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FISCAL YEAR 2005 SUMMARY REPORT OF THE NOAA ATMOSPHERIC SCIENCES MODELING DIVISION TO THE U.S. ENVIRONMENTAL PROTECTION AGENCY

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PREFACE

In September 2005, the Atmospheric Sciences Modeling Division (ASMD) celebrated its 50th Anniversary of the collaboration between the U.S. Department of Commerce s National Oceanic and Atmospheric Administration (NOAA) and the U.S. Environmental Protection Agency (EPA), and their predecessor agencies on air quality modeling research and its application. The relationship between NOAA and EPA began when the Air Pollution Unit of the Public Health Service, which later became part of the EPA, requested the Weather Bureau to provide it with meteorological expertise. Thus, in 1955, a special Weather Bureau air pollution unit was formed, integrated with the Public Health Service, and located in Cincinnati, Ohio, until it moved in 1969 to Raleigh, North Carolina. The unit is now the NOAA ARL ASMD, working within the framework of the Memorandum of Understanding and Memorandum of Agreement between the U.S. Department of Commerce and EPA. These agreements are implemented through long-term Interagency Agreements DW13938483 and DW13948634 between EPA and NOAA.

This report summarizes research and operational activities of the Division for the Fiscal Year 2005. The summary includes descriptions of research and operational efforts in air pollution meteorology, meteorology and air quality model development, model evaluation and applications, and air pollution abatement and compliance programs. ASMD serves as the vehicle for implementing the interagency collaboration on atmospheric research efforts. ASMD conducts research activities in-house and through contracts and cooperative agreements, and provides atmospheric sciences expertise, air quality forecasting support, and consultation and guidance on the meteorological and air quality modeling aspects of air quality management to various EPA offices, including the Office of Air Quality Planning and Standards, and to state and pollution control agencies. To provide these services, the Division is organized into four research Branches: Atmospheric Model Development Branch, Model Evaluation and Applications Research Branch, Air-Surface Processes Modeling Branch, and Applied Modeling Branch. This report is organized by major program themes reflecting the Division strategic plan, consistent with NOAA s mission and strategic goals.

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

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ABSTRACT. During Fiscal Year 2005, the Atmospheric Sciences Modeling Division s work on meteorological and air quality modeling, and policy guidance was accomplished in accordance with the memoranda signed by the U.S. Department of Commerce and the U.S. Environmental Protection Agency (EPA). This ranged from research studies and model applications to the provision of air quality forecast, policy advice, and guidance on air quality management. Research efforts emphasized the development, evaluation, and application of meteorological and air quality models. Among the research studies and results were the release of the Community Multiscale Air Quality version 4.5 (CMAQv4.5) modeling system; continued model improvement and evaluations; improvement of the SMOKE©[1] emission processing system; evaluation and improvement of the Eta-CMAQ modeling system for use in air quality forecasting; transition toward using the Weather Research and Forecasting (WRF) model for meteorological simulation; development of model evaluation tools; and the development of techniques for data analysis and interpretation.

1. INTRODUCTION

In Fiscal Year 2005, the Atmospheric Sciences Modeling Division (ASMD) continued its commitment for providing goal-oriented, high-quality research and development, and operational transfer of Division products in support of the missions and strategic goals of NOAA and EPA. Using an interdisciplinary approach emphasizing integration and partnership 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 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 communities. Division research is focused on five program areas: new developments in air quality modeling; climate change and its impact on regional air quality; multimedia modeling; data management and analysis; and air quality forecasting. The Division is organized to respond effectively to these research directions as more fully described in the following sections of the report.

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2. PROGRAM REVIEW

2.1 Fifty-Year Partnership between NOAA and EPA and their Predecessor Agencies

In FY-2005, the Atmospheric Sciences Modeling Division (ASMD) celebrated its 50-year partnership between NOAA and EPA and their predecessor agencies. To highlight the event, the American Meteorological Society (AMS) sponsored the highly successful *NOAA/EPA Golden Jubilee Symposium on Air Quality Modeling and Its Applications, September 19–20, 2005.* The 216 attendees participated in six sessions of oral presentations, two luncheons with distinguished keynote speakers, and an evening poster session and ceremony celebrating the occasion. The AMS will publish a special issue of the *Journal of Applied Meteorology and Climatology* (*JAMC*) for the papers presented at the symposium.

Dr. S.T. Rao, Director of the Atmospheric Sciences Modeling Division, opened the conference with introductory remarks, and a panel discussion of past, present, and future perspectives of the EPA-NOAA partnership followed. The panel consisted of Dr. Gary Foley, EPA; Dr. Kenneth Demerjian, State University of New York in Albany and former ASMD Director; Francis Schiermeier, retired ASMD Director; Thomas Curran, EPA; John Jones, Deputy Director, National Weather Service; Dr. Richard Rosen, NOAA Assistant Administrator for Oceanic and Atmospheric Research, and Bruce Hicks, Director, Air Resources Laboratory, NOAA.

Dr. James Mahoney, Assistant Secretary of Commerce for Oceans and Atmospheres and NOAA Deputy Administrator, was the Luncheon Keynote Speaker on the first day. He discussed the past and present building of partnerships and the future of research in NOAA. Dr. Lawrence Reiter, Director, EPA National Exposure Research Laboratory, was the Luncheon Keynote Speaker on the second day. He discussed the EPA perspective on building partnerships and his vision for expanding air quality modeling to include health related exposure and dosage estimates.

The 50th Anniversary Ceremony on the evening of the first day began with the presentation of awards to four retired members of the Division for their outstanding contributions to the field of air quality modeling and its applications. The award recipients were Dr. William Snyder, Dr. Gary Briggs, Mr. Bruce Turner, and Mr. Joseph Tikvart. This was followed by the cutting of a cake displaying the NOAA and EPA emblems by Drs. Gary Foley and Lawrence Reiter, representing EPA, and Dr. Richard Rosen, representing NOAA.

2.2 Atmospheric Model Development

This research is aimed at providing state-of-science air quality models and guidance for use in the implementation of National Ambient Air Quality Standards (NAAQS) for ozone and fine particulate matter ($PM_{2.5}$), for use in national and local assessments of toxic air

contaminants, and for air quality forecasting. The principal effort is to develop and improve the 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 chemical solvers development, aerosol representations in grid-based air quality models, subgrid-scale representations for large elevated sources of pollution, CMAQ code integration and efficiencies improvement, and air quality forecasting.

The objectives of this research program are to continuously improve the mesoscale (regional through urban scale) air quality simulation models, including CMAQ, as a tool for air quality management, NAAQS implementation, and forecast guidance. 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 meteorological models via improved process parameterizations.

By design, CMAQ is expected to be used by both scientists and policy-makers for various air quality 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 meteorological model. Tested model configurations can be established for use by the policy community to develop and analyze implementation strategies for air quality management. CMAQ utilizes the "one-atmosphere" approach to air quality modeling. It is capable of concurrently simulating concentrations of oxidants and fine particles, visibility degradation, air toxins, and acidic and nutrient deposition and loadings to ecosystems at urban and regional scales. As the understanding of the atmospheric processes, input data, and model formulations and parameterizations improves, it will be essential to continue to upgrade or provide science options through 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 that led to the September 2005 release of the CMAQ modeling system.

2.2.1 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 the meteorological fields for CMAQ. MM5 is widely used to generate meteorological characterizations of the atmosphere throughout the air-quality modeling community. For CMAQ, MM5 is applied to case studies (episodic, seasonal, and annual) at a variety of spatial scales using a series of one-way nested domains. Typically, MM5 is run retrospectively using four-dimensional data assimilation 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 Sparse Matrix Operator Kernel Emission (SMOKE)© (emissions) and CMAQ (chemistry) modules to describe the atmospheric state variables and characteristics of the planetary boundary layer.

During FY-2005, annual simulations were completed for 2002 and 2003 on a 36-km (horizontal grid-cell size) continental United States (CONUS) domain, and for 2002 on a 12-km eastern United States domain. These year-long MM5 simulations were used as input to annual CMAQ air quality simulations. These MM5 simulations are also being used to better understand the ability of MM5 to reproduce characteristics of the atmosphere that have an impact on the air quality model results. To date, the Division has three years of observed and modeled data for MM5 performance and diagnostic evaluations. Follow-on modeling with MM5 will extend the annual simulations to include 2004 and 2005.

Proof-of-concept research to implement urban canopy parameterizations in MM5 for modeling the effects of urban areas at horizontal grid spacings of ~1 km was developed (Dupont *et al.*, 2004; Otte *et al.*, 2004) in FY-2004. In FY-2005, simulations with and without the advanced urban canopy parameterization were completed for a two-week period of the 2000 Texas air quality study. A detailed evaluation of both the MM5 and CMAQ simulations will be conducted in FY-2006. Preliminary results indicate significant differences in the near-surface temperature, wind, and surface fluxes between the advanced urban and default simulations, which should lead to more accurate ozone and particulate matter predictions.

Also during FY-2005, efforts were made to transition to the Weather Research and Forecasting (WRF) model for meteorological simulations. WRF is the next-generation meteorological model that is intended to ultimately replace MM5, and it includes many of the features that are currently in MM5. It is attractive for air-quality modeling applications because, unlike MM5, it contains mass-conserving equations. Collaborative work focused on implementing a nudging-based four-dimensional data assimilation capability in WRF, as well as developing a version of the Pleim-Xiu Land-Surface Model (PX LSM) for WRF. Some preliminary simulations were conducted using WRF (without the nudging and without the PX LSM). The resulting data sets were compared to observations and to MM5 simulations for the same forecast region and time period. Initial evaluation efforts indicate that WRF performance is similar to MM5 for a number of meteorological variables, but WRF may be superior in simulating cloud and precipitation structures. However, the absence of nudging and a LSM in WRF was noticeable, as expected. It is anticipated that the transition to WRF will intensify as those capabilities, which are available in MM5 and typically used for air quality modeling simulations, become more fully integrated into WRF.

2.2.2 Linking Meteorology and Chemistry Models for Research Applications

The Meteorology-Chemistry Interface Processor (MCIP) creates the off-line linkage between meteorological models and the CMAQ model for research and regulatory applications. MCIP is compatible with upgrades to the meteorological models that are used by CMAQ to preserve numerical and physical consistency between the meteorology and chemistry models. In FY-2005, MCIP received a major upgrade to version 3.0 and included several new features. The most notable change was to allow meteorological fields to be input from either MM5 or WRF. There are new optional dry deposition species for chlorine and mercury with the ˜M3Dry™ scheme. Also, there is an option to use fractional land-use in MCIP if it is imported from an MM5v3 pre-processing file. Extensive testing and evaluation of MCIPv3.0 was initially conducted in-house, then reinforced through an external panel of beta testers. MCIPv3.0 was released to the public in September 2005.

2.2.3 Planetary Boundary Layer and Land Surface Modeling

Realistic simulation of land-surface and planetary boundary layer (PBL) processes is 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. Therefore, efforts in this area involve both meteorology and chemical transport models to develop realistic and consistent modeling of the surface and PBL processes.

Parameterizations of the vertical transport due to boundary-layer turbulence are among the most important components of meteorology and air quality models. However, the PBL schemes employed in the meteorological models and those used in the air quality models are often quite different. Part of the reason for this is simply different histories related to model development. However, the schemes that worked well in the meteorological models have not worked so well in the air quality models, and vice versa. Clearly, the vertical mixing of trace chemical species should be similar to the vertical mixing of heat and water vapor.

Mesoscale meteorological models typically include either simple non-local closure schemes or higher-order schemes that involve prognostic equations for turbulent kinetic energy (TKE) and sometimes to such other higher-order terms as turbulent dissipation or potential temperature variance. The non-local schemes, in particular, have been developed to address the inadequacies of local schemes that cannot produce realistic profiles of both first-order quantities and their fluxes in convective conditions. Air quality models typically use simple local closure (eddy diffusivity) although both non-local and higher-order schemes have been used. A difficulty for air quality models is that chemical profile data for evaluation, including ozonesondes and aircraft measurements, are very sparse. Therefore, ground-level concentration data are often used for evaluation, which may be affected by many other processes. Without extensive comparisons to PBL profiles of chemical measurements, it is difficult to know whether

an accurate simulation of ground-level concentrations represents realistic PBL mixing or results from compensating errors.

During the past two years, new PBL schemes have been developed for use in both meteorology and air quality models. Most notably, a more advanced version of the Asymmetric Convective Model (ACM) has been developed, tested, and evaluated. The new model, ACM2, is a combination of local- and non-local closure. Specifically, the ACM2 is a combination of the original ACM (Pleim and Chang, 1992) and eddy diffusion. The key is to match the two schemes at a certain height, in this case the top of the lowest model layer, and apportion the mixing rate between the two schemes such that the resultant flux is identical to that produced by either scheme running alone. The formulation of the ACM2 is described along with one-dimensional testing compared to large eddy simulations and field study data in an upcoming journal article (Pleim, in press).

ACM2 has been implemented in the MM5 and CMAQ models and work is underway for its implementation in the WRF model. Several MM5 and CMAQ simulations were made for the summer of 2004 to evaluate the effect of ACM2 on meteorological and chemical model results. Statistics for temperature, humidity, and winds are similar to previous MM5 simulations using the original ACM. ACM2 has been shown to accurately simulate PBL heights and vertical profiles of temperature and humidity through comparisons to PBL heights derived from radar wind profilers and vertical profiles derived from rawinsonde measurements. Future work will include evaluation of CMAQ model results using ACM2 through comparisons to the ICARTT (International Consortium for Atmospheric Research on Transport and Transformation) 2004 field observations, including vertical profiles and curtains derived from aircraft measurements.

The Pleim-Xiu Land Surface Model (PX LSM) is being implemented in the WRF model. The PX LSM code has been adapted to the WRF infrastructure. The WRF implementation includes a surface-flux parameterization and the ACM2 PBL model. In the WRF structure, the land-surface model, the surface-flux parameterization, and the PBL model are all in separate modules. Thus, any of these three components can be used with any other of the LSM/PBL component options in the WRF system. The indirect soil-moisture data-assimilation scheme awaits completion of a four-dimensional data assimilation ˜nudging™ implementation in the WRF model. Specifically, soil-moisture data assimilation requires surface analyses of observed 2-m temperature and relative humidity.

