory Data Analyzer (IDA), resulting in a functional reliable emission processor. Limited enhancements to the system included expanding the existing internal GIS (Geographic Information System) coverage to North America from Mexico north and the Carribean, and providing optional area-normalized processed emission reports that allow comparison of gridded emission data at different spatial resolutions.

- Work was completed on installation of the EPA Highway Vehicle Particulate Emission Modeling Software — PART 5 — in MEPPS. PART 5 is a companion to the Mobile 5a model which computes hourly gaseous emissions from vehicles. PART 5 is important because of the increasing need for accurate particulate emission inventory data for air quality modeling in support of the new, more stringent, particulate NAAQS.

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[5] Copyright 1999 MCNC-North Carolina Supercomputing Center, Research Triangle Park, NC.

- Extensive streamlining and modification of the SMOKE© processing system for use in the Models-3 framework were accomplished. SMOKE© was initially developed as a prototype by MCNC-North Carolina Supercomputing Center with cooperation from the Division. Its sparse matrix approach to the repetitive computations involving very large emission databases increases processing performance by at least an order of magnitude. SMOKE© will be fully incorporated within the Models-3 framework, unlike MEPPS, which is a SAS™[6]-based system that can only be partially integrated and requires much more data file space. Substantial data handling and quality control capability remains to be added to SMOKE© before it is fully functional in Models-3. Because SMOKE© cannot create its own input files and grids from diverse sets of raw data, an input file quality control and file formatting tool (SMOKE© Tool) is under development. SMOKE© Tool is a necessary and important component.

- Initial planning began on expanding the capability of Models-3 using SMOKE© to process emission data of agricultural pesticides for use in CMAQ.
- During late FY-1999, MEPPS began generating multiple emission data sets for evaluation runs of CMAQ, for July 2-18, 1995, with spatial domains covering the eastern half of the United States and Canada. These emission data sets are being produced at 36-km, 12-km, and 4-km spatial resolution, for both CB-IV and RADM2 chemical mechanisms.

2.3.2 Biogenic Emissions

The Division continues 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 will be integrated into the Biogenic Emissions Inventory System (BEIS), the third generation of which should be released during FY-2000. Focus areas during FY-1999 included isoprene for photochemical ozone modeling, and ammonia for modeling aerosols, visibility, and nitrogen deposition.

Pierce *et al.* (1999) reported on the OZark Isoprene Experiment (OZIE). The purpose of the experiment was to investigate isoprene levels near the Ozark Plateau, a region densely populated with high-isoprene emitting oak trees and experiencing abnormally high modeled isoprene concentrations (>250 ppbC). Measurement platforms during OZIE included an aircraft, two tethered balloons, seven surface sites (two state-operated). Excellent sampling conditions occurred during July 18–22, 1998, as temperatures peaked around 100 °F. Surface and aloft data were finalized for analysis by the study team, which includes NCAR, Boulder, Colorado, and Washington University, St. Louis, Missouri. A preliminary comparison of observed measurements to a Models-3/CMAQ simulation shows reasonably good agreement above 200 m,

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

with isoprene around 15 ppbC. The cause for CMAQ overestimation of near-surface concentration is still being investigated.

A paper on ammonia and nitric oxide emissions from agriculture will be presented at the Air & Waste Management Association Emission Inventory Conference in Raleigh, North Carolina. This work focused on recommending improved temporal characterization of ammonia emissions from fertilizer and livestock, and nitric oxide emissions from fertilized soils. Ammonia emissions from agricultural sources comprise ~85 percent of the total ammonia inventory in the United States, and better temporal resolution is needed for modeling aerosol formation and nitrogen deposition.

The basic building blocks for the third-generation Biogenic Emissions Inventory System (BEIS3) were completed. These include a 1-km vegetation cover database and an expanded emission factor table. Emission factors compiled for 213 vegetation categories and 35 hydrocarbon compounds significantly build on earlier emission factors that included 165 vegetation categories and 3 hydrocarbon classes. BEIS3 will also include a more sophisticated soil NO algorithm, which will account for precipitation, fertilizer application schedules, and canopy interception. This will allow for more realistic modeling of background NO_x values in regional photochemical modeling simulations.

A presentation at the Global Climate and Hydrology Center in Huntsville, Alabama, highlighted the possible importance of lightning-produced nitric oxide for regional air quality modeling. A simulation with RADM indicates that lightning may contribute ~10 percent of total nitrogen oxide (NO_x) emissions during the summer in the eastern United States. This finding could be important because lightning NO_x is not explicitly included in most regional model simulations.

International collaboration on biogenic emissions is evidenced by the paper by Simpson *et al.* (1999). More information on the Division's biogenic emissions research, slides of presentations, and access to data and computer algorithms can be obtained at http://www.epa.gov/asmdnerl/biogen.html.

2.3.3 Improvements in Vegetation Cover Data

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 (Pierce *et al.*, 1998). 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 ftp://monsoon.rtpnc.epa.gov/pub/beis2/landuse.

2.3.4 Technology Transfer

The release of Models-3/CMAQ version 3 occurred on June 30, 1999. Significant improvements were made to the installation procedures to eliminate difficulties for first time users. Users can elect to install the system from a single Digital Linear Tape, rather than from five 8 mm exebyte tapes. All users of Models-3/CMAQ on Sun workstations received version 3, a new installation document (Atmospheric Modeling Division, 1999a) and users manual (Atmospheric Modeling Division, 1999b). Nearly 40 users received the Models-3/CMAQ version 3 on tape. There is no count of the number who have downloaded and tested the stand-alone version from the web site. There are about 15 requests for the Models-3/CMAQ on untested computing platforms.

The release of Models-3/CMAQ version 3 included updated versions of other publicly available software where Y2K (Year 2000) compliance issues were addressed. The MM5 version 2.10, the standard for developing the meteorological input files for Models-3/CMAQ, is not Y2K compliant. A Y2K compliant version of MM5 is being tested to replace version 2.10. Models-3 documentation can be obtained at http://www.epa.gov/asmdnerl/models3.

2.3.4.1 Visualization and Analysis Tools

Visualization tools used for and provided with Models-3 were updated to more recent versions for both PAVE©[7] (Package for Analysis and Visualization) that is available at http://envpro.ncsc.org/EDSS/pave_doc/Pave.html and Vis5D©[8] that is available at http://www.ssec.wisc.edu/~billh/vis5d.html. The IBM DX®[9], which is also used by Models-3, is

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[7]Copyright 1997–2000 MCNC-North Carolina Supercomputing Center, Research Triangle Park, NC.

[8]Copyright 1990–1999 Bill Hibbard, Johan Kellum, Brian Paul, Dave Santek, and Andre Battaiola.

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

now publicly available at http://www.research.ibm.com/dci/software.html. For visualization in a Microsoft® Windows™ NT®[10] computing environment these tools are used with a Microsoft® Interix™[11] product that is available at http://www.interix.com/products/matrix.html. The Microsoft® Windows™ NT® version should be evaluated and released during FY-2000.

2.3.4.2 Training Sessions

Training sessions were held during FY-1999 to familiarize users with the science and operation of Models-3/CMAQ:

- January 1999 - Personnel from Research Triangle Park, North Carolina, were the focus of this training. EPA personnel from the Office of Air Quality Planning and Standards, NOAA/ARL scientists, post-doctoral students, visiting scientists and government contractors received training. Thirteen attended the emissions processing session on January 27–28, and 13 attended the CMAQ session on January 19–20. Three individuals attended both training sessions.

- March 1999 - Additional personnel from Research Triangle Park, North Carolina, along with representatives from EPA Region 3, University of Maryland, Canadian Research Council, Ottawa, Ontario, Canada, and NOAA/ARL, Silver Spring, Maryland, were the focus of this training. Twenty attended the CMAQ training on March 1–3, and 14 attended the emissions training on March 4–5.

- June 15–17, 1999 - Three groups who want to use the Models-3/CMAQ framework on SGI™[12] computing platform were the focus of the training. The CMAQ code will execute on SGI™ as will the database for the Models-3 framework. The only component that cannot reside on SGI™ is the user interface. The software required for this was ordered. The SGI™ can be used as a host and the user interface can reside on a Sun™ [13] workstation. The five attendees were from EPA Acid Rain Division, Office of Air and Radiation, Atmospheric Environment Service of Environment Canada, Downsview,

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Corporation; Open-source availability starting May 26, 1999.

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

[11]Interix is a trademark of Softway Systems, Inc.

[12] SGI is a trademark of Silicon Graphics, Inc.

[13] Sun is a trademark of Sun Microsystems.

Ontario, Canada, and a consortium of academic, government and private entities from the State of Washington.

2.3.4.3 Help Desk and Web Site

A Help Desk was established for Models-3/CMAQ along with assignments to individual scientists to answer user questions in specific areas. The telephone number for the Help Desk is 919-541-0157. The Models-3/CMAQ website (http://www.epa.gov/asmdnerl/models3/) was expanded to provide user support for a 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 that ingests the data sets for a second tutorial designed to use 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. A Models-3 *Public Forum* area was established on the SCRAM (Support Center for Regulatory Air Models) web site (http://www.epa.gov/scram001/) at EPA. The purpose of this area is to provide a central location for discussion of issues related to the operation and use of Models-3.

2.3.4.4 Computing Platforms for the Models-3 Framework

The Models-3 framework version 3 was released for use on Sun™ workstations. The science code can be run on a number of machines and operating systems, including Sun™, DEC™ Alpha™[14], Cray C90™, Cray T3E™, SGI™, and Microsoft® Windows™ NT®. The Models-3 framework was ported to an SGI™ computing platform with a single exception; the graphical user interface must be on a Sun™ workstation. Software was ordered to overcome this limitation. Models-3 framework and data sets are also being ported to the Microsoft® Windows™ NT® operating system. This implementation has problems with Orbix™[15], a commercial software component of the framework supporting distributed applications using object-oriented client-server technology. These problems must be overcome before Models-3/CMAQ can be fully tested for use with the Microsoft® Windows™ NT® operating system.

The scientific evaluation of CMAQ is being done on multiple computing platforms through the Models-3 framework. The modeling of emissions with MEPPS is being done on Sun workstations, and the MM5 simulations are being done on a Cray C90™. CMAQ runs on a Cray T3E™ with the initial and boundary conditions being executed on either a Sun workstation or a Cray C90™. The Fortran source code for the science modules is the same for multiple computing platforms, and is recompiled and linked on the host machine to create an executable for the

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[14]DEC and DEC Alpha are registered trademarks of Digital Equipment Corporation.

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

specific host hardware. The use of a single scientific source code simplifies the management and maintenance of the software.

2.3.5 Cross-Platform Implementation of CMAQ Chemistry-Transport Model

Hundreds of model runs are required, demanding rapid turnover for model evaluation, sensitivity studies and other applications. The only computing platform available that can provided the needed throughput is the CRAY T3E™, a distributed memory, high performance parallel computer. To take advantage of its performance capabilities, CCTM code was modified to run in parallel. The modifications are sufficiently general, using a standard message-passing protocol, so the code would run on any distributed memory architecture, including workstation farms.

The parallel implementation developed for CCTM requires a horizontal grid domain decomposition that involves near-neighbor communication (data transfer across adjacent processors) and file input/output (I/O) with data redistribution depending on processor location in the domain decomposition. The I/O is built on top of (layered on) the Models-3 I/O Application Programming Interface. To manage and simplify the near-neighbor communication from the user's point of view, a stencil exchange library was developed that contains standardized data communication calls, which can be inserted in the code.

The code modifications from the serial version necessary for the parallel version are not trivial, and the issue of code maintenance and control demanded a solution to the problem that arises from maintaining the same essential science algorithms, but implemented on different architectures. The solution developed for CCTM involves:

- A single source code that contains a few precompiler options that are selected for execution on either serial or parallel platforms.
- The use of parallel I/O and stencil exchange libraries linked in at the load step during code compilation.
- The additions of Fortran include files that contain the two horizontal grid parameters associated with the domain decomposition.
- The additional pre-compiler directives to select the appropriate stencil exchange and parallel I/O functions during the compile phase. For example, if targeting a serial platform, the stencil exchange functions linked into the executable are no-operation and simply return when called.

To simplify the compilation and linking for different platforms, UNIX®[16] C Shell scripts were developed, and the monocode was successfully tested on the CRAY T3E™ and CRAY T3D™, the CRAY C90™ and Sun™ workstations.

2.3.6 Multimedia Integrated Modeling

The Branch is involved in a long-term project to develop a Multimedia Integrated Modeling System (MIMS) with predictive capability for transport and fate of nutrients and chemical stressors over multiple scales to improve the environmental management community's ability to evaluate the impact of air quality and watershed management practices on stream and estuary conditions. This system will provide a computer-based problem solving environment for testing the understanding of such multimedia (atmosphere, land, water) environmental problems as the movement of chemicals through the hydrologic cycle, or the response of ecological systems to land-use change. The approach combines state-of-the-art in computer science, system design, and numerical analysis (*i.e.*, object-oriented analysis and design, numerical libraries including finite analytic elements) with the latest advancements in process level science (process chemistry, hydrology, and atmospheric and ecological science). The problem solving environment will embrace the watershed/airshed approach to environmental management, and build upon the latest technologies for environmental monitoring and geographic representation. MIMS will provide a common and open modeling framework for the university and government modeling communities.

Toward this goal several multimedia modeling workshops were held in North Carolina and Georgia to facilitate discussions among federal and state participants on critical MIMS science and design issues. Planning meetings were held with the Software Engineering Institute, Pittsburgh, Pennsylvania, on architecture design concepts for MIMS. A survey of data models and software for supporting complex scientific data was prepared to compare existing work on data models and software (Application Programming Interfaces and libraries) supporting efficient representation and operations on a wide variety of scientific data. The focus is on the practical suitability of such data models rather than an exploration of their mathematical details. Of particular interest is multi-language support for integrated analysis and visualization of large disparate spatial temporal data, and metadata in a distributed heterogeneous high-performance computing environment. Also, the environmental fluid dynamics code, selected as a starting point for surface water pollutant transport and fate, was converted to Fortran 95, modified to enable dynamic allocation of grid structures, and set-up for use in the Neuse River Basin program.

2.3.7 Training in Object Technology for Scientific Computing

A course, *Object Technology for Scientific Computing,* sponsored by the Division was held in Washington, DC, Athens, Georgia, and Research Triangle Park, North Carolina.

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

Approximately 100 scientists and managers from government and academia attended the course. Object technology is a proven method for building quality software with long-term maintainability, extendability, reliability, and reusability. These are valuable traits for scientific modeling and data-management software, which benefit from increased flexibility to adapt as the state-of-science grows. Attendees heard about applying object technology to scientific modeling and data from three leaders in the field.

A working meeting was held about two months after the training to provide a hands-on opportunity for the Division scientists to use these fundamental technologies to rethink the organization of CMAQ to increase its maintainability, extendability, reliability, and reusability. A meeting was also held with one of the course authors to better understand how these object-oriented fundamentals can be implemented in numerical models using Fortran 90, which is an updated version of the programming language used for CMAQ. Fortran 90 tools were presented that can be used to design object-based code, increase flexibility, reduce potential for error, and ease code modifications.

2.4 Applied Modeling Research Branch

The Applied Modeling Research Branch investigates and develops applied numerical simulation models of sources, transport, fate, and mitigation of air toxic pollutants in the near field and conducts research to develop and improve human exposure predictive models, focusing principally on urban environments where exposures are high. Databases are assembled and used to model development and research on flow characterization, dispersion modeling, and human exposure. Using the Fluid Modeling Facility (FMF), the Branch conducts simulations of atmospheric flow and pollutant dispersion in complex terrain, in and around such obstacles as buildings, in convective boundary layers and dense gas plumes, and in other situations not easily handled by mathematical models. The Facility consists of two wind tunnels and a convection tank. The large, meteorological wind tunnel has an overall length of 38 m with a test section 18.3 m long, 3.7 m wide, and 2.1 m high. It has an airflow speed range of 0.5 to 10 m/s, and is generally used for simulating transport and dispersion in the neutral atmospheric boundary layer. The small wind tunnel has a test section 1 m by 1 m in cross section, 4 m in length and capable of air speeds up to 20 m/s. It is suitable for both near-field dispersion studies using grid-generated turbulence and instrument calibrations. A convection tank measuring 1.2 m on each side and containing water to a depth of 0.4 m is used to study the convective boundary layer (CBL), and flow and dispersion under convective conditions. The tank is initially temperature stratified using an electrical heating grid. Convection is then initiated by heating the floor of the tank, producing a simulated convective boundary layer capped by an overlying inversion. Dispersion processes are simulated in the tank by releasing fluorescent dye into the CBL and measuring the resulting concentration distributions with a laser-induced-fluorescence system. Another activity of the FMF is the study of resuspension mechanics and wind erosion, primarily through experimental field measurements.

