AA Technical Memorandum OAR ARL-249

FISCAL YEAR 2002 SUMMARY REPORT OF THE NOAA ATMOSPHERIC SCIENCES MODELING DIVISION TO THE U.S. ENVIRONMENTAL PROTECTION AGENCY

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Air Resources Laboratory
Silver Spring, Maryland
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Research Triangle Park, North Carolina

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PREFACE

This report summarizes the Fiscal year 2002 research and operational activities of the Atmospheric Sciences Modeling Division (ASMD), Air Resources Laboratory, National Oceanic and Atmospheric Administration (NOAA), working under Interagency Agreements EPA DW13938483 and DW13948634 between the U.S. Environmental Protection Agency (EPA) and U.S. Department of Commerce. The summary includes descriptions of research and operational efforts in air pollution meteorology, meteorology and air quality model development and evaluation, and air pollution abatement and compliance programs.

Established in 1955, the Division serves as the vehicle for implementing the agreements with EPA, which funds the research efforts. ASMD conducts research activities in-house and through contract and cooperative agreements for the EPA National Exposure Research Laboratory and other EPA groups. With a staff consisting of NOAA and EPA employees, ASMD also provides technical information, observational and forecasting support, and consulting on all meteorological aspects of the air pollution control program to many EPA offices, including the Office of Air Quality Planning and Standards. ASMD is organized into three research Branches - Atmospheric Model Development Branch, Modeling Evaluation and Applications Research Branch, and Air-Surface Processes Modeling Branch, and an operational Branch - Air Policy Support Branch. The report is organized by major program themes reflecting the ASMD strategic plan.

Any inquiry on the research or support activities outlined in this report should be sent to the Director, Atmospheric Sciences Modeling Division, MD-E243-02, U.S. Environmental Protection Agency, 109 T.W. Alexander Drive, Research Triangle Park, NC 27711.

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ABSTRACT. During Fiscal Year 2002, the Atmospheric Sciences Modeling Division provided meteorological and air quality modeling assistance to the U.S. Environmental Protection Agency. This ranged from research studies and model applications to the provision of advice and guidance. Research efforts emphasized the development and application of meteorological and air quality simulation models. Among the research studies and results were the release of the latest version of the Community Multiscale Air Quality (CMAQ) modeling system in June 2002, continued development and improvement of CMAQ and its modules, wind tunnel modeling of the World Trade Center disaster site, estimation and characterization of the dispersion of particulate matter from the World Trade Center recovery site after September 11, 2001, study of the requirements for air quality modeling at fine or neighborhood scales, and initial work on an air quality forecasting system using the Eta model.

1. INTRODUCTION

In Fiscal Year (FY) 2002, the Atmospheric Sciences Modeling Division (ASMD) continued its commitment to providing goal-oriented, high quality research and development, and operational support to the U.S. Environmental Protection Agency (EPA). Using an interdisciplinary approach emphasizing integration and close cooperation with EPA and public and private research communities, the Division's primary efforts focused on studying processes affecting the dispersion of atmospheric pollutants through numerical modeling as well as physical modeling; and developing and evaluating meteorological and air quality models on all temporal and spatial scales. The research products developed by the Division are transferred to the public and private national and international user communities.

Division research is focused on five areas: new developments in air quality modeling; global climate change and its impact on regional air quality; multimedia modeling; data management and analysis; and air quality forecasting. The Division was reorganized to prepare it to respond effectively to these new research directions as more fully described in the following sections. A new version of the Community Multiscale Air Quality (CMAQ) modeling system, incorporating the latest advances in state-of-science in modeling ozone, fine particles, visibility, and other pollutants was released in June 2002. Research was initiated to develop and apply statistical techniques for evaluating air quality model performance in reproducing the spatial and temporal features embedded in the observational data. In collaboration with the NOAA National Weather Service and Office of Oceanic and Atmospheric Research, work was begun to link CMAQ with the NOAA operational meteorological model, Eta. To improve the simulation of the transport and fate of airborne agents in the near-field, a scale model of Lower Manhattan was designed for use in the wind tunnel to study the impact of pollutants released from ground zero. These studies will help improve the predictions using computational fluid dynamics models and mesoscale models to quantify the adverse impacts from the collapse of the World Trade Center.

2. PROGRAM REVIEW

2.1 Atmospheric Model Development

This research is aimed at providing state-of-science air quality models and guidance for their use in the implementation of National Ambient Air Quality Standards (NAAQS) for ozone and fine particulate matter ($PM_{2.5}$). The principal effort is to develop and improve the Models-3/Community Multiscale Air Quality (CMAQ) modeling system, a multiscale and multi-pollutant chemistry-transport model (CTM). Specific research components include: meteorological modeling, land-surface and planetary boundary layer (PBL) modeling, emissions modeling, gas-phase chemical mechanisms and solvers, aerosol representations in grid-based air quality models, plume-in-grid treatment for large elevated sources of pollution, CMAQ code integration and efficiencies, and air quality forecasting.

The objectives of this research program are to continuously develop and improve the mesoscale (regional through urban scale) air quality simulation models, including CMAQ, as air quality management and NAAQS implementation tools. The CMAQ CTM includes the necessary critical science process modules for handling atmospheric transport, deposition, cloud mixing, emissions, gas- and aqueous-phase chemical transformation processes, and aerosol dynamics and atmospheric chemistry. Research is conducted to develop and test appropriate chemical and physical mechanisms, improve the accuracy of emissions and dry deposition algorithms, and to develop and advance state-of-science meteorology models and contributing process parameterizations.

By design, CMAQ is expected to be used by both scientists and policy makers for assessment activities, research module developments, and detailed model evaluation studies. Scientists can thus incorporate additional air quality science process modules into the system. A generalized coordinate approach used in CMAQ allows the CMAQ CTM to be configured dynamically consistent with the driver meteorology model. Tested model configurations can be established for use by the policy community to develop and analyze implementation strategies for air quality management. CMAQ supports the vision of "one atmosphere" approach to air quality modeling. It is capable of concurrently simulating gridded fields of oxidants, fine particles, visibility degradation, and acidic and nutrient deposition and loadings to ecosystems at urban and regional scales. As our understanding of atmospheric processes, input data, and model formulations and parameterizations improve, it will be essential to continue to upgrade or provide science options for future releases of CMAQ. Therefore, activities that facilitate the maintenance and science process evolution within CMAQ will be required. The work described below includes additional model development and testing leading to the June 2002 release of the CMAQ modeling system.

2.1.1 Meteorological Modeling for CMAQ Applications

The Fifth-Generation Pennsylvania State University (PSU)/National Center for Atmospheric Research (NCAR) Mesoscale Model (MM5) is the primary tool for providing meteorological input for Models-3/CMAQ. MM5 is widely used to generate meteorological characterizations of the atmosphere throughout the air-quality modeling community. For Models-3/CMAQ, MM5 is applied to several case studies (both episodic and seasonal) at a variety of spatial scales using a series of one-way nested domains. MM5 is run retrospectively using four-dimensional data assimilation (FDDA) for a dynamic analysis of the simulation period. The output represents a dynamically-consistent multiscale meteorology simulation for various horizontal grid spacings ranging from continental to urban scales. The MM5 output is ultimately used in the SMOKE (emissions) and CMAQ (chemistry) modules to describe the atmospheric state variables and the planetary boundary layer characteristics.

Several projects were underway during FY-2002 using MM5 to support Models-3/CMAQ applications. MM5 Version 3 Release 5 (MM5v3.5) was made available to the modeling community by NCAR in December 2001. MM5v3.5 featured scientific revisions to the Pleim-Xiu land-surface model (Xiu and Pleim, 2001), as well as updated land-use and soil databases, all of which are of particular interest for air-quality modeling. During FY-2002, MM5v3.5 was tailored for air quality applications with minor modifications to the science algorithms and parameters, and it was used in various research projects.

During FY-2002, MM5 was used to drive CMAQ for a 10-week summer modeling period based on the photochemical field studies from the Southern Oxidants Study (SOS) in Nashville and Atlanta during the summer of 1999. Meteorological and chemical observations were made in Nashville during June and July 1999, and chemical observations were made in Atlanta during August 1999. The modeling of SOS 1999 consisted of a common domain with 32-km horizontal grid spacing and separate 8-km and 2-km domains over each of the focal cities. Preliminary results from the Nashville study have been summarized by Pleim *et al.* (2002).

In addition, modeling domains were established for simulating the periods observed during the 2000 Texas Air Quality Study of Houston (TexAQS 2000) and the 2002 Bay Regional Atmospheric Chemistry Experiment (BRACE) of Tampa , Florida. Tentatively, these modeling projects will use the same 32-km grid spacing that was used for the SOS 1999 studies and 8-km and 2-km domains over the focal cities. Some of the plans for the TexAQS 2000 application have been discussed by Ching *et al.* (2002). In-house modeling for TexAQS 2000 and BRACE is expected to commence in FY-2003.

Also in FY-2002, development continued on the implementation of alternate land-use databases in MM5v3. The alternate land-use databases theoretically will add value to the meteorology simulations through use of higher-resolution base data (on the order of meters rather than kilometers) and through more detailed categorization. Specifically, the Biogenic Emissions Land cover Database version 3 (BELD-3) has been selected for implementation in MM5 to facilitate linkage between the meteorology and emissions components of CMAQ. It is anticipated that these new databases will also be of particular benefit for the neighborhood-scale modeling activities.

Finally, preliminary plans for a transition from MM5 to the Weather Research and Forecast Model (WRF) were discussed. WRF is expected to be the next-generation meteorology model that will include many of the features currently in MM5. WRF is a developmental community model, and it is available to the modeling community for testing. WRF is attractive for air-quality modeling applications because it contains mass-conserving equations, whereas MM5 does not. The primary drawback of WRF is that there are no plans to develop MM5's FDDA system for WRF, and the FDDA would be a requirement for in-house WRF applications. WRF's developers have recognized the need for FDDA as an unfunded requirement. As a result, the ASMD transition to WRF has been tentatively postponed until late FY-2003, at the earliest.

2.1.2 Linking Meteorology and Chemistry Models

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

In FY-2002, the upgraded software program, MCIP Version 2 (MCIP2), was released to 30 beta testers in the CMAQ community representing federal and state regulatory agencies, industry, and academia. The beta-testing exercise enabled the creation of more test cases to build a more robust MCIP2, allowed users to become familiar with the new code structure, provided a vehicle for user feedback, and infused the new science into the user base. Three beta releases of MCIP2 were made in early FY-2002. The MCIP2 code was released to the community in March 2002, three months ahead of the remainder of the CMAQ system.

2.1.3 Land Surface and Planetary Boundary Layer Modeling

Realistic simulation of land surface and planetary boundary layer (PBL) processes are critically important for both meteorology and air quality modeling. Interactions between surface characterization, surface fluxes, and PBL processes are very tightly coupled. In addition, surface fluxes and PBL mixing of chemical constituents closely follow the meteorological processes. Hence, work involves both the meteorology and chemical transport models to develop realistic and consistent modeling of surface and PBL processes.

The bulk of this effort years has focused on the development, testing, and implementation of the Pleim Xiu land surface model (PX LSM) (Xiu and Pleim, 2001) in the MM5 and the M3dry dry deposition model in CMAQ. The M3dry scheme is linked to the PX LSM by use of the canopy (bulk stomatal) resistance and aerodynamic resistance directly from the PX LSM. These modules are now in public releases of both models (MM5 and CMAQ), providing the capability of using the same PBL scheme for both meteorological and chemical species. The Asymmetric Convective model (ACM) is part of the PX LSM implemented in MM5 and has also been added to CMAQ in the 2002 release.

2.1.4 Anthropogenic Emissions

During FY-2002, the Sparse Matrix Operator Kernel Emission (SMOKE)©[1] modeling system (www.emc.mcnc.org/products/smoke) was enhanced to allow user definition and grouping of major elevated point sources by stack parameters, emissions, emission rank, plant identification number, source identification number, calculated plume rise, or any combination of the preceding. A variety of software bugs were fixed. In addition, the Biogenic Emission Inventory System Version 3 (BEIS-3) and 1-km spatial resolution Biogenic Emission Land use Data Base (BELD) were installed in SMOKE©. SMOKE© development began under ASMD sponsorship, however, it has become a true community model. Development of SMOKE© is continuing with the contribution of several entities for modeling of wild fire emissions (ASMD and U.S. Forest Service), toxic emissions (EPA Office of Air Quality Planning and Standards (OAQPS)), and alternative land cover and wildfire emissions (Western Regional Air Partnership). ASMD is collaborating with OAQPS in defining the methodology by which SMOKE© will model toxic emission data for input to CMAQ. The initial estimation of toxic

[1]Copyright 1999 MCNC—North Carolina Supercomputing Center

emissions by SMOKE© will be limited to mobile sources, although application of the complete National Toxic Emission Inventory is planned in the near future.

The SMOKE© Tool was phased out during FY-2002 along with the old Models-3 modeling framework and graphical interface. The old framework was dependent on obsolete commercial software and had become problematic. The core Models-3 modeling components (CMAQ, MCIP, SMOKE) are often run independently and are not affected by the phase-out of the old framework and interface. The Tool was more tightly bound with the old framework. The SMOKE© Tool was used to define major elevated point sources and to grid emission data and related spatial surrogates for input to CMAQ. Point source definition is now done within SMOKE© and gridding may be accomplished using the new Spatial Allocator tool of the Multimedia Integrated Modeling System (MIMS). Unlike the SMOKE© Tool, the Spatial Allocator does not require the use of expensive SAS®[2] or Arc/Info®[3] software licenses. Finally, SMOKE© can be run either independently using scripts or with MIMS as a graphical interface. MIMS has been tested as a new, optional, robust interface for operation of SMOKE and CMAQ.

ASMD continued collaboration with the EPA National Risk Management Research Laboratory (NRMRL) on the development of a Modal Mobile Model for improved estimation of mobile source emissions. At the end of FY-2002, a detailed plan for completion of the coding and testing of the model was finished. The model will combine emission factors produced by the EPA Mobile6 mobile source emission model and spatial road network information following the approach of the spatially detailed Modal Model to produce spatially distributed mobile emission model results. The results will be more spatially refined than Mobile 6 outputs, but less input-date intensive than the Modal Model. The concepts testing with the Modal Mobile Model may be used in the new Multiscale Motor Vehicle and Equipment Emission System (MOVES), under development by the EPA Office of Transportation and Air Quality (OTAG), will eventually replace the regulatory mobile source emission model Mobile6. MOVES is designed as a modular model, thereby allowing components to be run individually or in combination. MOVES will accommodate modeling of mobile source emissions at various spatial scales, ranging from individual vehicles (micro-scale) to producing regionally-distributed mobile emission data suitable for use in such regional air quality transport models as CMAQ. MOVES will be a Geographic Information System (GIS)-based multiscale mobile emission model. MOVES version for greenhouse gases is planned for release in FY-2006.

2.1.5 Biogenic Emissions

Version 3.10 of the Biogenic Emissions Inventory System (BEIS) was introduced as part of an upgrade to CMAQ (Pierce *et al.*, 2002a). BEIS3.10 features a 1-km vegetation database for

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

[3]ARC/Info is a registered trademark of ESRI

the contiguous United States, which resolves forest canopy coverage by tree species; normalized emission factors for 34 chemicals, including 14 monoterpenes and methanol; a soil nitric oxide emissions algorithm that accounts for soil moisture, crop canopy coverage, and fertilizer application; and, speciation factors for the CB-IV, RADM2 (Regional Acid Deposition Model, version 2), and SAPRAC99 chemical mechanisms. During 2002, BEIS3.09 was formally imbedded as part of the SMOKE modeling system (Vukovich and Pierce, 2002).

In an effort to improve the characterization of vegetation cover for biogenic emissions and other air quality modeling processes, vegetation cover and isoprene emission estimates were compared with three contemporary databases (Pierce *et al*., 2002b). These databases included (1) the North American Land Cover Characteristics (NALCC) version 2 database, (2) the Biogenic Emissions Land cover Database (BELD3), and (3) the National Land Cover Database (NLCD). The NALCC database, which is released by the U.S. Geological Survey (USGS) and supported by the National Center for Atmospheric Research (NCAR) for use with MM5, consists of 1-km resolved land-cover classes derived from Advanced Very-High Resolution Radiometer (AVHRR) satellite data (U. S. Geological Survey, 2001). BELD3 provides vegetation data to the Biogenic Emissions Inventory System (U. S. Environmental Protection Agency, 2001). It combines the NALCC data with U.S. Forest Service (USFS) and U.S. Department of Agriculture databases so that tree and crop cover (by species) are resolved to 1-km. The NLCD was released by the Multi-Resolution Land Characteristics Consortium (U.S. Geological Survey, 2002). It is based on Landsat-TM data and available at ~30-m resolution. The relative distribution of forest and agriculture cover contained in the popular NALCC database was found to differ considerably from the two other contemporary databases across the mixed agricultural/forested region of the Tennessee Valley. Isoprene emission estimates varied by a factor of two depending on the source of vegetation data. Therefore, caution is urged in using such broadly-defined vegetation classes as those found in the NALCC data to derive biogenic emissions. Finally, it was recommended that future work consider the use of other databases, such as the NLCD, coupled with tree species distribution information to simulate other meteorologically-related processes that depend on the characterization of vegetation data.

2.1.6 Modeling Smoke Emissions From Fires

A prototype, stand-alone emissions processor is being developed that will introduce smoke from fires (prescribed and wildfires) into the Models-3/CMAQ modeling system. The goal of this project is to build a tool to generate emissions from forest burning for use in regional air quality modeling with the following characteristics:

- horizontal scale from regional to national with grid spacings ranging from 1 km to 36 km;
- temporal resolution ranging from hourly to multi-year;
- chemical species, including all NAAQS and visibility components and their precursors; and
- accuracy equivalent to other emissions estimates.

This prototype system, Community Smoke Emission Model, consists of a set of processors based on state-of science algorithms developed primarily by the USFS. This development is a cooperative effort with the U.S. National Park Service (USNPS) and includes principals at the Cooperative Institute for Research in the Atmosphere, Colorado State University, Fort Collins, Colorado. This project will serve to facilitate the use of Models-3/CMAQ 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. The effort to develop the smoke emission processor will involve introducing several major components, including:

- a system to identify fire boundaries determined from Geographic Information Systems (GIS) coverage;
- fuel models to introduce vegetation coverage and fuel loading data associated with the fires;
- a fuel moisture model;
- a fire generation processor based on spatial coverage of historical wildfire;
- a processor based on the USFS Consume[4] model for determining fire behavior or biomass consumption; and
- a processor for computing plume rise and providing emissions profiles for speciated wildfire emission pollutants.

The outputs and variables from these various modules are to be shared through linkages to the other CMAQ processors that are being set up for testing. An EPA/USNPS Interagency Agreement is in place to continue the collaborations and coordination for implementing the modeling system into the Models-3/CMAQ SMOKE emissions processor.

2.1.7 Fugitive Dust Modeling

Windblown and fugitive dust from on- and off-road activities, industrial and construction activities, and agricultural tillage practices are sources of PM_{10} in the atmosphere. These contributions are not incorporated in CMAQ because of a lack of an acceptable emission processing system to models these fluxes. Clearly, models for windblown and fugitive dust must involve complex atmospheric processes and linkages with spatially and temporally variable land surfaces, soil types, and soil conditions. Initial development of a prototype windblown dust model to be used in CMAQ at 36-km resolution was begun. The basis for the wind blowndust formulation is derived from use of threshold friction velocity parameterizations, and incorporation of gridded databases prepared with information on soil types, surface soil moisture content, weather, and vegetation type and coverages. Due to the variability of vegetation coverages, and the non-homogeneous distribution of wind-erodible land-use types, and the

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[4]A fuel consumption model, which predicts total smoldering fuel consumption during wildfires.

interception of uplifted dust particles by tree and vegetation canopies, a series of modeling sensitivity studies was performed. The purpose of these studies was to understand the model sensitivities to such input information such as percentage distribution of wind-erodible land-use types and vegetative coverage at fine grid resolutions in modifying the estimated dust flux at 36-km grid resolution. The development of an algorithm for determining the flux of dust from on/off road, construction, and agriculture tillage will result from the studies on windblown dust.

2.1.8 Effects of Desert Vegetation Type on Fugitive Dust Emissions

The objective of the investigation was to determine the effects of desert land vegetation type on the emissions of fugitive dust. The study area was the Jornada del Muerto located in the northern part of the Chihuahuan desert. A previous study showed that sandy soils have the lowest threshold friction velocities of any non-disturbed soil type, and consequently, have the greatest potential for sand movement. In the sandy soils, mesquite *(Prosopis glandulosa*) is the dominant plant, creosote (*Larrea tridentata*) is widespread, and black grama grass (*Bouteloua eriopoda*), dominant about 50 years ago, is still found. Other locally dominating vegetative types are tar bush, and mixed grass species found in topographic lows (playas). Both tar bush and playa vegetation are found in heavier soils, silty for tar bush and clay for playas, that are associated with larger threshold velocities for wind erosion.

Sand fluxes were measured at three different sites for five dominant plant types: mesquite, tar bush, creosote bush, black gramma grass, and mixed grasses on playas. For comparison, measurements were also made at a vegetation-free, flat site having sandy soil similar to that found at the mesquite sites.

The daily mean, Q, is a measure of the accumulated mass of sand movement. It is accumulated flux of sand transported through a surface having unit width, perpendicular to the ground and to the wind direction and extending to the height of the highest transported sand grain. Integrated, 3-month horizontal sand flux measurements (Q) were made for almost 3 years at 15 Net Primary Productivity sites having vegetation typical of the northern Chihuahuan Desert. A comparison site with no vegetation (Scrape Site) shows the effect of long-term removal of all vegetation on sand movement. Mean sand emission values for mesquite-dominated sites are higher than the mean emission rates for other kinds of vegetation (Figure 1). The other four means corresponding to different vegetation types are grouped by dominant plant type: creosote, tarbush, grama grass, and playa vegetation. Each of these means is composed of data from three individual sites.