2.2.4 Anthropogenic Emissions

During FY-2005, CMAQ began using the SMOKE$^{\pm}$ v2.2 modeling system (http://cf.unc.edu/cep/empd/products/smoke/version2.2/). Now recognized as a key emission processing tool for air quality management modeling, SMOKE$^{\pm}$ was initiated by the Division over a decade ago. During FY-2005, Division scientists provided upgrades to SMOKE$^{\pm}$ v2.2 for wildland fire emissions and plume rise. SMOKE$^{\pm}$ v2.2 is now compatible with the fire emission model included in the BlueSky modeling framework, a software package from the U.S. Forest

Service. SMOKE©v2.2 also includes a plume rise algorithm for fires that can be applied on a per fire basis using meteorological inputs from such models as MM5 or WRF. In addition, the traditional plume-rise calculation has been updated with several improvements: (1) use of the residual buoyancy flux (rather than the buoyancy flux) in the unstable plume rise function; (2) an option to use either the Turner approach or the Gillani approach for the plume-spread computation; (3) improvement to the numerical approach used to allocate the emissions to different model layers using the plume rise and plume spread information; and, (4) use of the friction velocity from the meteorological model in the neutral plume-rise equation. These plume-rise enhancements are consistent with the plume-rise calculations found in the Plume-in-Grid component of the CMAQ model.

2.2.5 Biogenic Emissions

Introduced in 1988, the Biogenic Emissions Inventory System (BEIS) provides hourly, gridded estimates of biogenic volatile organic compounds and soil NO emissions to such regional air quality models as CMAQ. During FY-2005, BEIS3.12 was upgraded to BEIS3.13 (Schwede *et al.*, 2005). BEIS3.13 includes updates to the radiation model used in the estimation of isoprene emissions and updates to the isoprene and monoterpene emission factors for spruce, hemlock, and douglas fir tree types. BEIS3.13 will be included in a future SMOKE© release.

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

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 dependent upon the validity of the gas-phase chemical interactions and transformations contained in the chemical mechanism that is used in the model. 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 in the chemical modules that have been used historically consume about 50 percent to 75 percent of the computer time required for model simulations, any substantial computational efficiencies that can be gained will significantly lower the computational time of CMAQ. Therefore, 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 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 atmospheric chemistry, while ensuring the practicality of using CMAQ as a modeling tool in regulatory and operational modeling applications by lowering the computational burden.

During FY-2005, an updated and expanded Carbon Bond mechanism (CB05) was developed and incorporated into the CMAQ model to more accurately simulate conditions in pristine areas, winter temperatures, and high altitude situations. The CB05 mechanism contains 52 chemical species. Additional species in the mechanism include ethane, internal olefins, terpenes, acetaldehyde, higher aldehydes (C3+ species), formic acid, acetic acid, methanol, ethanol, peroxyacetic acid, higher alkyl peroxy acetyl nitrate (PAN) analogues, methylhydroperoxide, methylperoxy radical, acetyl peroxy radical, higher peroxy acyl radical (C3+ species), and higher (C2+) organic peroxides. Details of the chemical mechanism containing 156 reactions are described by Yarwood *et al.* (2005). The changes in the CB05 mechanism relative to the CB-IV (Gery *et al.*, 1989) include the following categories: kinetic updates, photolysis updates, extended inorganic reaction set, and representation of atmospheric chemistry of simple alkanes, higher aldehydes, alkenes with internal double bonds, oxygenated products and intermediates, and terpene.

Model simulations were performed using both the CB05 and the CB-IV mechanisms for winter and summer of 2001. For winter simulations using the CB05 mechanism, ozone, aerosol nitrate, aerosol sulfate, and organic carbon concentrations were all within 3 percent of the results obtained using the CB-IV mechanism. However, formaldehyde and hydrogen peroxide concentrations were reduced significantly (27 percent and 33 percent) during winter when the CB05 mechanism was used. For summer simulations using the CB05 mechanism, ozone concentrations increased about 8 percent while aerosol nitrate, aerosol sulfate, and organic carbon concentrations decreased by about 10 percent or less, when compared with results using the CB-IV mechanism. As in winter, the concentrations of formaldehyde and hydrogen peroxide were reduced significantly (13 percent and 49 percent) during summer when using the CB05 mechanism. Comparisons of model predictions of ozone against observations show no significant differences between the two mechanisms.

The CMAQ model currently provides three different gas-phase chemistry solvers: the Sparse-Matrix Vectorized Gear Algorithm solver, the Rosenbrock solver, and the Euler Backward Iterative solver. Both the Sparse-Matrix Vectorized Gear Algorithm and Rosenbrock solvers are general chemistry solvers. The Euler Backward Iterative solver is dependent on the chemical mechanism; but it is faster than the other two solvers. Therefore, a special version must be developed for each new chemical mechanism. An Euler Backward Iterative solver was developed for the CB05 mechanism during FY-2005 based upon Hertel *et al.* (1993). A beta version of the CB05 mechanism and the associated Euler Backward Iterative solver will be released to the public with an interim CMAQ model release in spring 2006.

2.2.7 Aerosol Mechanism Improvements in CMAQ

In FY-2005, the CMAQ aerosol module was revised substantially to improve the underlying science and the numerical stability of the model. A new version of the aerosol module, AERO4, was developed to treat the emissions of sea salt and some chemical interactions between sea-salt particles and gaseous pollutants. The AERO4 module was released to the public as part of CMAQv4.5. To develop the module, a recent parameterization of wind-speed-dependent and size-resolved sea-spray flux (Gong, 2003) was fit to a bimodal distribution for incorporation into the accumulation and coarse modes of the CMAQ model. Rather than reading the sea-salt emissions from a pre-computed file, the emissions are calculated within the model during each time step so that the emission fluxes are consistent with the meteorological inputs used to drive the model. Particle sizes of fresh emissions are adjusted to ambient relative humidity in each grid cell (Zhang *et al.*, 2005). Fine sea-salt particles interact with the gaseous pollutants using the ISORROPIA (Greek for "equilibrium") thermodynamic equilibrium module, whereas coarse sea-salt particles are assumed to be inert. Further details of the AERO4 module are described by Shankar *et al.* (2005).

In addition to developing the new AERO4 module, development of the earlier version of the CMAQ aerosol module (*i.e.*, AERO3) continued during FY-2005. Modifications discussed in this section were made to the AERO3 and AERO4 modules. The numerical stability of the ISORROPIA module was improved by revising the Zdanovskii-Stokes-Robinson parameters and fixing an error in the retrieval of Kusik-Meissner binary activity coefficients. Further improvements to the numerical stability of ISORROPIA may be warranted, especially at high-elevation and in wintertime conditions. A new subroutine was added to calculate the volume fraction of each mode that is composed of particles smaller than 2.5 μm aerodynamic diameter. Following the methodology of Jiang *et al.* (in press), these new diagnostic output variables facilitate a more rigorous calculation of $PM_{2.5}$ than a simple summation of Aitken and accumulation modes. Summer and winter 36-km (horizontal grid-cell size) simulations with these new diagnostic calculations indicate that, on average, 10 percent to15 percent of the coarse mode aerosol falls within the $PM_{2.5}$ size range and up to 40 percent of the accumulation mode exceeds 2.5 μm in aerodynamic diameter. These and other updates to the CMAQ aerosol modules are described by Bhave *et al.* (2005) and are incorporated into CMAQv4.5.

In addition to the AERO3 and AERO4 modules, a pair of new model options was released in CMAQv4.5 that will enable users to probe the sources of modeled aerosol concentrations. With one tool, the ambient sulfate concentrations formed via different pathways (*e.g.*, direct emission, gas-phase oxidation, aqueous-phase oxidation) can be determined quantitatively. With a second diagnostic tool, one may calculate the contributions from individual emission source categories and/or geographic regions to the ambient primary carbonaceous aerosol burden.

2.2.8 Plume-in-Grid Modeling

The plume-in-grid (PinG) approach provides a subgrid scale treatment of the dynamic and chemical/aerosol processes governing gas-phase and particulate species in isolated, major point-source plumes within the CMAQ Eulerian grid modeling system. The CMAQ/PinG applies a Lagrangian approach that simulates plume growth in a gradual, real-world manner due to turbulence and wind shear processes. This treatment differs from the traditional Eulerian grid modeling method, which instantly mixes point-source emissions into an entire grid-cell volume. This overdilution effect becomes more pronounced with increasing horizontal grid size, especially for the coarse grid resolutions specified for regional- or continental-scale modeling domain applications. The key algorithms are a plume dynamics model processor and a Lagrangian reactive plume model (PinG module), which are designed to simulate the relevant plume processes at the proper spatial and temporal scales for CMAQ model domains with grid-cell sizes greater than 10 km. The PinG treatment is able to simulate plumes from multiple point sources and for the entire diurnal cycle. A continuous plume is represented by a series of plume sections, each of which has been released at a 1-hour interval. The horizontal dimension of each plume cross-section is internally resolved by an array of attached plume cells. The PinG module is fully integrated into the CMAQ grid model. It is exercised concurrently during a CMAQ-CTM model simulation and takes advantage of grid-cell concentrations as boundary conditions along each plume section edge. An important feedback occurs when a plume section reaches the model grid-cell size. At that time, the subgrid plume treatment ceases for the particular plume section and plume concentrations are incorporated into the Eulerian grid framework. A full description of the capabilities of the CMAQ/PinG modeling treatment and its technical formulation are described in Gillani and Godowitch (1999).

The aerosol algorithm version 3 (AE3) employed in the CMAQ-CTM was also incorporated and successfully tested in the PinG module. The 2005 public release of the CMAQ modeling system included the PinG module with the capability to perform aerosol formation in subgrid plumes. Currently, the PinG module treats aerosol species and $PM_{2.5}$ along with gas-phase photochemistry in subgrid plumes. A set of CMAQ/PinG simulations was successfully completed on a multi-processor computer system in a parallel processing mode. Model simulations were conducted with the PinG approach for January and July 2001 on a continental domain with a 36-km grid-cell size. There were 47 high emission NO_x and SO_2 point sources in the modeling domain. In the no-PinG simulations, these major point-source emissions were incorporated into the 3-dimensional emission data sets. Preliminary results of modeling aerosols in PinG revealed differences in aerosol sulfate (SO_4) concentrations in the vicinity of high NO_x and SO_2 point sources. For point sources with comparable SO_2 emissions, greater sulfate formation occurred in those subgrid plumes exhibiting a lower NO_x emission rate. These PinG results appeared to be supported by recent experimental aerosol data obtained in plumes, which indicated sulfate formation was inhibited in the plumes of high NO_x sources. Initial intercomparisons between the no-PinG and PinG simulation results on the grid-scale indicate, for example, higher ozone and SO_4 concentrations occur in grid cells in the vicinity of the major point sources, which is attributable to the rapid dilution and acceleration of photochemical and aerosol processes in the 36-km grid cells with the no-PinG approach. Further downwind,

concentration differences were small. In addition, an evaluation of modeled gaseous and aerosol species against surface monitoring network data was undertaken. Final results are anticipated in FY-2006.

2.2.9 Linkage of the CMAQ and HYSPLIT Modeling Systems

The development of software interface programs to link the CMAQ and HYSPLIT (HYbrid Single-Particle Lagrangian Integrated Trajectory) modeling systems has commenced in a collaborative effort between ASMD and ARL Headquarters' scientists. This research effort is expected to expand the capabilities of both systems and to provide better analysis tools to assist in investigations involving results produced by both the CMAQ-CTM and HYSPLIT. A key task for providing a software bridge linking the two modeling systems will involve the development of an interface program for the conversion of CMAQ meteorological data files into a HYSPLIT input data file format. The new interface program will retrieve selected meteorological fields required by HYSPLIT from data sets generated by CMAQ's MCIP. Subsequently, the new CMAQ/HYSPLIT interface program will create a compatible output data file for direct use in HYSPLIT modeling applications. Additional software conversion tools will also be designed to rewrite HYSPLIT trajectory and concentration outputs as CMAQ-type data files for importation into a CMAQ visualization tool. This development effort will allow data sets from both modeling systems to be utilized jointly in upcoming model analyses, evaluation, and visualization tasks.

An initial application planned for the new CMAQ/HYSPLIT interface program will be to generate HYSPLIT input data files from existing CMAQ meteorological data sets spanning the summer months of 2002 and 2004 in conjunction with an on-going CMAQ modeling study. The capabilities and strengths of both CMAQ and HYSPLIT modeling frameworks will be utilized to assess the impacts of recent emission reductions of nitrogen oxides (NO_x) from major-point sources on ozone concentrations in the eastern United States. Photochemical simulations by the CMAQ model on a large domain with a 12-km grid-cell size will be performed to generate ozone and other pollutant species for 92 days in June, July, and August of 2002 and 2004. Separate model simulations will be conducted with base case emissions for 2002 and with revised emissions reflecting the NO_x point-source emission reductions implemented for 2004. With the new interface tool linking the CMAQ and HYSPLIT modeling systems, the same meteorological fields used in the CMAQ simulations will be applied to exercise the HYSPLIT trajectory model in an effort to determine back trajectories starting from selected CASTNet (Clean Air Status and Trends Network) measurement sites situated throughout the modeling region. In this study, a HYSPLIT back trajectory will follow the same path taken by pollutants treated in the CMAQ simulations in an upwind manner in space and time in an effort to determine the origin of the air parcel containing the pollutant concentrations impacting the site. Another new CMAQ/HYSPLIT modeling tool will utilize the spatial coordinates of each HYSPLIT back trajectory to probe the 3-dimensional CMAQ concentration field to extract ozone and other pollutant values along each back trajectory path within the gridded domain. In particular, model results from cases with back trajectories passing through such notable major point-source regions

as the Ohio River Valley will be examined to assess maximum ozone concentration differences between the base case and reduced emission simulations. With the combined application of both modeling systems and the new software tools linking the CMAQ and HYSPLIT models, results to be obtained during FY-2006 from this investigation are expected to provide valuable quantitative information about the effectiveness of NO_x emission changes undertaken in particular source areas on decreasing maximum 8-hour ozone levels in downwind areas of the eastern United States.