During FY-1999, the FMF regained some of the support personnel lost during reductions in prior years, adding part-time support in the model shop and in the areas of software and data acquisition. Primary research efforts have continued to be focused in three areas: (1) continuation of analysis and reporting on results from studies of buoyant puff and plume dispersion in the convective boundary layer, (2) evaluations of instrumentation for investigating the physics of particle resuspension from grass-like surfaces, and (3) fundamental measurements of flow and dispersion within, over, and around an array of buildings. In addition to these in-house research areas, the FMF hosted a student from the University of Paris who participated in a cooperative study designed to characterize various surface roughness geometries in terms of roughness length.

2.4.1 Hazardous Waste Identification Rule

The EPA is developing a proposed amendment to its regulations under the Resource Conservation and Recovery Act (RCRA) by establishing constituent-specific exit criteria for low-risk solid wastes that are designated as hazardous because they are listed, or have been mixed with, derived from, or contain listed hazardous wastes. Listed waste with concentrations below the exit criteria would no longer be regulated by RCRA Subtitle C. The methodology under development for the Hazardous Waste Identification Rule (HWIR99) will estimate risks through an integrated multi-media, multiple pathway, and multiple receptor assessment that characterizes potential human health and ecological exposure and risk. The characterization of exposures and risks are intended to provide a national distribution of individual risk from individual constituents released from the following types of waste management units: industrial landfills, waste piles, land application units, surface impoundments, and tanks.

The atmospheric concentration and deposition of constituents can be determined in several ways. However, the selected procedure has to be computationally efficient to satisfy the HWIR99 requirements of numerous simulations within a Monte Carlo framework. Because the HWIR99 modeling is site-based, the steady-state Gaussian plume modeling approach was considered to be appropriate, and the Industrial Source Complex-Short Term (ISCST3) (U.S. Environmental Protection Agency, 1995) model was selected. The model provides estimates of contaminant concentration, dry deposition (particles only), and wet deposition (particles and gases) for user-specified averaging periods (*i.e.*, annually for HWIR99). ISCST3 does its calculations using an hourly time step. For the periods of simulation for HWIR99, this results in extensive runtimes. The long-term version of the model (ISCLT3) (U.S. Environmental Protection Agency, 1995) uses a joint frequency distribution instead of the hourly meteorological data. This offers a shorter runtime, but only provides long-term estimates of concentration and dry deposition. The wet deposition cannot be calculated since the necessary serial correlation between the precipitation and other meteorological data is not available.

One of the significant enhancements made to the ISCST3 model for use in HWIR99 pertains to the implementation of the Sampled Chronological Input Model (SCIM) (Koch and Thayer, 1974; Thayer and Koch, 1974) option. The SCIM option allows the sampling of a subset of the sequential hourly meteorological data based on a user-specified sampling interval. The purpose of this option is to allow the user to obtain a representative long-term estimate of pollutant impacts by only sampling a representative subset of the long-term meteorological data. It allows for the calculation of concentration, dry deposition, and wet deposition since it maintains the precipitation information for each hour sampled. Given that such an option is likely to introduce an added level of uncertainty, *i.e.*, uncertainty in addition to those inherent to the model, a study was performed in an attempt to characterize the uncertainty introduced by the use of the SCIM option.

To analyze the impact of ISCST3 estimates by using the sampled meteorological data, model runs were made using five area sources designed to be representative of possible HWIR sources. The source sizes were selected from the high end of the size distribution for each source category since larger units are expected to produce impacts farther downwind. The surface impoundment and aerated tank sources were modeled with vapor phase emissions only while the land application units (two sources, differing in their particle size distributions) and the waste pile sources included particulate emissions as well. Each source was run with five years of meteorological data from four stations: Lake Charles, Louisiana; Pittsburgh, Pennsylvania; Salem, Oregon; and Tucson, Arizona. The HWIR99 meteorological databases typically contain at least 10 years of data; the sites were selected to provide a diversity of climatological regimes. A polar grid of receptors was created with receptors along 16 evenly spaced radials at distances from the edge of the source out to several kilometers. Model runs were made using different sampling rates and comparisons were made with the results from using the entire meteorological database for each station.

The initial testing of the SCIM option used one sampling rate for each run and always started the sampling with the first hour. Maximum concentration, dry deposition, and wet deposition at each distance were analyzed and plotted. Since concentration and dry deposition patterns were the same, only the concentration plots were retained. The analysis was repeated for several sampling rates. The analysis found that a sampling rate of 193 hours (~ 8 days) produced annual average concentration and dry deposition estimates that were comparable to those obtained from the full data set.

Figure 1a shows that the method worked best for meteorological stations with frequent precipitation (*e.g.*, Salem), while Figure 1b shows that sites with infrequent precipitation (*e.g.*, Tucson) showed problems with wet deposition. To improve the estimates for dryer climates, a separate sampling frequency for the wet hours in the meteorological data was introduced. The concentration and dry deposition were calculated using the dry SCIM sampling, while wet deposition was calculated from hours sampled during wet SCIM sampling. To avoid double counting, precipitation was ignored during the dry SCIM sampling. A composite, weighted average was calculated at the end of the simulation to determine annual values. Figures 2a and 2b show that the addition of the second sampling rate did not significantly change the results for Salem, but improved the results for Tucson.

To examine the variability associated with the selection of the start hour of the sampling, model runs were made varying only the start hour of the dry SCIM from 1 to 24. An example plot of the highest, lowest, and average of the 24 maximum impacts at each distance is shown in Figure 3a. For concentration, the error bars are small close to the source and increase in size with distance. Model runs were made varying only the start hour of the wet SCIM from 1 to 8. Figure 3b shows an example plot of the highest, lowest, and average of the 8 maximum impacts at each distance. For wet deposition, the error bars increase with decreasing annual precipitation. The results of the analysis showed little bias in the estimates of concentration and deposition. Therefore, the method was judged to be satisfactory for HWIR.

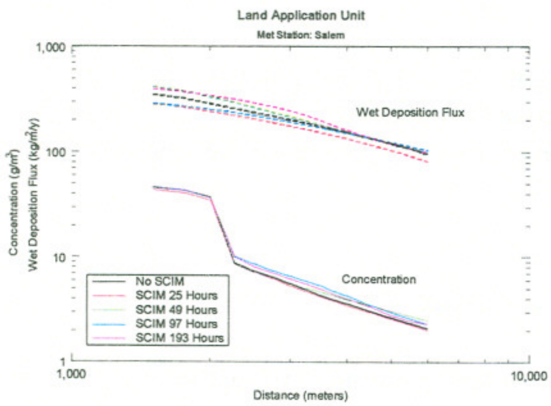

Figure 1a. Maximum concentration and wet deposition estimates at each distance for various sampling intervals using meteorological data for Salem, OR.

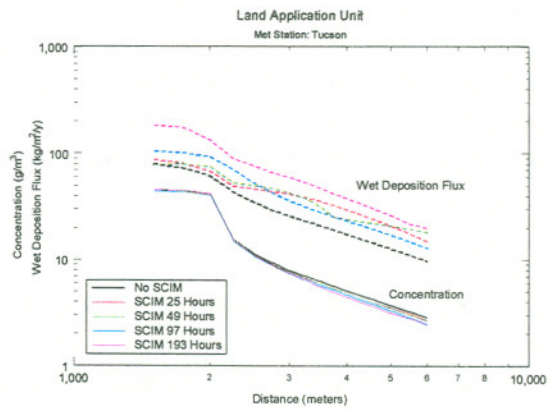

Figure 1b. Maximum concentration and wet deposition estimates at each distance for various sampling intervals using meteorological data for Tucson, AZ.

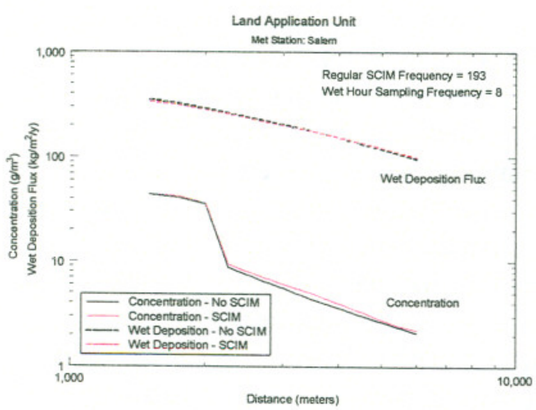

Figure 2a. Maximum concentration and wet deposition estimates at each distance using both separate dry and wet sampling rates and meteorological data for Salem, OR.

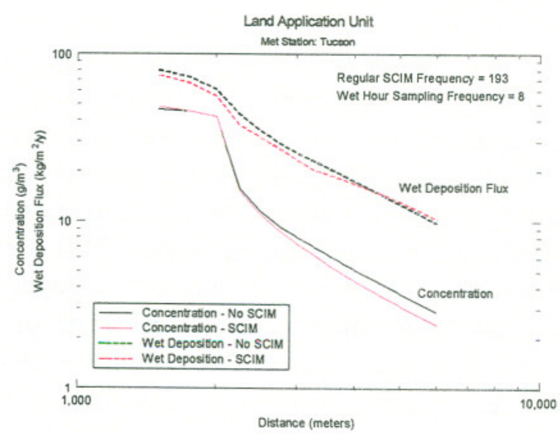

Figure 2b. Maximum concentration and wet deposition estimates at each distance using both separate dry and wet sampling rates and meteorological data for Tucson, AZ.

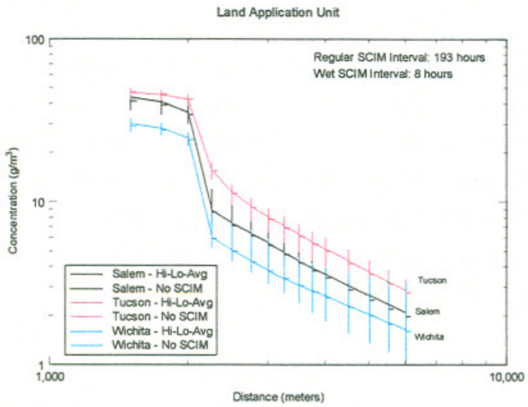

Figure 3a. High, low, and average concentration estimates at each distance from model runs with sampling starting hours 1-24.

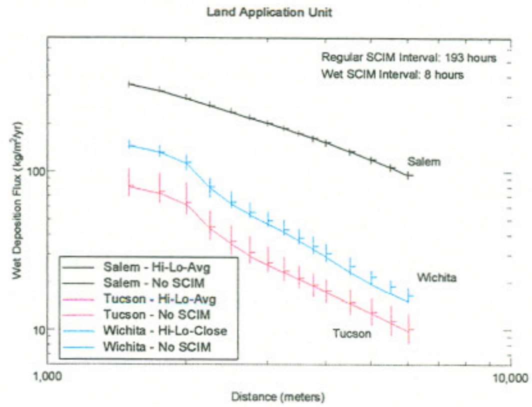

Figure 3b. High, low, and average wet deposition estimates at each distance from model runs with sampling starting hours 1-24.

2.4.2 Solar Radiation Exposure Modeling: A New Approach

During FY-1999, proof of concept was completed for the computer graphics-based solar radiation exposure modeling. Three-dimensional graphics modeling software is used to display a near-photographic quality human model, and illuminate the model with a simulated sun light source. The research goals of the modeling are to develop photobiology tools that enable quantification and anatomical resolution of sun exposure for scenarios of varying posture and duration. Lighting detail includes partitioning of direct beam and diffuse skylight, shadowing effects, and gradations in model surface illumination depending on model surface geometry and incident light angle.

The American Cancer Society reports that over 80 percent of skin cancers occur on the face, head, neck, and back of the hands (Scotto, 1996). Therefore, modeling human exposure to solar radiation demands that exposure calculation be anatomically resolved. The calculation of light illumination for various receptor points across the anatomy (shown as red patches in Figure 4) will provide information about differential exposure as a function of model posture, orientation relative to the sun, and sun elevation. During FY-2000, exposure research will be pushed to unprecedented precision. By integrating geodesic sun-tracking models with high resolution three-dimensional mathematical computer models of the human form, the instantaneous exposure [Watts per square meter] can be calculated, as well as the cumulative dose [Joules per square meter] received during a sun exposure scenario, at various monitoring areas on the anatomy. Illustration of exposure and/or cumulative dose is achieved using a false color rendering, mapping light intensity to color (see Figure 5). Such analysis is essential to determine the reduction in exposure gained by wearing a hat or sun glasses. This kind of research will provide the dose factor needed to develop dose-response functions for skin cancer, immune system suppression, and cataract formation.

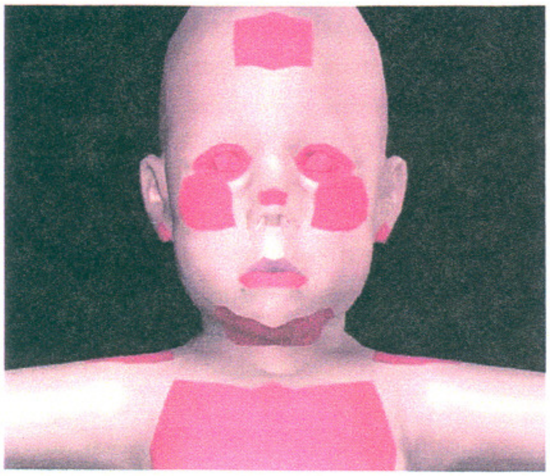

Figure 4. Three-dimensional graphic computer model with light monitoring receptor areas shown as red patches.

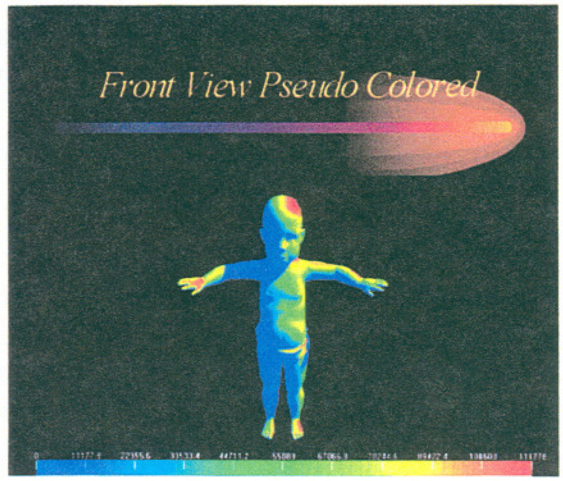

Figure 5. False color rendering of sun-illuminated model: mapping light intensity to color illustrates anatomical areas receiving greatest sunlight intensity.

2.4.3 Modeling Assessment of the Biological and Economic Impact of Increased UV-B Radiation on Loblolly Pine in the Mid-Atlantic States

This assessment required use of data and models from several disciplines, including U.S. Forest Service data, NASA projections of mid-latitude ozone depletion, radiative transfer models, biological exposure models, dose-response models, and economic cost models. A regional total column ozone regression model was developed from composite satellite and ground-based ozone measurements. This model was used to calculate current ozone as a function of Julian day, latitude, and longitude within the mid-Atlantic states region. A discreet-ordinate spectral radiative transfer model (libRadtran, version 0.13)[17] (Mayer *et al.,* 1997) was used to calculate the spectral flux [W/m^2/nm] for selected solar zenith angles, total column ozone levels, and elevations above sea level. Spectral flux was calculated at a resolution of 0.05 nm. Global (beam plus diffuse) radiation was used for exposure calculation. The biologically effective exposure [W/m^2]$_{be}$ was then calculated by convolution of the Caldwell generalized plant spectral weighting function (normalized at 300 nm) with the spectral flux. Spectral weighting functions, or action spectra, quantify the relative effectiveness, by wavelength, of incident light. Calculation of the biologically effective exposure for several solar zenith angles, ozone levels, and elevations, enabled the

[17]libRadtran is available at http://www.uio.no/~arveky/libRadtran.html under GNU General Public License http://www.linux.org/info/gnu.html.

development of a simple regression model of biologically effective exposure as a function of these input variables. This regression model was then incorporated into a sun tracking model with one-minute time resolution to calculate a daily biologically effective dose $[J/m^2]_{be}$ using an assumed linear dose metric. Figure 6 presents the 1999 dose profile for the mid-Atlantic states region for April and July; and Figure 7 presents a forecast percent change dose profile for April and July in year 2010 when stratospheric ozone levels are predicted to be a minimum. UV dose/response data for Loblolly pine were used to estimate growth rate reductions. A dose/response regression function was developed from field data and used to investigate possible growth rate reductions corresponding to two ozone depletion scenarios. Total Loblolly biomass by Hydrologic Unit Code (HUC) was reported for three size classes, as well as annual Loblolly biomass growth rate. Annual growth rate by HUC was determined, and future growth rate was estimated by applying the regressed dose/response function for projected ozone reductions. The economic assessment of growth rate reduction considered fixed stumpage price by tree size. Prices used in this assessment were fixed quotes for Virginia stumpage, published in Timber Mart-South (Timber Mart-South Market Newsletter, 1999). Annual biomass production was similarly assigned a dollar value within each watershed, and projected annual growth deficit due to UV-B stress was then evaluated in dollar terms.