Daily mean Q data for the vegetation types, tar bush, creosote, playa and grama, appear to be varying almost randomly with time, giving rough means of about 0.1 g/cm per day for the 3-month collections. The lack of correlation of Q for the non-mesquite vegetation types with the Q from the Scrape Site shows that non-mesquite site emissions have a weak relationship with the Scrape Site emissions. The mesquite Q means, however, seem to correlate quite well with the Scrape Site Q means (Figure 1). This was interpreted as evidence that response to wind at the

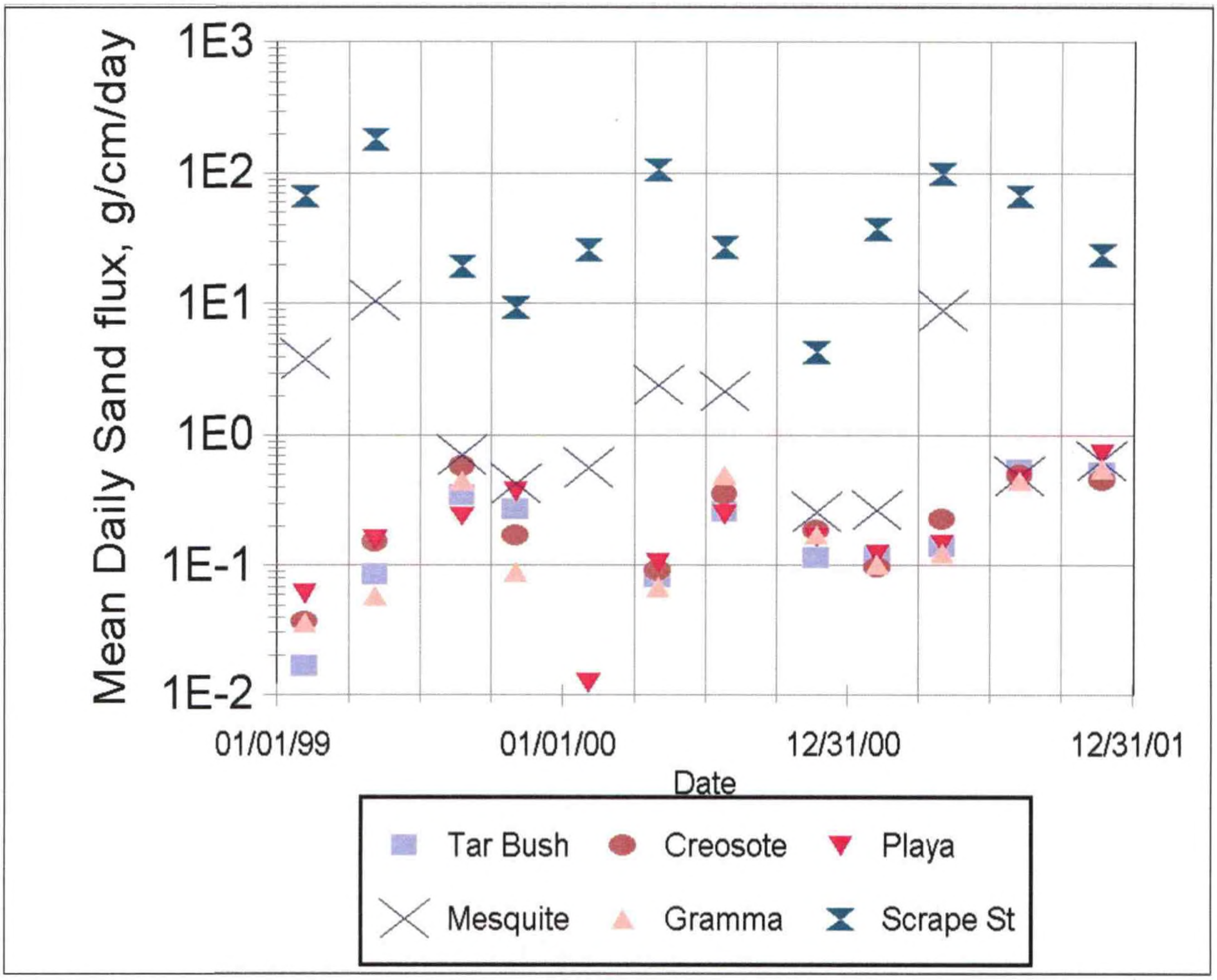

Figure 1. Mean daily sand mass horizontal flux versus date of collection for the means of five ecosystem types and the Scrape Site. The averaging period was approximately three months. Each mean is for values measured at three Net Primary Productivity sites having the same ecosystem type. The Scrape Site mean is for three measurements taken within an area usually dominated by mesquite bushes but having been scraped free of any vegetation. All sampled sites are located within a circle having a radius of 10 km centered at the headquarters of the U.S. Department of Agriculture, Jornada Experimental Range (JER), which is located between Las Cruces and Alamagordo, New Mexico.

mesquite site is roughly proportional to that at the Scrape Site. For the five lowest values of the Scrape Site Q, four of the mesquite Q means are almost the same as the means for the other vegetative sites. This may be showing that the threshold velocities for the mesquite sites are higher than those for the Scrape Site and that those threshold velocities were not exceeded or barely exceeded for those time periods, as was the case at the other vegetative sites. During these times, however, threshold velocity was exceeded at the Scrape Site. Lastly, except for the four of the time periods mentioned above, the mesquite Q are always higher than for any other vegetative type. The study may be summarized by the conclusion that land dominated by mesquite (*Prosopis glandulosa*) is the most important area for active sand movement at the Jornada Experimental Range.

2.1.9 Implementation and Testing of New and Refined Chemical Mechanisms and Chemical Solvers in CMAQ

The treatment of atmospheric, gas-phase chemistry is a critical component of the CMAQ modeling system. The ability of CMAQ to accurately predict ambient concentrations of trace gases in the atmosphere is fundamentally dependent upon the validity of the gas-phase chemical interactions and transformations contained in the chemical mechanism that is used in CMAQ. The accurate representation of gas-phase chemistry is also vital for the simulation of such other important atmospheric processes as the formation of aerosols, the chemical transformations taking place in the liquid phase, and the deposition of air contaminants to land and water surfaces. Commensurate with the need for an accurate chemistry representation is the need for gas-phase chemistry solution techniques that are both highly accurate and computationally-efficient. Since numerical solution techniques that have been used historically consume about 50 to 75 percent of the computer time required for model simulations, any substantial computational efficiencies that can be gained will significantly lower the computational requirements of the model. The underlying objectives of this research effort are twofold: (1) to improve and enhance the representation of atmospheric gas-phase chemistry in CMAQ by refining existing chemical mechanisms, by adding new chemical mechanisms, and by investigating new approaches for increasing chemical information in the model, and (2) to reduce computer time required to simulate gas-phase chemistry by enhancing the computational efficiency of existing solvers, by investigating new approaches that can be used in conjunction with existing solvers to lower computational requirements without sacrificing the numerical accuracy, and by testing and evaluating new chemistry solver algorithms. The results of this work will help improve the scientific integrity of CMAQ by incorporating new scientific knowledge in the area of atmospheric chemistry, and will increase the practicality of using CMAQ as a modeling tool in regulatory/operational modeling applications by lowering the computational burden.

During FY-2002, several enhancements have been made to the treatment of gas-phase chemistry in CMAQ. First, a new gas-phase chemical mechanism, SAPRC99, was added to the existing array of chemical mechanisms in CMAQ. SAPRC99, developed by researchers at the University of California Riverside, is a detailed mechanism of the reactions of volatile organic compounds (VOC) and nitrogen oxides (NO_x) that can be used for both urban and rural areas. It includes recent kinetic and mechanistic atmospheric chemistry data, and represents the state-of the-science in atmospheric chemistry mechanisms as of mid-1999. It has been fully implemented in CMAQ, including linkages to aerosol and aqueous chemistry to enable a "one-atmosphere" modeling approach. Second, a new form of gas-phase chemistry solver— the Modified Euler Backward Iterative (MEBI) method—was included. This solver is about two to three times faster than the solvers included with the original CMAQ modeling system. Because MEBI is not a generalized chemistry solver, a unique version must be formulated for each chemical mechanism with which it is to be used. Thus far, CMAQ MEBI solvers have been developed and released for the following chemical mechanisms: Carbon Bond-IV (CB-IV), RADM2 with 4-product isoprene chemistry, and SAPRC99. Since the MEBI solvers are more computationally-efficient, but still provide a relatively high level of accuracy, this class of solver is usually preferred for most CMAQ modeling applications. Their availability often enables the conduct of CMAQ model applications that are more detailed and extensive than those that could be performed using one of the slower solvers included in previous CMAQ releases.

2.1.10 Aerosol Mechanism Improvements in CMAQ

Ongoing development of the CMAQ aerosol module includes the investigation of sea salt dynamics for aerosols in a marine environment. Several sea spray generation functions (Andreas, 1998; Monahan *et al.*, 1986; Smith and Harrison, 1998; Smith *et al.*, 1993) were examined to determine the relative merits and drawbacks of each. The lognormal form of the Smith and Harrison (1998) function appears best-suited to CMAQ's modal approach to aerosol modeling and the necessary equations to calculate sea salt emissions according to Smith and Harrison (1998) have been coded into a stand-alone box model for testing. These equations include number, volume, and mass emissions; vertical wind profiles; and roughness length. To date, box model testing has included the investigation of wind profile functions for determining sea salt emissions; performance of a sensitivity analysis on selected input terms; examination of the dependence of sea spray generation on various values of friction velocity u_*; and whether or not equilibrium between the gas and aerosol phases may be assumed for marine environments (Allen *et al.*, 1989; Hildemann *et al.*, 1984; Nenes *et al.*, 1998; Quinn *et al.*, 1992). Upon sufficient testing of the box model, sea salt dynamics will then be added to the CMAQ model.

The most recent version of the aerosol component, AE3, has a new approach to calculating the secondary organic aerosol (SOA) mass produced by biogenic and anthropogenic precursors. The method used to calculate SOA is based upon work by Schell *et al.* (2001), modified to be consistent with the CMAQ modeling paradigm. The precursors of SOA considered in AE3 are aromatics, monoterpenes, internal alkenes, and high molecular weight alkanes. Schell *et al.*, (2001) considered a lumped class of precursor aromatics, and alpha pinene and limonene as separate precursors. AE3 considers toluene, xylene, and cresol as separate aromatic precursors, and a lumped class of monoterpenes, as well as long chain alkanes and internal alkenes. The partition coefficients for the biogenics were taken from Griffin *et al.* (1999); those for the aromatics, toluene and xylene, are from the high and low yield curves, respectively, in Odum *et al.* (1997). The partition coefficients for the alkanes and cresol are from Strader *et al.* (1999); those for the internal alkenes are from Kalberer *et al.*, (2000). Temperature corrections for the partition coefficients were made using the methodology of Sheehan and Bowman (2001), and the biogenics were lumped using the methodology of Bian and Bowman (2002). In lumping the biogenics, the fractional contribution of the biogenic species was taken as 0.4 alpha pinene, 0.25 beta pinene, 0.15 delta 3-carene, and 0.1 each for sabinene and limonene. These fractions reflect a national rather than a regional distribution of the species. The lumping scheme was provided for use in CMAQ by Professor Bowman (personal communication) prior to publication.

2.1.11 Plume-in-Grid Modeling

The plume-in-grid (PinG) approach contained in the CMAQ provides a realistic scientific treatment of the physical and chemical processes impacting pollutant concentrations in isolated, major point-source plumes. The PinG treatment simulates gradual plume growth due to dispersion processes, in contrast to instant mixing into the entire volume of a large Eulerian model grid cell in which the elevated point source is located, which can have a strong impact on the temporal evolution of photochemistry in the near-field. The description of the capabilities of the CMAQ/PinG modeling treatment and its technical formulation have been described in Gillani and Godowitch (1999). The key modeling algorithms are a plume dynamics model (PDM) and a Lagrangian reactive plume model (PinG module), which are designed to simulate the relevant plume processes at the proper spatial and temporal scales for CMAQ regional modeling domains with typical grid sizes of about 10-40 km. The PinG treatment is capable of simulating multiple point-source plumes with hourly emission releases. The PinG module is fully integrated into the CMAQ, and it is exercised concurrently during a simulation to use grid cell concentrations as boundary conditions for each plume section. An important feedback occurs when a plume section attains the model grid cell size, as the subgrid plume treatment ceases and plume concentrations are incorporated into the Eulerian grid system.

A notable FY-2002 update for the PinG module has been the inclusion of an aerosol/particulate modeling algorithm to simulate PM and aerosol species along with gas-phase pollutant species in the subgrid plumes. The Binkowski (1999) aerosol algorithm, which has been employed as the aerosol modeling component in the CTM grid model, was adapted and integrated into the PinG module. A series of model simulations were conducted with the RADM2 and CB-IV photochemical mechanisms and with the three available chemical solver methods: QSSA (quasi-steady state approximation), MEBI (modified Euler backward iterative), and Gear approaches to assess differences in aerosol species formation due to the choice of chemical mechanism and numerical solver approach. The Gear solver is the preferred method when applying either chemical mechanism with PinG. Model simulations were also performed for a set of major point-sources exhibiting a wide range of NO_x and SO_x emission rates within a regional grid model domain encompassing the greater Nashville, Tennessee, area. Preliminary model results presented in Godowitch (2002) revealed interesting differences in sulfate aerosol (SO_4) concentrations and PinG results appeared to agree with emerging observed plume aerosol data. For point sources with comparable SO_2 emissions, greater sulfate formation occurred in those plumes with lower NO_x emission rates. For the gas-phase species, previous PinG results at various downwind distances were encouraging with the modeled plume NO_x and ozone concentrations exhibiting the same evolutionary pattern found in real-world plume measurements (Godowitch and Young, 2000). An initial, limited comparison of PinG modeled plume concentrations against ozone, selected nitrogen species, and SO_2 data obtained from aircraft traverses across plumes was reported by Godowitch (2001). In addition, analyses of CTM results from 12-km and 36-km domains for a July 1995 period were performed from separate model simulations, which either included the PinG treatment or omitted it. Comparisons of modeled and observed hourly ozone concentrations indicated that the CTM/PinG results displayed better agreement and less bias than the CTM/NoPinG results, particularly in areas where numerous large point sources exist. Further modeling results are anticipated with modeled photochemical pollutant and aerosol species to be compared to available observed plume data collected by various airborne platforms during the SOS 1999 field experiments.

2.1.12 CMAQ Code Integration and 2002 Release

ASMD redesigned, and tested the CMAQ system code to optimize performance and assist with public releases of the CMAQ modeling system code. The main focus was on modifying CMAQ to maintain the high quality science processing, while restructuring code and data structures to speed up the computational time.

The latest version of CMAQ was released for public use in June 2002. The modeling system is available for downloading at ftp://ftp.epa.gov/amd/stand_alone_models3/cmaq/. The scripts for this release have been tested on Linux™[5] (specifically, Redhat®[6] Linux 2.1 with the Portland Group F90 compiler, pgf90 version 3.2). This version of CMAQ features several major changes:

1. Addition of a new aerosols module, AE3, which includes improved treatment for secondary organic aerosol formation by including semi-volatile compounds that partition between gas and aerosol phases, updated process for sulfate nucleation, heterogeneous conversion of N_2O_5 to nitric acid, and the ISORROPIA model for aerosol thermodynamics;

2. Incorporation of aerosol emissions in the vertical diffusion process;

3. Change in the order of the time splitting science processes, from chemistry -> clouds -> aerosols, to clouds -> chemistry -> aerosols, to provide a better linkage between gas-phase chemistry and aerosols;

4. Addition of the SAPRC-99 gas-phase mechanism;

5. Addition of the MEBI solver for all variants of CB-IV, SAPRC-99, and the RADM2-Carter-4-Product-Isoprene mechanisms;

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[5]Linux is a trademark of Linus Torvaldo

[6]Red Hat is a registered trademark of Red Hat, Inc.

6. Addition of a new optional vertical diffusion module, ACM;

7. Change to dynamically allocate the horizontal grid for the chemistry model and the initial and boundary concentrations pre-processors (ICON and BCON), thus allowing one executable to run any horizontal domain that CMAQ supports;

8. Ability for CMAQ to window from meteorology and emission data sets, so that runs on many subdomains can be executed using one data set that encompasses all those subdomains; and

9. Addition of an hour-average concentration output option for any chemical species.

2.1.13 Development and Testing of an Air Quality Forecast Model

As part of a joint NOAA-EPA project on air quality forecasting, an optimized version of the CMAQ model is being linked with the NOAA/National Weather Service (NWS) mesoscale Eta meteorological model. The project started toward the end of FY-2002, and will continue into FY-2003. Appropriate linkage software to drive CMAQ with the Eta model output will be developed and tested. Other objectives of this work will be to make significant improvements in the computational performance of the air quality model, which uses the CMAQ science. The current CMAQ was designed to be a highly flexible community modeling system, capable of running on various computer architectures including parallel processors. The main focus was not speed of execution, but generality and ease of facilitating model science versions for the general modeling community. The air quality forecast version of CMAQ, however, will aim towards a platform-specific air quality forecasting model that will trade off much of generality for computational speed.

The development of an air quality forecasting model will require significant performance improvements over the current version of CMAQ. To add to the challenge, some processing presently done in the meteorology-chemistry interface processor (*e.g.,* deposition velocity calculations) and some emissions processing that depends on dynamic meteorology (*e.g.,* biogenic emissions) will have to be included with the set of operator-splitting, science processes already done in CTM.

To achieve the necessary speedup structurally, it is envisioned that CMAQ will have to be changed in two major areas. First, a new model architecture is being developed that will be tuned for a specific parallel platform. Second, code modifications are being made to optimize use of such specific hardware features as memory access (cache) and hardware floating point units. In addition to structural modifications, ASMD is also looking at algorithms and data organization changes to achieve performance gains. The initial version of the forecast model

(FY-2003) will include ozone and photooxidants, but will not include prediction of PM, whose capability will be added to a subsequent version of the air quality forecast model.

2.1.14 AERMET

Work continued on necessary improvements and upgrades to the meteorological preprocessors, MPRM (Meteorological Preprocessor for Regulatory Modeling) and AERMET (American Meteorological Society and Environmental Protection Agency Regulatory Model for Meteorology). These programs process meteorological data for use with the EPA regulatory dispersion models. Upgrades to these programs are necessary from time-to-time to keep pace with changes to the meteorological data archives maintained by the NOAA National Climatic Data Center, and to support ongoing improvements in regulatory dispersion models. MPRM, the older of the two preprocessors, supports dispersion models that rely on Pasquill-Gifford dispersion coefficients (U.S. Environmental Protection Agency, 1996). EPA continues to support these older models; however, the intent is to eventually phase out such support.

AERMET, which supports the newest generation of dispersion models, is based on planetary boundary layer (PBL) theory. Important processes within the PBL (*e.g.,* the surface layer and the mixed layer) are modeled separately (U.S. Environmental Protection Agency, 1998). Similarity theory is used to model the surface layer. AERMET algorithms provide hourly estimates of the following surface and mixed layer parameters: Monin-Obukhov length, friction velocity, surface heat flux, and convective scaling velocity. Hourly estimates of convective and mechanical mixing heights are also provided. Upgrades and improvements to AERMET continued throughout FY-2002 in response to user comments on the beta versions of the software released in September 2001 and again in March 2002. In addition, support was also provided to the EPA OAQPS staff involved in evaluating and testing AERMOD. These evaluations, which are required for the promulagation of AERMOD, are being conducted using multiple test data sets and meteorological databases. The necessary preprocessing of these data provides an excellent opportunity for exercising AERMET.

2.1.15 Recommendations for Observations-Based Methods

The NARSTO Ozone Assessment of 2000 suggested the use of observations-based methods (OBMs) as diagnostic tools (1) to diagnose ozone production and production efficiency in both the real atmosphere and in the model-simulated atmosphere, and (2) to assess and help explain the effectiveness of emission controls over time. Diagnostic analyses and OBMs require a special set of non-routine measurements, because they typically involve ratios of special species. Earlier work (Tonnesen and Dennis, 2000a; 2000b) had identified a set of OBMs, which were refined and described subsequently in an EPA report (Dennis et al., 2001). During FY-2002, the main elements of the recommended set of OBMs, based on the measurement of O_3, NO+true $NO_2 = NO_X$, NO_Y, and NO_Y-$NO_X = NO_Z$, were tested for their ability to effectively and diagnostically compare CMAQ's results and measured ozone production. The test data sets came from SOS data taken in Nashville, Tennessee, in the summers of 1995 and 1999 and in Atlanta during August 1999. For Nashville, the OBM set worked well. However, for Atlanta, interpretation of the OBM measures turns out to be more complicated due to differences in air mass histories, and further interpretive work is planned. As data permit, other recommended measures are now being examined, to assess the overall robustness of the OBM measures.

2.2 Atmospheric Model Evaluation and Application Activities

2.2.1 Improve O_3 Vegetation-Atmosphere Exchange Models

Biologists and plant physiologists interested in studying the effects of pollutants on vegetation have learned that it is not sufficient to relate plant symptoms to local pollutant concentration. The air concentration above or near the plant canopy is not the same as the amount of pollutant that actually gets into the plant, or its exposure, which for the same concentration can vary depending on species, weather, time of day, season of the year, and health of the plant. While they do a good job of predicting exposure of the total canopy, normal deposition models are not designed to operate within the canopy at the leaf level where pollutant damage occurs. Yet understanding deposition at the leaf level is necessary if a complete understanding of the pollutant, plant-damage relationship is to be understood for the development of defensible secondary ambient air quality standards as required by the Clean Air Act (CAA). To estimate dosage and exposure, a model designed to estimate fluxes and plant exposure within a plant canopy is needed. However, a sub-canopy model is not simple. Because wind and pollutant profiles within a canopy are not log-linear as they are in the normal atmospheric boundary layer, simple gradient-transfer models are inappropriate, and it is necessary to use the more complex second-order closure models. These models have been developed for use in tree canopies from theoretical considerations, but have received little evaluation. For use in herbaceous perennials, which are frequently studied because of their sensitivity to pollutants, these models have never been evaluated. ASMD has started a model evaluation and improvement program for this reason, adapting a second order closure model developed by NOAA's Atmospheric Turbulence and Diffusion Division at Oak Ridge, Tennessee, and collaborating in the evaluation and improvement program. This study is part of a larger study of ozone damage to sensitive plants, with additional collaborators at Auburn University, Auburn, Alabama, University of Newcastle, United Kingdom, and Appalachian State University, Boone, North Carolina. The funding comes from the USNPS, the National Geographic Society, and other sources.

A first field study was completed in the summer of 2002 at Purchase Knob in the Great Smoky Mountains National Park, a high elevation location set aside by the USNPS for educational and scientific activities. Two study sites were selected, one on the outside edge of a forest, and one inside the forest where the plants grew in dappled shade. The species under study was Rudbeckia laciniata (cutleaf coneflower), which has been shown to be very sensitive to ozone. Populations of this plant are not uncommon in the park at higher elevations.