2.2.10 CMAQ Mercury Model Refinements and Evaluation

The final phase of a European intercomparison study of numerical models for long-range atmospheric transport of mercury was completed. This multi-phase European model intercomparison study was organized by the Meteorological Synthesizing Center - East in Moscow, Russia. The final phase of the intercomparison study involved full-scale simulations over Europe for periods of one month or more. Model simulation results were compared to observations of both air concentrations and wet deposition fluxes of mercury. The results generally showed moderate skill in all models for simulating air concentrations of elemental mercury and particulate mercury, but very limited skill for reactive-gaseous mercury, which is believed to be the most rapidly deposited form of mercury. The results also showed that the lateral boundary values for the air concentrations of elemental mercury had a large effect on the magnitude of the simulated mercury deposition flux across the interior of the model domain used by all of the participating models. A journal article is planned to describe the final phase study results.

During FY-2005, the Division collaborated with the EPA Office of Air Quality Planning and Standards (OAQPS) in the use of the CMAQ mercury model to support EPA's issuance of its Clean Air Mercury Rule (CAMR). This modeling was performed to assess the expected reduction in mercury deposition across most of North America due to various emission control options being considered for CAMR. Simulations were performed using calendar year 2001 meteorology to estimate current deposition patterns and deposition patterns expected in 2020 given a variety of mercury and criteria pollutant emission scenarios. All of the simulations used initial condition/boundary condition (IC/BC) inputs derived from a global-scale simulation of the GEOS-Chem model developed and applied by the Harvard University Department of Earth and Planetary Sciences (Bey *et al.*, 2001). A recent upgrade of the GEOS-Chem model resulted in significantly higher simulated elemental mercury air concentrations. Work is continuing to assess the impact of this boundary value change on simulated mercury deposition fluxes from the CMAQ mercury model.

During FY-2005, efforts continued on a mercury model intercomparison study for North America. This North American Mercury Model Intercomparison Study is designed to build upon the findings from the previous model intercomparison study in Europe. In the absence of comprehensive measurement networks, atmospheric mercury model developers have had to rely on model intercomparison studies to evaluate their modeling of various atmospheric processes, to

gauge the level of modeling uncertainty with respect to specific parameters and variables, and to collect evidence of the most important knowledge gaps leading to these uncertainties. Wet deposition of mercury is measured on a regular basis at a number of remote locations in North America through the Mercury Deposition Network (MDN); however, MDN was designed to detect long-term trends in regional mercury deposition and few of its monitors are located in areas of concentrated mercury emissions. While MDN may not provide sufficient observational closure for comprehensive model evaluation, it can provide information leading to a better understanding of why models differ in their simulations of wet deposition and various related atmospheric processes. The regional-scale atmospheric mercury models being applied are: a mercury-specific version of the CMAQ model by the Division, the Regional Modeling System for Aerosols and Deposition by Systems Applications International (SAI), and the Trace Element Analysis Model (TEAM) by Atmospheric and Environmental Research, Inc. (AER). The modeling domain for the study covers the 48 contiguous United States, southern Canada, northern Mexico, and Cuba. In a cooperative effort involving the Division, EPA's Office of Air and Radiation and Office of Water, Environment Canada, AER, Harvard University, and the New York State Department of Environmental Conservation, three separate global-scale atmospheric mercury models were applied to define three sets of IC/BC data for elemental mercury, reactive-gaseous mercury, and aerosol mercury air concentrations for the regional study area. The global models applied were: the Chemical Tracer Model by AER, the Global-Regional Atmospheric Heavy Metal model by Environment Canada, and the GEOS-Chem model by Harvard University. The regional-scale models are using each of these three IC/BC sets along with identical meteorological and pollutant emissions data to simulate atmospheric mercury transport and deposition across the same regional modeling domain. Through intercomparison and comparison of model results to available observations, the individual effects of IC/BC assumptions and science process treatments in the regional models can be better identified and quantified, and thus, provide guidance to the research community regarding which scientific uncertainties are contributing most to discrepancies in the modeling of source attribution for atmospheric mercury deposition. This effort in continuing into FY-2006.

2.2.11 CMAQ Code Integration and 2005 Release

The CMAQv4.5 model was released to the public in FY-2005. This version included: (1) sea salt aerosols (fine-mode equilibrium, but non-interactive coarse mode) and an updated aerosol dry deposition algorithm; (2) Carbon-Bond IV (CB-IV) chlorine chemistry, CB-IV air toxics, and SAPRC99 air toxics chemistry and associated Euler-Backward Iterative (EBI) solvers; (3) an updated minimum eddy diffusivity (K_z) to use the urban land use fraction; (4) a new subgrid cloud mixing algorithm/module (based on the Asymmetrical Convective Model); (5) a new mass continuity advection scheme; (6) run-time dynamic vertical layers; and (7) primary carbon-source apportionment and sulfate tracking capabilities. Another component of the CMAQ system, MCIPv3.0, was also revised and released in conjunction with the release of CMAQv4.5, which is publicly available from the Community Modeling and Analysis System center at www.cmascenter.org.

2.2.12 Development and Testing of an Air Quality Forecast Model

In FY-2003, NOAA and EPA signed a Memorandum of Agreement to collaborate on the design and implementation of a capability to produce daily air quality modeling forecast information for the United States. The National Centers for Environmental Prediction's (NCEP) Eta meteorological model and CMAQ were linked together to form the core of this forecast system. Testing of the system was conducted during the FY-2003 and FY-2004 ozone seasons for the northeastern United States, and the system became fully operational in September 2004. With additional development, testing, and verification of the air quality forecast (AQF) system, the coverage of the operational O_3 forecasts was expanded to include the entire eastern United States in September 2005. Over the next five years, the model domain will be expanded to the continental United States, and $PM_{2.5}$ will be added to the model forecast capability.

During the summer of 2005, the AQF system was exercised along four streams: (1) operational O_3 forecasts over the northeast United States (1x domain) for dissemination to the general public; (2) experimental forecasts of O_3 over an expanded eastern United States domain (3x domain) for dissemination to the general public; (3) developmental forecasts of O_3 over the entire continental United States domain (5x domain) for dissemination to a focus group of forecasters, and (4) developmental forecasts of both O_3 and particulate matter (PM) concentrations over the 3x domain for initial assessments of PM forecast capabilities. In the first three applications, aerosols were not simulated by CMAQ. In all applications, the CB-IV chemical kinetic mechanism was used, the horizontal grid-cell size was 12 km, while the vertical extent from the surface to 100 mb was discretized using 22 layers of variable thickness. The emission inventories used by the AQF system were updated to represent the 2005 forecast period. NO_x emissions from point sources were projected to 2005 (relative to a 2001 base inventory) using estimates derived from the annual energy outlook by the Department of Energy. Comparisons of NO_x emission estimates for 2003 and 2004 using this approach with measurements from the Continuous Emission Monitoring (CEM) database showed good agreement. Area source emissions were based on the 2001 National Emissions Inventory v3, while BEIS3.12 was used to estimate the biogenic emissions. Mobile emissions were estimated using a computationally-efficient, least-square regression-based approximation to the Mobile6 model, which utilized 2005 estimates for the vehicle fleet information and vehicle miles traveled data.

Based on performance of the AQF system in 2004 and additional retrospective testing, several enhancements were included in the CMAQ model, which were further tested in the different forecast streams described above. The turbulent mixing scheme in CMAQ was further enhanced to allow the minimum value of the surface layer vertical-eddy diffusivity (K_z) to vary spatially depending on the fraction of urban area in each grid cell. The approach allows for K_z in rural regions to fall off to a lower value than predominantly urban regions. This allows increased nighttime O_3 titration in rural areas, reducing modeled O_3 overpredictions. The approach also allows simulated nighttime precursor concentrations in urban areas from becoming too large. Examination of the AQF system's performance over time revealed a systematic pattern of varied accuracy that was attributed to the synoptic-scale meteorology impacting the domain. The model

performed very well during periods when anticyclones, characterized by clear skies, dominated the domain. Conversely, periods characterized by extensive cloud cover associated with fronts and/or cyclones resulted in poor model performance. Subsequent analysis revealed two main factors contributing to this overprediction. The first involved the excessive downward transport of O_3 rich air (specified in the model based on O_3 profiles derived from the Global Forecast System (GFS) model) via CMAQ's convective cloud scheme. The second factor involved too little attenuation of actinic flux by CMAQ's simulated cloud cover, resulting in too much photolysis, and subsequently, too much production of O_3. In combination, these factors resulted in the AQF system's systematic overprediction of O_3 in and around areas of cloud cover. To address these shortcomings, modifications were introduced both to the cloud mixing scheme as well as in the estimation of attenuation of photolysis rates due to the presence of clouds. A new in-cloud mixing scheme based on the ACM model was included and tested in the 5x developmental runs. To improve the estimation of the below-cloud photolysis attenuation as well as for closer linkage with the driving meteorological model's cloud and radiation fields, the below-cloud attenuation was derived from the ratio of the radiation reaching the surface to its clear-sky value. Approaches for specifying lateral boundary conditions to CMAQ based on typical "clean" tropospheric background values and based on using O_3 predictions from the GFS model in the upper troposphere were also further investigated.

2.2.13 Linking the North American Mesoscale Model with CMAQ for Air Quality Forecasting

A key component in the linkage between NCEP's North American Mesoscale (NAM) model (currently the Eta model) and CMAQ is PREMAQ, a new pre-processor for CMAQ that is largely equivalent to MCIP and parts of SMOKE© in the community version of the CMAQ modeling system. PREMAQ places the post-processed Eta model output into the required horizontal and vertical grids for CMAQ. Like MCIP, PREMAQ computes state variables and other derived variables (*e.g.*, air density, Jacobian, dry deposition velocities for chemical species) that are required by CMAQ. Unlike MCIP, PREMAQ also includes calculations of the meteorology-dependent emissions (*i.e.*, biogenic and mobile sources) adapted from SMOKE©. The output from PREMAQ includes the full set of meteorology and emissions files that are used by CMAQ. A description of PREMAQ can be found in Otte *et al.* (2005).

Modifications to PREMAQ were continued in FY-2005 to improve the coupling between the meteorological and chemistry transport model components of the AQF system. To improve the representation of below-cloud photolysis attenuation in the chemistry calculations in CMAQ, a new variable representing the attenuation factor (the ratio of the radiation reaching the surface to its clear sky value) was added to PREMAQ. Testing of this new methodology to represent photolysis attenuation showed lower bias in predicted ozone under cloudy conditions and provided better representation of the effects of clouds on the simulated photochemistry compared to the previously used empirical approach. Major enhancements in improving the computational efficiency of the PREMAQ code were also made, which resulted in reducing by half its required computational time. In addition, work is underway to modify PREMAQ to produce fields on the

vertical and horizontal grids that are native to the WRF-Non-Hydrostatic Mesoscale Model (WRF-NMM), which is projected to replace the Eta model as the NAM model. These modifications to PREMAQ are targeted to further improve coupling of the meteorological and chemistry transport model in a "one-way" linkage. This coupling is expected to be available for initial testing in FY-2006.

A manuscript which describes the process and software components that were used to link the Eta model and CMAQ was published in *Weather and Forecasting* (Otte *et al.*, 2005). The manuscript discusses several technical and logistical issues that were considered, and provides examples of ozone forecasts from the air quality forecasting system and relates them to the forecast meteorological fields.

2.2.14 Evaluation of Eta-CMAQ Forecast Predictions for Summer 2005

An important component of the AQF system was the development and implementation of an evaluation protocol. Accordingly, a suite of statistical metrics that facilitate evaluation of both *discrete-type* forecasts and *categorical-type* forecasts of O_3 concentrations was developed and applied to the system to characterize its performance. The continental United States was divided into six geographic regions (Figure 1) for which various statistical measures were examined. The results reveal that the AQF system performed reasonably well as indicated in Table 1. The model was biased high for all regions, though the magnitude of the bias varied from region to region. Comparison of model forecasts from the experimental and developmental forecast streams using different model configurations provided an opportunity to test and evaluate alternate process representations. These revealed consistently improved performance (lower O_3 bias) resulting from improvements made in the representation of cloud processes (mixing and photolysis attenuation) that were tested in the developmental forecast simulations.

Extensive evaluation of the forecast results from the summer of 2004 were conducted through comparisons with a variety of measurements from surface sites and aircraft deployed during the 2004 ICARTT field study. Comparisons of predicted vertical O_3 profiles with measurements from ozonesonde data collected during this study indicated overpredictions in modeled free-tropospheric O_3 concentrations at altitudes greater than 6 km. This overprediction was attributed to the use of the GFS-derived O_3 lateral boundary conditions at altitudes above 6 km. Comparison of Eta-CMAQ O_3 predictions with those from several forecast models operational during the ICARTT period showed performance comparable with other models (McKeen *et al.*, 2005).

Continuous evaluation of PM forecast results from the developmental simulations was performed. These include evaluation of predicted total $PM_{2.5}$ against measurements from the AIRNow network. The compositional characteristics of predicted particulate matter were evaluated against speciated PM measurements from the Speciated Trends Network (STN) and CASTNet data and showed model performance to be reasonable and comparable to previous

CMAQ assessment applications. Additional comparisons of PM constituent predictions with aircraft measurements from the ICARTT study are underway.