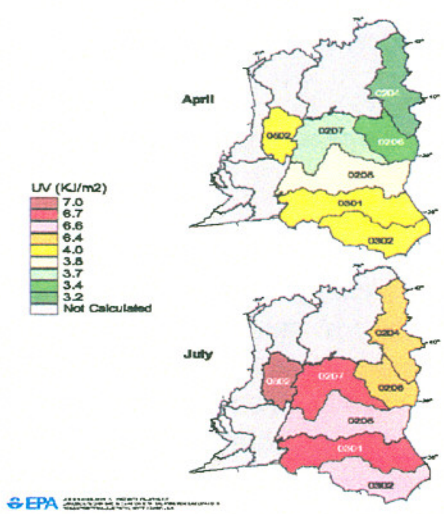

Figure 6. Average daily biologically effective dose of UV by Hydrologic Subregion for 1999. April and July are shown with legend presented in [KJ/m2].

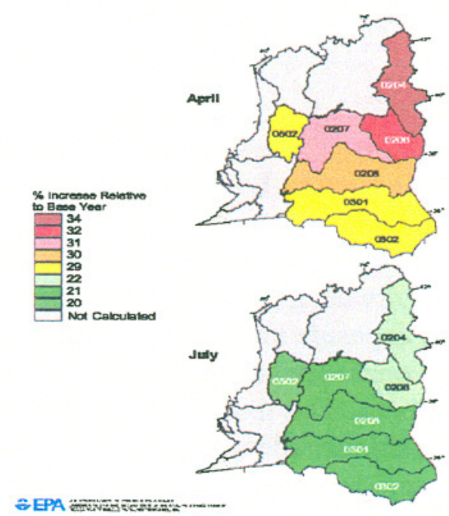

Figure 7. Year 2010 forecast of average daily biologically effective dose of UV by Hydrologic Subregion.

2.4.4 Model Characterization for Indoor Sources of Particulate Matter

Indoor sources of particulate matter (PM) contribute significantly to total human exposure due to the disproportionate time (upwards of 80 percent) that the population spends indoors. Indoor activities that generate PM include tobacco smoking, cooking, vacuuming, burning candles and incense, and walking (resuspension). Modeling the physical characteristics of these emissions is essential to predicting the magnitude and duration of indoor concentrations. Development work began in FY-1999 to model several of these sources. The completed model design includes simulation of emitted mass as a lognormal function of particle size and time; emitted particle count as a function of size and time; and constant or exponential decaying source strength. Calculation of mass aggregation into arbitrary particle size ranges allows comparison with specific measurement instruments or with regulatory standards. Required model inputs include total mass emitted, decay constant for exponential processes, and the geometric mean and standard deviation of particle size. Calibration of model against oven cooking data is in progress. Figure 8 illustrates the model output (mass as function of time and particle size) for a generic exponential source type. Figure 9 illustrates preliminary model simulation of indoor particle concentration during oven cooking.

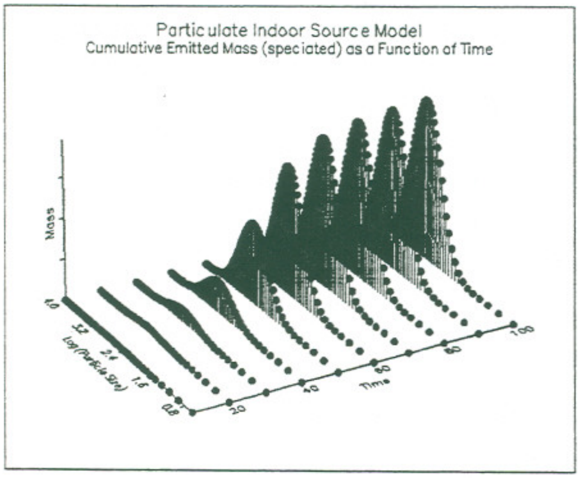

Figure 8. The Particulate Indoor Source Model simulates a source with exponentially decaying emission strength. Model output is presented as speciated mass (lognormal with size) as a function of time and particle size.

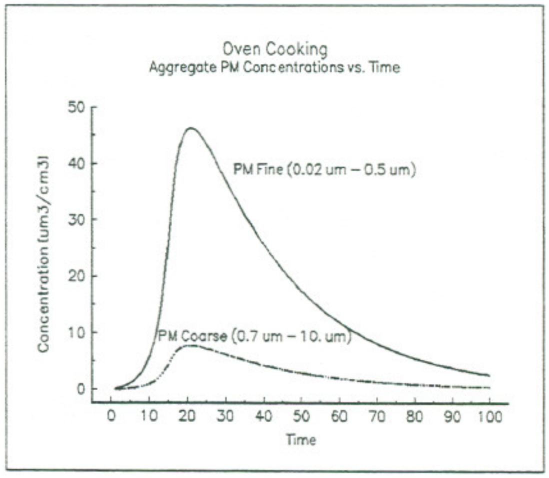

Figure 9. The Particulate Indoor Source Model simulation of fine (0.02um-0.5um) and coarse (0.7um-10.0um) aggregate fractions during oven cooking. The volumetric concentrations are calculated by incorporating the source model into a numerical indoor air model.

2.4.5 Modeling Pesticide Spray Drift from Agricultural Operations

As part of an ongoing Cooperative Research and Development Agreement (CRADA) involving scientists from NOAA, the EPA, U.S. Agricultural Research Service, and a consortium of about 40 pesticide chemical manufacturers, a number of field studies were performed to gather data for the purposes of developing a comprehensive database of primary (at the time of application) spray-drift related information from aerial, ground-based, orchard air-blast, and chemigation pesticide application methods. An initial version of the AgDRIFT spray drift dispersion and deposition model was developed from this extensive database.

The primary focus of the CRADA efforts was the development of a better understanding of the factors that influence the transport, dispersion, and deposition of pesticide material from the operation of air-blast sprayers that are unique to orchard applications. To obtain adequate efficacy and total coverage on plant material, pesticide laced droplets are blasted at extremely high speeds throughout the orchard canopy. This type of operation can result in significant over spray and subsequent spray drift from the intended target for certain application practices and meteorological conditions. An analysis of data from three major field studies in eight orchard types focused attention on several factors that are most important in influencing off-canopy drift. Of primary concern is the drop size distribution of the spray material leaving the air-blast sprayer, the architecture of the canopy (*i.e.,* planting density, leaf area index, and canopy height), and meteorological conditions (wind speed particularly, wet bulb depression, and atmospheric stability to a lesser extent) just above and downwind of the canopy. Meteorology just above the canopy is particularly important because air-blast spraying within moderate to dense canopies results in a significant portion of the drifting (over-spray) material to exit the canopy not at the lateral edges but rather vertically upward at which time the meteorology above the canopy (within one to three canopy heights) takes control of the transport and drift. The conclusions from this analysis are guiding future efforts in developing mechanistic algorithms within the AgDRIFT framework for pesticide drift from orchard canopies.

2.4.6 Lake Michigan Mass Balance Project - Atrazine

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

The ORTECH Pesticide Emissions Model©[18] modifications identified during the previous reporting period were incorporated. An hourly atrazine emission inventory for the period April 1 through July 16, 1995, was generated over a 36 km^2 model grid domain stretching from southern Canada to the Gulf of Mexico and from the Rocky Mountains eastward to the Atlantic. A database documentation report was prepared and published at http://www.epa.gov/asmdnerl/massb.html (Atmospheric Sciences Modeling Division, 1999c). Research was completed regarding the identification of wet deposition episodes most likely to facilitate comparison of the CMAQ transport and deposition model results with 28-day cumulative LMMB field samples collected during the summer of 1995 along the shores of Lake Michigan. Results of this research were presented at the annual meeting of the International Association of Great Lakes Research and a manuscript was prepared for a journal article. Another manuscript documenting atrazine source characterization required for emission inventory generation is in preparation. Other on-going work includes the expansion of the 36 km^2 database through August 3, 1995, generation of meteorological and emissions information for a 12 km^2 nested model grid centered over Lake Michigan and close coordination with CMAQ/Toxics model application development. Coordination of the fate and transport modeling portion of this research with related activities continues in the NOAA Air Resources Laboratory.

2.4.7 Retrieval and Dissemination of Data from the EPA Complex Terrain Model Development Field Studies, 1984-1986

At the request of investigators at the University Catholique de Louvain, Louvain, Belgium, and Lawrence National Livermore Laboratory, Livermore, California, data files of tracer gas experiments in complex terrain conducted by EPA at Cinder Cone Butte, Idaho (Truppi and Holzworth, 1984), Hogback Ridge, New Mexico (Truppi, 1986), and the Tracy Power Plant, Nevada (Truppi, 1987) were retrieved from computer archives and forwarded to the interested scientists by Internet file transfer protocol (FTP). User's guide documents to the data files were also forwarded. Since 1986, when the last experiment at the Tracy Power Plant in Nevada concluded, more than 150 foreign and domestic investigators have shared the data.

2.4.8 Simulation of Diffusion in a Laboratory Convection Tank

The FMF was awarded an internal grant to investigate dispersion in convective boundary layers. Previous work in the FMF convection tank has shown its value for the study of dispersion from both continuous point sources (plumes) and instantaneous buoyant releases (puffs). The internal grant supports continuation of measurements for additional combinations of the

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[18]Copyright to CGEIC ORTECH.

governing parameters. Upgrades were made to the convection tank system and equipment was purchased in anticipation of beginning the experimental measurements early in FY-2000.

The convective boundary layer (CBL) is characterized by the heating rate at the surface as represented by w_*, the convective velocity scale; z_i, the depth of the CBL; and the gradient of potential temperature above the CBL. Because of the turbulent nature of the CBL and the highly variable plume and puff trajectories, a large number of repetitions of each case must be made to obtain statistically stable results to describe the dispersion. Use of a convection tank in the laboratory makes controlled repetition of particular parameter combinations possible. Measurements at the FMF were for one value of w_* and one value of elevated temperature gradient. Ensembles of measurements were completed for puffs of three buoyancies and plumes of four buoyancies. Continuous point source releases were all made at one height in the CBL. To validate theoretical scaling relationships and extend the range of application of the algorithms, additional values and combinations of these parameters will be investigated.

Another aspect of the internal grant research involves making measurements of the turbulent velocity field in the CBL. To accomplish this a Digimage©[19] system was purchased. This system consists of a video camera, a video recorder, and a personal computer including image capture or a frame grabber board that were modified to work together with a software package. Tracer particles are tracked from frame to frame by the software to determine velocity fields.

In preparation for commencing the experimental program, all existing equipment was examined and upgraded. The 5-watt argon ion laser was sent out for inspection and recharge and upon its return, new front optics were installed that greatly improved its efficiency. The aging video camera used to record the fluorescent dye concentration tracer as it is illuminated by a laser light sheet was replaced by a more modern camera. The new camera, designed for scientific applications, has a switch setting for γ=1.0 which means that the camera output is linearly related to the intensity of the image. A key requirement of measuring dispersion in the convection tank is obtaining quantitative concentration fields. The linear output of this new camera makes the calibration process more straightforward than with the former camera. At the close of FY-1999, the new camera and laser upgrades were incorporated into the laboratory and the Digimage© system was delivered and setup. The tank was configured and ready for a series of puff experiments to commence.

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

This project is a three-year effort designed to develop methods for modeling of resuspension fluxes from vegetated surfaces. The working hypothesis is that resuspension from

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[19]Copyright 1992–1999 Stuart Dalziel, DL Research Partners.

surfaces of vegetation is primarily caused by the impaction and rubbing of the surfaces against each other, liberating particles that were deposited on the vegetation surfaces from the atmosphere.

The initial effort centered around finding and evaluating instrumentation to quantify the conversion of wind energy to mechanical energy by the impaction or rubbing of a single grass blade. After consideration of several experimental approaches, a dynamic measuring system was chosen to make this measurement. The instrument chosen, the SENSIT™[20], directly measures mechanical energy exchanges. The first-year accomplishments were calibration of the SENSIT™ instrument and demonstration that the movements of typical grass blades will elicit responses of the SENSIT™ in a linear sensitivity range.

The linear range of SENSIT™ response was found for mechanical energy inputs above 1×10^{-9} Joules to single impulse energy inputs of 1×10^{-7} Joules. Four organic filaments (three natural grass blades and one pine needle) were tested. Three of the filaments yielded data within the valid calibration range for the SENSIT™ but the fourth, a soft, pliable live grass only yielded data in the calibration range for an unusual movement. This pliable green grass is not expected to participate in resuspension, however, and the other three filaments are candidates for resuspension activity. The SENSIT™ instrument was found to be suitable for obtaining the kind of data needed for the resuspension experiment.

2.4.10 Flow Visualization and Quantitative Measurements of the Mean Flow and Turbulence Structure Around Two-Dimensional and Three-Dimensional Arrays of Buildings in a Wind Tunnel

The FMF has, under contract with the Los Alamos National Laboratory, Los Alamos, New Mexico, and the Lawrence Livermore National Laboratory, Livermore, California, performed physical modeling studies of flow and dispersion in and around an idealized urban area. The purpose of the studies was twofold: to gain insight into the fundamental physics of airflow in and around a complex urban environment and to develop a database for refinement and evaluation of numerical models of flow and dispersion in urban areas.

A series of flow visualization experiments was completed using both two-dimensional and three-dimensional building arrays (Figure 10), systematically varying the building geometry, source location and wind direction. Results were recorded with multiple video cameras and subsequently assembled into a summary video tape to facilitate analysis. Not unexpectedly, the flow visualization studies showed strong downwash effects when a smoke source was placed near the array. While flow separation from the upstream buildings in the array was clearly apparent, separation from the surfaces of the downstream buildings appeared to be retarded. When a single, high-rise building (three times the height of the surrounding buildings) was placed in the center of

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[20]SENSIT is the trademark of Sensit.

the three-dimensional building array, smoke released near the base of the high-rise building was drawn rapidly into the wake of the building. The smoke was then drawn rapidly upward along the downstream side of the building with most of the smoke appearing to escape the building wake near the top of the building. The impression was that this chimney-like effect may be very effective in ventilating urban areas characterized by buildings of relatively uniform height, separated by street canyons and interspersed with an occasional tall building.