To evaluate the sub-canopy deposition model, measurements of the important inputs and outputs were made. Along with the necessary routine meteorological variables, measurements of radiation and atmospheric turbulence directly above the coneflower canopy had to be made. Turbulence measurements were made with a fast-response sonic anemometer that measures the wind speed by recording the doppler shift in a sound wave traveling between two sensors located a few centimeters apart. Figure 2 displays the installation of the meteorological tripod and sonic anemometer at the site inside the forest canopy. The sonic anemometer is at the top of the tripod, the other sensors on the crossarms, and the dataloger is in the white box. Ozone was measured at four levels: one above, and three within the canopy. Along with observations of the meteorological variables, measurements of photosynthetic rate, water use, anthocyanin concentration, leaf area index, and stomatal conductance were made.

The field study was completed in July 2002. Data have been processed, screened, and put into a database for analysis. Much of the preliminary analysis and model evaluation has also been completed. Ozone values were measured at four heights at the site outside the forest (Figure 3). At the first height within the canopy (1.0 m) the vegetation is still very sparse, and the ozone hardly diminished at all from the levels measured above the canopy at 2.35 m. At the next level down (0.57 m) in the densest section of leaves, the ozone levels are much lower. And at the lowest levels, just 0.2 m above the ground, the ozone levels are lower yet.

Figure 2. Installation of the meteorological tripod and sonic anemometer at the site inside the forest canopy.

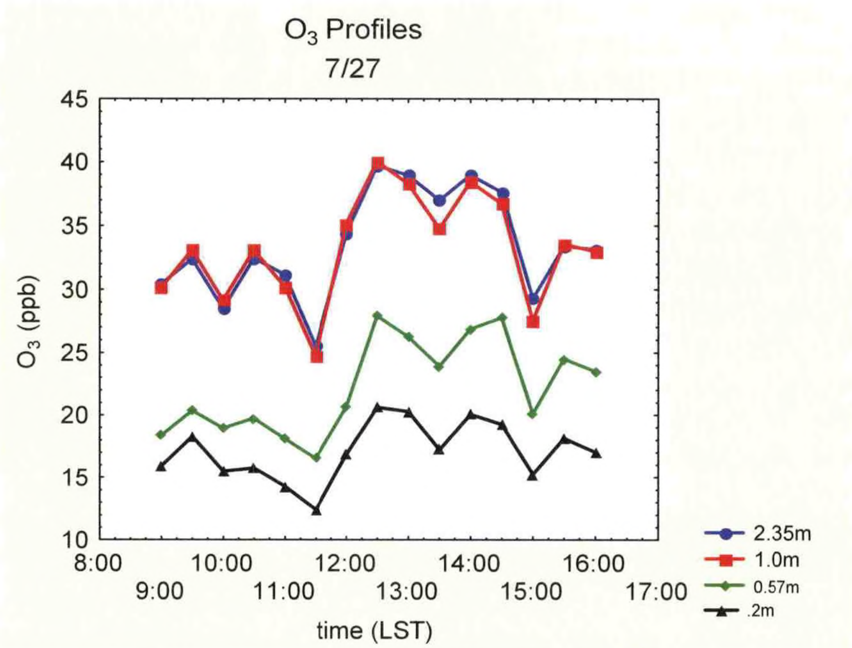

Figure 3. Ozone values measured at four heights outside the forest.

The task now is to run the model of subcanopy deposition to see if it can reproduce these measurements, determine its strengths and weaknesses, diagnose reasons for the weaknesses, and find improvements. In addition to ozone concentration, profiles of leaf conductance, photosynthethically active radiation, and higher moments of turbulence measured with the sonic anemometer will be compared with the model to test model performance. The database of observations from the field program will be put into a form accessible to the public, and located on the ASMD website (http://www.epa.gov/asmdnerl/).

2.2.2 Modeling Studies in Coastal Environments

Simulations with the Extended RADM were used in a joint effort with the USNPS to develop an environmental assessment for the Shenandoah National Park. Such an assessment is fairly unique in Park history. The first purpose of the assessment is to estimate how air pollution stressors will be reduced due to ozone and acid rain controls on air emissions that stem from the 1990 Clean Air Act Amendments (CAAA), estimate how ecosystem damage from ozone and acid rain will be changed or mitigated, and how air quality related values connected to visibility degradation will be affected. The second purpose is to provide an approximate sense of how much farther air emissions would need to be reduced to provide full protection of the ecosystems from ozone and acid rain damage. The Extended RADM was used to estimate the degree to which surrounding states and regions are responsible for multi-pollutant exposures of ecosystems of the Shenandoah National Park to acidic deposition, inorganic fine particle concentrations, and seasonal ozone. Airsheds for Shenandoah were found to be quite large, covering roughly 13 states. The Extended RADM was also used to explore the degree to which CAA regulations using two scenarios, and subsequent, significant emission reductions beyond the CAA using two additional scenarios, could reduce acidic deposition and seasonal ozone exposures to achieve ecosystem-protective levels of exposure. The Shenandoah assessment has undergone internal Park Service and external science review. Completion of the Shenandoah assessment report is expected during FY-2003. Besides the analyses for the assessment, a concise description of the Extended RADM as a multi-pollutant model was also written for an appendix, in response to reviewer requests, which serves as an aid to scientific documentation.

2.2.3 Chesapeake Bay 2005 Re-Evaluation

ASMD has established a long-term relationship with the EPA and NOAA Chesapeake Bay Programs to address multi-media environmental problems where the atmosphere is an important pathway. Atmospheric deposition of reduced and oxidized nitrogen is an important source of new nitrogen to coastal estuaries, contributing to eutrophication problems that have been growing, and Chesapeake Bay is a leader in using multi-media modeling. Two major Chesapeake Bay re-evaluations or assessments of required nitrogen load reductions to the Bay have already occurred. The next re-evaluation is slated for 2005 or shortly thereafter.

Chesapeake Bay has been placed on EPA's list of impaired waters. A 1999 court agreement set 2011 as the deadline for writing an enforceable cleanup plan, a TMDL (Total Maximum Daily Load) plan. The Chesapeake 2000 agreement calls for preempting the need for a TMDL plan by cleaning up the Bay by 2010. The Bay 2005 re-evaluation is a critical step in this process towards the 2010 cleanup and delisting, and ASMD is participating in the re-evaluation process. The best science is desired for the re-evaluations, and during the period between major re-evaluations, ASMD is changing its multi-media modeling of nitrogen from the Extended RADM to its new model, CMAQ. CMAQ has been sufficiently evaluated for deposition to show that it is an improvement over the Extended RADM. A newly designed aggregation data set with 40 cases has been developed for CMAQ that can directly address seasonal deposition, an improvement over the older aggregation set. The outer, continental grid resolution is 36-km, a significant reduction over the 80-km resolution used with the Extended RADM. For Chesapeake Bay multi-media simulations, a 12-km nest over the Northeast within the 36-km grid covering most of the Chesapeake Bay airshed has been developed. This inner nest will better resolved the Bay surface compared to the 20-km nest used with the Extended RADM. The MM5 meteorological runs for the 36-km aggregation set and the 12-km nest were completed during FY-2002. Prior to establishing new base cases with CMAQ, testing is now underway to determine the best method for parameterizing the mixing height, because the

CMAQ MCIP has new capabilities available. In FY-2002, post-analyses were completed to help tributaries and Bay states set the stage for the re-evaluation, based on current model runs using the Extended RADM. The relative contribution from each of the six main Bay states to nitrogen deposition to the watershed tributaries was calculated, using runs that coordinated with the Shenandoah assessment.

2.2.4 Bay Regional Atmospheric Chemistry Experiment: Evaluation and Assessment

The Tampa Bay Estuary Program and the Florida Department of Environment (FDEP) have asked EPA/National Exposure Research Laboratory (NERL) and NOAA/Air Resources Laboratory (ARL) to enter into a partnership to lead the application of CMAQ to help them understand the sources of nitrogen deposition affecting Tampa Bay. The majority (60 percent) of the nitrogen deposition to the estuary and watershed is estimated to come from sources local to Tampa Bay, which is unusually high, due to Tampa's isolation from other large source regions. ASMD was asked to work with the Tampa Bay National Estuary Program to assess the atmospheric contribution of nitrogen to Tampa Bay. Tampa Bay provides an important atmospheric multi-media problem significantly involving coarse particles and sea salt, and creates an excellent research opportunity to test advances in the science in CMAQ to deal with coastal nitrogen deposition. Two of the largest power plants in the nation, in terms of NO_X emissions, are on the shores of the Bay and there are serious questions as to how much of the atmospheric deposition is due to the power plants versus mobile sources in the area surrounding the Bay. CMAQ was selected as the model for the Tampa Bay Assessment, in part because CMAQ will incorporate sea salt in its fine particle module in FY-2003. Prior to any Tampa Bay assessment, it was agreed that CMAQ needs to be evaluated against high-quality local data and that the nitrogen budget around Tampa Bay needs to be more carefully characterized.

The Bay Regional Atmospheric Chemistry Experiment (BRACE) was designed for these two purposes. BRACE was conduced in May 2002. Division scientists, along with ARL colleagues, were significantly involved in the planning of BRACE. Division scientists played a major role in establishing the location of the BRACE supersite and in establishing the suite of measurements for the supersite and several surrounding measurement sites that would to the best degree feasible delineate the full nitrogen budget and photochemical processing behind the budget. ASMD scientists worked on deployment of true-NO_2 monitors and with Hillsborough and Pinellas Counties' air quality professional on deployment of NO_Y instruments. ASMD and NOAA ARL, Silver Spring, Maryland, scientists took the lead on siting three wind profilers around the Bay, and helped define the complete chemistry package of instruments for the NOAA Twin Otter aircraft.

2.2.5 Ammonia Budgets for Coastal Systems

An important fraction of atmospheric nitrogen deposition is reduced nitrogen (ammonia/ammonium). In the future, with successful implementation of the EPA regulations on

NO_x emissions for control of ozone and increases in animal operations in the eastern seaboard states, reduced nitrogen is expected to become a majority of the nitrogen deposited from the atmosphere. However, ammonia is not receiving the attention it deserves, in part, because many ecologists dealing with marine estuaries and watersheds believe ammonia deposits instantly so that none leaves the immediate area. Long-range transport of ammonia is ignored. ASMD has an opportunity to correct this misinterpretation of data through modeling and model-data interpretation studies using the regional models. Model atmospheric budget analyses were performed in FY-2002 for North Carolina ammonia emissions associated with the large increase in the hog population. The analysis, covering a short summer period and reported at the International N2001 Conference, show that only 5 to10 percent of the NH_x budget dry-deposits locally while most of the ammonia emissions are involved in long-range transport. This is contrary to conventional wisdom. The model results are consistent with spatial and temporal trends in the ammonia wet deposition data. A regional exploration of the ammonia budget was performed for the eastern United States using the Extended RADM. The conclusion thus far is that the conventional wisdom that assumes there is no long-range transport of ammonia is incorrect. Nonetheless, the conventional wisdom persists and distorts studies of nitrogen-cycling in coastal estuaries, introducing significant errors in them. Because it is important to correctly assess the ammonia/ammonium transport and deposition to coastal estuaries and coastal oceans, further analyses will be undertaken with new CMAQ simulations to build a case against the conventional wisdom.

2.2.6 Inverse Modeling for Ammonia

One of the key uncertainties affecting emissions-based air quality model predictions is the uncertainty in the emissions input. Ammonia emissions have one of the highest degrees of uncertainty as compared to other emissions, and they have a significant impact on fine particle predictions. Variations in ammonia emissions will cause large variations in predicted nitrate PM concentrations. The EPA National Emission Inventory (NEI) for ammonia emissions is based on a 1994 report where European emission factors were extrapolated for the United States. These emission estimates suggest that the largest source of ammonia emissions is animal husbandry, which comprises about 80 percent of the total. Fertilizer is also a substantial source. Both of these sources are expected to have seasonal variations because of the temperature dependence of ammonia volatilization from animal waste and because of the seasonal patterns in fertilizer application. However, the emission factors used in the NEI do not have any dependence on temperature, and great uncertainty exists in the factors themselves. For these reasons, the uncertainty in ammonia emissions is both with respect to their seasonality (they are expected to vary significantly between winter and summer) and in their overall annual magnitude.

Ammonia emission studies traditionally have been based on flux observations at individual sites, which are dependent on such local factors as the meteorological conditions, housing conditions, and feed for the animals studied. To evaluate the current ammonia emissions inventory on a regional scale, inverse modeling is used to estimate monthly ammonia emission fields for the eastern United States. Using the Kalman Filter technique with CMAQ, inverse modeling is used to estimate monthly ammonia emissions that produce optimized predictions of wet concentrations of ammonium for 1990. Further, uncertainties in the modeled precipitation have been accounted for by introducing the standard error of the precipitation estimate into the Kalman filter. As anticipated, results suggest that the emissions should be highest during summer conditions and lower during fall and winter. Findings from this study will be presented in a journal article.

As a next phase of this study, the inverse modeling of ammonia will be extended to the United States continental domain for a more current time period. Then the work will be extended to examine different sources of emissions that have different spatial patterns, such as cattle versus hogs. The objective is to assess whether a particular source has a greater degree of uncertainty than other sources and to consider spatial uncertainty in the emissions based on source-specific information. The ammonia emission estimates developed from this study support the wok of OAQPS, which is currently evaluating the NEI ammonia inventory and considering improvements. This work also supports the air quality modeling community whose modeling results can be detrimentally affected by large uncertainties in ammonia emission inputs to the model.

2.2.7 Diagnostic Metrics for Ozone and Particulate Matter

Diagnostic metrics enable us to examine the process side of the model to better examine the degree of reliability of control strategy predictions. They require a special set of non-routine measurements, because they typically involve ratios of species involved in photochemical production. Earlier work (Tonnesen and Dennis, 2000a; 2000b) had identified a set of metrics based on measurement of O_3, NO+true $NO_2 = NO_X$, NO_Y, and NO_Y-$NO_X = NO_Z$. These diagnostic tests were applied to CMAQ for Nashville, Tennessee, for the 1995 SOS field measurements. The model simulations examined for Nashville were at 12-km and 4-km resolutions. The modeling results from 36-km grid spacing were not examined because they were considered to be too coarse for ozone predictions for a moderate-sized urban area. The diagnostic metrics suggest that the 4-km grid cell size produces slightly better predictions relative to ozone process fidelity. The metrics also highlighted sites that were being influenced by local emissions sources that were missing in the model, pointing out sites where model prediction of ozone changes might be biased because of missing emissions (or extra emissions) in the model inputs. New statistical procedures for the assessment of ozone production efficiency were developed as part of this work because the metric used to define ozone production efficiency, the relationship between hourly O_3 and aged nitrogen oxides (NO_Z) (as typically illuminated in scatterplots) is curvilinear and involves effectively two independent variables, rather than dependent and independent variables. Thus, standard procedures are not appropriate. Also, approaches for partitioning the data into age and ozone productivity classes were developed for a cleaner comparison and interpretation of observataions and model predictions. The metrics are now being applied to other time periods (SOS Nashville 1999 data) and other cities (SOS Atlanta 1999) to test their robustness.

2.2.8 CMAQ Model Evaluation to Assess Readiness for State Implementation Plans

Model evaluation is an essential component of such science-based air quality models as CMAQ. Operational or performance evaluations examine the pollutant end-points that are of direct interest to client users of CMAQ and mostly relate to ozone, fine particles, and acidic and nitrogen deposition. Where possible, these performance evaluations are supported by diagnostic evaluations. ASMD has participated in the NARSTO model intercomparison for ozone. For this study, the comparison period of July 5–18, 1995, was resimulated with the new SMOKE emissions processor, using the 2001 release version of CMAQ to correct errors that had been uncovered. To make the comparisons more relevant, control strategy runs were also included in this round. To examine CMAQ's performance for deposition, wet deposition simulations for January and June 1990 were compared to the National Atmospheric Deposition Program measurements and reported at the Spring 2002 American Geophysical Union Conference in Washington, DC. The updates to the cloud module in CMAQ to better account for ice and snow improved the wintertime predictions over those using the older cloud formulation of RADM. The comparisons were quite reasonable although errors in predicted precipitation created significant scatter. In a sensitivity simulation to examine the importance of possible errors in the dry deposition rate for SO_2 it was found that wet deposition changed by about 10 to15 percent for a factor of 3 change in the SO_2 dry deposition rate.

A major evaluation task was the testing of CMAQ for the 2002 release. The evaluation was continental in scope for the 2-week period from June 30 to July 14, 1999. The focus was on ozone (against data from the AIRS sites) and fine particulate matter (against data from IMPROVE and CASTNet). The simulations were generated with a 32-km continental resolution and an 8-km grid over the Southeast. During the checkout, several errors were uncovered and corrected in the emissions processing by SMOKE. A bench run with the older 2001 science modules selected (RADM2 vs. SAPRC99; AE2 vs. AE3; BEIS2 vs. BEIS3) was included. In addition, several versions of CMAQ with incremental science changes were run on both domains to test the effect of the new science. Sulfate continued to be predicted well with the newer science, while the nitrate over-prediction bias increase and organic carbon predictions changed from an under-prediction to an over-prediction. Ozone is biased higher with the new chemical mechanism. A full 1999 evaluation from June 15 to August 31, 1999, was begun for full ozone evaluations against the Nashville 1999 data set (June 15–July 15, 1999) and full fine particle evaluations against the Atlanta 1999 supersite data set (August 3–August 31, 1999). Three grid structures will be available: 32-km (continental), 12-km (southeast), and 2-km (Nashville and Atlanta).

2.2.9 Sensitivity of CMAQ Control Strategy Predictions to Model Input Uncertainties for CMAQ and MM5 Configurations

Sensitivity analyses are important adjuncts to model-data comparisons. A key use of the air quality models is prediction of the effects of emission controls on air concentrations. These predictions can be affected by model input uncertainties, model parameter uncertainties, and structure of the model itself. The focus of the sensitivity analyses was principally on the chemical mechanism and vertical mixing algorithms, because a major new chemical mechanism, SAPRC99, was newly available for CMAQ. Grid size effects were also examined because finer grids have a large computational burden, limiting the number of analyses that can be performed. The results of this sensitivity work were reported at the U.S.-German Workshop in Bad Breisig, Germany, in October 2002. The key findings were:

- Differences in the type of vertical mixing (meteorology) create the largest differences in predicted daily peak 8-hour ozone, but differences in chemical mechanisms cause the largest difference in control strategy response, for the same grid resolution.

- The reduction in ozone from NO_X emission reductions is smaller with the older mechanisms, like RADM2, compared to the newer SAPRC99 mechanism, and may include ozone increases in certain locations. There is no difference in the VOC control response between mechanisms.

Additional sensitivities are underway to further explore the reason for the chemical mechanism differences and to provide user guidance regarding the sensitivity results. Further exploration of the influence of vertical mixing on control strategy predictions will be undertaken.

2.3 Air Toxics Modeling

2.3.1 CMAQ Extensions to New Air Toxics Gaseous Species

The 1990 CAAA identified nearly 200 individual compounds or mixtures of compounds as hazardous air pollutants that have the potential for causing adverse health effects. Air quality models for predicting ambient concentrations of these toxic compounds are needed to provide human exposure estimates for both risk assessment and risk management. To obtain accurate estimates of the ambient concentrations of these compounds, the important processes that control their fate must be properly simulated. For many compounds, this necessitates inclusion of the chemical reactions that lead to the formation and transformation of those compounds in the atmosphere. The objective of this work is to add to CMAQ the capability to model specific gaseous toxic compounds.

Two approaches are being evaluated for modifying CMAQ to include gaseous toxic compounds. The first approach involves treating each toxic compound explicitly by including its atmospheric chemical reactions directly in the CMAQ chemical mechanism. This approach provides the most accurate representation of the atmospheric chemistry, but has the disadvantage of requiring chemical mechanism and solver modifications for each toxic compound that is added. A second approach involves approximating the atmospheric chemistry of the toxic compounds outside the chemical mechanism. This approach is preferable because the need for modifications to the core chemistry mechanism and solver are lessened and because the computational expense is lowered by not including the compound directly in the chemistry computations. This approach is also more amenable to generalization, which would facilitate adding new gaseous toxic compounds in the future. The major disadvantage is that it may not be feasible for those toxic compounds that have many chemical production and loss pathways, or for those compounds that react very fast.

During FY-2002, initial work was completed on incorporating 18 toxic compounds explicitly in CMAQ . Model tests were conducted both with toxics included explicitly in the mechanism and with the reactions of several toxics approximated outside the chemical mechanism. The results of these tests have shown that, of the 18 toxics considered, 14 compounds can be modeled outside the chemical mechanism with little loss in accuracy. The exceptions identified thus far are formaldehyde and acetaldehyde which have numerous loss and production pathways, and hence, must always be included in the mechanism explicitly. Two others, acrolein and 1,3-butadiene, are also included explicitly in the chemical mechanism because of their interactions (the atmospheric reaction of 1,3-butadiene leads to the formation of acrolein). To conduct these tests, both the SAPRC99 and CB-IV chemical mechanisms and associated MEBI chemistry solvers in CMAQ were modified to accommodate the inclusion of the toxic compounds. For most compounds, virtually identical results were obtained with either mechanism. This effort has laid the foundation for conducting a comprehensive modeling assessment of these compounds in FY-2003.

2.3.2 CMAQ Extensions to Semi-Volatile and Involatile Compounds

During FY-2002, a version of CMAQ was developed that simulates air concentrations and deposition for toxic congeners of Poly-Chlorinated Dibenzo-Furans and Dibenzo-p-Dioxins (PCDF's and PCDD's). The effort expanded upon previous research on atrazine (Cooter and Hutzell 2002; Cooter *et al.*, 2002) with appropriate modifications for dry deposition and atmospheric chemistry. The model represents each congener's mass in gaseous and aerosol forms that exchange mass based on theoretical coefficients for gas to particle partitioning. Gaseous forms undergo chemical transformations based on congener-dependent rate constants and concentrations of hydroxyl radicals determined by a chemical mechanism within CMAQ. Dry deposition removes all forms; however, wet deposition removes only particulate forms because gaseous forms have extremely low solubility in water. Dry deposition velocities for gaseous forms do not include effects from organic factors because their contribution is still uncertain.

This version of CMAQ was evaluated through simulations that covered July 1999. One part of the evaluation compared model predictions against observed air concentrations from the National Dioxins Air Monitoring Network (Cleverly *et al.*, 2000). Model predictions had good correlations with observations for lower chlorinated congeners of PCDF's, but had poor correlations with most PCDD congeners. Emission inventories could be the cause of these problems because PCDF and PCDD emissions have been historically difficult to identify and quantify (Cohen *et al.*, 2002). Model results were also evaluated regarding observed partitioning between gaseous to particle forms. Predictions reproduced observed values within observational and modeling uncertainties. A project by the National Center for Environmental Assessment may support further evaluations of the developed model. The Center will inter-compare predictions between several models that use an improved emissions inventory (National Center for Environmental Assessment, 2001).