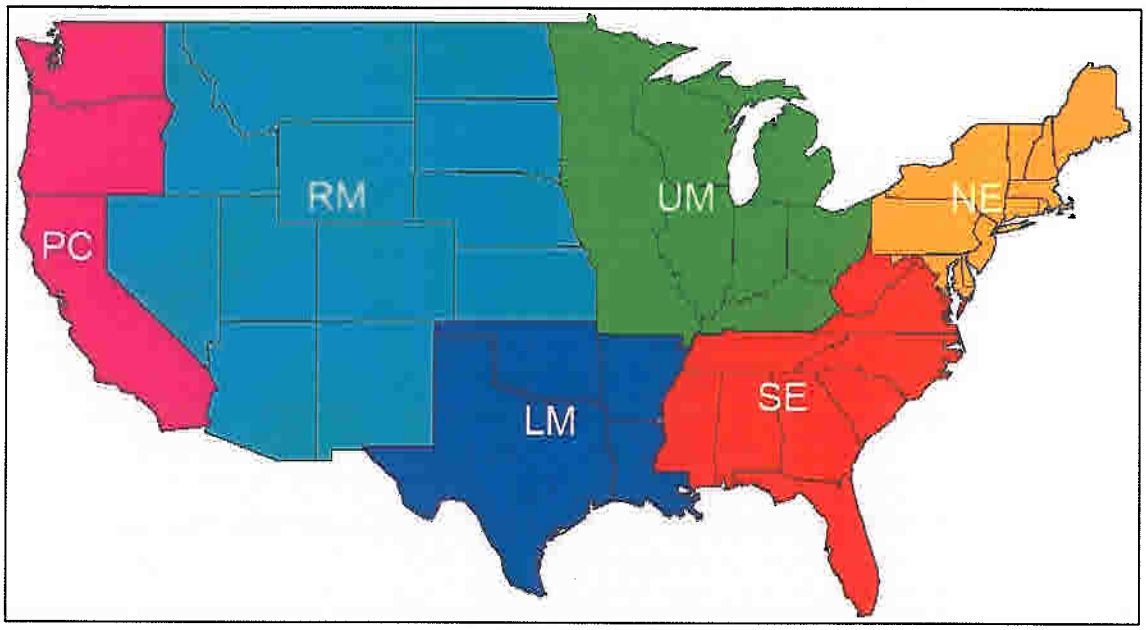

Figure 1. Analysis of sub-region for the continental United States air quality forecast applications.

Table 1. Summary of discrete statistics for maximum 8-hour ozone for the July-September 2005 period over the continental United States and sub-regions (N denotes the number of data points).

Region	N	Obs. (ppb)	Model (ppb)	RMSE (ppb)	NME (%)	MB (ppb)	NMB (%)	R
Domain	102356	48.8	56.0	14.3	23.3	7.2	14.7	0.70
NE	14723	48.8	57.5	14.6	23.4	8.6	14.7	0.73
SE	18916	47.3	56.6	14.8	25.0	9.3	19.6	0.73
UM	22675	51.1	64.1	13.6	20.3	7.9	15.5	0.74
LM	12117	48.3	54.0	14.6	23.8	5.6	11.7	0.69
RM	10439	53.2	59.9	14.1	20.4	6.7	12.5	0.53
PC	14698	52.7	53.8	14.9	22.6	1.2	2.2	0.64

2.3 Atmospheric Model Evaluation and Application Activities

2.3.1 Diagnostic Metrics for Ozone and Inorganic Particulate Matter

Diagnostic metrics enable the examination of model processes and consider the reliability of control strategy predictions. They require a special set of non-routine measurements, because they typically require ratios of species involved in photochemical production or aerosol equilibrium processes. Earlier work (Tonnesen and Dennis, 2000a; 2000b) identified O_3/(NO+true NO_2 = NO_X) as a metric to help assess the troposphere's photochemical state of the atmosphere relative to ozone production and to the expected magnitude and direction of a change in O_3 concentrations due to a change in hydrocarbon or nitrogen oxide emissions.

Current work is examining the Gas Ratio (GR) defined by Ansari and Pandis (1998) as a metric to assess the physical and chemical state of inorganic fine particles in the atmosphere. The inorganic fine particle system is a priority, because the inorganic fine particles represent a majority of the total fine mass in the eastern United States and the inorganic system has some important nonlinearities. The GR is equal to the free ammonia divided by total-nitrate. Free ammonia is defined as the moles of total ammonia (gaseous ammonia plus aerosol-phase ammonium) minus twice the moles of aerosol sulfate, and total nitrate equals nitric acid + aerosol-nitrate. The usefulness of the GR for evaluation of model-predicted inorganic fine aerosols and their nonlinear responses is being assessed. The first nonlinear response being studied is the degree to which aerosol nitrate will replace sulfate as SO_2 emissions are reduced. The conceptual model represented in the GR and articulated through thermodynamic calculations (Ansari and Pandis, 1998) indicates that the degree of nonlinearity in the PM response to sulfate reductions will depend on the GR value. For GR values much greater than 1 (*i.e.*, ammonia-rich regime), the decrease in inorganic PM is expected to be proportional to the sulfate reduction, because two moles of ammonium are removed along with each mole of sulfate. At GR values much less than 1 (*i.e.*, nitrate-rich regime), inorganic PM mass is expected to increase in response to a sulfate reduction, because two moles of nitrate will replace each mole of sulfate that is removed. At GR values close to 1, the inorganic PM mass response to a sulfate reduction is expected to be nonlinear.

Examination of CMAQ results for winter 2002 suggests that almost the entire eastern United States will be affected by the nonlinear response of the inorganic aerosol system. The winter 2002 nonlinear response was studied with CMAQ sensitivity analyses in terms of the nitrate relative response (Nitrate-RR), or percentage increase in nitrate, due to a 25 percent decrease in SO_2 emissions. The inorganic PM concentrations, the GR, and the Nitrate RR were all examined with respect to monthly averaged concentration to be consistent with model application practice. All model grid cells across the eastern United States with significant inorganic PM (*i.e.*, concentrations > 5$\mu g/m^3$) were included. An exploration of relationships between the Nitrate RR and other variables showed that the GR is the best predictor of the Nitrate RR, even for monthly averages. The GR is a better indicator than originally thought when examining CMAQ sensitivities at the Pittsburgh supersite alone. Model evaluation comparisons show that model inputs of total ammonia and total nitrate have a larger degree of

uncertainty than does sulfate. This input uncertainty will create an uncertainty in the CMAQ-predicted GR and, therefore, also the CMAQ-predicted Nitrate RR compared to real world values. A second part of the sensitivity analysis explored how large an uncertainty in the Nitrate RR might result from errors in the model inputs of total ammonia and total nitrate. It was found that the most important input uncertainty is the uncertainty in total ammonia. Further analyses are underway to link the monthly average GR and Nitrate RR behavior with the hourly behavior that is understood best in terms of theory. A publication on this work will be forthcoming.

2.3.2 Diagnostic Evaluation for Carbonaceous Aerosol Components

A substantial fraction of fine particulate matter across the United States is composed of carbon (Malm *et al.*, 2004). At routine monitoring sites, carbonaceous aerosol is segregated into organic carbon (OC) and elemental carbon (EC) based on its thermal and optical properties. The OC fraction may be subdivided further into primary organic carbon (OC_{pri}), which is emitted directly to the atmosphere in particulate form, and secondary organic carbon (OC_{sec}), which is formed in the atmosphere through oxidation of reactive organic gases and subsequent gas-to-particle conversion processes. It is important to determine the relative contributions of OC_{pri} and OC_{sec} to the ambient aerosol burden so that policymakers may decide which portion of the organic aerosol complex to target in their control strategy selection process. In FY-2005, the semi-empirical EC-tracer technique of Yu *et al.* (2004) was applied to estimate ambient concentrations of OC_{pri} and OC_{sec} throughout the 2001 calendar year at 142 monitoring sites across the United States. The semi-empirical estimates of OC_{sec} were compared with CMAQ model results of OC_{sec} at the same times and locations. This comparison revealed that the CMAQ model results of OC_{sec} are biased high by a factor of two during August and September in the west coast states and are biased low by a factor of two during June through August in the southeastern United States. Knowledge of these discrepancies will help guide the development of the next generation of secondary organic aerosol modules.

In the southeastern United States, carbonaceous aerosol is the largest component of fine particulate mass (Hansen *et al.*, 2003) and a significant portion of that carbon is of non-fossil-fuel origin (Lewis *et al.*, 2004). Radiocarbon (^{14}C) measurements quantitatively distinguish contemporary sources of carbon from fossil-fuel carbon. To date, ^{14}C data have received limited use in air quality model evaluations, because most models do not track contemporary carbon and fossil-fuel carbon separately. For example, carbonaceous aerosol in the CMAQ model is tracked as either EC, OC_{pri}, anthropogenic OC_{sec}, or biogenic OC_{sec}. Among these model species, both EC and OC_{pri} contain a mixture of contemporary and fossil-fuel carbon. Recently, Bhave *et al.* (2004) developed a version of CMAQ to track explicitly the EC and OC_{pri} contributions from individual source categories. In FY-2005, this model version was exercised over the continental United States for a 1999 summer simulation. Source-segregated model results were combined with anthropogenic and biogenic OC_{sec} concentrations to obtain CMAQ model estimates of contemporary- and fossil-fuel-carbon concentrations. These model estimates were compared against ^{14}C measurements collected in Nashville, Tennessee, during the same period (Bhave *et al.*, 2005). The comparisons reveal that the CMAQ model substantially underestimates

contemporary carbon (mean bias = -2.3 $\mu g/m^3$) and slightly underestimates fossil-fuel carbon (mean bias = -0.6 $\mu g/m^3$). This information in combination with the OC_{sec} comparisons described above suggests that a large fraction of the model underestimations of carbonaceous aerosol during summer in the southeastern United States may be due to biogenic OC_{sec}.

2.3.3 CMAQ Model Operational Evaluation to Assess Its Readiness for use in the Preparation of State Implementation Plans

An operational evaluation of CMAQv4.5 was performed in support of its September 2005 release. This evaluation included annual simulations at both 36-km x 36-km and 12-km x 12-km horizontal-grid resolution, and also a model-to-model comparison against the previous CMAQv4.4. A key result from the evaluation is a notable improvement in sulfate predictions for the 12 km x 12 km resolution as compared to last year's version, which is related to changes that were made to the CMAQ cloud scheme and dry deposition velocity estimates for fine particulates. While 8-hour maximum O_3 concentration predictions during the "O_3 season" (April through September) were quite good overall ® = 0.74, Normalized Mean Bias (NMB) = 1.62 percent; and Normalized Mean error (NME) = 17.4 percent), CMAQ underpredicted ozone for high observed concentrations (> 85 ppb) and overpredicted ozone for low observed concentrations (< 35 ppb). CMAQ also displayed a tendency to overpredict (NMB often > 30 percent) along coastal regions, which may be tied to poor representation of coastal boundary layers and their interaction with land/sea breezes. The performance of CMAQ's NO_3^- simulations continued to improve from previous versions of the model with the best performance for NO_3^- was in the winter and spring seasons. The quality of simulations of EC and OC also improved over the previous version of the model; however, much uncertainty in the emissions and the secondary formation of OC is still evident when looking at the evaluation results.

As identified in this evaluation, potential areas of research for model improvements include reducing uncertainties in emission inventories (especially the temporal allocation of NH_3 emissions and emissions associated with the carbonaceous species), proper representation of the meteorological fields, and improving our understanding of the aerosol dynamics in the CMAQ aerosol component. Underpredictions at high ozone concentrations must also be investigated to determine the cause of this bias. Results from this evaluation have been documented in a report that is available at the CMAS website.

2.3.4 Model Evaluation Tool Development

Significant effort is often required to compare observations and model results for operational evaluations, as well as extended analyses for diagnostic testing. Most off-the-shelf tools do not address the specialized needs encountered in model evaluation. The Atmospheric

Model Evaluation Tool (AMET) utilizes a MySQL®[2] database framework, combined with a web-based interface and R scripting to create a user friendly, fast method to aid model evaluation. The advantages of the AMET is that it offers an organized method for storing, retrieving and querying observational and model data through the use of a MySQL® database. The program offers a user friendly, web-based method to query and generate various plot and statistics. AMET has capabilities to evaluate both meteorological model predictions and air quality model predictions.

Air quality modeling predictions are strongly affected by errors in meteorological model predictions. AMET has been used to evaluate 2001, 2002, and 2003 meteorology simulations from the PSU/NCAR MM5 over the continental United States at a grid size of 36-km, and a similar simulation over the eastern United States with 12-km grid cells for 2001. Surface meteorological variables (2 m temperature, 10 m wind speed and direction, and mixing ratio), tropospheric wind profiles, and precipitation were evaluated, and results presented in various formats. The tool was used in other experiments, including 8-km and 2-km (horizontal grid size) meteorological MM5 simulations for the Bay and Regional Atmospheric Chemistry Experiment (BRACE), and several 12-km MM5 simulations during the summer of 2004 to aid in the development of a more accurate boundary-layer parameterization. The AMET system has been used to facilitate model evaluations presented in several peer-reviewed journal articles. Figure 2 is an example plot from the AMET system.

For the 2005 release of CMAQ, AMET was used extensively to create statistics and plots that were included in a comprehensive document covering the evaluation of the new air quality model. Model predictions were compared using AMET against five different observational networks to evaluate the ozone and aerosol species, including CASTNet, Interagency Monitoring of Protected Visual Environments (IMPROVE), Air Quality System (AQS), STN, and National Atmospheric Deposition Program (NADP) networks. Results have been presented and are currently being developed into a journal manuscript for submission.

In December 2005, a beta version of the AMET code was provided to the EPA OAQPS. In early 2006, the beta version of AMET will be shared with other beta testers, with the eventual goal of releasing a final version of AMET along with the 2006 release of CMAQ. All the components of the AMET system are open source and as such, the user community will be able to improve the code through additional codes and improvements in existing codes. Ongoing improvements to the AMET system will be made, including the addition of advanced model evaluation techniques as new code becomes available.

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[2]MySQL is a registered trademark of MySQL AB in the United States, the European Union and other countries.