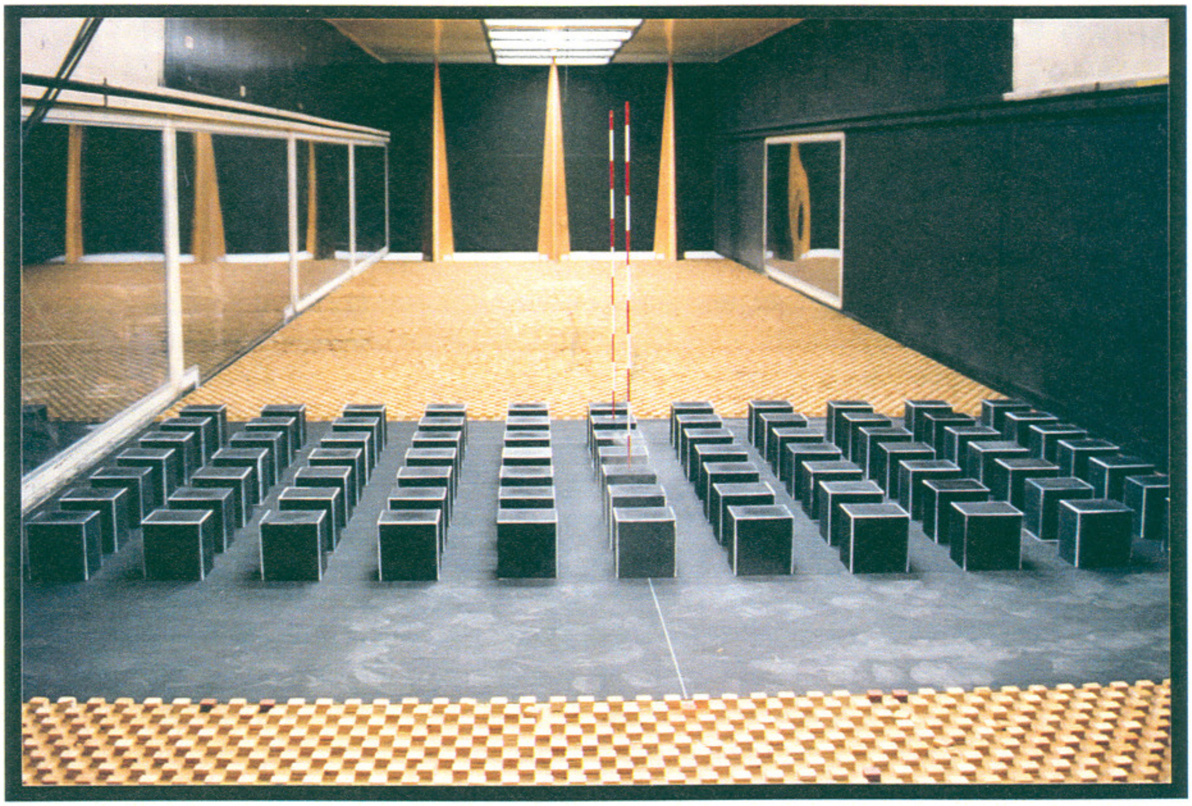

Figure 10. The three-dimensional building array as seen from the downstream end of the FMF wind tunnel.

Velocity measurements were completed along the vertical centerplane of the two-dimensional building array. A pulsed wire anemometer (PWA) was used to measure all three components of mean velocity and turbulence intensity at each of 1016 coordinate locations. The PWA uses a time-of-flight technique to unambiguously determine the flow speed and direction in areas of high turbulence intensity or flow reversal as is commonly encountered near obstacles. The PWA measurements were used to construct detailed high-resolution plots of the flow field upstream, downstream, over, and within the building array (Figure 11). The turbulence measurements were subsequently used to calculate the total kinetic energy for direct comparison with predicted the fields from numerical models. A conference paper (Brown *et al.*, accepted for publication) was prepared to summarize the measurements and present additional results and model comparisons.

In addition to velocity measurements, surface pressure measurements were obtained on the upstream face, downstream face, and top of each building in the two-dimensional array. The pressure coefficient obtained from these measurements compared favorably with measurements by Castro (1979) for a single two-dimensional obstacle, the differences indicating that the drag coefficient for the two-dimensional array was slightly higher.

2.4.11 Studies on Roughness Length for Low Roughness Densities and Several Porosities

The aerodynamic roughness height of the surface is an important parameter for a variety of surface process studies. One of its applications is the evaluation of the partition of wind force to natural obstacles (pebbles, gravels, etc.), which lie on a smoother surface and the wind force felt by the surface between the natural obstacles. A cooperative experiment between the Laboratoire Interuniversitaire des Systemes Atmospheriques (France) and the NOAA ARL (USA) had the purpose of evaluating aerodynamic roughness height, z_0 , versus the roughness density for differing forms of surface roughness.

This experiment was concerned only with low roughness densities with differing geometric placements and differing porosity of individual roughness elements. Individual roughness elements were formed from 2.55 cm-long dowel rods having diameters of 1 cm. Combinations of up to 8064 dowel rods were set into the 26.43 m^2 floor of the wind tunnel test section. Numerous tests were made for seven individual clusterings of roughness elements along with many repetitions of the reference case when no dowel rods were present. Aerodynamic roughness heights were estimated for many positions on the wind tunnel floor for each of the dowel rod clusterings by analysis of wind profiles. Turbulence intensities were also measured at the same points as wind profiles. Data from the experiment are presently being analyzed (Minvielle, 1999).

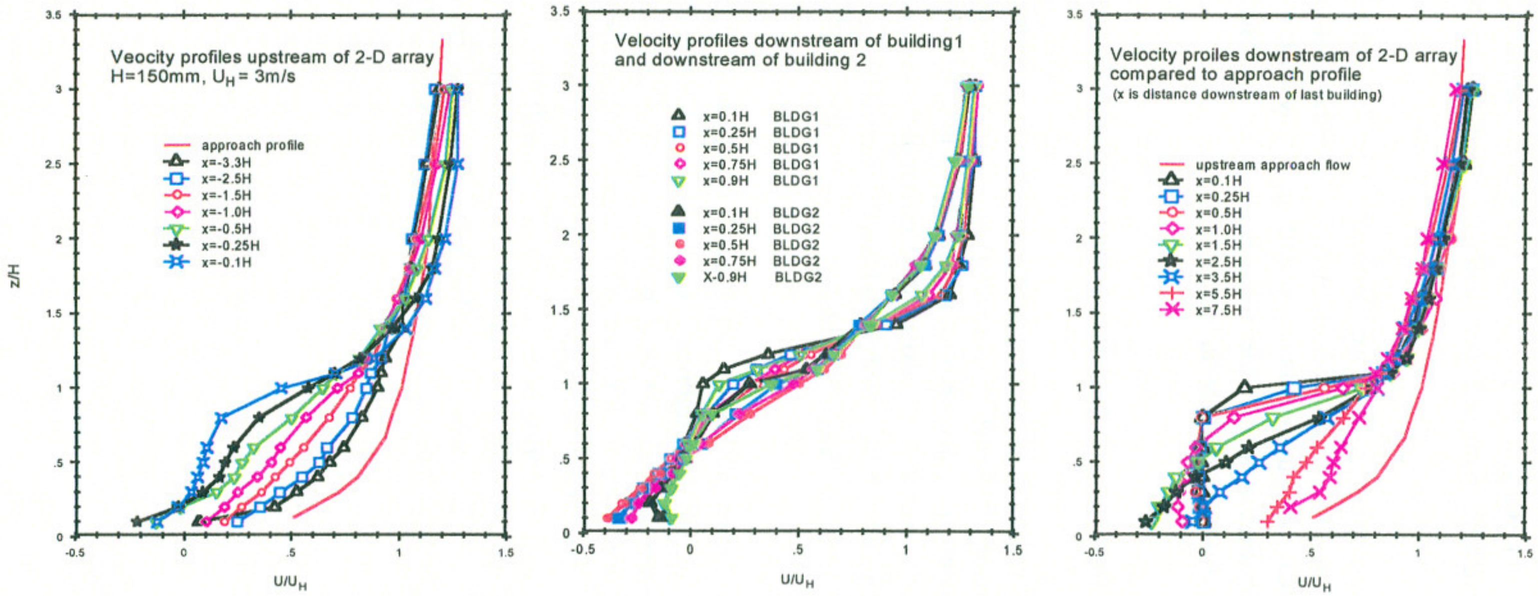

Figure11. Longitudinal component of mean velocity upstream, between and downstream of buildings in the two-dimensional array.

2.4.12 Contra Costa County, California, Environmental Monitoring for Public Access and Community Tracking

Important scientific assistance to both solve technical problems and provide analytical support for the ongoing community air toxics monitoring to the Contra Costa County California Hazardous Materials Division was initiated under the EPA Environmental Monitoring for Public Access and Community Tracking (EMPACT) program. The project is intended to enhance community air toxics monitoring, incident response, and response-planning capabilities by instrumenting a county mobile van supporting real-time measurements and modeling. This additional monitoring capability can provide refined temporal and spatial patterns of community ambient air toxic exposures both during routine days and during emergency episodes in support of the EMPACT program goals. The mobile van monitoring supplements already ongoing fixed site and fence-line monitoring in Contra Costa County. Real-time modeling is being installed on a laptop computer in the van to support the monitoring. The project includes real-time communications (cell phone voice and data) between the van and any Internet connected computer to support the potential application of information and modeling output not available from the laptop computer in the van. A GIS based on ArcView™[21] is being developed. The Army Research Laboratory's micrometeorological, High Resolution Wind model (Cionco, 1985) at a 100-m resolution is being tested to support the wind transport of air pollutants from nearby source locations downwind through neighborhoods whose air quality may be adversely impacted by such releases. The initial focus area of the project is the neighborhoods around a major petrochemical refinery, which is situated between the San Francisco Bay and large hills. Figure 12 shows an example display including the wind fields for this area.

In addition to providing support to the Contra Costa County monitoring program, this project is a pilot test for a real-time integrated geographical information system, networked communications, and networked prognostic and diagnostic modeling analyses of potential source-to-receptor relationships. The results of this proof of concept will be very helpful in targeting research priorities that could further enhance the goals of the EMPACT program as well as more general research on human exposures to urban air toxics.

2.4.13 Human Exposure Microenvironments

Computational Fluid Dynamics.

The development of microenvironmental models is ongoing to support the development of total human exposure models. Total human exposure is being separated into multi-pollutants within a sequence of microenvironments (*i.e.,* inside garage, inside automobile, outside near a roadway, inside an office) that humans sequentially experience each day. Applications using a Silicon Graphics Incorporated (SGI™) Onyx2™ with Fluent Incorporated Computational Fluid

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[21]ArcView is a registered trademark of the Environmental Systems Research Institute, Inc.

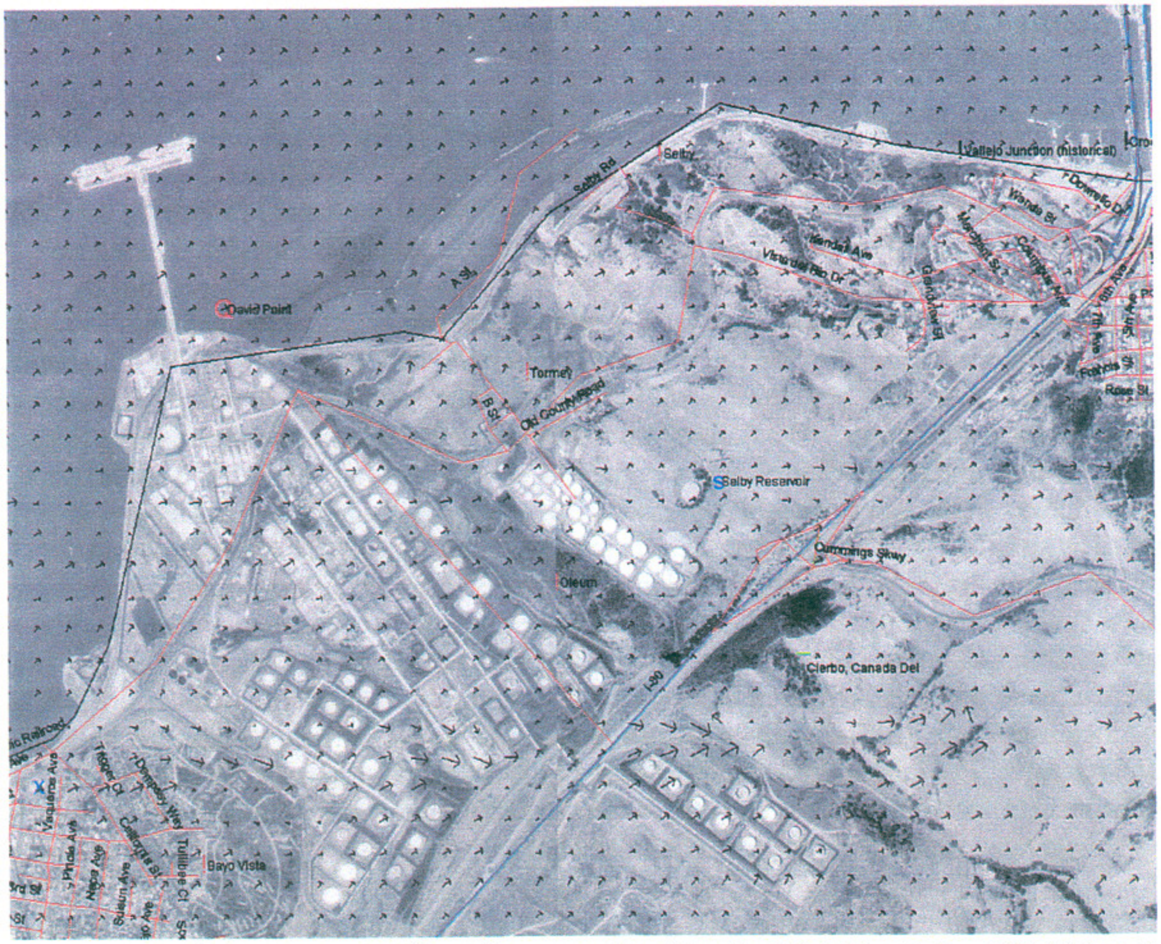

Figure 12. Wind vectors over the refinery produced by the High Resolution Wind Model with initial wind direction from SW.

Dynamics Software are being developed in support of the program. Modeling complex distributions of pollutant concentrations within each microenvironment is feasible using high performance computing. Output from high performance computing can be directly used to better understand exposure events and can lead to development of better simplified model approximations for general application. Specific projects modeling urban building complexes and the roadway microenviroment are ongoing. The studies include two vehicles moving in tandem along a roadway and a single vehicle moving in general roadway traffic. Collaborative applications with Fluent Incorporated are planned.

Mobile Source Specific Exposures.

A project to specifically improve the methodology for modeling human exposure to motor vehicle emission is ongoing. The overall project goal is to develop improved methods for modeling the source through the air pathway to human exposure in significant microenvironments of exposure.

A **micro**scale emission **fac**tor model for predicting real-world real-time motor vehicle **carbon monoxide** (MicroFacCO) emission was developed. It uses available information on the vehicle fleet composition. The algorithm used to calculate emission factors in MicroFacCO is disaggregated based on the on-road vehicle fleet. The emission factors are calculated from a real-time fleet at a specific location, rather than from a fleet-wide average estimated by vehicle-miles-traveled within a regional area as used in the EPA Mobile series of emission models. This model is being evaluated and will be incorporated into a roadway air concentration model. In collaboration with EPA scientists, roadside and in-vehicle measurements of automobile pollutants continue along major roadways in Research Triangle Park, North Carolina, to develop a database for future evaluation of the full modeling system.

Meteorological Measurements.

Meteorological measurements within the lower atmospheric boundary layer are important to initializing numerical simulation models of pollutant transport near pollutant sources within human exposure microenvironments. Meteorological instrumentation to support the measurements of the wind and turbulence in the lower boundary layer (up to 100 to 200m) was procured. The system includes a portable miniSODAR (4000MHz model) to provide a vertical profile of the wind velocity and turbulence from 15 meters up to 200 meters at 5 meter- height resolution and 10 minute averaging interval. The system will include a portable 10-meter tower instrumented for wind measurements at 2, 5, and 10 meters and temperature/humidity at 2 and 10 meters. These new instruments will complement the present midrange SODAR (2000Mhz model). Operation of these instruments is expected to begin during FY-2000. The SODAR system will be used to support the human exposure field projects as well as provide data for evaluating local scale diagnostic wind field models. Collaboration with research projects at the North Carolina State Climate Office, Raleigh, is planned.

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 simulation techniques that are used to assess, develop, or revise national, state, and local pollution control strategies for attainment and maintenance of National Ambient Air Quality Standards (NAAQS); and providing meteorological assistance and consultation to support OAQPS in developing and enforcing Federal regulations and standards and assisting the EPA Regional Offices.

2.5.1 Modeling Studies

2.5.1.1 Air Quality Assessment of Tier-2 Federal Motor Vehicle Control Program

As authorized under CAA Subsection 202(i), the EPA has proposed new regulations that will reduce the sulfur content of automotive fuels and reduce the direct emissions of nitrogen oxides (NO_x), reactive organics (ROG), and particulate matter (PM) from cars and light-duty trucks in an effort to reduce ambient concentrations of tropospheric ozone and particulates. These regulations are referred to as the Tier-2 program.