2.3.3 CMAQ Mercury Model Refinements and Evaluation

During FY-2002, the first phase of an intercomparison study of numerical models for long-range atmospheric transport of mercury was completed and a second phase was begun. This study is being sponsored by the European Monitoring and Evaluation Programme (EMEP) and is organized by EMEP's Meteorological Synthesizing Center - East in Moscow, Russia. The first phase of the intercomparison involved the simulation of mercury chemistry in a closed cloud volume given a variety of initial conditions. Results obtained from the CMAQ mercury (CMAQ-Hg) model and the other participating models from Russia, Germany, Sweden, Canada, and the United States were compared to identify key scientific and modeling uncertainties. A project report previously submitted to the EMEP governing body was published (Ryaboshapko *et al.*, 2002). The second phase of intercomparison involves full-scale model simulations of the emission, transport, transformation, and deposition of mercury over Europe and comparison of the modeling results to field measurements of elemental mercury gas, reactive gaseous mercury, and particulate mercury in air. Comparison of the various model results against observations, and between the models, will continue into FY-2003.

During FY-2002, a number of minor modifications were made to CMAQ Hg to more efficiently calculate the gas-phase and aqueous-phase mercury chemistry in concert with the chemistry mechanisms in the latest published versions of the standard CMAQ code. These modifications were made in anticipation of a planned public release of CMAQ Hg scheduled toward the end of FY-2003.

During FY-2002, the results from a comparison of CMAQ Hg simulations against observations of wet deposition of mercury were published (Bullock and Brehme, 2002). Measurements of the wet deposition of mercury obtained from the Mercury Deposition Network (MDN) (Lindberg and Vermette, 1995; Vermette *et al.*, 1995) at 11 locations in the central and eastern parts of the United States were compared to the CMAQ-Hg simulations during each week of two 4-week periods in 1995. The results showed relatively good agreement between modeled and observed weekly wet deposition of mercury during the period from April 4 to May 2, 1995. However, during the period from June 20 to July 18, 1995, the agreement was found to be much weaker due to the inability of the meteorological driver, MM5, to accurately define small-scale convective precipitation elements at the 36-km grid cell size employed. Further CMAQ-Hg evaluation will be performed against MDN data collected in 2001 as the necessary MM5-derived meteorological input data become available.

2.3.4 Estimating Background Concentrations

In the 1990 CAAA, Congress established a list of 188 toxic chemicals designated as hazardous air pollutants (HAPs), also known as air toxics. These pollutants are associated with a wide variety of adverse health and environmental effects. The sources of the air toxics include major point sources, area sources, mobile sources, and transport from other areas. As part of the implementation of the CAAA, EPA manages the National-Scale Air Toxics Assessment (NATA), a nationwide study of the potential inhalation exposures and health risks associated with 32 HAPs and diesel PM. To estimate total ambient concentrations, however, a value for background must be estimated and added to modeled concentrations. As defined, background accounts for natural sources, nearby sources (farther than 50 km), and unidentified sources.

In the recently completed NATA, corresponding to calendar year 1996 emissions and meteorological data, estimates for background were determined from open literature. There are two limitations to this approach. First, estimates based on literature or data correspond to points in time that were far removed from the 1996 temporal scope of the recent NATA study. Second, the literature was used to identify a constant, nationwide background estimate for each HAP under study. It is believed that such an approach may not be realistic for those HAPs that are expected to exhibit spatially heterogeneous backgrounds across the United States. New and improved values for background need to be determined.

A study (Bortnick *et al.*, 2002) uses statistical algorithms to estimate background levels at different localities. Estimates were obtained for such localities with available data as California, Texas, and parts of the Northeast and East Coast. The challenges ahead include extrapolating these finding to the rest of the United States where there are few or no available monitoring data.

2.3.5 Urban-Scale Analyses

The 1990 CAAA Section 112(k) requires EPA to reduce hazardous air pollutant (HAP) risks in urban areas. The EPA's strategy for reducing these risks is discussed in the Integrated Urban Air Toxics Strategy (U.S. Environmental Protection Agency, 2002). To help understand the air toxics problem in an urban area, it is necessary to know the concentrations of air toxics to which people are exposed. Unfortunately, air monitoring data are scarce and limited. Another means for estimating HAP concentrations is through the use of air quality models. Urban areas can vary greatly in terms of the types of emission sources and the legal enforcement options provided by state and local programs to control air toxics emissions. Air quality models allow state and local agencies to test the effectiveness of alternative control measures in reducing ambient levels of toxic contaminants.

The intent of urban-wide air toxics modeling applications is to provide data inputs for use in exposure and risk calculations and prioritization, obtain a higher degree of geographic resolution than those obtained from national-scale studies, identify data gaps and help allocate resources toward particular issues of interest or concern, and support the planning and implementation of ambient air monitoring programs. Regarding the higher geographic resolution of assessment results, an important benefit of refinement by an urban-scale application is illustrated by considering the methods by which emissions data are applied to the models. To achieve the objective of a national-scale assessment within a feasible scope of time and resources, assumptions about emissions allocation are typically made to simplify the modeling. An example would be the allocation of unknown emission source locations to the centroid of the census tract. While this approach allows the national-scale assessment to broadly identify pollutants of potential concern across large geographical areas, the assigning of source locations or other sensitive parameters limits resolution. The urban-scale modeling effort is more localized and can compliment the national-scale assessment by increase in specificity. However, the number of assumptions made in urban-scale modeling precludes the use in specifying the individual sources that contribute to the total concentrations or the impact of specific sources in specific areas such as a neighborhood. For determining impacts of specific sources, more detailed analysis than is warranted in an urban-scale application is needed.

Urban areas contain major sources, numerous smaller area sources, and mobile source. As a result, modeling analyses for large numbers of air toxics sources possess special challenges. Although most HAPs are emitted directly, some are produced and destroyed through reactions in the atmosphere. These issues, as well as receptor selection, meteorological data processing, and background concentration selection pose significant technical challenges to the air quality modeler. Although many air quality models can be used for estimating urban wide ambient concentrations, this document deals with the applications of the Industrial Source Complex (ISCST3) model, a model that can estimate close distance impacts from industrial facilities. This model has been extensively used in analyzing impacts from a single or a few facilities and this report should help provide transition to the more complex issues associated with urban-wide applications. Several conclusions can be drawn from the results of this study:

- Increasing the receptor density near high emission sources changed the location of maximum concentrations between ISCST3 base and ISCST3 fine grid. The ISCST3 fine grid results also illustrated the concentration gradients that can occur near high emission sources. These findings illustrate the importance of the receptor placement and receptor density to model performance.

- Allocating the onroad mobile emissions to road segments can improve the model predicted concentrations when compared to monitor observations. The benzene ISCST3 base underpredicted the average concentrations at the seven monitors. Road segment allocation (ISCST3 Roads) resulted in better model-monitor agreement and also changed the location of maximum concentrations when compared to ISCST3 base. Allocating onroad mobile emissions to road segments also increased the maximum total concentration for formaldehyde but as seen in Figure 4, the nonroad mobile concentrations still dominated the maximum total concentration.

- Higher concentrations are located near the higher emission regions for the five HAPs presented. A majority of the high emissions were located in eastern and northern Harris County, as were the higher concentrations. Among the five HAPs, the trend is that the HAPs with higher emissions also have higher maximum concentrations in the near-field.

- It is important that emission inventory development continue to be refined in order to define emission parameters, sources, emission amounts, and locations for input into dispersion models. This will aid in improving model predictions and their use in assessing exposure to toxic pollutants and designing emission control strategies for toxic air contaminants.

2.4 Fine-Scale Modeling

2.4.1 Urban Canopy Parameterization in MM5

Urban canopy parameterizations (UCPs) are being developed and implemented in MM5 to improve fine-scale (~1-km grid spacing) simulations. This effort is important to ultimately improve the pollutant transport for neighborhood-scale CMAQ simulations that will be linked to modeling human exposure to airborne toxic pollutants. The UCPs involve changes to the momentum and energy budgets in MM5, as well as acquisition and implementation of various databases on the urban morphology of the modeled cities. The UCPs in MM5 leverage the published work of international scientists.

In FY-2002, research continued on a UCP that was initially developed and implemented in MM5 in the previous fiscal year. This UCP is targeted for applications of MM5 that are on the order of 1-km horizontal grid spacing. This UCP accounts for the drag exerted by urban structures, the increase of turbulent kinetic energy particularly near the tops of buildings, and the changes to the energy budget due to anthropogenic heating and the absorption and emission of radiation within the urban canopy (*i.e.*, from the surface to the tops of buildings). In FY-2002, the energy treatment was extended, and a preliminary evaluation of the UCP on Philadelphia was performed. Details of the UCP and preliminary results from the application on Philadelphia are described in Lacser and Otte (2002) and Otte and Lacser (2002). In addition, development began of an advanced UCP that includes coupling with an urban soil model, SM2-U, to add a more sophisticated and specific treatment of the energy balance in the urban areas as well as a treatment of vegetation and rural zones within the modeling domain. Initial tests of the advanced UCP in MM5 used the same Philadelphia study as the UCP described above. A more rigorous evaluation of the advanced UCP is planned for FY-2003 using Houston.

In preparation for the Texas 2000 modeling study, a detailed database of the urban morphology for Houston and the surrounding areas was purchased. Several key parameters were identified (*e.g.*, building density and height, vegetation density and height, plan area density, and many more). The processing of the morphology database is expected to be completed in early FY-2003.

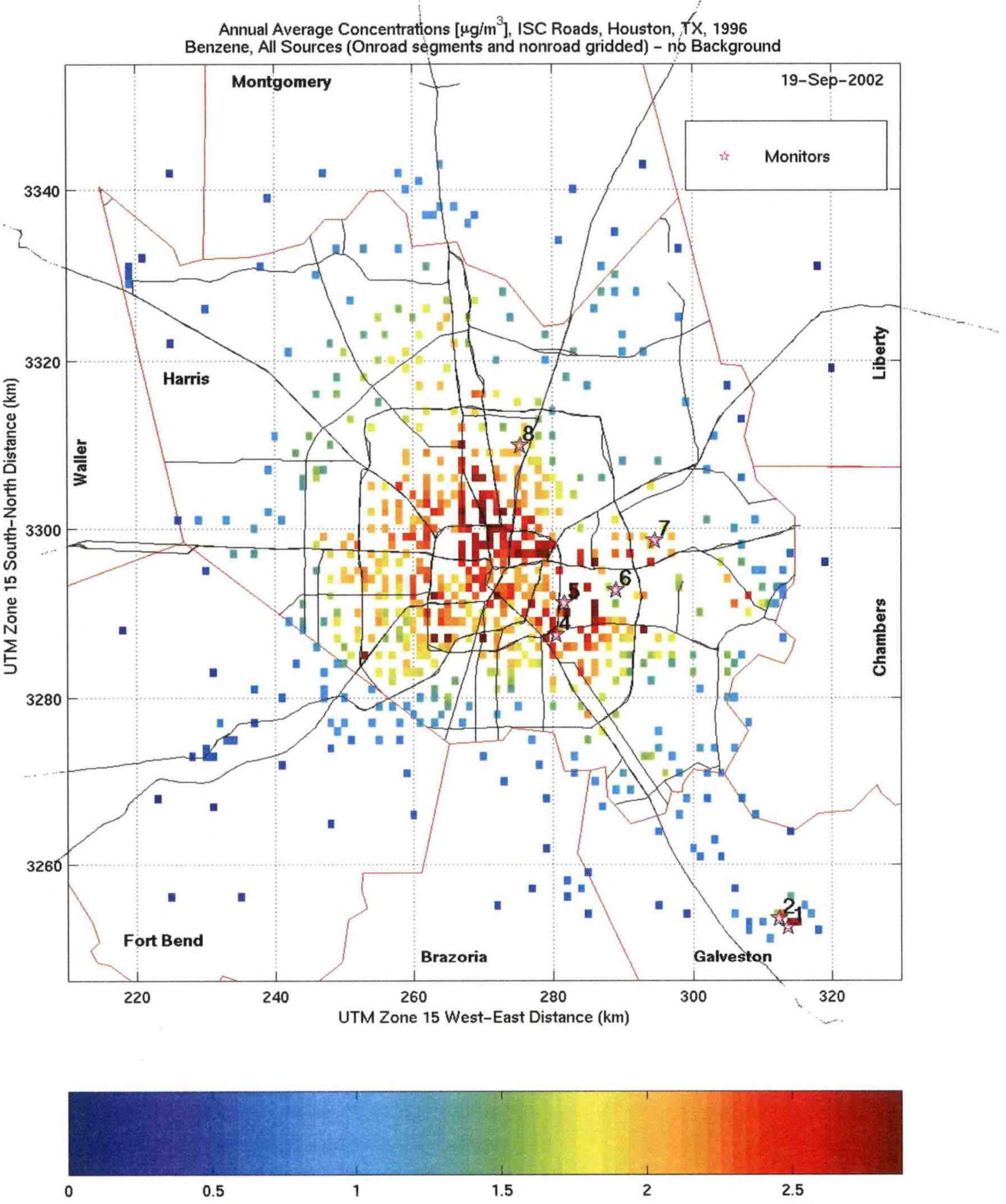

Figure 4. Annual average concentrations using ISC Roads for Houston, Texas, 1996, benzene, all sources (onroad segments and nonroad gridded) with no background.

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

Air quality simulation models provide a basis for developing and implementing the NAAQS and are tools for performing risk-based assessments for air toxics and developing and testing environmental management strategies. Both $PM_{2.5}$ and airborne air toxic pollutants have characteristically different degrees of spatial and temporal variability, especially in urban areas and different geographical-climatic regimes. The performance of human exposure assessments requires the capability for air quality model simulations at neighborhood scales for situations where pollutants can exhibit higher spatial and temporal variability than currently modeled. Exposure models will need concentration fields at neighborhood scale resolution to address such issues as environmental justice and community-based risk assessments, and conduct hot spot analyses. The Models-3/CMAQ system has been used in multiscale simulations to span a range of grid resolutions from 36 (or 32) km to 4 km to provide concentration distributions at regional to urban scales respectively. Also, exposure models are currently using either limited amounts of monitoring data and or crude dispersion modeling tools. Thus, there is a need to improve the capability of the modeling tools to provide accurate simulations at neighborhood scale resolutions.

In this study, the requirements are explored for modeling air quality at neighborhood scales. This effort investigates the science and operational requirements for running CMAQ at about 1-km grid resolution. Another requirement is the development of stochastic methods to handle additional concentration variability that arise from within grid sources and atmospheric processes. Recognizing that much of the attention for exposure assessments will be focused in urban areas, it is important to ensure that the flow fields in urban areas are accurately modeled, including the effects of heterogeneous building features in urban areas. A prototype UCP at neighborhood scales (~1 km horizontal grid spacing) was introduced into the PSU/NCAR Mesoscale Model Version 5, (MM5), which provides the meteorological fields for the chemistry-transport model in CMAQ. UCP is based on the drag approach, and is applied to grid cells in MM5 that have a non-zero fraction of urban land use. For this investigation, a model domain and study area were centered on the Philadelphia Metropolitan Area and MM5 and CMAQ were run for simulations at horizontal grid dimensions of 36 km, 12 km, 4 km, and 1.33 km. The 1.33-km simulation represents the neighborhood scale. The introduction of the UCP parameterization produced significant differences in the predicted mean and turbulent fields within the urban canopy, especially in areas characterized by high density of tall buildings. The MM5, with UCP, simulations of vertical profiles of wind speed and turbulent kinetic energy were highly consistent with results from wind tunnel studies. Results illustrate the importance of accounting for the urban morphological structures in modeling the flow in urban areas. It provides a basis for more accurately resolving the magnitude and spatial details of the modeled air quality fields, especially for pollutant species that may have fine spatial gradients that are important for human exposure assessment.

During the course of the study, it was found that the introduction of a new mixing length parameterization applied to the basic urban canopy parameterizations provided a means to eliminate spurious wave-like features in the meteorological fields and subsequent pollutant fields at 1.33-km grid resolution. Thus, with UCP in MM5, a limited set of pollutant concentration fields using CMAQ were examined, including NO_x, ozone, several PM species (including particle numbers for fine and accumulation modes), formaldehyde, and acetaldehyde. It was found that the spatial representation of the concentration fields to enhanced grid resolution was different for different pollutant species. For most pollutant species, the increased grid resolution from 4-km to 1.33-km resulted in enhancements to coarse resolution features and the emergence of additional spatial features, accompanied by an increase in the magnitude of the concentration distribution pattern. For example, in the simulation for NO_x, the concentration features for the areas of dense mobile sources and point sources were considerably sharpened both in terms of horizontal gradients and magnitude at 1.33-km resolution. Consequently, the simulations showed a corresponding decrease in ozone due to the effect of titration from the high NO features. While the simulations for PM mass were relatively insensitive to increased grid resolution, the number of aitken mode particles as predicted by the model exhibited spatial enhancements. The simulation of formaldehyde and acetaldehyde demonstrated that modeling these (and other toxic pollutants) at fine resolution can lead to identification and details of toxic pollutant hot spots. This project is a multi-year study. Several ongoing efforts underway are:

- refinements to modeling UCP at neighborhood scales,
- development of subgrid parameterizations, and
- model evaluation studies.

A new set of UCPs will be introduced into an advanced urban-soil canopy-air model, SM2-U (Dupont, 2001), to be subsequently implemented in MM5/CMAQ. These refinements will be applied to the Houston, Texas, area and tests performed against the Texas 2000 air quality study database. An important component of this study is the production of a new set of gridded, high resolution urban canopy parameters needed by the SM2-U model, and is to be based on building and tree canopies data for Harris County and the Houston Ship Channel area (derived from airborne lidar measurements). This effort is underway under a contract with the University of Arkansas, Fayetteville, Arkansas. The effort to formulate methodologies to produce the sub-grid concentration distributions is directed towards development of probability density functions (PDFs) for the CMAQ grids. Studies continue on deriving the PDFs for the sub-grid scale variability from turbulence-induced concentration fluctuations using large-eddy simulation (LES) techniques (Herwehe, 2000) and dispersion of point and area sources from street canyon flows, using a combination of computational fluid dynamics (CFD) and wind tunnel modeling techniques. Ultimately, using these modeled PDFs, various statistical parameters (*e.g.,* peak-to-mean ratios) and spatial structure functions of the variability as a function of the building morphology will compliment the CMAQ grid predictions. Initial results to date have focused on the results of using the coupled LES with the chemistry model (LESchem). They provide indications that this form of variability is governed by the chemical reactivity of the species, the atmospheric pollutant mixture, and the turbulent intensity and structure of the mixed layer. In addition to the Texas 2000 study, a collaboration was begun with the Ecole Centrale Nationale of the University of Nantes, France, for studies relevant to the neighborhood scale modeling project. This effort involves evaluation of neighborhood scale modeling techniques using a special database called ESCOMPTE, a major European sponsored intensive field study program. The

ESCOMPTE database (Mesteyer, 2002) contains specialized urban-canopy scale boundary layer and chemical measurements made in Marseilles, France, in 2001.

2.4.3 Modeling the World Trade Center Disaster Site

The September 11, 2001, destruction of the World Trade Center (WTC) in New York City resulted in the release of a large volume of airborne pollutants in the form of fugitive PM and various combustion products. These emissions persisted at varying degrees for weeks and months after the initial catastrophic event. This event has elevated the need for reliable models to predict concentrations of such contaminants within complex urban areas. Pollutant monitoring alone cannot provide the temporal and spatial details generally needed for exposure assessments and associated risks due to unplanned releases in urban regions. Models are critical for providing timely and reliable estimates of human exposures. The successful development and evaluation of such models demands relevant laboratory and/or field measurements of flow and dispersion in a variety of urban settings. Toward this database development goal, a laboratory study has been initiated in the Fluid Modeling Facility's meteorological wind tunnel to characterize the near and mid-range distribution of concentrations of pollutants emitted from the WTC site. The study will provide both flow and concentration fields for comparison against those estimated by CFD models being developed and tested both within the Division and by collaborators in other national laboratories. This site-specific and detailed study of the WTC surroundings, in conjunction with previous (and more generic) building-array, wind-tunnel studies, is integral in the attempts to understand the variability of concentrations in complex urban areas as part of the neighborhood scales program (Ching *et al.*, 2002). The laboratory study consists of eight main components:

1. study design;
2. preparation of the wind tunnel instrumentation and development of an appropriate approach flow boundary layer;
3. construction of the scale model of Lower Manhattan and the WTC rubble-pile source area, and installation on the turntable within the meteorological wind tunnel;
4. establishment of Reynolds number independence within the narrow street canyons of Manhattan;
5. extensive visible and laser-enhanced smoke visualizations of releases from the WTC site;
6. vertical profiles of flow (velocities, turbulence, Reynold stresses) at approximately 30 to 40 selected locations within the city;
7. tracer releases and associated concentration measurements throughout and downwind of Lower Manhattan; and
8. analysis and documentation.

The current study design includes data collection for three wind directions relevant to the climatology of the Lower Manhattan area during the months following September 11, 2001.

During mid to late FY-2002, the first four study components were completed and the smoke visualizations were initiated. A 1:600 scale model of Lower Manhattan has been constructed and placed into the Meteorological Wind Tunnel (Figure 5). This model represents the full width (Hudson to East Rivers) of the southern most 2 kilometers of Manhattan Island. In addition to the many buildings, structures, and general roughness features of the city, the model includes an emulation of the WTC rubble pile with smoke emissions that were common for weeks after the collapse (Figure 6). The approach flow boundary layer has a depth of approximately 1.8 m with a 0.16 power law wind profile. The wind profile and approach flow roughness elements relate to a full scale roughness length of approximately 0.1 m. For the wind directions of this study, the actual approach to Manhattan is first over the relatively flat areas of suburban New Jersey followed by 1 to 3 kilometers of water.

Figure 5. A 1:600 scale model of Lower Manhattan as it appears on the turntable within the Meteorological Wind Tunnel.

Figure 6. Neutrally-buoyant smoke released from nine positions within the simulated World Trade Center rubble pile.