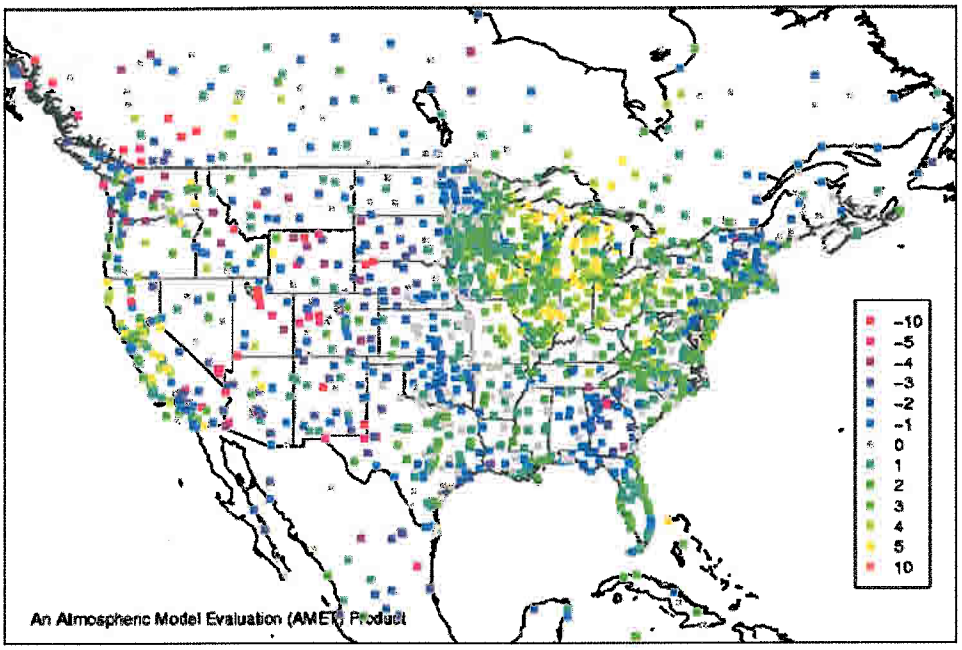

Figure 2. An AMET statistical plot depicting the difference between simulated and observed minimum temperature (K) on August 8, 2002.

2.3.5 Spatial and Temporal Analysis of CASTNet Air Concentration Data

As required by the Clean Air Act Amendments (CAAA) of 1990, CASTNet was implemented by EPA to establish an effective rural monitoring and assessment network. The network's primary purpose is to identify and characterize broad-scale spatial and temporal trends of various air pollutants and their environmental effects. Accordingly, the purpose of this research is to facilitate such identification and characterization across a variety of spatial and temporal scales, focusing on the ambient air concentration patterns of SO_2, SO_4^{2-}, HNO_3, NO_3^- and NH_4^+. This is achieved through the application of principal component analysis, in conjunction with spectral density analysis, to the weekly air concentration data obtained from CASTNet, covering the period October 24, 1989, through August 15, 1995.

These analyses have allowed for the identification and subsequent characterization of homogeneous "influence regimes" associated with each of the five species. Depending on the species, either two (NO_3^-); three (SO_2, SO_4^{2-}, NH_4^+); or four (HNO_3) influence regimes were identified by the principal component analysis. Examination of the temporal variability of these homogeneous influence regimes through spectral density analysis revealed various seasonal and annual cycles of differing strengths and timing. The identification of homogeneity across sites has added to the "weight of evidence" supporting regionality of behavior of each of the species, which have historically been difficult to estimate and understand because of complicating factors, both meteorological and chemical.

2.3.6 Model Evaluation Using Advanced Spatial Statistical Models

A typical model evaluation for CMAQ includes the comparison of each monitoring value with the value simulated by CMAQ for the grid cell in which the monitor lies. Based on these paired values, various analyses can be performed based on simple scatterplots, measures of correlation, and estimates of bias. Such methods allow large amounts of data to be processed quickly and produce easily understandable summary plots and statistics. However, for a detailed study of a particular pollutant and/or region, these traditional methods can be inadequate, especially when monitoring data is relatively scarce. In addition, formal statistical inferences are limited by inherent spatial and/or temporal correlation in the data.

More advanced statistical methods can be used to account for the spatial correlation structure inherent in the atmospheric process. For example, Bayesian spatial modeling techniques can be used to produce estimates of pollution for each grid-cell and the likely errors associated with these estimates based on the data collected by sparsely located monitors. These estimates can be compared with the actual simulated values provided by CMAQ. If the difference between an estimated grid-cell value and the CMAQ-simulated value is substantially larger than the error associated with the statistical estimate, the grid cell is identified for further inspection.

This statistical method was used to assess CMAQ's ability to simulate aerosol sulfate in a portion of the Mid-Atlantic region of the United States during two four-week periods in the winter and summer of 2001. During the summer period (17 July 2001–14 August 2001), average sulfate concentrations simulated by CMAQ largely agreed with the estimates made by the statistical model based on monitoring data collected during the period. However, during the winter period (02 January 2001–30 January 2001), there were many grid cells in the focus region for which the CMAQ-simulated values fell outside the 95 percent credible intervals yielded by the statistical model for average sulfate concentrations.

This statistical method was also used to investigate the impact of precipitation inputs from MM5 on the ability of CMAQ to simulate ammonium wet deposition amounts. This study focused on two eight-week periods, one in winter (02 January 2001–27 February 2001) and one in summer (05 June 2001–31 July 2001). For each season, two sets of statistical estimates of ammonium wet deposition were produced. One set was based on deposition monitoring data collected by the NADP monitoring sites and on observed precipitation from the National Weather Service U.S. Cooperative Observer Program network. The second set utilized the same deposition monitoring data, but used MM5-simulated precipitation. Each of these sets of statistical estimates was compared with the CMAQ-simulated ammonium wet deposition amounts, and significant differences were identified. In the winter period, the patterns of these differences are similar using both sets of statistical estimates, which implies that discrepancies between observed precipitation amounts and MM5-simulated precipitation amounts are not major factors in CMAQ's ability to simulate ammonium wet deposition. However, in the summer period, the patterns of significant differences using the two sets of statistical estimates differ. This allowed the identification of particular areas in which CMAQ's ability to simulate

ammonium wet deposition may have been affected by the accuracy of the precipitation information it received.

2.3.7 Bay Regional Atmospheric Chemistry Experiment Model Evaluation

The Tampa Bay Estuary Program and the Florida Department of Environment asked NOAA and EPA to enter into a partnership to apply CMAQ to 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. Tampa Bay provides an important coastal atmospheric problem involving coarse particles and sea salt. CMAQ was selected as the model for the Tampa Bay Assessment primarily for two reasons. One, CMAQ will incorporate sea salt in its aerosol module in FY-2006. Two, the University of California, Davis (UCD), developed a dynamic sectional model for CMAQ incorporating sea salt in its calculations. The Wexler sectional aerosol model, Aerosol Inorganic Model (AIM) was implemented into the 2004 release of CMAQ, and re-named CMAQ-UCD. Prior to any Tampa Bay assessment, it was agreed that CMAQ, starting with CMAQ-UCD, should be evaluated against high-quality local data.

BRACE, designed for the above purpose, was conducted during May 2002. Division scientists and ARL colleagues were involved in the planning of BRACE. ASMD and ARL scientists helped site three wind profilers around the Bay, and helped define the complete chemistry package of instruments for the NOAA Twin Otter aircraft flown by ARL. Analysis of the May 2002 data showed a large discrepancy in the measurement of HNO_3. ASMD scientists took the lead in organizing and conducting a HNO_3 intercomparison study during October 2003. The intercomparison showed that there was an inlet problem during May 2002. The October 2003 results have provided the ASMD modelers with crucial guidance in how to create a best estimate of the nitrogen budget for comparisons against CMAQ.

The MM5 simulations for the May 2002 period at 8-km and 2-km resolutions were evaluated, especially with respect to the ability to replicate the sea breeze. At the close of FY-2004, the MM5 simulations were deemed adequate, allowing the CMAQ-UCD evaluation to proceed. The evaluation of CMAQ-UCD against surface sites used diagnostic indicators to probe the nitrogen chemistry and sectional data to test the aerosol physics in CMAQ-UCD. The FY-2005 evaluation focused on the 8-km grid predictions. Ozone production efficiency curves in CMAQ-UCD agree well with those observed at the Sydney supersite, which is in the Tampa area. Performance of the new UCD aerosol module is judged to be adequate. Aerosol sulfate, ammonium, sodium, and chloride were all predicted to within a factor of 2 at three sites. Size segregation maxima were correct to within 2 size bins every day, sulfate and ammonium being in the fine sections and sodium and chloride being in the coarse sections. The evaluation established confidence in the surface-level performance of CMAQ-UCD for application to the Tampa Bay nitrogen deposition assessment.

2.3.8 Analysis of the NO_x State Implementation Plan Call: Accountability and Dynamic Evaluation

The NO_x Initiative project is a first phase of a long-term accountability program to develop innovative methodologies and analytical tools to assess emission control strategy effectiveness. It also provides an ideal venue for dynamic evaluation of the CMAQ model, where the model's air quality response to observed changes can be tested. Accountability is a growing area of needed research to demonstrate the effectiveness of required emission controls given the significant costs of emission control measures. Substantial reductions in NO_x emissions from stationary sources have occurred in the eastern United States, and additional reductions are anticipated. This first phase project focuses on the time period during which the NO_x State Implementation Plan (SIP) call required reductions in NO_x emissions from major-utility sources in the eastern United States, from approximately 1999 through 2004.

The conceptual framework of accountability involves the tracking of observed changes in relevant air quality endpoints and emissions and testing model abilities to replicate the observed air quality changes. The NO_x initiative project introduced an integrated approach toward assessing and documenting relationships between emissions, air quality, atmospheric deposition, and effects to public health and ecosystems through the following steps:

1. *Analysis of Continuous Emissions Monitoring (CEMs) Data.* Since the 1990 Clean Air Act Amendments, a greater number of stationary sources of SO_2 and NO_x emissions have installed continuous emissions monitoring systems. These CEM data provide the only ground-truth direct observations of NO_x emissions, and since these are measurements of emissions from major stationary sources, CEM data are directly relevant to emission reductions from the NO_x SIP call reductions that were required from the utility sector by 2004.

2. *Analysis of Observed Ozone Changes.* Using several methods to remove meteorology influences from ozone trends, time-series analyses of observed ozone data were performed from 1990 through 2004. Ozone data from AQS and CASTNet were included in this analysis. Results from this analysis did show a decrease in ozone concentrations (1 hour maximum values) over the same time period as the NO_x SIP call.

3. *Air Quality Modeling.* Since air quality models are used in the development of air quality management rulemaking, it is important to include air quality modeling in an accountability study. To consider the sensitivity of ozone predictions to meteorology, two series of air quality simulations were conducted for the years 2002 and 2004, since they represent an hotter, ozone-producing summer and a cooler, wetter summer, respectively. CMAQ simulations were conducted for both summers. CEM data were included for the emissions, so that the directly measured reductions in the utility sector were introduced into the simulations. CMAQ simulations were also conducted where the emissions for 2004, after NO_x SIP call reductions were introduced, were introduced to 2002 meteorology, and visa versa.

4. *Trajectory Modeling to Track Source Area Influences.* Since the NO_x SIP call was intended to reduce the amount of ozone and ozone precursors transported, it is important to consider the relationship between ozone concentration changes and change in emissions in other areas. The HYSPLIT model was used to separate summer days during the periods of 1998-1999 and 2002-2004 when monitors were downwind of the Ohio River Valley from days when they were not downwind. Analysis of the CEM data shows that some of the largest emission reductions during the NO_x SIP call occurred in the Ohio River Valley. This approach demonstrated that a larger ozone reduction was evident after the NO_x SIP call at many rural CASTNet monitors when only considering days downwind of the Ohio River Valley. A similar approach is planned for analyzing the CMAQ simulations where HYSPLIT will use the meteorological model fields that drove the CMAQ simulations.

A new task that will build upon the products of this initiative will be proposed to further address the development and use of tools that will enable and enhance air quality management accountability programs. Future work may focus on implementation and effectiveness of the Clean Air Interstate Rule (CAIR) and proposed rules to control air toxins.

2.3.9 Remote Sensing and Air Quality Modeling: Fire Emission Estimates

Major wildfire events can be an important source of airborne $PM_{2.5}$) emissions in the form of elemental carbon (EC) and organic carbon (OC). In the current National Emissions Inventory (NEI), fire-related emission estimates are spatially and temporally resolved to the monthly scale for most states, so that the emissions are constant for the entire month. Further, the locations have not been reported for some states, so that the spatial distribution of the fires must be crudely approximated without additional information. The purpose of this study is to test the usefulness of the National Aeronautics and Space Administration (NASA) MODerate Resolution Imaging Spectroradiometer (MODIS) Rapid Response (RR) fire-detection satellite product for improving the NEI emission estimates from wildland fires and predicting the $PM_{2.5}$ concentrations. May and August 2001 showed very high emissions from wildfires with two major fire events: May 14–29, 2001, in Lafayette County, Florida, popularly known as the Mallory Swamp fire", and August 13–21, 2001, in Cascade Range in northern Washington. In May 2001, wildfires in the state of Florida alone accounted for approximately 56 percent of the annual fire-related emissions in the NEI for the CONtiguous United States (CONUS). The impact of the wildfire-related emissions from the northwestern (NW) states of California, Oregon, Idaho, Montana, and Washington combined during the month of August 2001 is about 55 percent of the annual fire-related emissions in the NEI for the NW part of the CONUS. During these two months, emissions from wildland fires accounted for more than 15 percent of the total $PM_{2.5}$ emissions from all sources in the NEI. The MODIS RR active fire product is used for reallocation of the NEI, and the ground-based EC and OC data from the IMPROVE network are compared with the corresponding CMAQ time-series predictions of total carbon. Aerosol Optical Depth (AOD) and single scattering albedo computed from the CMAQ compositional mass are also analyzed in

conjunction with MODIS AOD columns to infer the aerosol property and to verify whether CMAQ responds well to the wildfire activity in time and space domain.