An extensive air quality modeling analysis was performed during FY-1999 to estimate the expected future benefits of Tier-2 on ozone and PM concentration. This modeling effort included the development of a nationwide inventory of emissions of ozone and PM precursor pollutants (*i.e.*, NO_x, ROG, SO_2, PM, and ammonia) for 1996. This base year inventory was projected to 2007 and 2030 to create two future baseline scenarios designed to reflect expected emissions without the Tier-2 program. The Tier-2 controls were then applied to each baseline to provide control scenarios for each future year. An analysis of the emission data indicates that control programs are expected to offset growth out to 2007 whereby emissions will decline between the base case and 2007. Beyond approximately 2013 emissions are expected to rise as growth outpaces the ability of the existing control programs to reduce emissions. By 2030 emissions are forecast to substantially exceed those in 2007. The Tier-2 regulations, which begin in 2004, will provide relatively modest additional emission reductions by 2007 with more substantial reductions by 2030 as more and more of the Tier-2 compliant cars are in use.

Air quality modeling was performed for five emission scenarios for 1996 base year, 2007 and 2030 baselines, and 2007 and 2030 Tier-2 control cases for ozone and PM. The ozone modeling included applications of UAM-V to simulate ozone concentrations across two large domains, one covering the eastern United States from the Plains States to the East Coast and the other covering the remainder lower 48 states to the West Coast. In the eastern domain, simulations were performed for 3-multi-day periods comprising 30 days in the summer of 1995. In the western domain, simulations were performed for 2 periods with a total of 27 days in July of 1996. These periods were selected because they contain episodes of high ambient ozone concentrations at levels posing a health risk to the public. The meteorological data used to drive the 1995 episode modeling were obtained from applications of the Regional Atmospheric Modeling System (RAMS), whereas the 1996 meteorological data were based on MM5. The results of the ozone modeling indicate that despite the reduction in emissions provided by control programs, unhealthy levels of ozone may still exist in some areas in 2007 and worsen in 2030, and the Tier-2 controls will provide increasing benefits from 2007 to 2030 towards lowering ozone levels. For example, Figure 13 shows a composite picture of the maximum reductions in ozone concentrations across the East that are expected to result from the Tier-2 control program in 2030. These reductions are significant relative to the NAAQS for ozone.

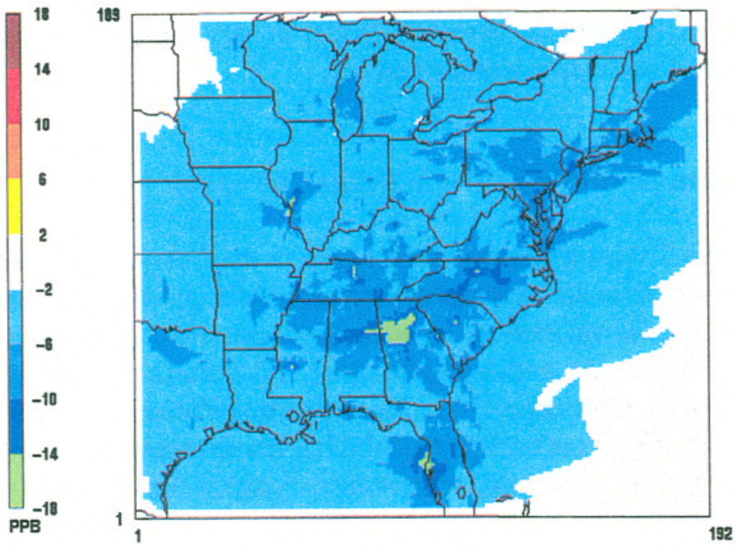

Figure 13. Impact on ozone of Tier-2 Program in 2030 — maximum reduction in peak ozone concentrations.

Simulations to estimate the impacts of Tier-2 controls on PM were obtained using the Regulatory Modeling System for Aerosols and Deposition (REMSAD). This model was applied for the 1996 base case and 2030 baseline and control scenarios for a year of meteorological data to estimate annual particulate concentrations with and without the Tier-2 program. The results of these simulations are being analyzed and interpreted to quantify the expected benefits of Tier-2. The full suite of ozone and PM modeling results will provide the air quality basis for the Regulatory Impact Analysis portion of the Tier-2 regulation, which is to be signed by the EPA Administrator by the end of 1999.

2.5.1.2 A Model for National Assessment of Air Toxics

Air toxics are those pollutants known to or suspected of causing cancer or other serious health effects. In 1990, Congress substantially strengthened the air toxics provisions in the CAA. To implement the requirements of the CAA, the Assessment System for Population Exposure Nationwide (ASPEN) (Systems Applications International, 1998) was used for the first time to provide a screening level estimate of 188 toxic air pollutant concentrations across the nation. An emissions pre-processing system was developed and is being tested for preparing the EPA's 1996 air toxics emissions inventory for use in ASPEN to get nationwide baseline ambient air concentration estimates for these toxic pollutants. Surface and upper air meteorological data from 214 National Weather Service Stations were processed for use in ASPEN.

Future activities include using ASPEN to test the myriads of EPA control strategy options and support the Government Performance Review Act goals. Other activities include such additional improvements to the scientific basis of ASPEN as improving the deposition algorithms and addressing the impact of secondary transformations.

2.5.1.3 An Assessment of Air Toxics in Urbanized Areas

The EPA Urban Air Toxics strategy is in response to the Congressional mandate in the CAA to reduce public exposure to air toxics in urban areas. In support of this effort, the Branch conducted a model study to estimate ambient air toxics concentrations in two pilot cities, Phoenix, Arizona, and Houston, Texas, of five pollutants: Benzene, 1,3 Butadiene, Formaldehyde, Polycyclic Organic Matter, and Chromium (U.S. Environmental Protection Agency, 1999a). Running the Industrial Source Complex (ISC) model (U.S. Environment Protection Agency, 1995) for such an application provided many technical challenges. A statistical technique was developed to reduce the number of receptors in the urban areas. A simplified approach was tested to estimate impact due to secondary production of formaldehyde. Results from research on pollutant half life was compiled and documented. (U.S. Environmental Protection Agency, 1999a)

Study results showed that air toxics impacts are very localized and that models should be able to estimate concentrations as close as plant fence line distances when the commensurate emissions inventory input is available. Peer reviewer comments (available from http://www.epa.gov/scram001/t29.htm#calpuff) were incorporated into the final report (U.S. Environmental Protection Agency, 1999a), which provides guidance to state and local air pollution agencies on performing air toxics model applications in urban areas.

2.5.1.4 Estimating Secondary Transformations of Hazardous Air Pollutants

Hazardous air pollutants (HAP) are found in the atmosphere as a result of primary emissions or from the transformation of organic compounds emitted into the atmosphere. Several very complex models exist that can 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. A goal of the completed study (ManTech, 1999) was to explore whether a simplified approach could provide useful estimates of total HAP concentrations. The approach taken was to estimate secondary HAP with a stand-alone model, run in a personal computing environment, that incorporated such non-dispersive processes as photochemistry. The results from this model would then be coupled to such a relatively simple dispersion model as ISC, which uses primary emissions.

2.5.1.5 Statistical Evaluation of Model Performance

Within the American Society for Testing and Materials (ASTM) a Standard Guide (Z6849Z) is being developed to provide guidance on construction of objective statistical procedures for comparing air quality simulation modeling results with tracer field data. The ASTM Guide defines a framework to describe the differences to be seen between that which is modeled and that which is observed. The observed concentrations are envisioned to be equal to an ensemble average (for the conditions specified), plus an error term due to sampling uncertainty and stochastic fluctuations (natural variability) that represents the ignorance of all the unresolved physical proceeses. The modeled concentrations are envisioned to be equal to an ensemble average (for the conditions specified), plus an error term due to uncertainty in specifying the model input and another error term due to errors in the model formulations.

It is assumed that for research field studies, every effort is made to minimize the effects of measurement uncertainty. It is assumed the average of the measurement uncertainty and unresolved variations is essentially zero. Then to perform an evaluation of modeling skill, the observations and modeling results over a series of nonoverlapping limited-ranges of the model input values are averaged. Averaging the observations provides an empirical estimate of what the model is attempting to simulate, namely, the ensemble average (for the conditions specified). Averaging the modeling results provides an empirical estimate of the modeled ensemble average, plus the average error due to input uncertainty and model formulation error. A comparison of the respective observed and modeled averages over a series of groups provides an empirical estimate of the combined deterministic error associated with input uncertainty and formulation errors.

With this framework in mind, the ASTM Guide recommends that evaluation procedures involve comparisons of separately derived averages over a series of groups. These averages can consist of any definable feature or characteristic in the concentration pattern (lateral extent, centerline concentration maximum, variance of centerline concentrations, etc.). This process is not without problems. The variance due to natural variability is of the order of magnitude of the ensemble averages (Hanna, 1993), hence small sample sizes in the groups will lead to large uncertainties in the estimates of the ensemble averages. The variance due to input uncertainty is quite large (Irwin *et al.,* 1987), hence small sample sizes in the groups will lead to large uncertainties in the estimates of the deterministic error in each group. Grouping data together for analysis requires large data sets, of which there are few. Nevertheless, this process does avoid making inappropriate comparisons in determining modeling skill.

As envisioned in the ASTM framework, it can be concluded that the modeled and observed concentrations (not averaged) have different sources of variance. A direct comparison of the two distributions, using cumulative frequency plots or Quantile-Quantile plots, assumes that the observed and modeled concentration distributions should agree, but the ASTM framework argues there is no valid reason for them to agree. The modeled distribution is a distribution of averages, whereas the observed distribution is a distribution of individual realizations. If the model has perfect input and no formulation errors, the modeled distribution would be expected to have a smaller variance than that observed; thus, the modeled distribution would have smaller maxima than observed and larger minima than observed. Therefore, unless working with one of the very few models that attempts to simulate the effects of natural variability, any agreement in the upper (or lower) percentile values of the respective cumulative frequency distribution can be attributed to happenstance, that is, the effects of model input uncertainty and model formulation errors are making up for the lack of characterization of unresolved physical processes in the modeling.

Thus far, those most involved in the development of this ASTM guide are scientists within the European community, where there is still strong interest in development of standard methods for assessing air quality modeling skill. To focus the discussion, a draft evaluation procedure was constructed that attempts to assess how well short-range dispersion models characterize the variation of the centerline maximum concentration at the surface with transport distance and stability (Irwin, 1998; Irwin and Rosu,1998). The example evaluation procedure envisions, but does not require, that if a dispersive situation were charted many times and all the observed lateral distributions superimposed along an arc on top of one another (using the observed center of mass from each trial as a common reference point), the graph might result in a bell-shaped lateral concentration profile, with the maximum average concentration at the center of mass. But the procedure makes no assumptions regarding what the actual crosswind distribution might look like.

In attempting to craft this procedure, a scheme was devised to select those values observed along a sampling arc that are so near to the centerline position that it is assumed they behave as centerline concentration values. This has stimulated an interesting debate as some of the problems reported with the procedure stem from preconceived notions that suggest concentration distributions along the arc are bell-shaped and concentration values at (or near) the centerline must not be zero. What happens in reality is that the lateral distributions are not bell-shaped but are skewed right or left; or in many instances the lateral distribution is broken into segments that are separated by zero concentration values. Hence, even though the conceptual model is readily accepted, the consequences are unexpected and sometimes unsettling to some.

Further exploration is underway of the sensitivity of the example evaluation procedure to uncertainties in grouping data, and sampling uncertainties resulting from having a limited number of samplers along an arc. These results will be presented at the *6th International Conference on Harmonization Within Atmospheric Dispersion Modeling for Regulatory Purposes*, October 11–14, 1999, at Rouen, France. A workshop is planned during this conference for participants to further discuss results and ideas.

2.5.1.6 The Krakow Urban Air Pollution Project

Local urban air pollution, including pollution from mobile sources, was recognized by the Environment for Europe Ministerial Conference as an area of high priority for the countries of the region. The EPA and Polish Ministry of Environment made this environmental problem one of six focal points for their cooperation. By focusing on the City of Krakow, Poland, this project seeks to build upon five years of cooperation between Poland and the United States in improving the air quality in the Krakow Metropolitan Area. The Krakow Urban Air Pollution project, under the sponsorship of the U.S. Agency for International Development, will assist local authorities to identify, quantify, and develop mitigation strategies for the control of air pollution in the City of Krakow, primarily from the transportation sector. It also will develop an approach for controlling urban air pollution that can be applied to other Polish cities, and with some modifications, to other cities in the region.

This project builds on the EPA Office of International Activities work in the Krakow area, which assisted in the identification, quantification, and dissemination of air pollution information in Krakow, primarily from stationary sources and low-level emitters. Over the last few years, it has become evident to Krakow, as well as to other urban and national level environmental officials, that the share of non-point and mobile sources of airborne pollution was increasing in Polish cities and will continue to rise as new roads develop and the number of private automobiles increases. The Polish government at the national level is considering alternative transportation control policies and strategies, including a program to phase out lead in gasoline over the next several years. At the heart of this project is the task of training staff in the local authorities to conduct air quality modeling studies. This would allow the local authorities to assess their air pollution problems caused by the increase in mobile source pollution, while establishing a basis for more informed national decision-making through the use of improved data, analytical tools (such as improved modeling techniques), and transportation control options.

To initiate the training on air quality modeling, the Branch was asked to develop a training course on the operation and running of a dispersion modeling system that would be suitable for use in the Krakow area. The training course was conducted in December 1998. It was envisioned that a series of training sessions would be scheduled during the following 18 months. This would allow the students to first learn the basics, and then gradually allow the training to become hands-on training in the initial application of the modeling system to characterize pollutant impacts in the Krakow area.

From an inspection of the monitoring data for Krakow, it was concluded that the pollutants of concern would be sulfur-dioxide (SO_2), carbon monoxide (CO), and particulate matter less than 10 microns in size (PM_{10}). The observed ozone concentrations were below the levels of concern, and thus were considered of secondary interest in this initial model training endeavor. From an inspection of the meteorological conditions that occur when high pollution concentrations are observed in Krakow, it was concluded that the standard plume models in common use in the United States and elsewhere would not prove to be very satisfactory for Krakow. The meteorological climatology for Krakow has too many extended period of near calm winds, and the wind fields are likely strongly influenced by the hills and mountains in the region.

Gaussian plume/line models provide good definition of which sources are responsible for the modeled impacts, and thus are the first choice for use in designing how emissions are to be managed to meet a specified reduction in pollutant impact. But the plume/line models do not provide estimates if the winds are near-calm. UAM is a photochemical grid model that estimates ozone impacts, and some have used it for large-scale city-wide estimates of CO impacts. UAM can handle near-calm stagnation conditions, but grid models do not provide clear definition of which sources are responsible for the modeled impacts. Furthermore, for impacts from primary emissions (*e.g.*, SO_2, CO and PM_{10}), grid models are very sensitive to modeling assumptions regarding the near-surface grid spacing and depths.

It was concluded that the most effective model for initial training was the CALMET/CALPUFF modeling system (Scire *et al.*, 1999a; 1999b). When first built in 1990, it was designed for modeling impacts resulting from transport and dispersion over distances beyond 30 km, and for applications with very complex wind flows (narrow twisting valleys). However, many enhancements were made including:

- CALPUFF can mimic steady-state dispersion plume modeling results for downwind distances from 1 meter to any distance downwind.

- The four source types (point, area, volume, line) were enhanced to allow diurnal or seasonal, or seasonal and diurnal, or wind speed/stability variation (scaling up and down) of the emissions. Additionally, any of these source types can have the emissions specified arbitrarily as a function of time.

- A buoyant plume rise algorithm was added to the area sources to allow treatment of forest fires.

- CALMET was enhanced to better simulate decoupling of meteorological conditions within deep valleys from the external winds aloft.

Following the initial training in December 1998, the administrative structure in Poland was reorganized, with the voivods decreasing from 49 to16. The Krakow Voivod was renamed the Malopolska Voivod, and increased in size. There are now districts within voivods, called pawiats, which are further subdivided in gminas. In the Malopolska Voivod there are 22 pawiats and 186 gminas. Some delays were experienced in the training activities, as the government sorted out which jobs belonged to the newly formed pawiats and voivods.

In March and again in July 1999, training visits were made to Krakow. In June and again in October 1999, Polish participants in the training traveled to the United States for specialized training in the CALPUFF modeling system. Tasks completed include a mobile source inventory adapted for use in CALPUFF; a point source inventory developed, tested and corrections developed for deficiencies found; and CALMET simulations tested using upper air and surface weather observations available for December 1997. The schedule calls for finalizing the 1997 and

1998 meteorology data for processing by CALMET by February 2000, and to conduct comprehensive CALPUFF modeling runs by March 2000. Results from these runs will be compared with monitoring data available from six sites in Krakow for discussion at a June 2000 workshop in Krakow.