Prior to including the scale model in the wind tunnel, a series of experiments were performed (Heist, 2002) to examine the flow and turbulence characteristics within some generic urban-like landscapes. This preliminary study was focused on an investigation of the Reynolds number independence within street canyons similar to the most extreme ones found in Manhattan (very narrow and deep). For the street canyon widths as little as 5 to 6 cm in this urban model, the study suggests that a freestream velocity of 4.0 ms^{-1} is needed to maintain sufficiently high Reynolds numbers (approximately 10,000) for flow independence. Smoke visualization for the first wind direction was initiated in late FY-2002. These qualitative studies will help in identifying the important flow features and in the final design of the flow and dispersion sampling arrays. Figures 7 depicts a neutrally-buoyant smoke release from the WTC site with flow from left to right and with visible light illuminating the smoke. This example, for a wind direction of 270 degrees, shows plume material almost immediately vented upward by the flow features associated with the tallest buildings in the vicinity of the site. Because of this, much of the resultant plume is lofted well above the buildings by the time the material passes beyond the downwind urban boundary. The laboratory study is expected to be concluded in mid FY-2003 with data made available for model comparisons by late FY-2003.

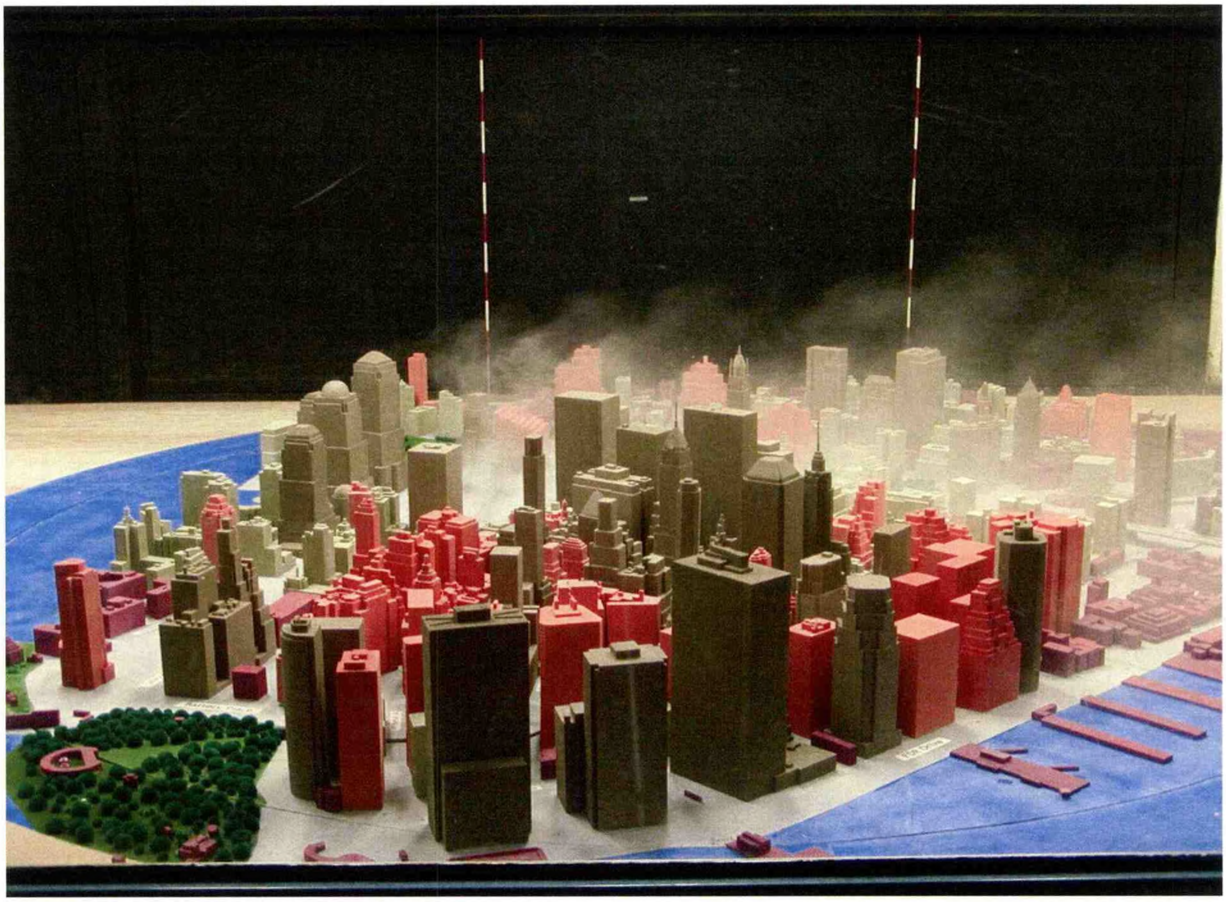

Figure 7. Smoke visualization for neutrally buoyant release from the simulated World Trade Center site (release area just left of center in this photo); flow is from left to right.

2.4.4 Meteorological Measurements Near the World Trade Center

The Meteorological Instrumentation Cluster of 3 (MIC3) portable trailers (10-m Tower instrumented for winds and temperature at 3 levels; AV Model 4000 miniSODAR; and AV Model 2000 SODAR) operated on Pier 25 near ground zero in Lower Manhattan from November 2001 through April 2002 (Figures 8 and 9). Observations from this equipment are being used to supplement routine meteorological observations and model applications for the surrounding New York City area to support assessments of the environmental impact of emissions from ground zero. These measurements provide the only data above the surface for assessing meteorological models and for providing boundary conditions for fine scale numerical simulations necessary to support human exposure assessment studies.

2.4.5 Estimating the Plume from the World Trade Center Recovery Site

A general characterization of the dispersion of the PM from the WTC recovery site in the ambient air during the three months following the September 11, 2001, events was completed. Hourly estimates of plume transport and unit source dilution were made using a blended observational and dispersion modeling approach. A derivative of the CALMET-CALPUFF dispersion model was employed to simulate the plume dilution for a 50-km x 50-km square area surrounding Lower Manhattan. This modeling was completed in collaboration with the North Carolina State Climate Office at North Carolina State University, Raleigh, North Carolina. An example hour-average plume and the plume averaged over the full study period are presented in Figures 10 and 11. The results of this 3-month simulation were developed to support the 2002 assessment of the environmental impact of the events following September 11, 2001. The plume characterization study has been very valuable in supporting the human health assessment studies.

A digital model replication of all buildings south of Canal Street in lower Manhattan was developed using licensed digital information from Vexcel Corporation, Boulder, Colorado. Meteorological information from both the EPA (two SODAR's and a 10-m tower) and U.S. Bureau of Land Management sites (six 2-m stations) in Lower Manhattan are being displayed with monitored PM concentrations to examine the influences of meteorology on air pollution concentration levels. Figure 12 displays a 1-hour example of these data within the building model. The lower left hand corner of the picture includes the winds reported at the five National Weather Service sites in the metropolitan area. A digital model of each building has been developed to support construction for wind tunnel model studies and the computation fluid dynamics numerical simulations studies of the fine-scale pollution dispersion near ground zero, which will be completed during FY-2003.

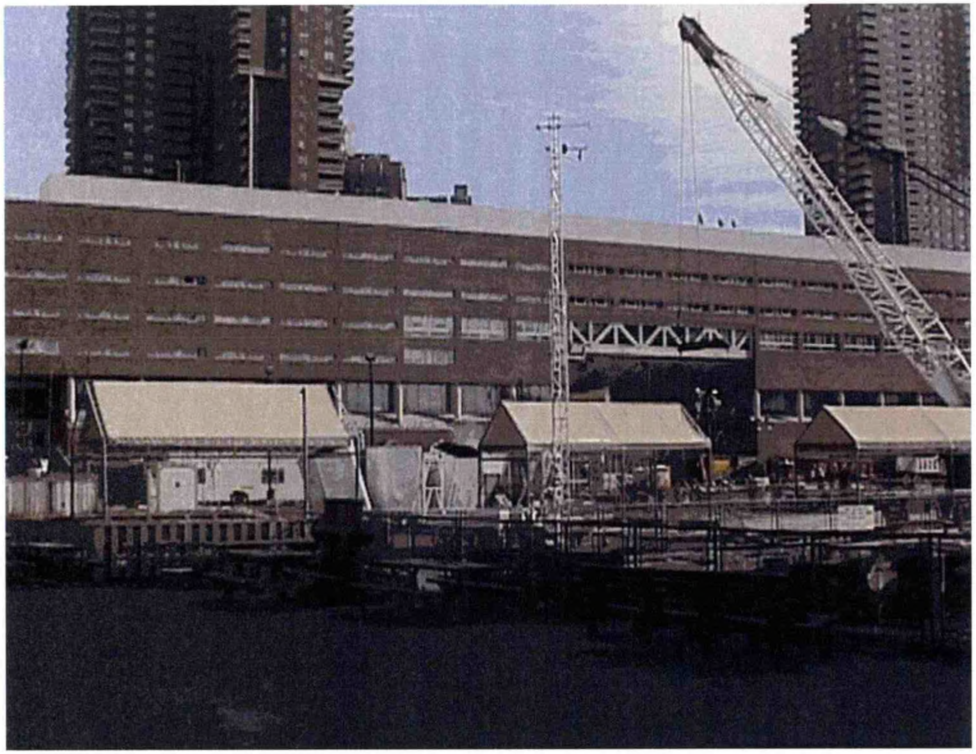

Figure 8. View of the Meteorological Instrumentation Cluster along the Hudson River looking Southeast.

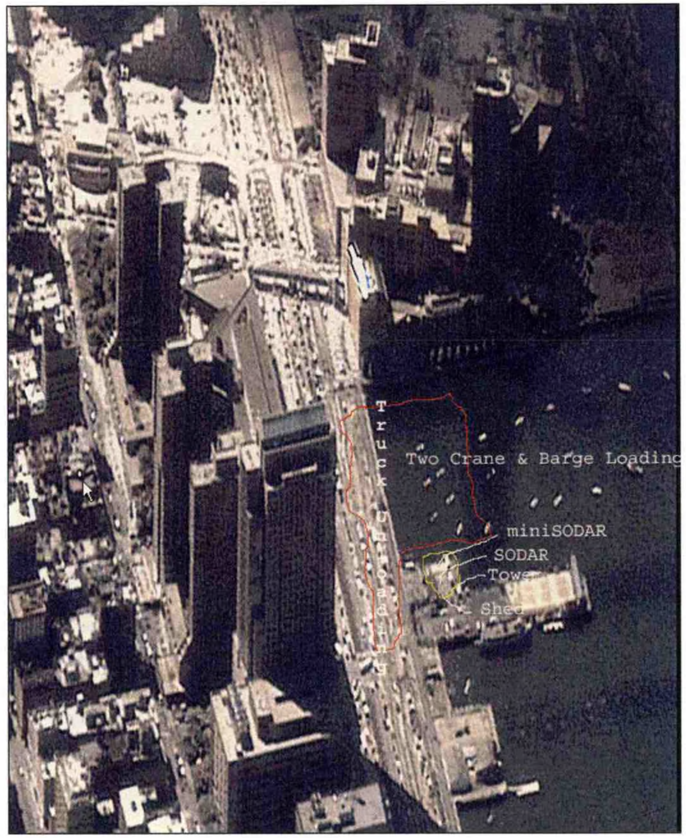

Figure 9. View of the Meteorological Instrumentation Cluster from above Pier 25.

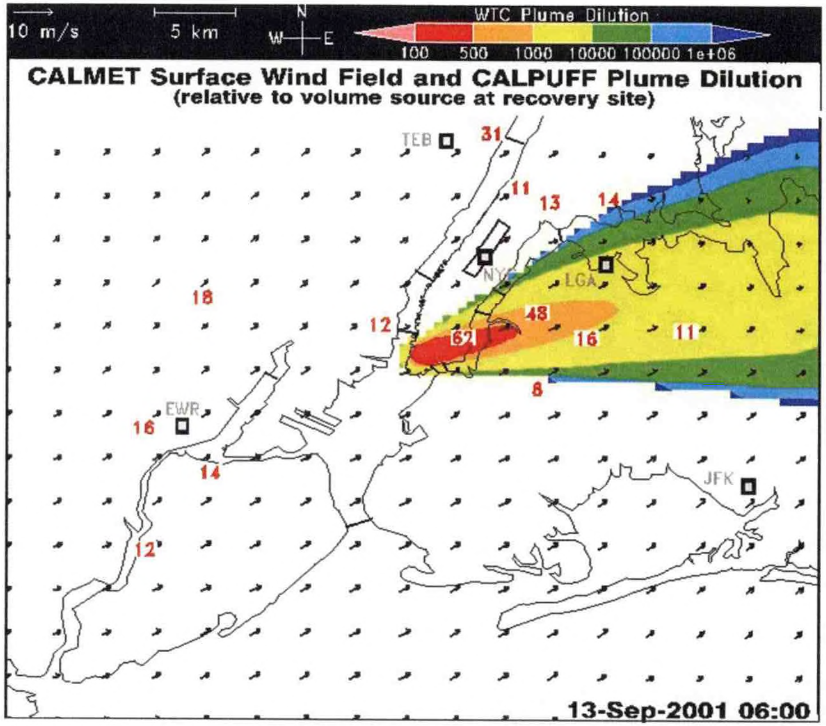

Figure 10. Map (50-km by 50-km centered on ground zero) of example 1-hour averaged plume dilution of a volume source from ground zero. Red numbers are $PM_{2.5}$ hourly measurements.

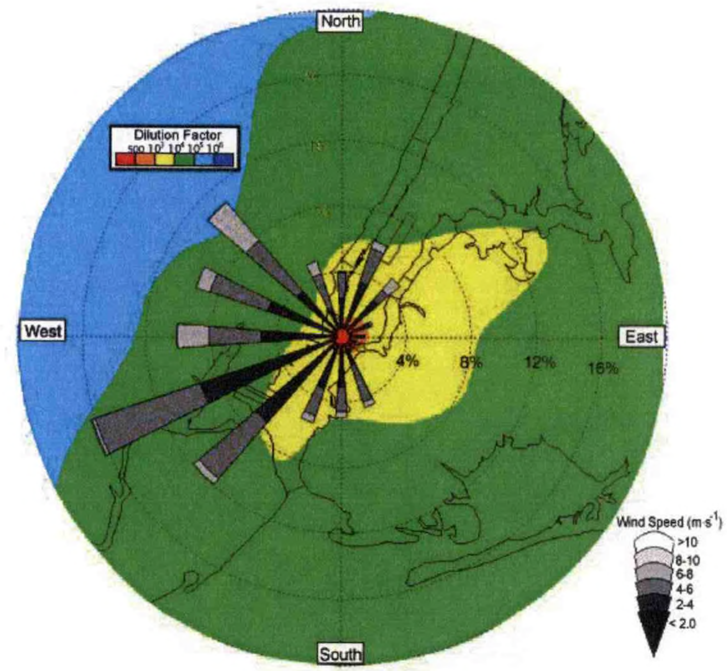

Figure 11. Map of September 11, 2001, through December 8, 2001, averaged plume dilution of a volume source from ground zero. The wind rose is presented for this same period.

Figure 12. An example display of meteorological and particulate matter concentrations with the 3-dimensional model of buildings for the Lower Manhattan area.

2.5 Multimedia Modeling

2.5.1 Develop Tools to Support Sensitivity and Uncertainty Studies

Estimating the sensitivity of models to their inputs and the effect of input uncertainties on model results provides valuable information for model developers and decision makers. Unfortunately, estimating such values can be difficult, typically requiring the execution of numerous simulations and the interpretation of their results. An even more common challenge is to execute simulations for many different situations, such as time periods, management strategies, or locations. In this case, the analysis of the results might not be as complex as it is for sensitivity and uncertainty analysis, but the management of simulations can still be a significant problem.

To support modelers who perform modeling studies that require repetitive computations, ASMD developed new capabilities for the Multimedia Integrated Modeling System (MIMS). MIMS supports the composition, configuration, application, and evaluation of complex systems of models. MIMS addresses some of the data management, software engineering, and mechanical bottlenecks that limit people's ability to perform large modeling studies, allowing them to focus more attention on essential policy, scientific, and modeling issues. The primary new capabilities that support repetitive simulations are composite models, general approaches for iteration, and the ability to execute models on remote computers.

Often a set of models and/or associated processors versus a single model are required to address an issue. This set of models forms a conceptual unit that is used in larger studies. For instance, a set of models that predicts the response of an estuary to watershed management practices might then be used as part of a sensitivity study to identify management actions that have a significant effect on the estuary's health. To simplify the process of composing models, the MIMS team developed capabilities that allow modelers to identify a set of models and programs that should be treated as one model. This allows modelers to compose complex simulations from hierarchical units, similar to how programmers organize functionality into subroutines.

Sensitivity analysis, uncertainty analysis, calibration, optimization, and application of a model to a series of data sets all have the common aspect of running a model repeatedly for different input data. To support all of these activities, the MIMS team designed and implemented generic support for iteration in the form of an abstract class that provides the common behaviors required for iteration. These common behaviors include providing user interfaces to connect inputs and outputs and managing the execution of simulations. Specific types of iteration are implemented by extending the abstract class and specifying three primary behaviors: 1) initialization of the iteration, 2) processing the result of one simulation, and 3) finishing the iteration. The first two behaviors can specify inputs for simulations that should be performed. When there are no more simulations to be performed, the third behavior is invoked. This design supports all types of iteration and allows developers to easily add new types of iteration to MIMS. To evaluate this design, the team implemented iterators for Monteo Carlo studies and for list of values. The team also worked with collaborators who are developing an urban drainage decision support system prototype in MIMS, to help them implement advanced uncertainty and nonlinear optimization iterators in MIMS. Iterators can apply to any model, which can include composite models consisting of a number of programs.

For some types of studies, thousands of model executions might be required. When inputs for multiple simulations can be specified simultaneously, it is possible to expedite such studies by utilizing multiple computers. Monte Carlo studies, sensitivity studies, and simulations of different, independent locations are examples of problems where task parallel processing can be beneficial. To support task parallelism on multiple computers in MIMS, the team created a general design for executing programs that allows easy implementation of new approaches for working with remote computers. This design allows users to easily specify that their simulations should be executed on multiple computers. The team implemented support for MIMS controlling computations on remote computers via secure shell. Additional methods for distributing computations, such as utilizing Condor®[7](http://www.cs.wisc.edu/condor/),will be supported in the future.

The MIMS team has also developed a variety of capabilities that were required to support applications in MIMS. These capabilities included generating model control text files by combining a user-supplied template and model input parameters, reading and writing columnar files containing time-series data, and basic plotting.

2.5.2 Development of Compartmental Modeling Tools for Toxics

The release, transformation, transport, and environmental fate of toxic pollutants are an inherently multimedia chain of events. FY-2002 multimedia research, regarding fully coupled, multimedia, dynamic, hybrid compartmental models, focused on the development and implementation of a pilot compartmental modeling tool under the MIMS framework. Programming support was provided by the Argonne National Laboratory and consultative assistance was provided by Multimedia Envirosoft Corporation, Los Angeles, California. The Three Compartment Model (3cm) application builds, solves, and displays the results of a system of ordinary differential equations (ODEs), describing the dynamic movement of chemical mass through multiple media (Figure 13)—a significant functional extension of the previous MIMS framework.

The 3cm multimedia system includes uniform air, water, and biota (fish) compartments. The initial test case follows the movement of chlorobenzene, a volatile organic chemical used as a solvent and in the production of other chemicals, through air and water media to Alewife (prey) and Salmon (predator) endpoints. The initial simulation period spans 3-summer months (~2160 hours) for a water body with geographic characteristics similar to Lake Michigan and climatological conditions similar to Detroit, Michigan. The 3cm is not intended to accurately reproduce observed chemical concentrations, but 1) to test the ability to implement the modeling approach under the MIMS framework, 2) begin modification of an existing commercial model configuration, MEND-TOX (Cohen and Cooter, 2002a; 2002b) to facilitate integration with air quality model development research, and 3) facilitate comparison of pilot results to a previous modeling study. The 3cm makes extensive use of the general approach described in Cohen and Cooter (2002a), but was developed entirely in-house, *i.e.*, no propriatary code. Modifications to Cohen and Cooter (2002a) include the addition of a linear food-chain model, use of alternative algorithms to increase compatibility with other ASMD modeling activities, and the introduction of dynamic time varying media volumes and meteorology. The biota model includes fish growth, uptake of chemical in the water via the gills, mechanical uptake via feeding, egestion and degradation. The published MEND-TOX model employs air/water mass transfer algorithms valid only for a neutral atmosphere. This was replaced with a more flexible stability-dependant

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[7]Condor is a trademark of Condor Team, University of Wisconsin-Madison

estimate similar to that used by CMAQ. Effects of water surface roughness (characterized by Reynolds number) on mass transfer and temperature dependent chemical diffusivity, neither of which are prominent in CMAQ (U.S. Environmental Protection Agency, 1999) but present in MEND-TOX, were included in the 3cm. The use of dynamic (hourly) boundary layer height and meteorological conditions is a marked departure from the traditional application of the compartmental modeling approach, but compliments other ASMD research.

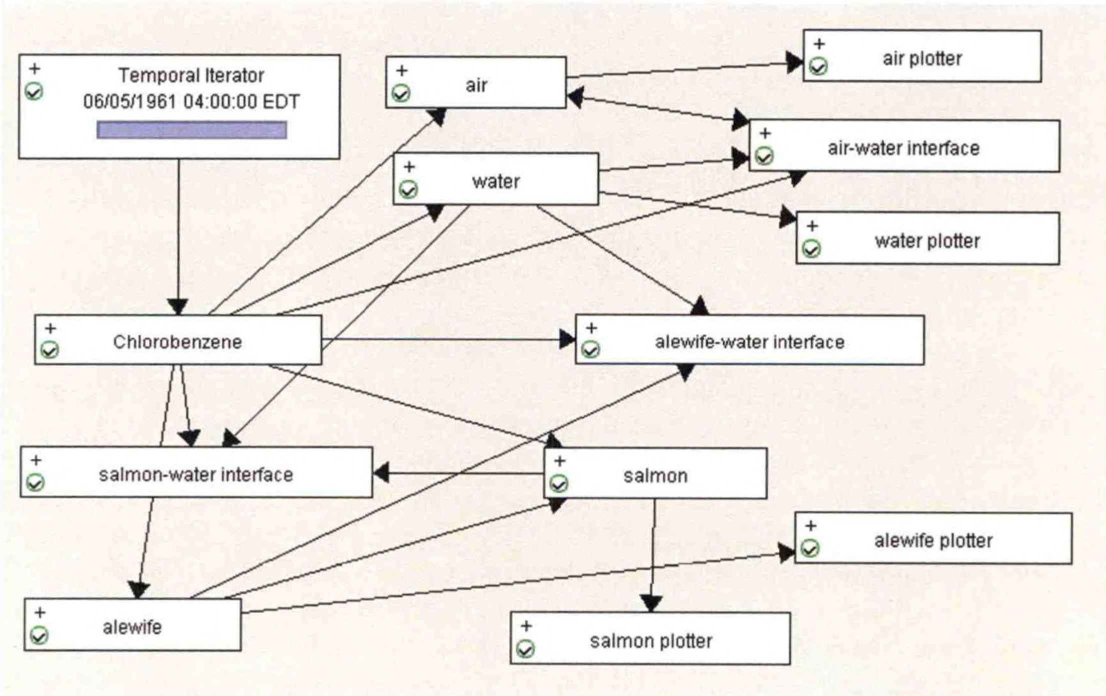

Figure 13. The pilot Three Compartment Model (3cm) as implemented under the MIMS framework.