The results suggest that the reallocation procedure can help improve the predictions of temporal variability in total carbon aerosol concentrations, but an overprediction is evident at some monitoring locations. While the satellite information does help to characterize the variability in carbonaceous aerosol predictions, additional work is needed to create more realistic emission distributions. It is also inferred that emissions reallocation could reduce biases in the base-case simulation of total carbon (OC+EC) during the non-fire periods, and consequently by applying the MODIS wildfire signature-based reallocated NEI for the CMAQ simulations show a better correlation with the IMPROVE total carbon data obtained from locations having a significant separation from the wildland fire. Also, during the fire events, emissions reallocation could result in overprediction of total carbon concentration at the grid cell with the wild fire itself when compared with observed total carbon concentration from an IMPROVE site in the adjacent grid cell located about 34 km from the fire. Figure 3 shows a monthly average of the modeled total carbon concentrations overlaid with IMPROVE observed total carbon. Figure 3 also includes scatter plots to show how the observed total carbon concentrations compare with the total carbon data obtained before and after emissions reallocation for the southeastern United States during May 2001, and for the northwestern United States during the month of August 2001 (Roy *et al.*, in press).

CMAQ predicted carbon-monoxide (CO) total columns obtained from model runs using satellite fire-count based reallocated emissions have also been compared with another satellite based data product obtained from the Measurement Of Pollution In The Troposphere (MOPITT) sensor. A preliminary comparison was done for the period August 22›25, and August 31, 2001. This study suggests a fair agreement between the model and MOPITT CO columnar observations. This could be inferred from the August 31, 2001, plots (Figures 4(a) and 4(b)). A slightly improved CO data is obtained for comparison with the MOPITT product after using the wild-fire reallocate model run CO profile (Figure 4(c)). In general, it is found that CMAQ underestimates CO compared to MOPITT data. Hence, it would be important to study the model—s responsiveness to convective outflow of CO from the planetary boundary layer to the free troposphere based on studies by Li *et al.* (2005) as mentioned in Choi *et al.* (2005). Using MOPITT data, it would also be possible to ascertain a factor by which CMAQ actually underestimates the observations on a seasonal basis. Since MOPITT provides data globally, it would also be important to estimate influx of CO due to intercontinental transport from outside the CMAQ boundary in the western part of the United States.

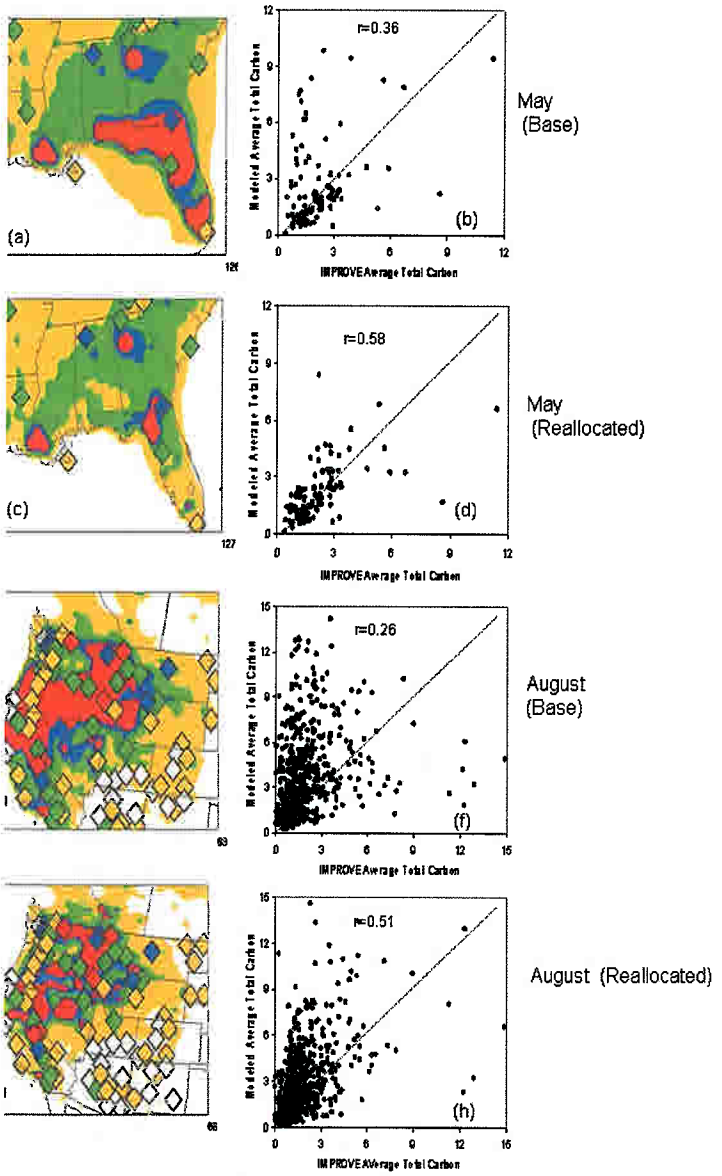

Figure 3 (a) Monthly average spatial plot of CMAQ total carbon concentration in μg m^{-3} before emission reallocation along with overlaid colored diamonds showing the IMPROVE measured average (of 10 samples) total carbon concentration obtained during the month of May 2001 in the SE region; (b) Scatter plot of daily observed and base case modeled total carbon concentration data along with the 1:1 line; (c) Same as in 1 (a) except plotted with model predictions averaged after emissions reallocation; (d) Same as in 1(b) but for the reallocated emissions case; (e-h) Same as in (a-d) respectively but for the NW region during August 2001.

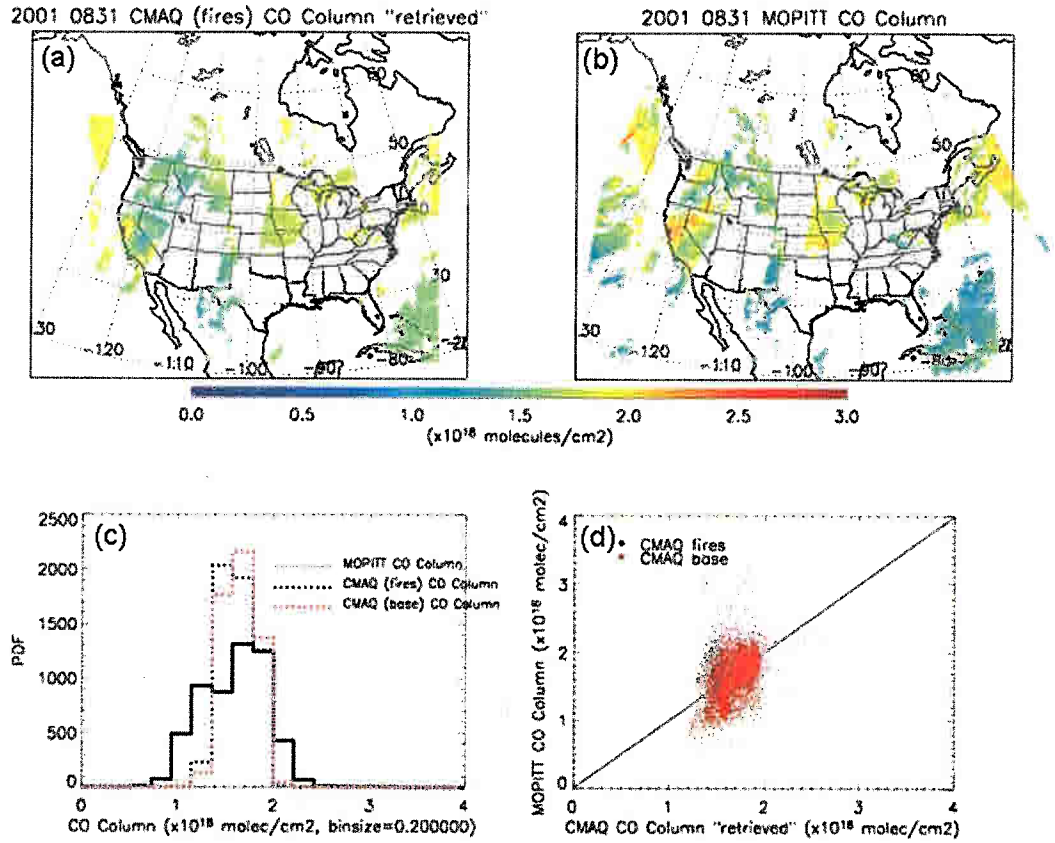

Figure 4. (a) Shows the CMAQ derived CO columnar average concentration (molec. cm^{-2}) along each the 640-km MOPITT swath for August 31, 2001 Terra scenes over the CONUS. The columnar averages are obtained after application of averaging kernels to the original 14-layer CO concentration data predicted by using the MODIS fire-count based reallocated emissions as input for the CMAQ input; (b) Shows the MOPITT CO average concentration data obtained directly from the MOP02 product; (c) Shows the frequency distribution of the average concentrations of CO derived using MOPITT, CMAQ (base case) and CMAQ fire-emissions reallocated case; (d) Scatter plots showing the CMAQ CO retrieved columns (after application of averaging kernel) and respective MOPITT CO data.

2.3.10 Remote Sensing and Air Quality Modeling: Aerosol Optical Depth

Aerosols have direct radiative forcing because they scatter and absorb solar and infrared radiation in the atmosphere (Penner *et al.*, 2002). Aerosols may include many different types of primary and secondary species (*e.g.*, sulfates (SO_4^-), ammonium (NH_4^+), nitrates (NO_3^-), organic carbon (OC) species, and black or elemental carbon (BC) from different types of sources). Air

quality models play a key role in developing emission control strategies for $PM_{2.5}$ and, hence, require extensive evaluation against observed concentrations of its components. To assess the usefulness of satellite observed AOD data as additional information for $PM_{2.5}$ model evaluation, the MODIS observed AOD data were compared with AOD values derived from the CMAQ model. The MODIS, IMPROVE, and AErosol RObotic NETwork (AERONET) sun-photometer ground-truth AOD data sets were used for an intercomparison study against CMAQ estimates. For performance verification purpose, the preliminarily quality-controlled IMPROVE nephelometer measured surface-scattering extinctions due to suspended particles obtained from Colorado State University"s Cooperative Institute for Research in the Atmosphere were compared with CMAQ surface-layer particle-scattering extinction, and total extinction values were averaged on a monthly basis. The importance of aerosols to the chemical and radiative processes in the atmosphere was studied using the ground-based chemical measurements and using AERONET sun-photometer data. Results from this study suggest that further analyses and comparisons with MODIS AOD, as well as the ground-based AERONET and IMPROVE parameters, should be conducted before including AOD as an additional data source for model evaluation.

2.4 Modeling Toxic Air Pollutants

The CAAA of 1990 identified almost 200 individual compounds or mixtures of compounds as toxic air pollutants or hazardous air pollutants (HAPs) having the potential to cause 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, there must be a proper accounting of the important, unique physical and chemical processes that control the fate of each individual compound. The objective of this work is to develop the capability to model toxic compounds at urban and regional scales using the CMAQ modeling system, and at finer scales using both probabilistic and deterministic approaches. These models are used to develop spatially and temporally variable estimates of concentrations of important toxic air pollutants at the appropriate resolutions, and to evaluate the model predictions. This task is closely linked to other tasks that involve the development and evaluation of the CMAQ modeling system, improvements in chemical and physical characterization of air toxins, and the measurement of ambient air toxics concentrations.

2.4.1 Extending CMAQ to New Species of Toxic Air Pollutants

To assess and manage the risk from HAPs to human health and ecosystems, it is important to know how their ambient concentrations and atmospheric deposition vary over location and time. The best way to obtain this information over a national domain at a high spatial and temporal resolution is the use of air quality models to simulate the chemical and physical processes that control the fate of emitted HAPs. Historically, Gaussian plume models have been used to compute concentrations of HAPs; however, the EPA Science Advisory Board

concluded that this approach inadequately accounted for long-range transport of less reactive HAPs and atmospheric photochemistry. In response to these problems, the CMAQ modeling system was modified to simulate HAP concentrations across the continental United States.

During FY-2005, research was performed to expand two chemical mechanisms, CB-IV and SAPRC99 (Statewide Air Pollution Research Center), and to use them to simulate the photochemistry of HAPs. These expanded mechanisms allow simulation of HAPs concentrations (Table 2) as well as concentrations of criteria particulate matter and ozone. Work also resulted in a new Euler Backward Iterative (EBI) solvers for the new CB-IV-based and SAPRC99-based HAPs mechanisms. Besides producing EBI solvers, the Gear and Rosenbrock numerical solvers in the CMAQ model were adapted to work for all the HAP mechanisms. The public release of the expanded mechanisms for HAPs, as a part of CMAQv4.5, was a major accomplishment. This is the first comprehensive, documented, ozone/particulate matter/HAPs mechanism made available in a public forum, which will allow researchers and regulators to assess the concentrations of criteria and hazardous air pollutants simultaneously.

Table 2. Toxic air pollutant species modeled explicitly in CMAQ during FY-2005.

Compound Name	CAS number
formaldehyde	50-00-0
1,3-butadiene	106-99-0
napthalene	91-20-3
acrolein	107-02-8
acetaldehyde	75-07-0
1,3-dichloropropene	542-75-6
quinoline	91-22-5
vinyl chloride	75-01-4
acrylonitrile	107-13-1
trichloroethylene	79-01-6
benzene	71-43-2
1,2-dichloropropane	78-87-5
ethylene oxide	75-21-8
1,2-dibromoethane	106-93-4
1,2-dichloroethane	107-06-2
tetrachloroethylene	127-18-4
carbon tetrachloride	56-23-5
dichloromethane	75-09-2
1,1,2,2-tetrachloroethane	79-34-5
chloroform	67-66-3

2.4.2 A Comprehensive Version of CMAQ for National and Local Assessments of Toxic Air Pollutants

National air toxics assessments are performed to help EPA, state, local, and tribal governments, and the public better understand the air toxics problem in the United States. A national-scale assessment includes four steps:

1. Compiling an inventory of air toxic emissions;
2. Estimating the annual average outdoor air toxic concentrations;
3. Estimating the exposure (what people are estimated to breathe); and
4. Characterizing potential public health risks.

In general, larger urban areas appear to carry greater risk than smaller urban and rural areas, because the air toxic emissions tend to be higher in areas having more people, but this trend is not universal, and can vary from pollutant to pollutant, according to their sources. Although large uncertainties (*e.g.*, emission levels, exposure, toxicity) are inherent in this analysis, EPA uses these results to answer such questions as which pollutants or source sectors may be associated with higher risks than others (*e.g.*, priority setting for data collection).