2.5.2 Modeling Guidance

2.5.2.1 Support Center for Regulatory Air Models

During FY-1999, several noteworthy activities were accomplished by the SCRAM (Support Center for Regulatory Air Models) web site manager. An area was established entitled *7th Modeling Conference* as a repository for models, user's guides, scientific documentation, and related information being proposed as new modeling techniques for inclusion into *Appendix W* (formerly the *Guideline on Air Quality Models*). In addition, a Models-3 presence was established to provide easy access to the Division web site, which contains the latest Models-3 release. The SCRAM Forum area was enhanced to provide more control by the webmaster, particularly for the topic areas. Approximately 35 items were updated during FY-1999, including models, programs, related documentation, and guidance information.

2.5.2.2 Meteorological Monitoring Guidance for Regulatory Modeling Applications

The Branch updated the 1987 meteorological monitoring guidance document (U.S. Environmental Protection Agency, 1987; 1999b). The new document contains more comprehensive guidance on remote sensing and conventional radiosonde technologies for use in upper-air meteorological monitoring. Previously, this section provided guidance on the use of sodar technology. Another significant change is the addition of material covering data validation for upper-air meteorological measurements. These changes incorporate guidance developed during the workshop on upper-air meteorological monitoring in July 1998.

The updated document provides guidance on the collection of meteorological data for use in regulatory modeling applications. It is intended to guide the EPA Regional Offices and States in reviewing proposed meteorological monitoring plans, and as the basis for advice and direction given to applicants by the Regional Offices and States. To facilitate this process, recommendations applicable to regulatory modeling applications are summarized at the end of each section. Editorial changes were made to ensure consistency with recent changes in *Appendix W to 40 CFR Part 51* (*Guideline on Air Quality Models*, 1997). The document was restructured to provide space for the addition of guidance in support of air quality dispersion models, which incorporate boundary layer scaling techniques.

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APPENDIX A: ACRONYMS, ABBREVIATIONS, AND DEFINITIONS

ACM	Asymmetric Convective Model
AgDRIFT	Agricultural spray DRIFT model
AMV	Air Management Version of Models-3/CMAQ
AQMF	Air Quality Modeling Forum
ARL	Air Resources Laboratory
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
BASC	Board on Atmospheric Sciences and Climate (NAS/NRC)
BCON	Boundary CONditions processor
BEIS	Biogenic Emissions Inventory System
CAA	Clean Air Act of 1970
CAAA	Clean Air Act Amendments of 1990
CALMET	CALifornia METeorological model
CALPUFF	CALifornia PUFF model
CAPITA	Center for Air Pollution Impacts and Trends Analysis
CASTNet	Clean Air Status and Trends Network
CB-IV	Carbon Bond-IV
CBL	Convective Boundary Layer
CCTM	CMAQ Chemistry-Transport Model
CD-ROM	Compact Disk - Read Only Memory
CMAQ	Community Multiscale Air Quality model
CRADA	Cooperative Research and Development Agreement
CTM	Chemistry-Transport Model
CCTM	CMAQ Chemical Transport Model
ECIP	Emissions-Chemistry Interface Processor
EMEP	European Monitoring and Evaluation Program
EMPACT	Environmental Monitoring for Public Access and Community Tracking
EPA	Environmental Protection Agency
Extended RADM	RADM with full dynamics of secondary inorganic fine particle formation taken from the RPM
FAMS	Florida Atmospheric Mercury Study
FCMSSR	Federal Committee for Meteorological Services and Supporting Research
FDDA	Four-Dimensional Data Assimilation
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
HUC	Hydrologic Unit Code
HWIR	Hazardous Waste Identification Rule
ICMSSR	Interdepartmental Committee for Meteorological Services and Supporting Research
ICON	Initial CONditions processor
IDA	Inventory Data Analyzer
I/O API	Input/Output Applications Program Interface
ISC	Industrial Source Complex model
ISCST	Industrial Source Complex - Short Term model
ITM	International Technical Meeting
JPROC	Photolysis rate processor
LMMB	Lake Michigan Mass Balance project
LULC	Land Use/Land Cover
MCIP	Meteorology-Chemistry Interface Processor
MEPPS	Models-3 Emission Processing and Projection System
MicroFacCO	Microscale emission Factor model for motor vehicle carbon monoxide
MIMS	Multimedia Integrated Modeling System
MIRAGE	Megacity Impact on Regional And Global Environments
MM5	Mesoscale Model - Version 5
MM5PX	Modified MM5 for land-surface effects
Models-3	Third generation air quality modeling system
NAAQS	National Ambient Air Quality Standards
NAPAP	National Acid Precipitation Assessment Program
NARSTO	North American Research Strategy for Tropospheric Ozone
NARSTO-NE	NARSTO-NorthEast
NASA	National Aeronautics and Space Administration
NATO/CCMS	North Atlantic Treaty Organization Committee on the Challenges of Modern Society
NCAR	National Center for Atmospheric Research
NERL	National Exposure Research Laboratory
NEXRAD	NEXt generation RADar
NOAA	National Oceanic and Atmospheric Administration
NPS	National Park Service
NSF	National Science Foundation
NWS	National Weather Service
OAQPS	Office of Air Quality Planning and Standards (EPA)
OMB	Office of Management and Budget
OZIE	OZark Isoprene Experiment
PAVE	Package for Analysis and Visualization
PBL	Planetary Boundary Layer
PDM	Plume Dynamics Model

PinG	Plume-in-Grid algorithm
PDM	Plume Dynamics Model
PM	Particulate Matter
PM	Particulate Matter of size 2.5 microns or less
PM_{10}	Particulate Matter of size 10 microns or less
PWA	Pulsed Wire Anemometer
RADM	Regional Acid Deposition Model
RAMS	Regional Atmospheric Modeling System
RCRA	Resource Conservation and Recovery Act
RELMAP	REgional Lagrangian Model of Air Pollution
REMSAD	Regulatory Modeling System for Aerosols and Deposition
RFF	Resources For the Future
RGM	Reactive Gaseous Mercury
RHR	Regional Haze Rule
ROG	Reactive OrGanics
RPM	Regional Particulate Model
SASWG	Standing Air Simulation Work Group
SCIM	Sampled Chronological Input Model
SCRAM	Support Center for Regulatory Air quality Models
SGI	Silicon Graphics Incorporated computing platform
SIP	State Implementation Plan
SMOKE	Sparse Matrix Operator Kernel Emission
SODAR	Sound Detection And Ranging
SoFAMMS	South Florida Atmospheric Mercury Monitoring Study
SOS	Southern Oxidants Study
TOMS	Total Ozone Mapping Spectrometer
UAM	Urban Airshed Model
UAM-V	Urban Airshed Model - Variable grid
URMM	Urban-Regional Multiscale Model
USGS	U.S. Geological Survey
US/USSR	United States/Union of Soviet Socialist Republics
UV	Ultraviolet
UV-B	Electromagnetic radiation of wavelengths in the 280 to 315 nm range
Vis5D	Visualizing five dimensional gridded data sets
WRAP	Western Regional Air Partnership
WWW	World-Wide Web
Y2K	Year 2000

APPENDIX B: PUBLICATIONS

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Young, J. Integration of science codes into Models-3. In *Science algorithms* of the EPA Models-3 Community Multiscale Air Quality (CMAQ) modeling system. Chapter 18. D.W. Byun, and J.K.S. Ching (Eds.). EPA/600/R-99/030, National Exposure Research Laboratory, Research Triangle Park, NC, 1–25 (1999).

Young, J. Program control processing in Models-3. In *Science algorithms of the EPA Models-3 Community Multiscale Air Quality (CMAQ) modeling system.* Chapter 15. D.W. Byun, and J.K.S. Ching (Eds.). EPA/600/R-99/030, National Exposure Research Laboratory, Research Triangle Park, NC, 1–17 (1999).

APPENDIX C: PRESENTATIONS

Atkinson, D.G. Meteorological projects. Presentation via telephone to the Region 4 State/Local Modeling Workshop, Atlanta, GA, October 27, 1998.

Benjey, W.G. Processing of emission data with the Models-3 Emission Processing and Projection System (MEPPS). Presentation at the EPA Models-3 training course, Research Triangle Park, NC, January 27, 1999.

Benjey, W.G. Processing of emission data with the Models-3 Emission Processing and Projection System (MEPPS). Presentation at the EPA Models-3 training course, Research Triangle Park, NC, March 4, 1999.

Binkowski, F.S. Modeling particulate matter with the EPA Models-3 Community Multiscale Air Quality (CMAQ) modeling system. Presentation at Ford Forschungszentrum, Aachen, Germany, September 2, 1999.

Binkowski, F.S. Prediction of aerosol surface area with a modal aerosol dynamics model development in three dimensions. Presentation at the European Aerosol Conference, Prague, Czech Republic, September 8, 1999.

Bullock, O.R., Jr. Modeling assessment of transport and deposition patterns of mercury air emissions from the U.S. and Canada. Presentation at the 5th International Conference on Mercury, Rio de Janeiro, Brazil, May 26, 1999.

Bullock, O.R., Jr. Mercury modeling/measurements and their source control implications. Presentation at the Hg Source and Ambient Monitoring Workshop, Minneapolis, MN, September 13, 1999.

Bullock, O.R., Jr. Current methods and research strategies for modeling atmospheric mercury. Presentation at the Conference on Air Quality: Mercury, Trace Elements in Particulate Matter, McLean, VA, December 3, 1998.

Byun, D.W. One-atmosphere concept; MCIP/CMAQ CTM. Presentation at the EPA Models-3/CMAQ training course, Research Triangle Park, NC, January 20, 1999.

Byun, D.W. One-atmosphere concept; MCIP/CMAQ CTM. Presentation at the EPA Models-3/CMAQ training course, Research Triangle Park, NC, March 3, 1999.

Byun, D.W. CMAQ overview. Presentation at the SOS Modeling Workshop, Research Triangle Park, NC, April 7, 1999.

Byun, D.W. Models-3/CMAQ modeling system. Presentation at the Office of Economy and Environment, Headquarters, U.S. Environmental Protection Agency, Washington, DC, April 13, 1999.

Byun, D.W. Multiscale dynamics description in EPA's Models-3 Community Multiscale Air Quality (CMAQ) modeling system. Presentation at the Korea Meteorological Administration, Seoul, Korea, August 23, 1999.

Byun, D.W. EPA's next generation air quality modeling system: Models-3/CMAQ. Presentation at the Korean Society for Atmospheric Environment Workshop, Chuncheon, Korea, August 26, 1999.

Byun, D.W. Ozone forecasting methods. Presentation at the Korean Society for Atmospheric Environment Workshop, Chuncheon, Korea, August 26, 1999.

Ching, J.K.S. Modeling particulate matter using the U.S. EPA Models-3 Community Multiscale Air Quality (CMAQ) modeling system. Presentation at the Atmospheric Sciences and Applications to Air Quality Conference, Beijing, China, November 5, 1998.

Ching, J.K.S. Modeling particulate matter using the U.S. EPA Models-3 Community Multiscale Air Quality (CMAQ) modeling system. Presentation at the Chinese Academy of Science, Institute of Atmospheric Sciences, Beijing, China, November 6, 1998.

Ching, J.K.S. Regional and urban PM and air quality modeling using Models-3/CMAQ. Presentation at the Taiwan National University, Taipei, Taiwan, November 10, 1998.

Ching, J.K.S. Regional and urban PM and air quality modeling using Models-3/CMAQ. Presentation at the Taiwan Central University, Taipei, Taiwan, November 11, 1998.

Ching, J.K.S. Models-3/CMAQ and fine scale modeling of PM. Presentation at the Seminar on High Resolution Modeling of Urban Aerosols for Human Exposure Studies, Huntsville, AL, January 6, 1999.

Ching, J.K.S. Neighborhood scale and CMAQ modeling. Presentation at the Arizona State University, Phoenix, AZ, February 24, 1999.

Ching, J.K.S. Neighborhood scale and CMAQ modeling. Presentation at the Arizona Department of Environmental Quality, Phoenix, AZ, February 25, 1999.

Ching, J.K.S. Models-3/CMAQ implementation. Presentation at the WRAP Modeling Forum for Regional Haze Rules Meeting, Seattle, WA, June 17, 1999.

Ching, J.K.S. Models-3/CMAQ and neighborhood scale modeling. Presentation at the United States-Taiwan Bilateral Meeting, Baltimore, MD, July 9, 1999.

Cooter, E.J. Application of air mass analysis to atrazine transport to Lake Michigan. Presentation at the International Association of Great Lakes Research (IAGLR), Cleveland, OH, May 25, 1999.

Cooter, E.J. Development of toxics version of CMAQ. Presentation at the Third Annual GMU/DTRA Transport on Dispersion Modeling Workshop, George Mason University, Fairfax, VA, July 28, 1999.

Dennis, R.L. Modeling tools — atmospheric models. Presentation at the Atmospheric Deposition Workshop for EPA's National Estuary Program, Solomons, MD, October 20, 1998.

Dennis, R.L. Linking air and water for coastal estuaries: Getting acquainted. Presentation at the University of North Carolina at Chapel Hill Marine Sciences Seminar, Chapel Hill, NC, November 4, 1998.

Dennis, R.L. Airshed modeling for the Chesapeake Bay. Presentation at the Chesapeake Bay Modeling Workshop, St. Michaels, MD, May 19, 1999.

Dennis, R.L. Nitrogen deposition airsheds for East Coast watersheds: Development for oxidized nitrogen and preliminary estimate for reduced nitrogen. Presentation at the Atmospheric Nitrogen Compounds II: Emissions, Transport, Transformation and Assessment Workshop, Chapel Hill, NC, June 8, 1999.

Dennis, R.L. Facing prediction and multimedia modeling; Model evaluation is a science and knowledge task: Recommendations from air quality modeling. Presentation at the Workshop on Quality Assurance of Environmental Models, Seattle, WA, September 8, 1999.

Dennis, R.L. NARSTO ozone model intercomparison plans. Presentation at the U.S. - Canada Workshop on Air Quality Modelling for Particulate Matter, Toronto, Canada, September 21, 1999.

Dennis, R.L. Models-3/CMAQ aggregation and episodic selection scheme. Presentation at the U.S. - Canada Workshop on Air Quality Modelling for Particulate Matter, Toronto, Canada, September 21, 1999.

Dennis, R.L. U.S. modeling activities: RADM/RPM, Extended RADM, Models-3/CMAQ. Presentation at the U.S. - Canada Workshop on Air Quality Modelling for Particulate Matter, Toronto, Canada, September 21, 1999.

Dennis, R.L. CMAQ model evaluation plans. Presentation at the U.S. - Canada Workshop on Air Quality Modelling for Particulate Matter, Toronto, Canada, September 21, 1999.

Eder, B.K. An aggregation and episode selection scheme designed to support Models-3/CMAQ. Presentation at the PM Modeling Scientist-to-Scientist Meeting, Research Triangle Park, NC, October 29, 1998.

Eder, B.K. El Nino impacts on North Carolina. Invited Speaker for an Honors Class at North Carolina State University, Raleigh, NC, February 25, 1999.

Eder, B.K. Weather and me. Presentation at Kirk of Kildaire Preschool, Cary, NC, March 26, 1999.

Eder, B.K. Severe weather. Presentation to the second grade at Kingswood Elementary, Cary, NC, May 14, 1999.

Eder, B.K. Aggregation applications for Models-3/CMAQ. Presentation for the Office of Air Quality Planning and Standards, Research Triangle Park, NC, July 14, 1999.

Gillette, D.A. Resuspension research. Presentation at Texas Technical University, Lubbock, TX, October 29, 1998.

Gillette, D.A. The importance of mesquite bushes in desert dust emission. Presentation at the Annual Meeting of the Jornada Symposium, New Mexico State University, Las Cruces, NM, June 23, 1999.

Gillette, D.A. Dust emissions in the Arabian Peninsula. Seminar presented at the Air Resources Laboratory, Silver Spring, MD, October 15, 1999.

Godowitch, J.M. Plume-in-grid modeling in CMAQ. Presentation at the EPA Models-3/CMAQ training course, Research Triangle Park, NC, March 3, 1999.

Huber, A.H. EPA EMPACT project in Contra Costa County, CA. Presentation at the Contra Costa County Hazardous Materials Commission Meeting, Contra Costa County, CA, August 26, 1999.

LeDuc, S.K. Air pollution. Presentation to first grade at Memorial School, Paris, IL, November 13, 1998.