Model building activities during FY-2002 included code checking and quality assurance, installation and testing of the public domain ODE solver LSODE (Livermore Solver for Ordinary Differential Equations) under the MIMS framework, and several multimedia system performance checks to establish that at chemical steady state agreement exists between numerical and analytical solutions. This later test revealed additional coding errors that were corrected, and established appropriate error tolerance limits for the ODE solver.

There are still several outstanding implementation issues. For instance, initial interest in this modeling approach stemmed from its combination of significant mechanistic detail with simulation speed. The 3cm application simulation is unacceptably slow. The original 3cm pilot was overly input/output bound and coding errors resulted in LSODE convergence errors. Once corrected, some speed improvement has been achieved, but the system is still much slower than the more complete Fortan 90 MEND-TOX implementation. This shortcoming will need to be resolved to achieve the system performance required for the long-time period, large-domain applications required by ASMD clients. A second unanswered question is the impact of dynamic media volumes and meteorology on the assumption of local equilibrium. Similar questions have arisen with regards to the semi-volatile partitioning model developed for the CMAQ toxics. Their solution will be studied for possible adaptation in the 3cm. A final question concerns variable process time-steps across media. This issue has been raised, but has not been adequately answered by the 3cm model. It gains importance as the FY-2003 task begins of adding multi-phase, non-uniform media to the pilot system, *e.g.,* sediment, soils. Coupling of uniform and non-uniform media will require definition of a new system of partial differential equations (PDEs) whose solution will require implementation of a PDE solver in MIMS, the definition of appropriate boundary condition expressions and development of an acceptable uniform/non-uniform media coupling paradigm.

2.5.3 Urban Drainage Decision Support System Prototype

A 2-year cooperative agreement was awarded in FY-2002 to develop and test the integration of the Storm Water Management Model (SWMM) with decision support tools to identify cost-effective and reliable watershed management strategies. A team of scientists from MCNC Environmental Programs, North Carolina State University, and University of North Carolina at Chapel Hill are the recipients of the cooperative agreement. The team is using the MIMS framework as an integration platform for developing the prototype urban watershed decision support tools. The prototype is being designed with local and city planners who manage urban point and non-point sources as potential users.

During the first year of the cooperative agreement, work was underway to design and implement the decision support and analysis tools. Included are such uncertainty analysis tools as a Monte Carlo and Latin Hypercube approach for uncertainty propagation, importance sampling, and uncertainty importance estimation. Several optimization approaches based on genetic algorithms are being tested as well. These uncertainty and optimization tools will be integrated into the MIMS framework during FY-2003 for use with SWMM and other models within MIMS. Also during FY-2002, code development, testing, and management approaches were established for quality assurance and control of the software development. Finally, the integration of SWMM with the uncertainty and optimization tools is planned for FY-2003 along with the testing of the coupled system in a case study of Rouge River near Detroit, Michigan. This case study will address many of the use-case scenarios for which the system is designed.

2.6 Global Climate Change Impacts on Air Quality

This project was initiated in FY-2002 and will directly contribute to the EPA Global Change Research Program's (EPA GCRP) assessment of global climate change impacts on air quality. The Division's role in the assessment is to simulate regional emissions and air quality, specifically ozone and PM, using CMAQ. The planned products for this effort are designed to provide results and analysis in a timely manner for the EPA GCRP 2007 air quality assessment report. FY-2002 activities included:

EPA GCRP Workshop on Global Climate Change Impacts on Air Quality. During December 5–2001, an EPA GCRP workshop was held that included scientists from universities, national laboratories, and other research organizations. Approaches for studying the influence of global climate change on air quality were discussed. It was decided that an incremental analysis would be necessary. In the first phase, the impact of climate change would be assessed without the added influence of future scenarios of emissions and land use. In the second phase, future emission scenarios would be included in the CMAQ simulations to consider the additive effects. It was also determined that multi-year simulations would be necessary during current and future periods to capture the climate change signals. Based on these points, a detailed methodology was developed during FY-2002 for the first incremental analysis of the air quality assessment, where all other factors except climate change remain unaffected.

STAR Request for Assistance. ASMD worked closely with the EPA GCRP in the development of a Request for Assistance (RFA) funding solicitation on global climate change and air quality. Cooperative agreements will be awarded in FY-2003 to groups doing research with global climate models and chemical transport models. Collaboration with recipients of this RFA will be necessary for linkages with CMAQ and the air quality assessment.

Regional Climate Downscaling Effort. To support this project and ultimately the air quality assessment, EPA GCRP is funding the Department of Energy's (DOE) Pacific Northwest National Laboratory (PNNL) to develop current and future regional climate simulations. These simulations will rely on MM5 with initial and boundary conditions from global climate simulations under current and future Intergovernmental Panel on Climate Change (IPCC) greenhouse gas scenarios.

Based on these activities, the primary outcome for FY-2002 was to finalize the approach for the assessment of climate change on air quality. The project approach will first focus on developing linkages of the meteorology with Global Climate Models (GCMs). DOE's PNNL will be performing regional climate modeling simulations using MM5 with information from several GCMs, including the NASA (National Aeronautics and Space Administration) GISS (Goddard Institute for Space Studies) models as boundary conditions and large-scale input. Simulations will be performed for a reference period (*e.g.*, 1995 ± 5 years) and a future period under climate change conditions (*e.g.*, 2050 ± 5 years). As regional climate modeling simulations become available, ASMD will archive the data and develop the model-ready meteorology fields needed for CMAQ and the emissions processor SMOKE (Sparse Matrix Operator Kernel Emission)[8].

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[8]Copyright 2000 MCNC - Environmental Modeling Center

During FY-2003, test simulations will be performed with the NASA GISS GCM under a future IPCC greenhouse gas emission scenario. By analyzing GCM output from a current year through 2050, it will be determined how many years of CMAQ simulation are needed to separate out the influence of climate change trends from interannual variability. The GISS simulations will include passive tracers to follow stagnation events in addition to a standard analysis of temperature and mixing height changes. Results from this analysis will be used to finalize the decision regarding the number of years of CMAQ simulation necessary for the analysis of climate change impacts on air quality.

Once the EPA STAR cooperative agreements are awarded in FY-2003, ASMD will identify collaborators for linking global chemical transport model (GCTM) results with CMAQ. It is anticipated that a GCTM will be used to provide initial and boundary conditions for ozone, PM, and related precursors. These activities will be ongoing during FY-2003–04, followed by the development of model-ready emissions for CMAQ based on base emission factors for current conditions and the regional climate simulations for current and future periods. CMAQ simulations for the first incremental analysis of global climate change effects on air quality without future air quality emission scenarios will then be performed and analyzed during FY-2005–07 for the 2007 EPA GCRP assessment report.

2.7 Specialized Client Support

2.7.1 Community Modeling and Analysis System Center

In FY-2002, efforts continued under the cooperative agreement between EPA and the MCNC North Carolina Supercomputing Center to establish and operate the Community Modeling and Analysis System (CMAS) in support of the Models-3/CMAQ modeling system. CMAS is crucial to the growth and sustenance of the CMAQ user community for collaboration in model improvements, training, and support. During FY-2002, CMAS staff established the basis for operation, including an 18 member External Advisory Committee (EAC) representing the user community, an Internet support site featuring model documentation, e-mail based user support, and online links to relevant modeling news (www.cmascenter.org). EAC consists of members representing state regulatory agencies, academia, industry, air quality consultants, foreign users, and ex officio EPA members. The web site provides a community-based Models-3/CMAQ Help Desk. Supported Models-3/CMAQ features include the CMAQ CTM, SMOKE, the Input Output/Applications Programming Interface convention that allows Models-3 system components to pass information, and MIMS interface for optional use with CMAQ and SMOKE. To guide the efforts, protocols were prepared and reviewed by EAC for intellectual property, testing, and acceptance of new Models-3/CMAQ components, membership, and user support. Recognition of CMAS by the Models-3/CMAQ user community has grown substantially. There are now users in at least 25 states and 6 foreign countries. In addition, a complementary Models-3/CMAQ applications support center is being established at the University of Waterloo in Waterloo, Ontario, Canada. CMAS planned a CMAQ User's Workshop and training courses for CMAQ, SMOKE, and MIMS, for October 21–23, 2002.

2.7.2 American Meteorological Society/Environmental Protection Agency Regulatory Model Screening Tool

During FY-2001 and FY-2002, an effort was underway to develop a procedure based on AERMOD that would be easy to implement and would provide worst-case surface concentration estimates of inert species released from a point source, where relatively simple transport and diffusion plume models are appropriate. The procedure would provide concentration values that would in general be greater than AERMOD would predict, if the application of AERMOD was tailored to the particular location and terrain (*i.e.,* run in a refined mode). Such screening tools have traditionally been used to provide a fast estimate of worst-case concentration values from which one can assess whether a more refined modeling assessment is needed.

Given the treatment of the interplay between the seasonal variation of local land-use and its effect on the profiles of wind and temperature within the AERMOD modeling system, it was decided to replace the meteorological processing requirements with the screening tool for AERMOD. A two-step plan was devised. In step one, a team of Federal and State air quality modelers proficient in the refined application of AERMOD applied the AERMOD modeling system to over 20 locations in the United States and its territories. From these analyses, a database of worst-case meteorology was complied for the sources simulated, which ranged from area and volume sources to point sources with various stack heights and buoyancy release conditions. In the second step, a Fortran-based program called MakeMet was developed that would generate worst-case meteorology, which were to be close to that determined through the actual application of AERMOD.

In conducting the analyses, it became apparent that novice users of AERMOD would have difficulty determining the characteristics of the land use and the variation of these land use characteristics over a 1-year period. To resolve this, another team was formed to develop a Fortran program called AirSurface that would compute the land-use characteristics for inhomogeneous (*e.g.,* is a mixtures of forested areas, water bodies, urbanize areas), and provide effective values of the land-use characteristics averaged over the domain of application of the AERMOD modeling system. Following the investigations of Batchvarova and Gryning (2001) and Batchvarova *et al.* (2001), methods were derived for computing these effective values. To complete this analysis, an uncertainty assessment was conducted to determine the number of significant figures needing to be reported so as to provide a realistic expectation of when differences are significant. It was determined that one significant figure is likely sufficient, especially since it is difficult to specify these inputs to less than 30 percent uncertainty even with on-site instrumentation and from land-use maps. Work is ongoing to develop and test the programs MakeMet and AirSurface. It is anticipated that versions of these programs will be released for public testing and evaluation during the Summer of 2003.

2.7.3 Joint Action Group for Selection and Evaluation of Atmospheric Transport and Diffusion Models

In December 2001, the Office of the Federal Coordinator for Meteorology (OFCM) hosted the *Workshop on Effective Emergency Response-Selecting a Suitable Dispersion Model for a Given Application.* The participants considered what kinds of models are used in specific situations and how atmospheric transport and diffusion (ATD) modeling systems are evaluated. The goal of the workshop was to define a framework for supporting the objective determination of the most appropriate dispersion modeling system to be used in a given situation. This workshop served as the impetus for the OFCM to lead the Federal ATD modeling community in a concerted effort to evaluate the ATD models available to address typical threats.

In January 2002, OFCM formed the Joint Action Group for Selection and Evaluation of Atmospheric Transport and Diffusion Models (JAG/SEATD) and charged the participants with the following tasks: review the ATD modeling systems in use by the Federal agencies at operational modeling centers; conduct a preliminary analysis of gaps in understanding of the processes on which the modeling systems are constructed; recommend areas for research and development to improve the Nation's capabilities to use ATD modeling systems in response to the terrorist threat; review the ATD model evaluation processes used by the agencies; and review plans to conduct field experiments. JAG was constituted from representatives of all Federal agencies actively employing atmospheric dispersion models for emergency response applications. The agencies included several arms of the Departments of Defense and Energy, the Environmental Protection Agency, the Federal Emergency Management Administration, Nuclear Regulatory Commission, and NOAA. The JAG/SEATD met monthly through July 2002, and summarized its findings in a report (Hicks *et al.*, 2002).

The JAG/SEATD members coordinated with modelers, emergency managers, and first-responders to understand the needs of decision makers and the end-users. The emergency managers and first-responders require the best available information regarding the spatial extent and timing of hazardous areas. Key decisions are usually made within the first hour of an incident. Therefore, because timeliness of dispersion forecasts is critical, the dispersion services and products that are needed must be available in time to be used in the decision-making process. The modeler requires the best available information regarding the characterization of the source and the physical environment.

While there are over 140 documented ATD models that are used for regulatory purposes, research and development, and emergency operations, the JAG/SEATD narrowed the list to only 29 non-proprietary modeling systems that are used operationally either by first-responders and/or at the Federal operational modeling centers. These 29 modeling systems were the focus of the JAG/SEATD's evaluation. The JAG/SEATD noted that there are differences among the operational modeling systems and that none encompassed the entire breadth of needs. Moreover, the JAG/SEATD noted important differences between the basic requirements confronting military and civilian developers of the dispersion forecasting methodologies. It was further noted that the two major civilian capabilities operate from opposite shores, with the DOE capability operating from California and the NOAA system from the Washington, DC, area.

After careful examination of the end-user and decision-maker's needs, eight scenarios were developed for review. The scenarios covered a wide range of potential threats and exercised a variety of model capabilities. For each scenario, individual modeling system applicability was evaluated over two spatial scales (local and mesoscale), two modeling environments (urban and rural), and three temporal scales (immediate response, intermediate response and short-term planning, and recovery and long-term planning). The evaluation included an assessment of the availability of data for model evaluation.

The analysis of the gaps in the understanding and capabilities of the ATD modeling systems yielded factors that require further research and development. The factors range from source characterization to the study of the effects of complex terrain, coastal influences, and urban areas. Four barriers to progress were identified: the not invented here barrier, the military-civilian barrier, the education barrier, and the emergency response/public communications barrier. Efforts to bridge those barriers are addressed in the JAG/SEATD report. Modeling system evaluation procedures were reviewed, and general guidelines of what needs to be considered in the evaluation of ATD models were developed. The JAG/SEATD concluded that the quality assurance planning, documentation, and scrutiny should be consistent with the intended use.

2.7.4 AERMOD Screening Model Comparison

A series of SCREEN3 model runs were performed using the cavity option to compare results from the SCREEN3 cavity concentration with AERMOD cavity concentrations. The purpose of this effort was to assess the cavity results from both models, since the AERMOD screening model, AERSCREEN, may not be ready when AERMOD is released. About 38 SCREEN3 model runs were made with different building sizes, urban/rural options, and other specifications. Preliminary comparisons indicate SCREEN3 cavity results are both higher and lower than the AERMOD cavity results. On-going study is required to detect patterns or trends in the various building configurations and their results.

2.7.5 Modeling Significant Increases in Concentrations of $PM_{2.5}$

Analyses were performed of modeling the concentration of $PM_{2.5}$ to determine the increase in emissions needed to affect a significant increase in concentrations for a range of point, area, and volume sources. Estimates were provided for both primary particulate emissions and precursor emissions (SO_2 for ammonium sulfate and NO_X for ammonium nitrate). The latter is a unique and, perhaps, a first time application of the precursor option in CALPUFF. These analyses were completed in support of policy making for the New Source Review. Similar analyses are anticipated in support of the EPA's Regional Haze Regulations.

2.7.6 Developing Statistical Forecasting Methods for $PM_{2.5}$

Public saturation of real-time ozone mapping and forecasting programs have fueled the demand for increased coverage of air quality and health information. Providing advanced warning of unhealthy air quality to the public is becoming increasingly important for EPA, as well as for state and local air quality agencies. Ozone forecasts now appear regularly in *USA TODAY*, or on *The Weather Channel*, and in other local media for many parts of the United States during the ozone season.

Division staff are managing a project designed to extend the forecasting efforts to fine PM by developing city-specific air quality forecasting techniques for 21 major metropolitan areas in the United States. The goal is to develop statistical models relating the increasingly available, continuous, real-time $PM_{2.5}$ ambient data to various meteorological scenarios, with an eye toward generation of next-day public health advisories using the EPA's Air Quality Index. In addition to the development of the regression-based forecasting tools, the project is in the process of transferring the relevant software and knowledge bases to the state and local air quality agencies that will be ultimately responsible for issuing air quality alerts.

2.7.7 NARSTO Program Support

The NARSTO program is a multinational, public/private partnership of over 70 organizations sponsoring and participating in ozone and particulate air quality research in North America. The coordination of communication and planning activities for air quality research, science plans, and state-of-science assessments with the NARSTO membership are important tasks performed by the NARSTO managers. ASMD provides a full-time associate management coordinator for the NARSTO program. Part of the management function includes project officer duties on an interagency agreement with the DOE's Oak Ridge National Laboratory to provide infrastructure support to the NARSTO program, assistance agreements related to the SOS program, contracts for technical support, and grants to the National Research Council. The associate management coordinator also provides technical assistance and leadership to the NARSTO Quality System Science Center, which is charged with developing and maintaining the NARSTO permanent data archive as well as a comprehensive quality management system.

An ASMD scientist serves as a co-chair of the NARSTO Modeling and Chemistry Team. As part of those duties, several NARSTO document reviews were conducted, including the internal review of the NARSTO PM Assessment and a review of a major report done under a Coordinating Research Council contract for NARSTO in which several ozone models were compared. The scientist was invited to write a descriptive analysis (conceptual model) for particulate concentrations in the northeastern United States for the NARSTO PM Assessment Report.

The principal authors of the NARSTO state-of-science suspended PM assessment met at the University of Minnesota in Minneapolis to discuss the comments from the National Research

Council's (NRC) review of the draft NARSTO report. NARSTO received the NRC review report in September and with all the comments received, the Assessment team began the process of producing a final report. All comments were discussed at the intensive meeting and each author was given the task of responding to the comments as determined by the team. The 500 page report, to be available on CD, will be formally released at the American Association for Aerosol Research meeting on March 30, 2003, in Pittsburgh, Pennsylvania.

2.7.8 European Monitoring and Evaluation Program

A Division scientist serves as the United States representative to the European Monitoring and Evaluation Program (EMEP) that oversees the cooperative program for monitoring and evaluation of the long-range transmission of air pollutants in Europe. The primary goal of EMEP is to use regional air quality models to produce assessments evaluating the influence of one country's emissions on another country's air concentrations or deposition. The emphasis has shifted from acidic deposition to ozone and there is now interest in fine particulates and toxic chemicals. The United States and Canadian representatives report on North American activities related to long-range transport. The Division scientist also evaluates European studies of special relevance to the program, providing technical critiques of the EMEP work during formal and informal interactions, and develops and coordinates such programs with EMEP as the modeling studies of the Modeling Synthesizing Center West at the Norwegian Meteorological Institute in Oslo, Norway.

2.8 Regulatory Support

2.8.1 Support Center for Regulatory Air Models

During FY-2002, the SCRAM (Support Center for Regulatory Air Models) website was modified to comply with the official EPA web page template, as directed by the Office of Environmental Information. Although the web site files and technical materials within SCRAM remained nearly the same, infrastructure modifications affected all web pages. Some additional links were created to provide easier maneuvering to specific models and related files. Thirteen SCRAM products were added and/or modified during FY-2002. Most of these changes were beta test files related to the work resulting from the *7th Modeling Conference for Air Quality Modeling* (http://www.epa.gov/scram001/tt26.htm). SCRAM serves as the sole Internet source for the EPA's air quality dispersion models, guidance, and related programs and information.

2.8.2 Trajectory Analyses

A plan was developed to use the HYSPLIT4 (Hybrid Single-Particle Lagrangian Integrated Trajectory) model to help determine possible source locations for high PM fine values for some of the EPA trends network. Initially, as part of the plan, the HYSPLIT4 model was run over several sites and a number of time periods using EDAS (Eta Data Assimilation System) and FNL (Final) meteorological data. These data were plotted simultaneously and analyzed to determine the approximate differences in running the model utilizing different meteorological fields.

The execution of the plan was completed for three sites. Trajectories were run for an approximate 2-year time period over the years 2001 and 2002 using the EDAS data set as the primary data and FNL as a backup. This involved running the trajectory model numerous times at different levels and different starting times within a 24-hour period. Analyses were then performed on the trajectories to help determine source locations of high PM fine values.

2.8.3 Effects of Additional VOC/NO_x Reductions in 2010

A series of modeling analyses were completed to examine the impact of further precursor reductions on future levels of 8-hour ozone over the eastern United States. The air quality model used to conduct the analyses was the Comprehensive Air Quality Model with Extensions version 3.10 (CAMx). Three sets of additional precursor reductions were layered atop the proposed 2010 Clear Skies Initiative control scenario. The modeling analyses were intended to answer three main questions:

1. How effective will additional low-level anthropogenic NO_x, anthropogenic VOC, or combined emissions reductions be in reducing 8-hour ozone concentrations from the levels to be achieved through existing and planned regional and national controls?

Based on the modeling analyses, it was determined that additional low-level anthropogenic NO_x, anthropogenic VOC, and/or combined emission reductions will generally be effective in reducing 8-hour ozone concentrations above and beyond the levels to be achieved through existing and planned controls. For instance, the number of projected nonattainment areas is decreased from 53 in the 2010 Clear Skies control case, to 40 areas after 35 percent low-level anthropogenic VOC control, to 27 areas after 35 percent low-level anthropogenic NO_x control, and to 19 areas after a 35 percent combined strategy.

2. Will reducing anthropogenic VOC help to reduce ozone in all projected 8-hour ozone areas?

Major metropolitan areas in the northern United States are expected to be responsive to additional VOC control. For example, the extent of the projected nonattainment area is reduced by 22 percent in Boston and 18 percent in Chicago after the imposition of a 35 percent low-level anthropogenic VOC reduction. Conversely, urban areas in the southern United States, which generally contain large quantities of biogenic VOC, are less responsive to VOC controls. For instance, modeled ozone levels in Atlanta are only reduced by 1 to 3 percent when low-level anthropogenic VOC emissions are cut by 35 percent. Other southeastern metropolitan areas essentially show no change when VOC is reduced.