The Division~~'s~~ contribution to these assessments is to provide spatially- and temporally-varying estimates of the outdoor concentrations of toxic air pollutants using the CMAQ model. This approach provides an accurate, state-of-the-science description of all relevant chemical and physical processes that can affect the concentrations of toxic pollutants. In FY-2004, the CMAQ system was used to develop concentrations and deposition for 20 HAPs during 2001 over the continental United States; in FY-2005, a regional/urban scale assessment was done for the Philadelphia metropolitan area.

During FY-2005, the focus was on planning and preparing inputs for an updated toxic pollutant assessment covering the year 2002. This included assessing which pollutants (both gas phase and aerosol phase) are expected to contribute the highest risk to the United States population, and determining whether to include them in the updated assessment. To follow up this work, plans for a 2002 multi-pollutant assessment include improving on the previous analysis by including additional toxic species and developing ways to account for local ~hot spots™ of high concentration.

2.4.3 Advancing the Neighborhood-Scale Version of CMAQ

Air quality simulation models need a more advanced capability for application at fine scales and to serve as a tool for performing exposure and risk assessments in urban areas (Touma *et al.*, in press). While grid-models are the model platform of choice for simulation of atmospheric chemistry and fate of airborne pollutants, there are various transport and diffusion models (often called dispersion models) that have been developed to simulate the fate of those airborne pollutants that are relatively chemically inert. Not having to treat atmospheric chemistry

of mixtures, dispersion models can provide detailed resolution of the spatial variations in hourly-average (1st moment) concentrations of airborne pollutants. Examples of such dispersion models include AMS/EPA Regulatory Model (AERMOD) (Cimorelli *et al.*, 2005; Perry *et al.*, 2005), Assessment System for Population Exposure Nationwide (ASPEN) (U.S. Environmental Protection Agency, 2000), and Industrial Source Complex Short-Term (ISCST) (U.S. Environmental Protection Agency, 1995). To date, local-scale dispersion models have been relied upon to provide detailed descriptions of concentration patterns. However, local-scale dispersion models cannot properly treat photochemical effects. Many of the air toxic pollutants listed in the National Toxics Assessment (U.S. Environmental Protection Agency, 2000) are identified as having a photochemical origin or being strongly affected by photochemical processes. Also, local-scale models need an estimate of background concentration levels, which is provided directly by CMAQ. It is desirable to combine the capabilities of chemical grid and dispersion models into one model, but this is a yet evolving area of research and development.

In collaboration with the EPA OAQPS, EPA Region 3, and the State of Delaware, the Division has developed a new approach to combine local-scale and regional model results. This approach was applied to Philadelphia using CMAQ as the chemical grid model and ASPEN as the dispersion model. Two pollutants were treated, benzene and formaldehyde. The CMAQ concentrations enhanced with local details from ASPEN for the two pollutants, benzene and formaldehyde, are shown in Figure 5. Benzene is considered an inert pollutant, while formaldehyde is chemically reactive. For chemically reactive species, the ˜adjustments™ provided by the ASPEN dispersion model reflect the effects of direct emissions of formaldehyde. It was found that the formaldehyde concentrations are dominated by secondary-formed contributions from CMAQ. For both chemicals, local details are important, and the approach provides a ˜texture™ on top of CMAQ results. The modeling approah will be further evaluated with the Hazardous Air Pollutant Exposure Model (HAPEM) and a refined modeling methodology will be used for a 2002 national air toxics assessment.

Further, given that spatial concentration distribution is dependent on distance from sources, which is true in the case of roadways, we would expect to find parameterizations to describe the relationships between annual concentrations and two major parameters: emissions Q, and inverse-receptor distance r. As an example, a simple parameterization has been developed based on the modeled benzene concentrations from Philadelphia. While further study is needed to support the development of simple parametric formulations, it seems, at least for benzene, that the possibility of deriving relatively simple parameterization for the subgrid variability (SGV) component to augment background values from grid models such as CMAQ is promising.

Additional studies are planned for FY-2006 to examine the use of the developed parameterizations. Working in collaboration with scientists from ARL, the Division plans to test the feasibility of an urban hybrid CMAQ/HYSPLIT modeling approach. In this system, grid modeling air chemistry would be conducted by such models as WRF and CMAQ. The fine scale urban meteorological fields from MM5 would be used to drive multiple HYSPLIT trajectories from multiple source locations within the urban area to define a probabilistic envelope of

trajectory ensembles and resulting dispersed pollutant concentrations. The contribution of CMAQ-s-deterministic concentration fields and HYSPLIT-s-ensemble probabilistic concentration fields can then be used to describe dispersion within an urban area with a robust modeling framework.

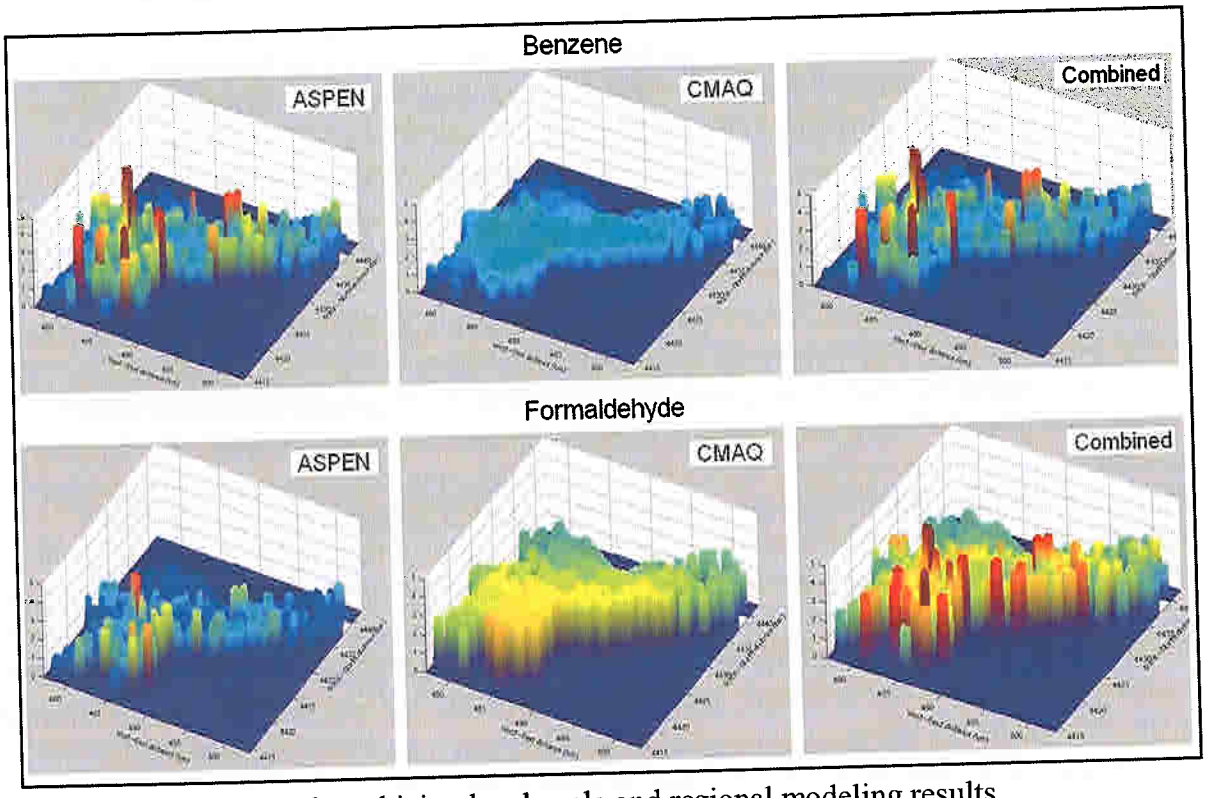

Figure 5. Examples of combining local-scale and regional modeling results.

2.4.4 Linking CMAQ to a Human Exposure Model in an Urban Area

The Division completed a pilot study to develop the capability to provide advanced photochemical grid-model air-toxic concentrations to a human exposure model. Human exposure assessments can be strongly affected by the level of detail provided in resolving the time and spatial variation of airborne pollutant concentration values. While grid-models are the model platform of choice for simulation of atmospheric chemistry and fate of airborne pollutants, dispersion models can provide the desired detailed description of the concentration pattern on local-scale for relatively chemically inert pollutants. The main objective of this study is to develop and evaluate a new approach to combine local-scale and regional model results to adjust for near-field concentration gradients, and then to use these subgrid ˜adjustments™ to CMAQ (Byun and Ching, 1999) results as input to the HAPEM5 (U.S. Environmental Protection

Agency, 2005) and Stochastic Human Exposure and Dose Simulation (SHEDS) (Graham and Burke, 2003) models. The technique has been evaluated using a combination of CMAQ and EPA regulatory dispersion models ASPEN (U.S. Environmental Protection Agency, 2000), ISCST3 (U.S. Environmental Protection Agency, 1995), and AERMOD (Cimorelli, *et al.*, 2005; Perry *et al.*, 2005) in Philadelphia, Pennsylvania. This modeling approach will be further evaluated in different areas (Houston, Detroit, and Los Angeles).

The study consisted of (1) extending an air toxics version of the CMAQ modeling system to a modeling domain centered over Philadelphia at 36-, 12-, and 4-km grid meshes; (2) performing model simulations for the year 2001; (3) combining the modeling results with local details from dispersion models; (4) reformatting the modeling results into the 3-hour annual averages needed for input to HAPEM5 (U.S. Environmental Protection Agency, 2005); and, (5) assessing the practicality of using CMAQ for estimating air toxics for human exposure assessments by examining the computational requirements needed for this exercise.

The pilot study demonstrated that CMAQ can be a useful tool to simulate the air toxic concentration fields needed to drive a human exposure model. For this pilot study, air toxic concentrations generated by the CMAQ modeling system for a 4-km grid mesh overlaying Philadelphia were successfully formatted for direct use in HAPEM5. Examples of simulated ambient concentrations and exposures for benzene in Philadelphia are shown in Figure 6. Based of these results, CMAQ is being considered for application for EPA—s National Air Toxics Assessment (NATA) program (U.S. Environmental Protection Agency, 2000).

The next phase of this research effort will focus on enhancing the CMAQ modeling system with fine-scale details from the Gaussian dispersion model AERMOD (Cimorelli, *et al.*, 2005) or the Lagrangian particle model HYSPLIT (Draxler and Hess, 1997). In addition, CMAQ applications are being performed for Houston, which is an excellent urban test bed for further development because it has a detailed building morphology database to test the urban parameterizations for meteorological modeling, and it has detailed air toxic concentration data from such field studies as the Texas Air Quality Study 2000 that can be used for extensive model evaluation.

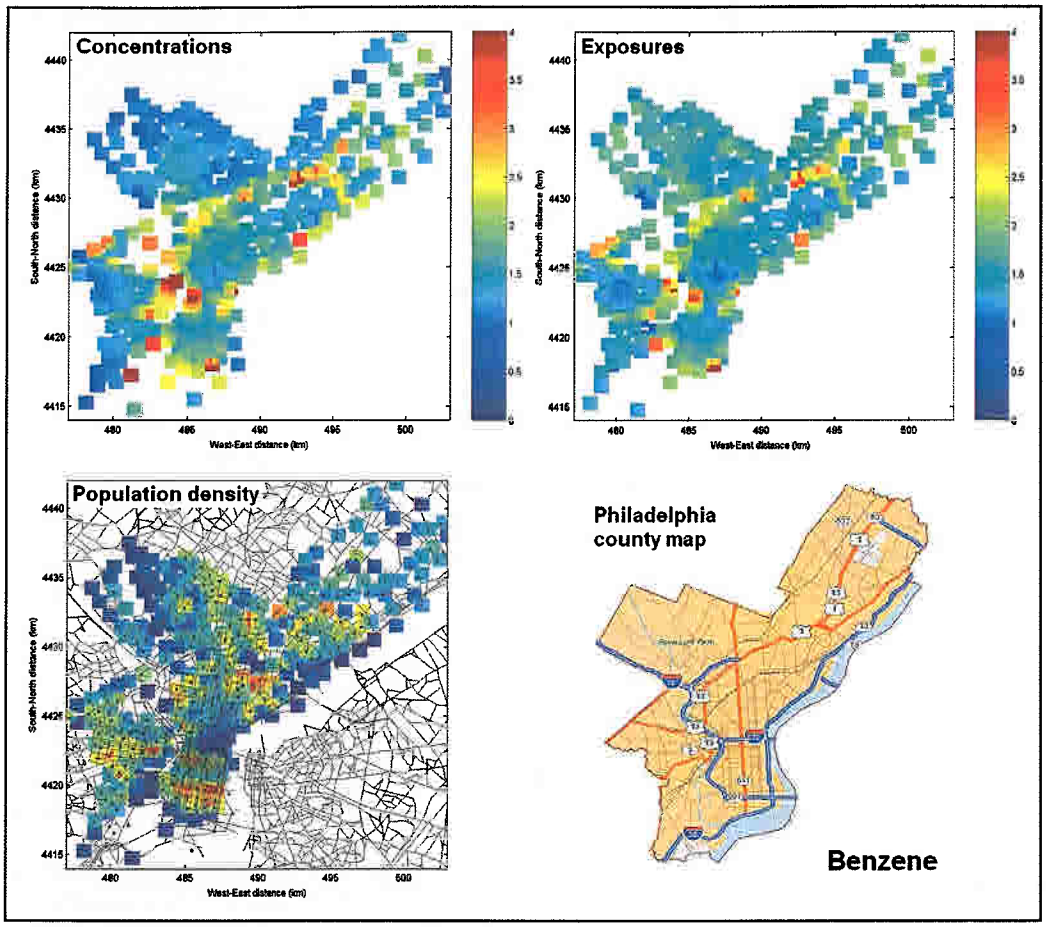

Figure 6. Annual benzene concentrations, inhalation exposures, and population density in Philadelphia.