LeDuc, S.K. Metric measures. Demonstrations to third grade at Swift Creek Elementary School, Raleigh, NC, January 9, 1999.

LeDuc, S.K. From tutorial to new application. Presentation at the EPA Models-3/CMAQ training course, Research Triangle Park, NC, January 19, 1999.

LeDuc, S.K. Data preparation and statistics. Presentation at the EPA Models-3/CMAQ training course, Research Triangle Park, NC, January 21, 1999.

LeDuc, S.K. Finding the results. Presentation at the EPA Models-3/CMAQ training course, Research Triangle Park, NC, January 21, 1999.

LeDuc, S.K. Understanding modeling options and the steps required. Presentation at the EPA Models-3/CMAQ training course, Research Triangle Park, NC, January 21, 1999.

LeDuc, S.K. Metric measures. Demonstrations to fifth grade at Wiley Elementary School, Raleigh, NC, February 5, 1999.

LeDuc, S.K. Demonstration of visualizations of air quality information. Presentation at EPA Scientific Visualization Center to 18 minority students and 4 teachers involved in the Washington, DC, Link and Learn Environmental Challenge Program, Research Triangle Park, NC, June 7, 1999.

Novak, J.H. Evolving towards a common modeling framework. Presentation at the EPA Office of Research and Development Eco-Camp Workshop, Washington, DC, November 4, 1998.

Novak, J.H. Application needs for a supercomputer acquisition. Presentation to the EPA Comptroller, Washington, DC, December 10, 1998.

Novak, J.H. Fundamentals of modular software design. Presentation at MIMS and Subsurface Geohydrology Workshop, Atlanta, GA. February 5, 1999.

Novak, J.H. Client view of supercomputing. Presentation at the EPA Office of Information and Resources Management, Supercomputing Recognition Ceremony, Research Triangle Park, NC, February 8, 1999.

Novak, J.H. Evolution toward a common modeling framework for watershed and airshed risk management. Presentation for the EPA Science Advisory Board, Washington, DC, February 23, 1999.

Novak, J.H. Evolution toward a common problem solving environment. Multimedia Modeling Workshop, Research Triangle Park, NC, March 23, 1999.

Novak, J.H. EPA's proposed collaboratory application. Virtual Laboratories Workshop, Research Triangle Park, NC, April 15, 1999.

Novak, J.H. Multimedia Integrated Modeling System (MIMS). Presentation at the EPA/NSF/USDA Partnership for Environmental Research Water and Watersheds Program Review, Washington, DC, April 19, 1999.

Novak, J.H. Multimedia Integrated Modeling System (MIMS). Presentation at the Air Resources Laboratory Retreat, Research Triangle Park, NC, April 27, 1999.

Novak, J.H. Evolution toward a common modeling framework for watershed and airshed risk management. Presentation at the 3rd Annual RCI Federal Government Special Interest Group Executive Conference, Washington, DC, May 4, 1999.

Novak, J.H. EPA HPCC/CIC R&D program. Presentation at the HPCC/CIC Annual Spring Strategy Meeting, Washington, DC, May 10, 1999.

Novak, J.H. Evolution toward a common modeling framework for watershed and airshed risk management. Presentation for the Coordinating Alliance of Super Computer Centers, Research Triangle Park, NC, September 22, 1999.

Novak, J.H., and F.A. Schiermeier. Modeling requirements for T3E supercomputer. Briefing for the EPA Comptroller and ORD Deputy Assistant Administrator, Washington, DC, December 10, 1998.

Novak, J.H., and F.A. Schiermeier. Modeling requirements for T3E supercomputer. Briefing for the EPA Chief Financial Officer, EPA Comptroller, and ORD Deputy Assistant Administrator, Washington, DC, February 25, 1999.

Otte, T.L. Use of a mesoscale model with CMAQ. Presentation at the EPA Models-3/CMAQ training course, Research Triangle Park, NC, January 19, 1999.

Otte, T.L. Mean and normal temperatures. Presentation for sixth and eighth grades probability and statistics elective, Carnage Middle School, Raleigh, NC, February 26, 1999.

Otte, T.L. Use of a meteorological model with CMAQ. Presentation at the EPA Models-3/CMAQ training course, Research Triangle Park, NC, March 1, 1999.

Otte, T.L. Weather in the news. Presentation at the Expanding Your Horizons Workshop, North Carolina State University, Raleigh, NC, March 9, 1999.

Otte, T.L. Symmetry in weather. Presentation to the third grade at Wiley Elementary School, Raleigh, NC, March 22, 1999.

Otte, T.L. Use of MM5 with CMAQ. Presentation at the SOS Modeling Workshop, Research Triangle Park, NC, April 7, 1999.

Otte, T.L. Weather basics. Presentation to the second grade at Timber Drive Elementary, Garner, NC, May 7, 1999.

Otte, T.L. Weather basics. Presentation to a fifth grade at West Lake Elementary School, Apex, NC, September 10, 1999.

Perry, S.G. Review of spray drift task force orchard airblast field data. Presentation at the EPA Office of Pesticide Programs Workshop on Pesticide Spray Drift by Ground, Airblast, and Chemigation, Arlington, VA, December 12, 1998.

Pierce, T.E. Preliminary modeling analysis for the OZark Isoprene Experiment (OZIE). Presentation at Washington University, St. Louis, MO, November 19, 1998.

Pierce. T.E. Meteorology. Presentation to fourth grade at Green Elementary School, Raleigh, NC, September 14, 1998.

Pierce. T.E. Meteorology. Presentation to fourth grade at Green Elementary School, Raleigh, NC, October 13, 1998.

Pleim, J.E. An inferential method for estimating dry deposition velocities based on similarity with latent heat flux. Presentation at the Atmospheric Sciences and Applications to Air Quality Conference, Beijing, China, November 4, 1998.

Pleim, J.E. Air-surface exchange modeling. Presentation at the Multi-media Modeling Workshop, MCNC, Research Triangle Park, NC, March 23, 1999.

Pleim, J.E. Land-surface and dry deposition modeling in CMAQ. Presentation at the SOS Modeling Workshop, Research Triangle Park, NC, April 7, 1999.

Poole-Kober, E.M. Sharing resources through collaboration using technology. Presentation at the Atmospheric Science Librarians International Meeting, Dallas, TX, January 14, 1999.

Poole-Kober, E.M. The benefits of doing collaborative research with foreign university graduate students. Presentation to School of Information and Library Science graduate students at the University of North Carolina at Chapel Hill, Chapel Hill, NC, August 19, 1999.

Poole-Kober, E.M. Career choices: Making and changing careers. Presentation at the University of North Carolina at Chapel Hill Alumni Association, Chapel Hill, NC, November 18, 1999.

Roselle, S.J. Preparing photolysis rates for CMAQ. Presentation at the EPA Models-3/CMAQ training course, Research Triangle Park, NC, March 3, 1999.

Roselle, S.J. The photolysis rate processor and Models-3/CMAQ. Presentation at the EPA Models-3/CMAQ course, Research Triangle Park, NC, January 20, 1999.

Schere, K.L. Models-3/CMAQ and PM modeling. Presentation at the EPA PM Modeling Scientist-to-Scientist Meeting, Research Triangle Park, NC, October 28, 1998.

Schere, K.L. Models-3/CMAQ demonstration runs. Presentation to the EPA Office of Air Quality Planning and Standards, Research Triangle Park, NC, January 15, 1999.

Schere, K.L. CMAQ modeling in the northeast United States. Presentation at the Science Workshop of the Northeast Oxidant and Particle Study, Pennsylvania State University, State College, PA, April 13, 1999.

Schere, K.L. Status of Models-3/CMAQ. Presentation at the Ozone/PM/Regional Haze Modeling Workshop, Arlington, VA, June 8, 1999.

Schiermeier, F.A. Closing address regarding support of future ITMs. Presentation at the Twenty-Third NATO/CCMS International Technical Meeting on Air Pollution Modelling and Its Application, Varna, Bulgaria, October 2, 1998.

Schiermeier, F.A. Update on ORD research activities in support of Program Office needs. Presentation at the Standing Air Simulation Work Group Meeting, Snow Bird, UT, October 9, 1998.

Schiermeier, F.A. EPA FY-99 atmospheric sciences budgets and programs. Presentation to the NRC Board on Atmospheric Sciences and Climate, Washington, DC, October 13, 1998.

Schiermeier, F.A. Demonstration of Supercomputing Center and Scientific Visualization Laboratory. Presentation for the EPA/ORD Assistant Administrator, Research Triangle Park, NC, January 14, 1999.

Schiermeier, F.A. Demonstration of Supercomputing Center and Scientific Visualization Laboratory. Presentation for the EPA Deputy Administrator and ORD Assistant Administrator, Research Triangle Park, NC, February 17, 1999.

Schiermeier, F.A. Demonstration of Supercomputing Center and Scientific Visualization Laboratory. Presentation for the Legislative Aide to U.S. Representative David Price, Research Triangle Park, NC, March 1, 1999.

Schiermeier, F.A. The EPA Models-3 and Community Multiscale Air Quality Modeling System. Presentation at the International Scientific Conference on Problems of Hydrometeorology and the Environment at the Turn of the XXI Century, Main Geophysical Observatory, St. Petersburg, Russia, June 25, 1999.

Schiermeier, F.A. EPA atmospheric sciences research programs. Presentation for the Committee for Cooperative Research, Interdepartmental Committee for Meteorological Services and Supporting Research, Washington, DC, August 18, 1999.

Schiermeier, F.A. Demonstration of Supercomputing Center and Scientific Visualization Laboratory. Presentation for U.S. Representative David Price, and the EPA/ORD and EPA/OARM Assistant Administrators, Research Triangle Park, NC, September 2, 1999.

Schiermeier, F.A., K.L. Schere, and J.A. Tikvart. Current status, problems, and plans for the Models-3/CMAQ modeling system. Briefing for OAQPS Senior Management Officials, Durham, NC, March 30, 1999.

Schiermeier, F.A., K.L. Schere, and J.A. Tikvart. Current status, problems, and plans for the Models-3/CMAQ modeling system. Briefing for OAQPS Senior Management Officials, Durham, NC, June 17, 1999.

Schiermeier, F.A., K.L. Schere, and J.A. Tikvart. Current status, problems, and plans for the Models-3/CMAQ modeling system. Briefing for OAQPS Senior Management Officials, Durham, NC, September 15, 1999.

Schwede. D.B. Introduction to the metric system. Presentation at the Farmington Woods Elementary School, Cary, NC, March 16, 1999.

Streicher, J.J. Graphics applications in education. Presentation to the North Carolina Department of Health and Human Services, Raleigh, NC, March 1, 1999.

Streicher, J.J. Advances in human exposure modeling. Presentation at the Air Resources Laboratory Management Retreat, Research Triangle Park, NC, April 27, 1999.

Streicher, J.J. Acute exposure and dose modeling. Presentation at the Workshop on the Research Uses of the EPA UV Monitoring Network, Albuquerque, NM, June 6, 1999.

Streicher, J.J. Biological and economic impact of increased UV-B radiation on Loblolly pine in the mid-Atlantic states region. Presentation at the International Congress on Ecosystem Health, Sacramento, CA, August 16, 1999.

Streicher, J.J. Emerging UV technologies. Presentation at the Climate Change and Ozone Protection Conference, Washington, DC, September 29, 1999.

Streicher, J.J., R.M. Nagatani, and J.H. Shreffler. A comparison of total column ozone from EPA's Brewer Spectrophotometer Network with SBUV/2 satellite data: Applications to mid-Atlantic UV Stressor Profiles. Presentation to the Modeling and Measuring the Vulnerability of Ecosystems at Regional Scales for Use in Ecological risk Assessment and Risk Management, Seattle, WA, August 17-20, 1998.

APPENDIX D: WORKSHOPS AND MEETINGS

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

R.L. Dennis

Science Experts Workshop on Mercury, Las Vegas, NV, October 5–9, 1998.

O.R. Bullock, Jr.

Standing Air Emission Working Group, Snow Bird, Utah, October 17–19, 1998.

W.G. Benjey

Standing Air Simulation Working Group, Snow Bird, Utah, October 17–19, 1998.

F.A. Schiermeier

Southern Oxidants Study Nashville 1999 Field Campaign Planning Meeting, Nashville, TN, October 19–21, 1998.

K.L. Schere

National Research Center for Statistics and the Environment Particulate Methodology Workshop, Seattle, WA, October 19–22, 1998.

J.K.S. Ching

Atmospheric Deposition Workshop for EPA's National Estuary Programs (NEP's), Solomons, MD, October 20–21, 1998.

R.L. Dennis

PM Modeling Scientist-to-Scientist Meeting, Research Triangle Park, NC , October 29, 1998.

D.W. Byun
J.K.S. Ching
B.K. Eder
K.L. Schere

Atmospheric Sciences and Applications to Air Quality 6th International Conference, Beijing, China, November 3–5, 1998.

J.K.S. Ching
J.E. Pleim

U.S. EPA Work Assignment Manager Course, Research Triangle Park, NC, November 3–5, 1998.

T.L. Otte

EPA Office of Research and Development Eco-Camp Workshop, Washington, DC, November 4–6, 1998.

R.L. Dennis
J.H. Novak
K.L. Schere
F.A. Schiermeier

OZark Isoprene Experiment (OZIE) Workshop, St. Louis, MO, November 19–20, 1998.

T.E. Pierce

NARSTO Meeting, Pasco, WA, November 19–21, 1998.

K.L. Schere

NARSTO Reactivity Workshop, Durham, NC, December 1–2, 1998.

K.L. Schere

REVA Ecological Research Strategy Workshop, Research Triangle Park, NC, December 8–9, 1998.

J.J. Streicher

Atmospheric Science Librarians International Meeting, Dallas, TX, January 13–15, 1999.

E.M. Poole-Kober

EPA Models-3/CMAQ Training Workshop, Research Triangle Park, NC, January 19–21, 1999.

O.R. Bullock, Jr.
J.K.S. Ching
E.J. Cooter
M.L. Evangelista
A.B. Gilliland
A.H. Huber
W.T. Hutzell
T.E. Pierce
N.C. Possiel, Jr.
K.L. Schere
J.S. Touma

EPA Models-3 Emissions Training Workshop, Research Triangle Park, NC, January 27–28, 1999.

O.R. Bullock, Jr.	A.B. Gilliland	W.T. Hutzell
D.W. Byun	G.L. Gipson	T.E. Pierce
E.J. Cooter	J.M. Godowitch	J.S. Touma
M.L. Evangelista	A.H. Huber	

NARSTO Fine-Particle Science Workshop, Crystal City, Arlington, VA, January 27–29, 1999.

F.S. Binkowski
J.K.S. Ching
K.L. Schere

Subsurface Geohydrology Within A Multimedia Integrated Modeling System (MIMS) Workshop, Atlanta, GA, February 5–6, 1999.

J.H. Novak

PM Supersite Planning Meeting, Georgia Institute of Technology, Atlanta, GA, February 8–10, 1999.

J.K.S. Ching

HWIR Module Developers Meeting, Research Triangle Park, NC, February 22–26, 1999.

D.B. Schwede

National Park Service Workshop on Shenandoah Assessment, Reston, VA, February 24–25, 1999.

R.L. Dennis

EPA Models-3/CMAQ and Emissions Training Workshop, Research Triangle Park, NC, March 1–5, 1999.

D.A. Atkinson	E.J. Cooter	T.L. Otte
W.G. Benjey	J.M. Godowitch	T.E. Pierce
O.R. Bullock, Jr.	A.H. Huber	K.L. Schere
J.K.S. Ching	S.K. LeDuc	

HWIR Module Developers Meeting, Research Triangle Park, NC, March 8–10, 1999.

D.B. Schwede

Expanding Your Horizons Workshop, North Carolina State University, Raleigh, NC, March 9, 1999.

T.L. Otte

Virtual Laboratories Workshop, Research Triangle Park, NC, March 10, 1999.

J.H. Novak

EPA-EOHSI-LBL Cooporative Partners Meeting on Particulate Matter Research Collaboration, Research Triangle Park, NC, March 16–17, 1999.

J.J. Streicher

Multimedia Modeling Workshop, Research Triangle Park, NC, March 23–24, 1999.

W.G. Benjey
T.A. Davis
R.L. Dennis
A.B Gilliland
S.C. Howard
S.K. LeDuc
J.H. Novak
T.L. Otte
T.E. Pierce
J.E. Pleim
F.A. Schiermeier
D.B. Schwede
J.O. Young

Water Resources Research Institute Research Conference, Raleigh, NC, March 25, 1999.