3. In 2010, are there areas where further NO_x reductions beyond existing and planned controls might result in increased ozone?

There are some areas where further NO_x reductions beyond existing and planned controls might result in increased ozone. In particular, the urban centers of Chicago, Detroit, and New York City showed increases in projected future ozone peaks when NO_x alone was reduced by 35 percent. That said, regional NO_x control is generally beneficial. For example, the extent of the projected nonattainment area (grid cells >= 85 ppb) is reduced by 65 percent in Boston and 19 percent in Chicago after the imposition of a 35 percent low-level NO_x.

2.8.4 Operational Evaluation of Proposed Clear Skies Initiative Ozone Modeling

EPA is applying CAMx to estimate the degree of future year ozone nonattainment of the NAAQS with and without the emissions reductions associated with the proposed Clear Skies Initiative. As part of this analysis, three 1995 base case episodes were simulated at resolutions of 36 km and 12 km. An operational evaluation was completed consisting entirely of comparisons against surface ozone data for the entire domain, as well as several dozen subregions.

At the synoptic scale, the model was found to exhibit little overall bias (-2.1 percent) or error (21.1 percent). However, for some of the individual subregions, particularly those that included coastal areas, model biases and errors approached +/- 40 percent. Unlike similar regional modeling applications, the model did not appear to exhibit any trend in bias over the course of the episodes. Ultimately, the model was deemed acceptable for use in a relative sense, *i.e.,* for projecting changes in future year air quality.

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APPENDIX A: ACRONYMS, ABBREVIATIONS, AND DEFINITIONS

ACM	Asymmetric Convective Model
AE3	Aerosols component version 3
AERMIC	American Meteorological Society/Environmental Protection Agency Regulatory Model Improvement Committee
AERMET	AERMOD Meteorological Preprocessor
AERMOD	AERMIC Model
AERSCREEN	AERMOD screening model
ARL	Air Resources Laboratory
ASMD	Atmospheric Sciences Modeling Division
ASPEN	Assessment System for Population Exposure Nationwide
ATDD	Atmospheric Turbulence and Diffusion Division, NOAA
AVHRR	Advanced Very High Resolution Radiometer
BCON	Boundary Concentrations
BELD	Biogenic Emissions Land cover Database
BELD-3	Biogenic Emissions Land cover Database version 3
BEIS-3	Biogenic Emissions Inventory System version 3
BRACE	Bay Regional Atmospheric Chemistry Experiment
CAA	Clean Air Act
CAAA	Clean Air Act Amendments
CALMET-CALPUFF	A diagnostic meteorological model/puff dispersion model
CAMx	Comprehensive Air Quality Model with extensions
CB-IV	Carbon Bond version 4
CCM	Community Climate Model
CIRA	Cooperative Institute for Research in the Atmosphere
CMAQ	Community Multiscale Air Quality modeling system
CMAQ-Hg	Community Multiscale Air Quality modeling system mercury model
CMAS	Community Modeling and Analysis System
CONSUME	A fuel consumption model, which predicts total smoldering fuel consumption during wild fires.
CSEM	Community Smoke Emission Model
CTM	Chemistry-Transport Model
DOE	Department of Energy
EDAS	Eta Data Assimilation System
EMEP	European Monitoring and Evaluation Program
EPA	Environmental Protection Agency
ESCOMPTE	A European sponsored intensive field study program
Eta	National Center for Environmental Prediction Mesoscale Model
Extended RADM	Regional Acid Deposition Model with full dynamics of secondary inorganic fine particle formation taken from the RPM
FDDA	Four-Dimensional Data Assimilation

FY	Fiscal Year
GCM	Global Climate Models
GCRP	Global Change Research Program
GCTM	Global Chemical Transport Model
GIS	Geographic Information System
GISS	Goddard Institute for Space Studies
HAP	Hazardous Air Pollutant
HYSPLIT4	Hybrid Single-Particle Lagrangian Integrated Trajectory model
ICON	Initial Concentrations
IPCC	Intergovernmental Panel on Climate Change
ISORROPIA	A computationally efficient thermodynamic model
LADCO	Lake Michigan Air Directors Consortium
LES	Large-eddy simulation
LESchem	LES with the chemistry model
LSODE	Livermore Solver for Ordinary Differential Equation
M3DRY	Models-3 Dry Deposition Scheme
MARAMA	Mid-Atlantic Regional Air Management Association
MCIP	Meteorology-Chemistry Interface Processor
MCIP2	Meteorology-Chemistry Interface Processor version 2
MDN	Mercury Deposition Network
MEBI	Modified Euler Backward Iterative
MEND-TOX	Multimedia Environmental Distribution of TOXics
MIC3	Meteorological Instrumentation Cluster of 3
MIMS	Multimedia Integrated Modeling System
MM5	Mesoscale Model - version 5
Mobile6	Mobile Source Emission Model
MOVES	**M**ultiscale m**O**tor **V**ehicle and equipment **E**mission **S**ystem
MPRM	Meteorological Preprocessor for Regulatory Modeling
NAAQS	National Ambient Air Quality Standards
NALCC	North American Land Cover Characteristics
NASA	National Aeronautics and Space Administration
NATA	National Air Toxics Assessment
NCAR	National Center for Atmospheric Research
NEI	National Emission Inventory
NERL	National Exposure Research Laboratory
NHEERL	National Health and Environmental Effects Research Laboratory
NLCD	National Land Cover Database
NOAA	National Oceanic and Atmospheric Administration
NO_x	Nitrogen oxides
NPS	National Park Service
NRMRL	National Risk Management Research Laboratory
NSR	New Source Review
NWS	National Weather Service
OBMs	Observations-Based Methods

ODE	Ordinary Differential Equation
OFCM	Office of the Federal Coordinator for Meteorology
OTAG	Office of Transportation and Air Quality
PBL	Planetary Boundary Layer
PCDF's	Poly-Chlorinated Dibenzo-Furans
PCDD's	Poly-Chlorinated Dibenzo-p-Dioxins
PCM	Parallel Climate Model
PDE	Partial Differential Equation
PDFs	Probability Density Functions
PDM	Plume Dynamics Model
PinG	Plume-in-Grid
PinG Module	Plume-in-Grid Model
PM	Particulate Matter
PNNL	Pacific Northwest National Laboratory
PX LSM	Pleim Xiu Land-Surface Model
QSSA	Quasi-Steady State Approximation
RADM2	Regional Acid Deposition Model version 2
RFA	Request for Assistance
RPM	Regional Particulate Model
SAPRC99	A gas-phase chemical mechanism
SCRAM	Support Center for Regulatory Air Models
SM2-U	An urban soil model
SMOKE	Sparse Matrix Operator Kernel Emission model
SOA	Secondary Organic Aerosol
SOS	Southern Oxidants Study
SWMM	Storm Water Management Model
TexAQS	Texas Air Quality Study of Houston
TKE	Turbulent Kinetic Energy
TMDL	Total Maximum Daily Loan
TTCP-CBD	The Technical Cooperation Program (TTCP) Chemical, Biological and Radiological Defense (CBD)
UCPs	Urban Canopy Parameterizations
USFS	U.S. Forest Service
USGS	U.S. Geological Survey
VOC	Volatile Organic Compounds
WRF	Weather Research and Forecast
WTC	World Trade Center

APPENDIX B: PUBLICATIONS

Athanassiadis, G., S.T. Rao, J.Y. Ku, and R. Clark. Boundary layer evolution and its effects on ground-level ozone concentrations. *Preprints, 4th Conference on Atmospheric Chemistry: Urban, Regional and Global-Scale Impacts of Air Pollutants, January 13–17, 2002, Orlando, Florida.* American Meteorological Society, Boston, 97–102 (2002).

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APPENDIX C: PRESENTATIONS

Benjey, W.G. Status and support: Community Multiscale Air Quality model. Presentation at the Department of Physical Chemistry, University of Waterloo, Ontario, Canada, November 2, 2001.

Benjey, W.G. Models-3/CMAQ and SMOKE status. Presentation to the NARSTO Reactivity Research Working Group, Research Triangle Park, NC, January 17, 2002.

Benjey, W.G. CMAS status and emission modeling progress. Presentation to the Standing Air Emission Working Group, Coeur d'Alene, ID, April 3, 2002.

Benjey, W.G. Community Analysis and Modeling System (CMAS) Center progress and support to the modeling community. Presentation at the U.S. Department of Agriculture, Forest Service Research and Development, Atmospheric Sciences Research Program Meeting, Fairfax, VA, August 14, 2002.

Benjey, W.G. Overview of SMOKE updates. Presentation to the Standing Air Emission Working Group, Stowe, VT, September 25, 2002.

Bullock, O.R., Jr. CMAQ-Hg model simulations of mercury in the closed cloud volume. Presentation at the 6th International Conference on Mercury as a Global Pollutant, Minamata, Japan, October 18, 2001.

Bullock, O.R., Jr. Atmospheric mercury—Modeling the source media of a multi-media problem. Mercury Roundtable (monthly multi-agency conference call), November 20, 2001.

Bullock, O.R., Jr. Eulerian-type atmospheric mercury model development at the U.S. EPA Office of Research and Development, CEC/IJC (North American Commission for Environmental Cooperation/International Joint Commission) Workshop on Atmospheric Mercury: Science and Policy, Research Triangle Park, NC, December 14, 2001.

Bullock, O.R., Jr. Atmospheric mercury model development at the U.S. EPA, Office of Research and Development. Combustion Assistance Teleconference for Support (conference call organized by the Combustion Technical Assistance Center, January 17, 2002.

Bullock, O.R., Jr. Accuracy and sensitivity of atmospheric mercury simulations using CMAQ. Presentation at the Air & Waste Management Association Speciality Conference, Mercury: Consequences for Environment and Health, Montreal, Canada, March 5, 2002.

Bullock, O.R., Jr. Modeling atmospheric mercury emission, transport, transformation and deposition. Presentation at the Committee on Environment and Natural Resources, Air Quality Research Subcommittee Meeting, White House Conference Center, Washington DC, April 18, 2002.

Ching, J.K.S. Air toxics-PM modeling at neighborhood scales. Presentation at the French-American Workshop on Air Quality Modeling, Rice University, Houston, TX, October 4, 2001.

Ching, J.K.S. Neighborhood scale air toxics and exposure modeling. Presentation at the ISEA 2001 Symposium, Charleston, SC, November 7, 2001.

Ching, J.K.S. Neighborhood scale modeling project. Seminar presented at the Atmospheric Sciences Modeling Division, Research Triangle Park, NC, November 27, 2001.

Ching, J.K.S. Information issues for urban scale modeling. Presentation at the Office of Federal Coordinator for Meteorology Workshop on Strategy for Providing Atmospheric Information, Urban Air Quality Modeling, Crystal City, VA, December 3, 2001.

Ching, J.K.S. Air toxics modeling at neighborhood scales to support human exposure. Presentation at the Coordinating Research Council Air Toxics Modeling Workshop, The Woodland, TX, February 27, 2002.

Ching, J.K.S. Air quality modeling at neighborhood scales: A conceptual framework. Presentation at the University of Houston, Houston, TX, February 28, 2002.

Ching, J.K.S. Neighborhood scale air toxics modeling (Prototype) for human exposure and community-based assessments. Poster presentation at the Environmental Protection Agency, Research Triangle Park, NC, June 11, 2002.

Ching, J.K.S. Modeling sub-grid air pollution concentration distributions in air quality models. Presentation at George Mason University, Fairfax. VA, July 10, 2002.

Ching, J.K.S. Neighborhood scale modeling. Briefing for the Air Toxics Modeling Group, Office of Air Quality Planning and Standards, Environmental Protection Agency, Research Triangle Park, NC, August 20, 2002.

Ching, J.K.S. Neighborhood scale modeling project. Presentation at the University of Nantes (Ecole Centrale Nationale), France, September 19, 2002.

Dennis, R.L. Ammonia deposition and airsheds and their relation to inorganic nitrogen deposition. Presentation at The Second International Nitrogen Conference: Optimizing Nitrogen Management in Food and Energy Production and Environmental Protection—N2001, Potomac, MD, October 15, 2001.

Dennis, R.L. Atmospheric nitrogen deposition and coastal systems. Presentation at the EPRI Air Quality Area Council Meeting, Washington, DC, October 24, 2001.

Dennis, R.L. Effects of the Clean Air Act, Phase 1, controls on sulfate air concentrations and the ability of CMAQ to replicate the changes. Presentation at the Lake Michigan Air Directors Consortium Regional Planning Organization Meeting, Chicago, IL, November 8, 2001.

Dennis, R.L. Preliminary evaluation of CMAQ on visibility. Presentation at the Lake Michigan Air Directors Consortium Regional Planning Organization Meeting, Chicago, IL, November 8, 2001.

Dennis, R.L. Preliminary evaluation of CMAQ for fine particulate. Presentation at the Lake Michigan Air Directors Consortium Regional Planning Organization Meeting, Chicago, IL, November 8, 2001.

Dennis, R.L. Preliminary results of the diagnostic evaluation of CMAQ for ozone. Presentation at the Lake Michigan Air Directors Consortium Regional Planning Organization Meeting, Chicago, IL, November 8, 2001.

Dennis, R.L. Inverse modeling of ammonia emissions. Presentation at the Lake Michigan Air Directors Consortium Regional Planning Organization Meeting, Chicago, IL, November 8, 2001.

Dennis, R.L. Oxidized-nitrogen and reduced-nitrogen budgets and airsheds. Presentation at the Nitrogen Research Workshop, University of Maryland Center for Environmental Science, Frostburg, MD, December 11, 2001.

Dennis. R.L. Atmospheric deposition of nitrogen as a contributor to coastal eutrophication: How far away it comes. Presentation at the 82nd Annual Meeting of the American Meteorological Society, Orlando, FL, January 15, 2002.

Dennis, R.L. Background on MM5 and CMAQ for the BRACE study. Presentation at the BRACE (Bay Regional Atmospheric Chemistry Experiment) Workshop, University South Florida College of Public Health, Tampa Bay, FL, February 19, 2002.

Dennis, R.L. PM model evaluation studies: Air quality model evaluation. Presentation at the National Research Council Implementation Panel Review, Research Triangle Park, March 12, 2002.

Dennis, R.L. Model evaluation of CMAQ for acidic deposition and fine particles. Seminar at the U.S. EPA Clean Air Markets Division, Washington, DC, May 29, 2002.

Dennis, R.L. Evaluation of the acidic wet deposition predictions of CMAQ. Presentation at the 2002 Spring American Geophysical Union Meeting, Washington, DC, May 31, 2002.

Dennis, R.L. Delineating the connection between airshed and watershed pathways. Presentation at the Air & Waste Management Association Section Meeting, Jupiter, FL, September 16, 2002.

Dolwick, P.D. CMAQ modeling at U.S. EPA Office of Air Quality Planning and Standards: Proof of concept modeling. Presentation at the Midwest Regional Planning Organization, Des Plaines, IL, November 8, 2001.

Dolwick, P.D. OAQPS CMAQ modeling: Review, preliminary results, next steps. Briefing for the Director, Office of Air Quality Planning and Standards, Environmental Protection Agency, Research Triangle Park, NC, October 22, 2001.

Dolwick, P.D. U.S. EPA meteorological modeling activities. Presentation at the Midwest Regional Planning Organization, Des Plaines, IL, November 8, 2001.

Dolwick, P.D. U.S. EPA Office of Air Quality Planning and Standards meteorological modeling activities. Presentation at the Ad Hoc Meteorological Modeling Group, Des Plaines, IL, July 30, 2002.

Dolwick, P.D. Summary of Clear Skies Initiative ozone performance evaluation. Presentation to the Regional Planning Organizations (by phone), August 20, 2002.

Dolwick, P.D. U.S. EPA Office of Air Quality Planning and Standards meteorological modeling activities. Presentation at the U.S. EPA/OAQPS Regional/State/Local Modelers Workshop, Research Triangle Park, NC, August 22, 2002.

Dolwick, P.D. Summary of VOC/NO_x CAM_x sensitivity modeling completed for the eight-hour ozone implemenation team. Briefing for the Director, Air Quality Strategies and Standards Division, Office of Air Quality Planning and Standards, Research Triangle Park, NC, August 27, 2002.

Dolwick, P.D. Fine PM forecasting: Office of Air Quality Planning and Standards support to state/local agencies. Presentation at the Fall 2002 Standing Air Simulation Working Group Meeting (by phone), Stowe, VT, September 27, 2002.

Eder, B.K. Lightning. Presentation at Kingswood Elementary School, Cary, NC, October 1, 2001.

Eder, B.K. Air quality forecasting evaluation. Presentation at the University of New Hampshire, Durham, NH, October 30, 2001.

Eder, B.K. Rotated principal component analysis in environmental studies. Presentation at the Office of Air Quality Planning and Standards' Spatial Analysis Workshop, Research Triangle Park, NC, December 3, 2001.

Eder, B.K. Air quality forecasting evaluation. Presentation at the NOAA Aeronomy Laboratory, Boulder, CO, December 17, 2001.

Eder, B.K. Preliminary evaluation of CMAQ for aerosols and visibility parameters. Presentation at the Mid-Atlantic Regional Air Management Association Meeting, Baltimore, MD, January 23, 2002.

Gillette, D.A. The long-distance transportable fraction of the vertical flux of wind-transported dust. Presentation at the Fifth International Conference on Aeolian Research /Global Change and Terrestial Ecosystem—Soil Erosion Network Joint Meeting, Lubbock, TX, July 22, 2002.

Gillette, D.A. Modeling of wind blown dust emissions at Owens Lake, California. Presentation at the Fifth International Conference on Aeolian Research /Global Change and Terrestial Ecosystem—Soil Erosion Network Joint Meeting, Lubbock, TX, July 24, 2002.

Gilliland, A.B. Estimating seasonal NH_3 emissions using inverse modeling. Presentation at the Second International Nitrogen Conference—N2001, Potomac, MD, October 15, 2001.

Gilliland, A.B. Monthly and annual bias in weekly (NADP/NTN) versus daily (AIRMoN) precipitation chemistry data in the eastern USA. Presentation at The Second International Nitrogen Conference—N2001, Potamac, MD, October 15, 2001.

Gilliland, A.B. Inverse modeling applications for air quality. Invited presentation to the Harvard Atmospheric Chemistry Modeling Group, Cambridge, MA, March 24, 2002.

Gilliland, A.B. Evaluating air quality emissions with inverse modeling. Presentation at the Center for Integrating Statistical Environmental Sciences Inaugural Workshop, Chicago, IL, September 19, 2002.

Huber, A.H. Meteorological measurements and modeling in support of human exposure modeling: Microenvironmental factors, Coordinating Research Council Air Toxics Modeling Workshop, The Woodland, Texas, February 25 2002.

Huber, A.H. Characterizing meteorology and air pollution dispersion in urban environments: A case study in New York City post September 11, 2001. Presentation at the 2002 EPA Science Forum, Washington, DC, May 2, 2002.

Huber, A.H. Cooperative research and development for application of CFD to estimating human exposures to environmental pollutants. Presentation at the 2002 Fluent Users' Group Meeting, Manchester, NH, June 11, 2002.

Huber, A.H. Summary of the meteorological measurements/modeling studies and the initial mapping of plumes from ground zero in support of the EPA initial World Trade Center exposure assessment studies. Presentation at the National Academy of Science Workshop Tools for Tracking Chemical/Biological/Nuclear Releases in the Atmosphere Implications for Homeland Security, Woods Hole, MA, July 22, 2002.

Huber, A.H. Estimating the plume from the World Trade Center recovery site following September 11, 2001. Presentation at the New York State Health Department and New York City Health Department, New York City, NY, July 29, 2002.

Huber, A.H. World Trade Center Studies and CFD update. Presentation at the U.S. EPA/OAQPS Regional/State/Local Modelers' Workshop, Research Triangle Park, NC, August 22, 2002.

Irwin, J.S. Issues/concerns to be addressed in simulating atmospheric processes. U.S. Weather Research Program Prospectus Development Team (PDT-11) Meeting: Meteorological Research Needs for Improved Air Quality Forecasting, Palm Springs, CA , November 6, 2001.

Irwin, J.S. First define the information needed, then select a course of action. Presentation at the Workshop on Effective Emergency Response—Selecting a Suitable Dispersion Model for a Given Application, Washington, DC, December 5, 2001. Available at http://www.ofcm.gov/atd2/presentations/linking_list.htm (accessed October 2002).

Irwin, J.S. Evaluate earth science models for what they are—cartoons of reality. Presentation at the Workshop on Effective Emergency Response—Selecting a Suitable Dispersion Model for a Given Application, Washington, DC, December 6, 2001. Available at http://www.ofcm.gov/atd2/presentations/linking_list.htm (accessed October 2002).

Irwin, J.S. Issues/concerns to be addressed in dispersion model evaluations. California Energy Commission Short-Range Dispersion Modeling Workshop, Sacramento, California, January 24, 2002.

Irwin, J.S. Uncertainty in air quality modeling for risk calculations. Coordinating Research Council Air Toxics Modeling Workshop, The Woodland, Texas, February 26, 2002.

Irwin, J.S. Review of D6589 ASTM model evaluation procedure. Presentation at the U.S. EPA/OAQPS Regional/State/Local Modelers Workshop, Research Triangle Park, North Carolina, August 22, 2002.

Otte, T.L. Preparing science fair projects. Presentations to 5th Grade (five sessions), Olive Chapel Elementary School, Apex, NC, February 13, 2002.

Otte, T.L. Implementation of an urban canopy parameterization in MM5. Presented to representatives from the Japan Center for Air Pollution, Research Triangle Park, NC, March 5, 2002.

Otte, T.L. Weather Jeopardy. Two sessions. Presented at the 10th Expanding Your Horizons Workshop, North Carolina State University, Raleigh, NC, March 12, 2002.

Otte, T.L. Weather basics: Evaporation and condensation. Presentation to 2nd Grade (four sessions), Olive Chapel Elementary School, Apex, NC, April 12, 2002.

Otte, T.L. Weather basics: Evaporation and condensation. Presentation to 2nd Grade (four sessions), West Lake Elementary School, Apex, NC, April 19, 2002.

Otte, T.L. Weather basics: Evaporation and condensation. Presentation to 2nd Grade (four sessions), West Lake Elementary School, Apex, NC, May 9, 2002.

Otte, T.L. Weather basics: Evaporation and condensation. Presentation to 2nd Grade (four sessions), Olive Chapel Elementary School, Apex, NC, May 15, 2002.