R.L. Dennis

NERL ERD-Athens Ecological Integration Modeling Workshop, Athens, GA, March 29–April 1, 1999.

J.H. Novak

Southern Oxidants Study (SOS) Modeling Workshop, Research Triangle Park, NC, April 7–8, 1999.

D.W. Byun
R.L. Dennis
J.M. Godowitch
T.L. Otte
T.E. Pierce
J.E. Pleim
K.L. Schere

Science Workshop of the Northeast Oxidant and Particle Study, Pennsylvania State University, State College, PA, April 12-14, 1999.

K.L. Schere

NOAA Library Conference and Workshop, Silver Spring, MD, April 12–14, 1999.

E.M. Poole-Kober

Virtual Laboratories Workshop, Research Triangle Park, NC, April 15, 1999.

J.H. Novak

EPA STAR Waters and Watershed Meeting, Washington, DC, April 19–21, 1999.

R.L. Dennis
J.H. Novak

Annual ASTM Committee Meetings, Seattle, WA, April 19-22, 1999.

J. S. Irwin

TTN Web Managers Meeting, Research Triangle Park, NC, April 20, 1999.

D.G. Atkinson

Modeling Software Architecture Workshop, Research Triangle Park, NC, April 21–23, 1999.

A.B Gilliland
J.H. Novak

Joint Research Planning Meeting (for Exposure Modeling), Research Triangle Park, NC, April 27–28, 1999.

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

NOAA/ARL Laboratory Retreat for Management Personnel, Research Triangle Park, NC, April 27–28, 1999.

M.L. Evangelista
R.E. Lawson, Jr.
J.H. Novak
W.B. Petersen
K.L. Schere
F.A. Schiermeier
R.S. Thompson

Hyperspectral Imagery and Water Quality Management Workshop, Raleigh, NC, April 29, 1999.

R.L. Dennis
A.B Gilliland
J.H Novak

Western Regional Air Partnership (WRAP), Modeling Town Meeting, Albuquerque, NM, May 5–7, 1999.

J.K.S. Ching

Toxics Deposition Workshop, Chicago, IL, May 6–7, 1999.

O.R. Bullock, Jr.

Standing Air Emission Working Group, Tempe, Arizona, May 14–16, 1999.

W.G. Benjey

Standing Air Simulation Working Group, Tempe, Arizona, May 14–16, 1999.

F.A. Schiermeier

Chesapeake Bay Monitoring Strategy Workshop, Annapolis, MD, May 17, 1999.

R.L. Dennis

Advanced Monitoring Initiative Workshop, Langley, VA, May 17–18, 1999.

J.K.S. Ching

NOAA Weather Research Workshop: Challenges facing NOAA weather research and services as we enter a new century, Silver Spring, Maryland, May 18–19, 1999.

B.K. Eder

Chesapeake Bay Modeling Workshop: Higher Trophic Level Modeling, Annapolis, MD, May 18–20, 1999.

R.L. Dennis

SMOKE Workshop, Research Triangle Park, NC, May 20, 1999.

W.G Benjey	J.H. Novak
D.W Byun	J.O. Young

Fifth International Conference on Mercury, Rio de Janeiro, Brazil, May 23–29, 1999.

O.R. Bullock, Jr.

Tropospheric Aerosol Program Workshop, Brookhaven National Laboratory, Upton, NY, June 1–4, 1999.

F.S. Binkowski

Workshop on the Research Uses of the EPA UV Monitoring Network, Albuquerque, NM, June 6–7, 1999.

J.J. Streicher

Third Colloquium on Particulate Air Pollution and Human Health, Durham, NC, June 6–8, 1999.

J.K.S. Ching

Workshop on Atmospheric Nitrogen Compounds II: Emissions, Transport, Transformation, Deposition, and Assessment, Chapel Hill, NC, June 7–9, 1999.

D.W. Byun	T.E. Pierce
E.J. Cooter	J.E. Pleim
R.L. Dennis	D.B. Schwede
P.L. Finkelstein	

Particulate Matter/Regional Haze/Ozone Modeling Workshop, Arlington, VA, June 7–10, 1999.

S.J. Roselle
K.L. Schere

Soil Properties Influencing the Emission of Dust by Wind: Workshop on Mineral Dust, Boulder, CO, June 9–11, 1999.

D.A. Gillette

Gordon Research Conference, Newport, RI, June 11–18, 1999.

F.S. Binkowski

Western Governor's Air Partnership (WRAP) Modeling Forum Meetings, Seattle, WA, June 15–18, 1999.

J.K.S. Ching

Three-Dimensional Variational Assimilation Short Course, Ninth MM5 User's Workshop, and Land-Surface Modeling Workshop, Boulder, CO, June 22–25, 1999.

T.L. Otte

Jornada Symposium: The Importance of Mesquite Bushes in Desert Dust Emissions, New Mexico State University, Las Cruces, NM, June 24, 1999.

D.A. Gillette

Object Technology for Scientific Computing Workshop, Research Triangle Park, NC, July 12–16, 1999.

W.G Benjey
D.W. Byun
A.B. Gilliland
S.C. Howard
S.K. LeDuc
J.H. Novak
T.L. Otte
T.E. Pierce
S.J. Roselle
D.B. Schwede
A.R. Torian
G.L. Walter
J.O. Young

Chesapeake Bay Modeling Workshop: Watershed Modeling, St. Michaels, MD, July 13–15, 1999.

R.L. Dennis

National Climatic Data Center Meeting, Asheville, NC, July 23, 1999.

D.G. Atkinson

Air Pollution 99 Conference, San Francisco, CA, July 26–30, 1999.

D.W. Byun

Third Annual GMU/DTRA Transport on Dispersion Modeling Workshop, George Mason University, Fairfax, VA, July 28, 1999.

E.J. Cooter

Western Regional Air Partnership (WRAP) Modeling Forum Meeting, Albuquerque, NM, August 3–5, 1999.

J.K.S. Ching

Korean Society for Atmospheric Environment Workshop, Seoul, Korea, August 20–30, 1999.

D.W. Byun

Quality Assurance of Environmental Models Workshop, Seattle, WA, September 7–10, 1999.

J.R. Arnold
R.L. Dennis
B.K. Eder

HWIR Steering Committee Meeting, Athens, GA, September 9–11, 1999.

D.B. Schwede

Hg Source/Ambient Monitoring Workshop, Minneapolis, MN, September 13–15, 1999.

O.R. Bullock, Jr.

Planning Meeting for the U.S. DOE Vertical Transport and Mixing (VTMx) Program, Salt Lake City, UT, September 14–16, 1999.

D.W. Byun

TTN Web Managers Meeting, Research Triangle Park, NC, September 21, 1999.

D.G. Atkinson

U.S. - Canada Workshop on Air Quality Modelling for Particulate Matter, Toronto, Canada, September 21–22, 1999.

R.L. Dennis

Ecological Society of America Workshop on Where Air and Water Meet: the Role of Atmospheric Deposition in the Gulf of Mexico, New Orleans, LA, September 26, 1999.

R.L. Dennis

APPENDIX E: VISITING SCIENTISTS

1. Dr. Julius Chang
   Atmospheric Science Research Center
   State University of New York
   Albany, NY

Dr. Julius Chang visited the Division on December 7, 1998, and presented a seminar on fast and efficient numerical solvers for gas-phase chemistry in air quality models.

2. Dr. Jonathan Fink
   Vice President for Research
   Arizona State University
   Tempe, AZ

Dr. Fink visited the Division on November 18, 1998, to discuss urban research and modeling.

3. Jack Fishman
   NASA Langley Research Center
   Hampton, VA

Mr. Fishman visited the Division on October 28, 1998, for a meeting to discuss the joint modeling and observational study of tropospheric ozone.

4. Prof. Evgueni Genikhovich
   Main Geophysical Observatory
   St. Petersburg, Russia

In his role as Working Group Co-Chairman, Prof. Genikhovich visited the Division from March 7 to 13, 1999, to conduct an Annual Meeting of the United States/Russia Working Group 02.01-10 on Air Pollution Modeling, Instrumentation, and Measurement Methodology.

5. Dr. Hiroshi Kanzawa
   Head, Atmospheric Physics Section
   National Institute of Environmental Sciences
   Tsukuba, Japan

Dr. Kanzawa visited the Division on March 4, 1999, and presented a seminar discussing on-going research projects at the National Institute of Environmental Sciences.

6. Mr. Nobuhiro Kino
Air Quality Bureau
Japan Environment Agency
Tokyo, Japan

Mr. Kino visited the Division on March 16, 1999, and had discussions on air quality modeling and the implementation of new U.S. ozone and fine particle standards.

7. Dr. Richard T. McNider
University of Alabama-Huntsville
Huntsville, AL

Dr. McNider visited the Division on March 10, 1999, to discuss using satellite data in specifying cloud fields for computing photolysis rates.

8. Dr. Beatrice Marticorena
LISA University of Paris 12
Paris, France

Dr. Marticorena visited the FMF from March 16 to 22, 1999, in a joint project relating aerodynamic roughness length to physical roughness geometry.

9. Miss Fanny Minvielle
LISA University of Paris 12
Paris, France

Miss Minvielle visited the FMF from March 16 to May 15, 1999, in a joint project relating aerodynamic roughness length to physical roughness geometry.

10. Dr. R.S. Patil
Indian Institute of Technology
Bombay, India

Dr. Patil visited the Division on June 16, 1999, to discuss numerical dispersion models.

11. Drs. Sara C. Pryor, and Rebecca Barthelmie
Indiana University
Bloomington, IN

Drs. Pryor and Barthelmie visited the Division on May 3 and 4, 1999, and presented seminars on *Modeling Aerosol from Biogenic Secondary Organic Species* and *Dry Deposition of Nitrogen Species in a Coastal Environment*.

12. Dr. D. Graeme Ross
Monash University
Caulfield, Australia

Dr. Ross visited the Division on February 18, 1999, for discussions on windfield modeling and air quality modeling.

13. Dr. Elena Rusina
Arctic Institute and Main Geophysical Observatory
St. Petersburg, Russia

Dr. Rusina visited the Division from March 7 to13, 1999, to discuss possible United States/Russia cooperation concerning measurements of solar radiation, including UV measurements and aerosol optical depths, at the Global Atmospheric Watch (GAW) stations in Russia.

14. Dr. Seiji Sugata
Takezono 1-803-506
Tsukuba, Ibaraki, 305-0032
Japan

Dr. Seiji Sugata worked at the Division from October 1, 1998 to October 1, 1999, on developing RAMS interface to Models-3/CMAQ.

15. Prof. Itsushi Uno
Kyushu University
Tsukuba, Japan

Dr. Uno visited the Division to discuss RAMS/CMAQ linkage from June 19 to 23, 1999.

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

Dr. Kondragunta worked with the Division from January 1998 through June 1999 as a postdoc. Her research concentrated on linking aerosol predictions and photolysis rate calculations within CMAQ. She visited on December 10, 1998. and made a presentation on *Predicting Aerosol Optical Properties for Multimodal Size Distributions Using Neural Networks*.

3. Dr. Qinyuan Song
   Atmospheric Environment Service
   Ontario, Canada

Dr. Song worked with the Division during FY-1999. His research focused on development of a grid-resolved cloud model for CMAQ. He visited the Division from May 25 to 26, 1999, and gave a seminar on the resolved cloud model. He visited again from August 26 to September 10, 1999, to work with the Division on integrating the resolved cloud model into CMAQ.

4. 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 those designated EPA, who are employees of the Environmental Protection Agency; PHS, who are members of the Public Health Service Commissioned Corps.; or SEEP, who are part of the Senior Environmental Employment Program.

Office of the Director

Francis A. Schiermeier, Supervisory Meteorologist, Director
Herbert J. Viebrock, Meteorologist, Assistant to the Director
Dr. Robin L. Dennis, Physical Scientist
Dr. Basil Dimitriades (EPA), Physical Scientist
Dr. Peter L. Finkelstein, Physical Scientist
Bruce W. Gay, Jr. (EPA), Program Manager
Evelyn M. Poole-Kober, Librarian
Jarrett Barber (EPA), Physical Science Technician (Summer)
Barbara R. Hinton (EPA), Secretary
B. Ann Warnick, Secretary (Until June 1999)

Atmospheric Model Development Branch

Kenneth L. Schere, Supervisory Meteorologist, Chief
Dr. Francis S. Binkowski, Meteorologist
O. Russell Bullock, Jr., Meteorologist
Dr. Daewon W. Byun, Physical Scientist
Dr. Jason K.S. Ching, Meteorologist
Dr. Brian K. Eder, Meteorologist
Gerald L. Gipson (EPA), Physical Scientist
James M. Godowitch, Meteorologist
Dr. William T. Hutzell (EPA), Physical Scientist
Dr. Michelle R. Mebust (EPA), Physical Scientist (Since August 1999)
Tanya L. Otte, Meteorologist
Dr. Jonathan E. Pleim, Physical Scientist
Shawn J. Roselle, Meteorologist
Thomas Szymkiewicz (EPA), Physical Science Technician (Summer)
Tanya L. McDuffie, Secretary

Modeling Systems Analysis Branch

Joan H. Novak, Supervisory Computer Specialist, Chief
Dr. William G. Benjey, Physical Scientist
Dr. Alice B. Gilliland, Physical Science Administrator (Since March 1999)
Steven C. Howard, Computer Specialist
Dr. Sharon K. LeDuc, Physical Scientist
Thomas E. Pierce, Meteorologist
John H. Rudisill, III, Equipment Specialist
Alfreida R. Torian, Computer Specialist
Gary L. Walter, Computer Scientist
Dr. Jeffrey O. Young, Mathematician
Carol C. Paramore, Secretary

Applied Modeling Research Branch

William B. Petersen, Supervisory Physical Scientist, Chief
Dr. Ellen J. Cooter, Meteorologist
Dr. Dale A. Gillette, Physical Scientist
Dr. Alan H. Huber, Physical Scientist
Robert E. Lawson, Jr., Physical Scientist
Dr. Steven G. Perry, Meteorologist
Donna B. Schwede, Physical Scientist
John J. Streicher, Physical Scientist
CDR. Roger S. Thompson (PHS), Environmental Engineer
Lawrence E. Truppi, Meteorologist
Jonathan Petters (EPA), Engineering Technician (Summer)
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 (Since June 1999)
John S. Irwin, Meteorologist
Brian L. Orndorff, Meteorologist
Norman C. Possiel, Jr., Meteorologist
Jawad S. Touma, Meteorologist

FY 1999 AWARDS

Exceptional Support to EPA/ORD for Outstanding Leadership of NOAA Division
Francis A. Schiermeier

NOAA Administrator's Award for Division Leadership
Francis A. Schiermeier

NOAA Air Resources Laboratory Paper-of-the-Year Award
Peter L. Finkelstein

NOAA Air Resources Laboratory Accomplishment-of-the-Year Award
Steven G. Perry

EPA Scientific Achievement Award for Chesapeake Bay Nutrient Modeling
Robin L. Dennis

EPA James W. Akerman Award for Pesticides Spray Drift Modeling
Steven G. Perry

EPA/OSW Team Excellence Awards for Multimedia Risk Assessment Methodologies
Sharon K. LeDuc
Donna b. Schwede

EPA/OSWER Team Excellence Awards for Hazardous Waste Risk Assessment
Sharon K. LeDuc
Donna B. Schwede

U.S. Environmental Protection Agency Gold Medal for Model Applications for the NO_x *SIP Call Rulemaking*
Norman C. Possiel, Jr.

U.S. Environmental Protection Agency Silver Medal for Mercury Study Team for Congressional Mercury Report
O. Russell Bullock, Jr.

U.S. Environmental Protection Agency Silver Medals for Development and Evaluation of Models-3/CMAQ
Daewon Byun
Joan H. Novak
Jeffrey O. Young

U.S. Environmental Protection Agency Bronze Medal for Fluid Modeling Simulation of WTI Waste Incinerator

William H. Snyder

U.S. Environmental Protection Agency Bronze Medal for Development and Evaluation of Models-3/CMAQ

William H. Benjey	Brian K. Eder	Sharon K. LeDuc	Shawn J. Roselle
Frank S. Binkowski	Gerald L. Gipson	Tanya S. Otte	Kenneth L. Schere
Jason K.S. Ching	James G. Godowitch	Thomas E. Pierce	Alfreida R. Torian
Robin L. Dennis	Steven C. Howard	Jonathan E. Pleim	Gary L. Walter