Otte, T.L. Implementation of an urban canopy parameterization in MM5: Preliminary results. Presentation at the 6th George Mason University Workshop on Transport and Dispersion, George Mason University, Fairfax, VA, July 10, 2002.

Otte, T.L. Neighborhood scale modeling. Presentation at the 3rd Ad Hoc Meteorological Modeling Workshop, Lake Michigan Air Directors Consortium, Des Plaines, IL, July 31, 2002.

Otte, T.L. MM5 overview. Presentation at the U.S. EPA/OAQPS Regional/State/Local Modelers' Workshop, Research Triangle Park, NC, August 22, 2002.

Pierce, T.E. The wonders of weather. Presentation at the Morrisville Elementary School, Raleigh, NC, March 15, 2002.

Pierce, T.E. The importance of biogenic emissions for air quality modeling, EPA Science Forum, Washington, DC, May 2, 2002. (http://www.epa.gov/asmdnerl/epa_science_forum2.PDF)

Pierce, T.E. Intercomparison of alternative vegetation databases for regional air quality modeling, Gordon Research Conference on Biogenic Hydrocarbons and the Atmosphere, Oxford, England, September 2, 2002.

Pleim, J.E. Modeling for air quality forecasting. U.S. Weather Research Program Prospectus Development Team (PDT-11) Meeting: Meteorological Research Needs for Improved Air Quality Forecasting, Palm Springs, CA , November 6, 2001.

Pleim, J.E. Application of MM5 to air quality modeling of SOS/Nashville 1999. Presentation at the Twelfth PSU/NCAR Mesoscale Model Users' Workshop, Boulder, CO, June 25, 2002.

Pleim, J.E. The Models-3/Community Multiscale Air Quality (CMAQ) model: 2002 Release—Description and testing. Presentation at the U.S. EPA/OAQPS Regional/State/Local Modelers' Workshop, Research Triangle Park, NC, August 22, 2002.

Pleim, J.E. Weather research and forecast (WRF) model. Presentation at the U.S. EPA/OAQPS Regional/State/Local Modelers' Workshop, Research Triangle Park, NC, August 22, 2002.

Pleim, J.E. Overview of the Models-3/Community Multiscale Air Quality (CMAQ) model. Presentation at the Environmental Modeling Center modelers meeting at the National Center for Environmental Prediction, Camp Springs, MD, September 17, 2002.

Rao, S.T. Integrating observations and model predictions in designing emission control strategies. Invited talk at the EMEP/LOOP Workshop, Bern, Switzerland, December 4, 2001.

Rao, S.T. Using air quality models for emissions management decisions. Invited talk at the Uncertainty Treatment in Integrated Assessment Modelling Workshop of the UN/ECE Task Force on Integrated Assessment Modelling, IIASA, Laxenburg, Austria, January 24, 2002.

Rao, S.T. Probabilistic assessment of regional scale ozone pollution in the eastern United States. Invited presentation at the NATO-Advanced Research Workshop, Halkidi, Greece, June 11, 2002.

Rao, S.T. Examination of model predictions at different horizontal grid resolutions: Approaches, findings, and challenges. Invited presentation at the RAMS Workshop, University of Athens, Santorini Island, Greece, September 30, 2002.

Schere, K.L. Environmental Protection Agency's Community Multiscale Air Quality modeling system. Presentation at the American Meteorological Society-Central North Carolina Chapter, Research Triangle Park, NC, November 15, 2001.

Schere, K.L. Preliminary model evaluation of CMAQ for particulate matter. Presentation at the Environmental Protection Agency, Office of Air and Radiation, Office of Research and Development Air Progress Review, Research Triangle Park, NC, November 30, 2001.

Schere, K.L. Environmental Protection Agency's multi-pollutant Models3/Community Multiscale Air Quality (CMAQ) model. Presentation at the Workshop on the Effects of Global Climate Change on Regional Air Quality, Research Triangle Park, NC, December 5, 2001.

Schere, K.L. NERL's modeling and chemistry program in particulate matter. Presentation at the EPA NRC Committee on Research Priorities for Airborne Particulate Matter, Research Triangle Park, NC, March 12, 2002.

Schere, K.L. Environmental Protection Agency's Community Multiscale Air Quality (CMAQ) model. Poster presentation at the Environmental Protection Agency Science Forum 2002: Meeting the Challenges, Washington, DC, May 1, 2002.

Schere, K.L. NOAA/EPA-ASMD air quality forecasting program: The Models-3/CMAQ model—2002 Release: Description, testing, support. Presentation at the Standing Air Simulation Work Group Meeting, Stowe, VT, September 28, 2002.

Schwede, D.B. Thinking like a scientist. Presentation at the Leadmine Elementary School, Raleigh, NC, March 1, 2002.

Schwede, D.B. Thinking like a scientist. Presentation at the Olive Chapel Elementary School, Apex, NC, February 7, 2002.

West, J.L. NARSTO/NERL. Poster presentation at the Environmental Protection Agency Building Dedication, Research Triangle Park, NC, May 29, 2002.

APPENDIX D: WORKSHOPS AND MEETINGS

Texas Air Research Center Proposal Review Meeting, Houston, TX, October 2–3, 2001.

R.L. Dennis

NARSTO PM Assessment Meeting, Sacramento, CA, October 11–14, 2001.

J.L. West

Time Management, Planning and Prioritization for Special Librarians, GlaxoSmithKline, Research Triangle Park, NC, October 12, 2001.

E.M. Poole-Kober

Fall 2001 Standing Air Emissions Working Group, Nebraska City, NE, October 12–13, 2001.

W.G. Benjey

The Second International Nitrogen Conference: Optimizing Nitrogen Management in Food and Energy Production and Environmental Protection—N2001, Potomac, MD, October 14–18, 2001.

R.L. Dennis

NARSTO Quality Systems Science Center—Data Management, Knoxville, TN, October 24, 2001.

J.L. West

EPRI Air Quality Area Council Meeting, Washington, DC, October 24, 2001.

R.L. Dennis

BRACE Planning Meeting (Bay Regional Atmospheric Chemistry Experiment), Research Triangle Park, NC, October 25, 2001.

R.L. Dennis

25th Anniversary of the North Carolina State Climate Office, North Carolina State University, Raleigh, NC, October 26, 2001.

B.K. Eder

New England Air Quality Study Planning Meeting, University of New Hampshire, Durham, NH, October 29–30, 2001.

B.K. Eder

Lake Michigan Air Directors Consortium Regional Planning Organization Meeting, Chicago, IL, November 7–8, 2001.

R. Dennis

Super Sites Workshop, Research Triangle Park, NC, November 13–14, 2001.

B.K. Eder
K.L. Schere

United States-Canada Subcommittee 2 Workshop of PM Modeling, Research Triangle Park, NC, November 27–28, 2001.

R.L. Dennis

Office of Air Quality and Planning Standard's Spatial Analysis Workshop, Research Triangle Park, NC, December 3–5, 2001.

B.K. Eder

Office of Federal Coordinator for Meteorology Workshop on Effective Emergency Response, Crystal City, VA, December 3–5, 2001.

J.K.S. Ching
J.S. Irwin

Office of Federal Coordinator for Meteorology, Workshop on Strategy for Providing Atmospheric Information, Urban Meteorology and Air Quality Session, Co-Chair, Crystal City, VA, December 3–5, 2001.

J.K.S. Ching

Workshop on Climate Change and Air Quality: Part I: Intercontinental Transport and Climatic Effects of Pollutants, Research Triangle Park, NC, December 3–5, 2001.

J.M. Godowitch
K.L. Schere

Workshop on the Effects of Global Climate Change on Regional Air Quality, Research Triangle Park, NC, December 5–7, 2001.

E.J. Cooter
J.M. Godowitch
J.E. Pleim
K.L. Schere

Nitrogen Research Workshop, sponsored by the University of Maryland, Center for Environmental Science, Frostburg, MD, December 11–12, 2001.

R.L. Dennis

CEC/IJC (North American Commission for Environmental Cooperation/International Joint Commission) Workshop on Atmospheric Mercury: Science and Policy, Research Triangle Park, NC, December 13–14, 2001.

O.R. Bullock, Jr.

Air Quality Forecasting Evaluation, NOAA Aeronomy Laboratory, Boulder, CO, December 17–19, 2001.

B.K. Eder
K.L. Schere

Environmental Protection Agency, Office of Research and Development Board of Scientific Counselors Review, Research Triangle Park, NC, December 18, 2001.

T.L. Otte

The 82nd Annual Meeting of the American Meteorological Society, Orlando, FL, January 13–17, 2002.

R.L. Dennis
B.K. Eder
E.M. Poole-Kober

Fifth Annual Atmospheric Science Librarians International Conference, Orlando, FL, January 16–17, 2002.

E.M. Poole-Kober

Mid-Atlantic Regional Air Management Association Modeling and Data Analysis Workshop, Baltimore, MD, January 22–23, 2001.

B.K. Eder

Short Range Dispersion Modeling Workshop, California Air Resources Board and California Energy Commission, Sacramento, CA, January 24–25, 2002.

J.K.S. Ching

The Technical Cooperation Program, Chemical, Biological and Radiological Defense Technical Panel 9 Meeting, Dispersion Modeling Workshop, Sacramento, CA, January 28–30, 2002.

J.K.S. Ching

14th Annual Alumni Student Career Connection, UNC General Alumni Association, University of North Carolina at Chapel Hill, Chapel Hill, NC, January 29, 2002.

E.M. Poole-Kober

U.S. EPA's National Air Quality Conference: Forecasting and Public Outreach, San Francisco, CA., February 2–6, 2002.

K.L. Schere

International Mercury Model Intercomparison Meeting, Moscow, Russia, February 14–15, 2002.

O.R. Bullock, Jr.

BRACE Workshop (Bay Regional Atmospheric Chemistry Experiment), University of South Florida College of Public Health, Tampa Bay, FL, February 19–20, 2002.

R.L. Dennis

External Advisory Committee Meeting, Columbia University Global Climate STAR Grant, New York, NY, February 22, 2002.

K.L. Schere

Coordinating Research Council, Air Toxics Workshop, The Woodland, TX, February 26–27, 2002.

J.K.S. Ching

Japan Center for Air Pollution Meeting, Environmental Protection Agency, Research Triangle Park, NC, March 5, 2002.

T.L. Otte

Japan Clean Air Program-II, Environmental Protection Agency, Research Triangle Park, NC, March 6, 2002.

J.K.S. Ching

10th Expanding Your Horizons Workshop, North Carolina State University, Raleigh, NC, March 12, 2002.

T.L. Otte

National Research Council PM Implementation Panel Review, Environmental Protection Agency, Research Triangle Park, NC, March 12–13, 2002.

R.L. Dennis

Spring 2002 Standing Air Emissions Working Group, Coeurd'Alene, ID, April 3–4, 2002.

W.G. Benjey

$PM_{2.5}$ and Electric Power Generation: Recent Findings and Implications, Pittsburgh, PA, April 9–10, 2002.

J.M. Godowitch

American Society for Testing and Materials Committee Week, Philadelphia, Pennsylvania, April 15–18, 2002.

J.S. Irwin

Eleventh International Emission Inventory Conference, Atlanta, GA, April 16–28, 2002.

W.G. Benjey

Environmental Protection Agency National PBT (Persistent Bioaccumulative Toxics) Monitoring Workshop, Raleigh, NC, April 22-24, 2002.

O.R. Bullock, Jr.

CASTNet Technical Advisory Committee, U.S. EPA Office of Air and Radiation, Office of Air Quality Planning and Standards, Research Triangle Park, NC, April 24–25, 2002

D.B. Schwede

Environmental Protection Agency Science Forum 2002: Meeting the Challenges, Washington, DC, May 1–2, 2002.

K.L. Schere

Workshop on Validation Data Sets for Modeling Mineral Aerosol in Global Climate Cycles, Max-Planck Institute for Biochemistry, Jena, Germany, May 2–4, 2002.

D.A. Gillette

BRACE (Bay Regional Atmospheric Chemistry Experiment) Field Study Visit, Tampa Bay, FL, May 7–12, 2002.

R.L. Dennis

12th Annual SAIL (Southeast Affiliate of IAMSLIC Libraries) Meeting, Gloucester Point, VA, May 14–17, 2002.

E.M. Poole-Kober

NARSTO Reactivity Research Workgroup Meeting: Atmospheric Chemistry, Research Triangle Park, NC, May 15–16, 2002.

J.L. West

Air Quality and Human Health Under Climate Change, Canadian Lung Association, Moncton, New Brunswick, Canada, May 15–17, 2002.

E.J. Cooter

American Meteorological Society's Board of Urban Environment Annual Meeting, Norfolk, VA, May 20, 2002.

J.K.S. Ching

2002 Spring Meeting, American Geophysical Union, Washington, DC, May 28–31, 2002.

R.L. Dennis

U.S. EPA Clean Air Markets Division Seminar, Washington, DC, May 29, 2002.

R.L. Dennis

Air Toxics Implementation Planning Workshop, National Health and Environmental Effects Laboratory, Environmental Protection Agency, Research Triangle Park, NC, June 11–12, 2002.

J.K.S. Ching

95th Annual Conference of the Air & Waste Management Association, Baltimore, MD, June 23–27, 2002.

J.L. West

Twelfth PSU/NCAR Mesoscale Model Users' Workshop, Boulder, CO, June 24–26, 2002.

T.L. Otte
J.E. Pleim

2nd Annual Weather Research and Forecast Workshop, Boulder, CO, June 27–28, 2002.

T.L. Otte
J.E. Pleim

Weather Research and Forecast Tutorial, Boulder, CO, June 27–28, 2002.

T.L. Otte

George Mason University Transport and Dispersion Modeling Workshop, Fairfax, VA, July 9–12, 2002.

J.K.S. Ching
T.L. Otte

12th Annual Jornada Symposium, New Mexico State University, Las Cruces, NM, July11, 2002.

D.A. Gillette

Fifth International Conference on Aeolian Research and the Global Change and Terrestrial Ecosystem-Soil Erosion Network, sponsored by U.S. Department of Agricultural Research Service and Texas Tech University, Lubbock, TX, July 22–25, 2002.

D.A. Gillette

3rd Ad Hoc Meteorological Modeling Workshop, Lake Michigan Air Directors Consortium, Des Plaines, IL, July 30–31, 2002.

T.L. Otte

Design Workshop for EPA's Causal Analysis Diagnosis Decision Information System (CADDIS) Environmental Protection Agency, Mt. Sterling, OH, August 26–28, 2002.

S.S. Fine

NARSTO Reactivity Research Work Group, Photochemical Reactivity, Research Triangle Park, NC, August 28–29, 2002.

J.L. West

U.S. Environmental Protection Agency, Office of Air Quality Planning and Standards Regional/State/Local Modelers' Workshop, Research Triangle Park, NC, August 22, 2002.

T.L. Otte

EMEP Steering Body, Geneva, Switzerland, September 2-4, 2002.

R.L. Dennis

United Nations' Environment Program, Global Mercury Assessment Work Group Meeting, Geneva, Switzerland, September 9–13, 2002.

O.R. Bullock, Jr.

Air & Waste Management Association Section Meeting, Jupiter, FL, September 15–17, 2002.

R. Dennis

National Academy of Science, Review of the NARSTO Assessment of the Atmospheric Science on Particulate Matter, Washington DC, September 25, 2002.

J.L. West

U.S. Forest Service Research Workshop, Fire Emission Modeling for CMAQ, George Mason University, Fairfax VA, August 13–14, 2002.

J.K.S. Ching

Air Quality Forecasting Meeting, National Oceanic and Atmospheric Administration, National Center for Environmental Prediction, Camp Springs, MD, September 17, 2002.

T.L. Otte
J.E. Pleim
K.L. Schere
J.O. Young

Fall 2002 Standing Air Emissions Working Group, Stowe, VT, September 26–27, 2002.

W.G. Benjey

Standing Air Simulation Workgroup, Stowe, VT, September 27–28, 2002.

K.L. Schere

Models-3/CMAQ Annual Workshop, Research Triangle Park, NC, October 22–24, 2002.

D.A. Atkinson
P. D. Dolwick
M.L. Evangelista
J. S. Irwin
B.L. Orndorff

APPENDIX E: VISITING SCIENTISTS

9. Messrs. Mike Abraczinskas, George Bridgers, and John White
North Carolina Division of Air Quality
Raleigh, NC

Messrs. Abraczinskas, Bridgers, and White visited the Division on December 11, 2001, to present a seminar on air quality forecasting for North Carolina.

10. Dr. Kiran Alapaty
MCNC Environmental Modeling Center
Research Triangle Park, NC

Dr. Alapaty visited the Division on October 31, 2001, and presented a seminar entitled *The flux-adjusting surface data assimilation system (FASDAS) for meteorological applications.*

3 Dr. Nancy Brown
Chief Scientist
Lawrence Berkeley National Laboratory
Berkeley, CA

Dr. Brown visited ASMD to learn ASMD's research in air quality model development and model performance evaluation in March 2002.

4. Dr Steven Burian
University of Arkansas
Fayetteville, AR

Dr. Burian visited the Division on January 4, 2002, for collaboration on urban morphology studies, and again on February 21, 2002, to assist in the development of urban morphological parameterizations.

5. Mr. Satoru Chatani
Toyota Central Research and Development Laboratories
Nagakute, Japan

Mr Chatani visited the Division on August 5, 2002, to discuss Japan Clean Air Program and to learn the latest status of the CMAQ model.

6. Dr. Joshua Fu
University of Tennessee
Knoxville, TN

Dr. Fu visited the Division from July 30-31, 2002, to obtain assistance with Models-3/CMAQ.

7. Dr. Christian Hogrefe
Division of Air Resources
New York Department of Environmental Conservation
Albany, NY

Dr. Hogrefe visited the Division on April 11, 2002, to learn about emissions processing for air quality simulation models.

8. Mr. Mike Moss
U.S. Air Force Reserves
Tyndall Air Force Base, FL

Mr. Moss visited the Division on July 18, 2002, to learn about Models-3/CMAQ for potential Air Force applications.

8. Dr. James Sloan
Professor of Physical Chemistry
Department of Chemistry
University of Waterloo
Waterloo, Ontario, Canada

Dr. James Sloan visited the Division on July 18, 2002, to present and discuss the formation of a Models-3/CMAQ application center at the University of Waterloo, Ontario, Canada.

9. Pam Tsai
U.S. Environmental Protection Agency, Region 9
75 Hawthorne Street
San Francisco, CA

Pam Tsai visited the Division on April 12, 2002, to discuss CMAQ modeling in the United States.

10. Dr. Satoshi Yamazaki (Toyota Research), Dr. Hitoshi Kunimi (Nissan Research), Dr. Shinji Kobayashi (National Institute for Environmental Sciences-Japan), Mr. Hayashi from Japan Clean Air Promotions Department, Mr. Shinichi Doki from Japan Clean Air Promotions Department, Japan Clean Air Program
Tokyo, Japan

Drs. Yamazaki, Kunimi, and Kobayashi, and Messrs. Hayashi, and Doki visited the Division on March 5 and 6, 2002, to discuss collaboration on CMAQ modeling in the United States and Japan.

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

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

Dr. Arnold, a postdoctoral researcher, is in his fourth 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 make weight of evidence approaches objective.

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

Dr. He, a post-doctoral researcher, is working with the Division on air quality model evaluation for particulate matter. He began a 2-year visit with the Division on August 21, 2000.

APPENDIX G: ATMOSPHERIC SCIENCES MODELING DIVISION STAFF AND AWARDS

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

Office of the Director

Dr. S.T. Rao, Supervisory Meteorologist, Director
Randy M. Brady (EPA), Deputy Director
Herbert J. Viebrock, Meteorologist, Assistant to the Director
Linda Green (EPA), Budget Analyst
Dr. Jay Messer (EPA), Physical Scientist
Evelyn M. Poole-Kober, Librarian
Dr. Basil Dimitriades (SEEP), Physical Scientist
Barbara Hinton (EPA), Secretary

Atmospheric Model Development Branch

Kenneth L. Schere, Supervisory Meteorologist, Chief
Dr. Francis S. Binkowski, Meteorologist (Until January 2002)
O. Russell Bullock, Jr., Meteorologist
Gerald L. Gipson (EPA), Physical Scientist
James M. Godowitch, Meteorologist
Dr. Alan H. Huber, Physical Scientist
Dr. William T. Hutzell (EPA), Physical Scientist
Dr. Michelle R. Mebust (EPA), Physical Scientist
Tanya L. Otte, Meteorologist
Dr. Jonathan E. Pleim, Physical Scientist
Shawn J. Roselle, Meteorologist
Dr. Jeffrey O. Young, Mathematician
Patricia F. McGhee, Secretary

Model Evaluation and Applications Research Branch

William B. Petersen, Supervisory Physical Scientist, Chief
Dr. Robin L. Dennis, Physical Scientist
Dr. Brian K. Eder, Meteorologist
Dr. Steven S. Fine, IT Specialist
Dr. Peter L. Finkelstein, Physical Scientist
Dr. Alice B. Gilliland, Physical Science Administrator
Steven C. Howard, IT Specialist
John H. Rudisill, III, Equipment Specialist
Alfreida R. Torian, IT Specialist
Gary L. Walter, Computer Scientist
Jeffrey L. West, Physical Science Administrator
Sherry A. Brown, Secretary

Air-Surface Processes Modeling Branch

Thomas E. Pierce, Supervisory Physical Scientist, Chief
Dr. William G. Benjey, Physical Scientist
Dr. Jason K.S. Ching, Meteorologist
Dr. Ellen J. Cooter, Meteorologist
Dr. Dale A. Gillette, Physical Scientist
Dr. Steven G. Perry, Meteorologist
Dr. George A. Pouliot, Physical Scientist
Donna B. Schwede, Physical Scientist
John J. Streicher, Physical Scientist
Roger S. Thompson, Physical Scientist
Lawrence E. Truppi, Meteorologist (Until January 2002)
Bruce Pagnani (SEEP), Computer Programmer
Ashok Patel (SEEP), Engineer
John Rose (SEEP), Machinist/Model Maker
Ruby S. Borden, (SEEP), Secretary

Air Policy Support Branch

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

Alan Huber received the EPA/ORD Science and Technology Award for exceptional/Outstanding Technical Assistance to the Regions or Program Offices in recognition of outstanding support provided to enhance the use of sound science in Agency decisions by playing a key role in developing exposure study requirements for emission and exposure studies for MMT and MTBE and for reviewing the study protocols submitted by industry in response to the requirements.

Alan Huber received a special EPA commemorative medallion and a letter of appreciation from the EPA Administrator, Governor Whitman, for excellence in response to September 11, 2001, events as part of the EPA ORD Monitoring and Exposure Assessment Team.