2.4.5 Modeling Subgrid-Scale Variability

A property of such chemical-grid models as CMAQ is that near-source concentration distributions from point, line, and area sources are not explicitly treated. Instead, emissions from these local sources are instantaneously dispersed throughout the grid volume. Thus, near-source modeled concentrations fields from Gaussian-type models are higher than those from Eulerian grid models, and consequently, exposure assessments based on models like CMAQ will, in general, underestimate the potential levels of human exposures in the near field. Thus, there is a need to augment CMAQ with information about this additional source of variability. The approach taken during FY-2005 was (1) to apply an urbanized version of MM5 and the toxics version of the CMAQ modeling system to grid sizes as small as 1 km; (2) to begin to utilize suites of local-scale dispersion, coupled-chemistry dynamics, and CFD modeling to produce sub-kilometer scale concentration fields to complement the CMAQ fields; and, (3) to develop subgrid scale concentration descriptors, including distribution functions from fine scale modeling results.

During FY-2005, SGV results were obtained from incorporation of a hybrid local scale modeling techniques developed for the annual Philadelphia CMAQ simulations. Also, simulations for hourly, 1-km CMAQ runs for July 2001 were produced as part of a collaborative effort with the Delaware Department of Natural Resources and Environmental Conservation. Finally, efforts to model the entire Texas 2000 study period (August 22–September 3) at neighborhood scales (~1-km grid size) were begun by extending the modeling results beyond the previously studied August 30, 2000, case study simulation for Houston.

Results for these three modeling studies are providing the basis for a proof-of-concept study to explore approaches to incorporate SGV information into CMAQ. For this effort, several implementations based on statistical parameters of the SGV distribution were examined, including gridded coefficient of variation, 95th percentile, and peak-to-mean values. It is hoped that this information on SGV can be used to improve assessments with human exposure models.

During FY-2005, the Division participated in the Enhanced Delaware Air Toxics Assessment Study (EDATAS), a collaborative effort that included participants from EPA's OAQPS, EPA Region 3, and the State of Delaware, University of Delaware, and Duke University. The motivation for the Division's participation was to gain a better understanding of the distributions of ambient concentrations within a modeled-grid cell by using results from monitoring studies. The EDATAS study aims to gain a better understanding of ambient concentrations of hazardous air pollutants throughout Delaware, exposure to those air toxics, and the health risks associated with that exposure based on nationally-accepted health benchmarks.

During FY-2005, the Duke University team performed mobile measurements of PM water-soluble chromium species, gas-phase formaldehyde, and aerosol number size distributions to provide information on the spatial distribution of pollutants throughout the city as well as variability within neighborhoods with the spatial scale of the order of 100 meters. An example of spatial distributions of formaldehyde measured throughout the city of Wilmington is shown in Figure 7. Additional studies are planned for FY-2006 to examine SGV in air toxics modeling applications to support exposure and risk assessments. A new saturation monitoring study will be conducted in Southern California near Los Angeles. This will be a collaborative effort between the California Energy Commission, California Air Resources Board, and the Division to identify hot spots of pollutant concentrations on a neighborhood scale.

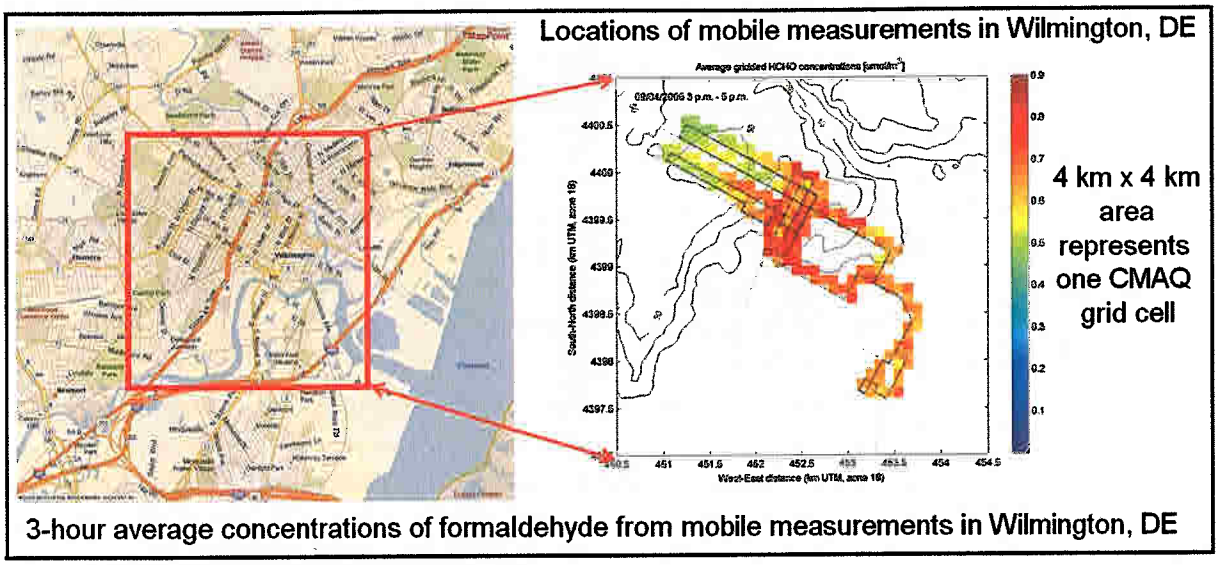

Figure 7. An example of locations of mobile measurements and of spatial distributions of formaldehyde throughout the city of Wilmington, Delaware.

2.4.6 Developing and Applying Computational Fluid Dynamics Simulations of Pollutant Transport and Dispersion

Developments and applications of Computational Fluid Dynamics (CFD) are ongoing for support of urban air toxics assessments and homeland security issues. CFD modeling has emerged as a promising technology for simulating wind flow and pollutant dispersion in urban microenvironments. Development and applications are linked closely with the advancing capabilities of both software and hardware. In addition to using EPA computing resources, cooperation has been established with the Department of Energy's Argonne National Laboratory for use of their large Linux cluster and at the Army's Major Shared Resources Center. Access to the Army's large graphical computing workstations has made it possible to examine critical issues when working with large numbers of buildings. Much is being learned about how best to set up CFD simulations to support environmental simulations and the issues that most affect comparability with physical model studies and field measurement studies. The choice of boundary conditions, grid resolution and structure, and turbulence models affect the outcome of a solution significantly. Transport and dispersion can be well simulated for flat plate like atmospheric boundary layers. No work has been done for stable stratified flows. Transport and dispersion simulations are more complicated for atmospheric flows due to the complex temporal-spatial wind fluctuations. The project has focused on the Reynolds-Averaged Navier-Stokes steady-state solutions and the standard k-e (turbulent kinetic energy and turbulent energy dissipation rate) turbulence models. This study is being extended to include unsteady solutions and higher order turbulence models. A method for setting up CFD simulations of wide ranging atmospheric boundary layers has been developed (Tang *et al.,* 2005) with an example provided by Figure 8. While setting up a working model of the extremely complex building environments

for New York City has been a challenging exercise, there were many lessons learned that should make it easier to set up similarly complex urban environments in the future. Understanding the pathway of toxic air pollutants from source to human exposure in urban areas finds immediate application for both routine air pollution assessments and in support of homeland security (Huber *et al.*, 2005).

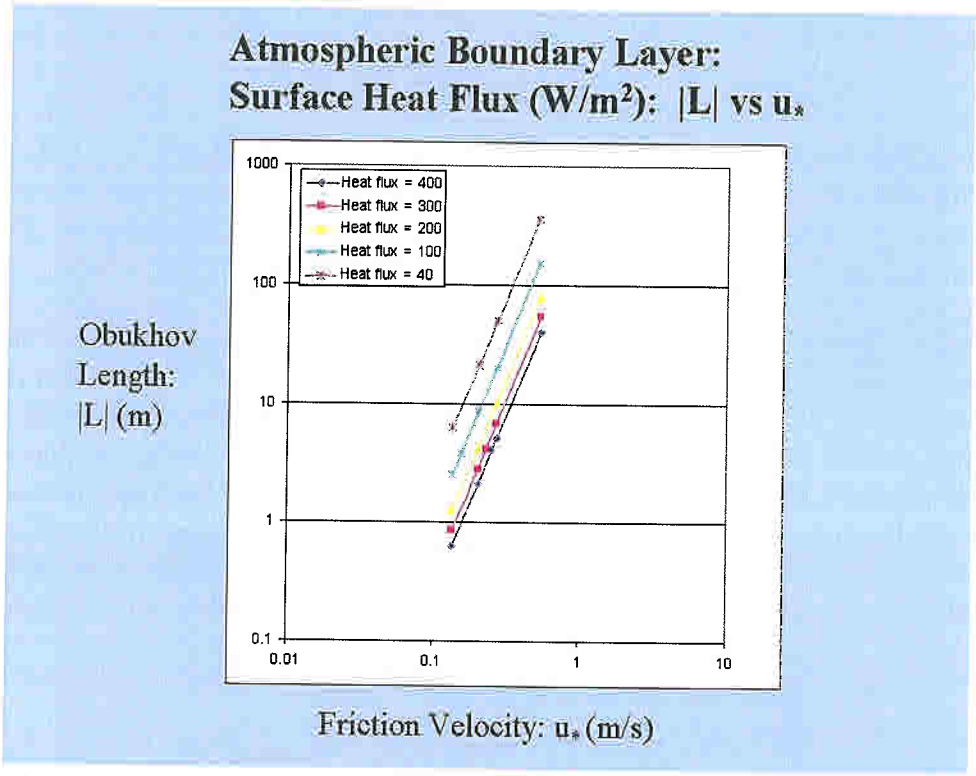

Figure 8. Monin-Obukhov theory applied to a range of CFD case studies.

The collapse of the New York World Trade Center towers on September 11, 2001, demonstrated some of the shortcomings in conducting rapid exposure and risk analyses in urban areas where the understanding of airflow around large buildings is poor. While problem-specific applications of CFD may not be feasible in "real-time" support, there is a major role for CFD simulations to be run for developing archives that could be tabularized for supporting real-time applications. Also, CFD simulations should have a significant role in supporting field studies in urban environments, which could be used to develop performance verification. Future research and development, including CFD simulations, could lead to the development of reliable simplified models (or databases) as needed to support emergency responders.

CFD simulations can be used to support necessary post-event analyses as is being done in support of post 9/11 studies. CFD modeling is being extended as part of multi-agency support for the Department of Homeland Security's New York City Urban Dispersion Program (UDP). Participation with the UDP program provided a good opportunity to demonstrate potential uses for CFD simulations and major field measurement campaigns and physical modeling will help evaluate the CFD model results.

CFD simulations for conditions with winds from South to Southwest were completed to support the UDP field measurement studies conducted during August 8–24, 2005, in a domain that includes areas around Times Square and Rockefeller Center. In this domain, the wide avenues are aligned generally North-South and the much narrower streets aligned East-West. The vertical motions (up and down) induced by the buildings lead to complex patterns of airflow through the streets of New York City. For example, Figure 9 presents CFD-modeled surface winds at 5 m above ground level (Z=25 m ASL). The displayed wind vectors represent only a 10 percent sample of the solution's cells (size approximately 1.7 m near the surface). Rockefeller Center is located in the center of Figure 9.

Evaluation of these preliminary results should be possible from several of the field study intensity measurement periods. Additional CFD simulations will be completed for the specific boundary conditions for several of the six intensive measurement periods. Even the intensity measurement periods will not provide the spatial resolution in anemometer measurements needed to fully evaluate the CFD wind-pattern simulations. To better understand the field wind patterns, Division staff developed a routine walking pathway through the core area of the study domain to observe patterns of soap bubbles. Figure 10 presents an example of the process. In general, very distinct patterns were observed, which in many cases support the complex features seen in the CFD simulations. Hand drawn patterns from the observed soap bubble pathways will be compared with the CFD simulations.

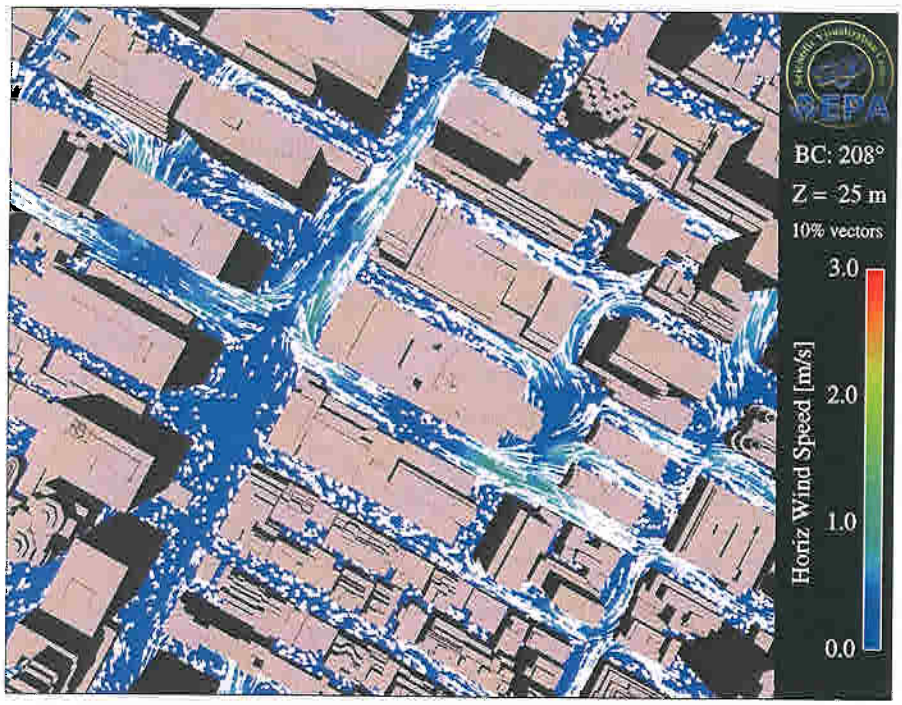

Figure 9. Surface wind pattern modeled with a CFD in the Rockefeller Center area for oncoming winds parallel to the New York City Avenues.

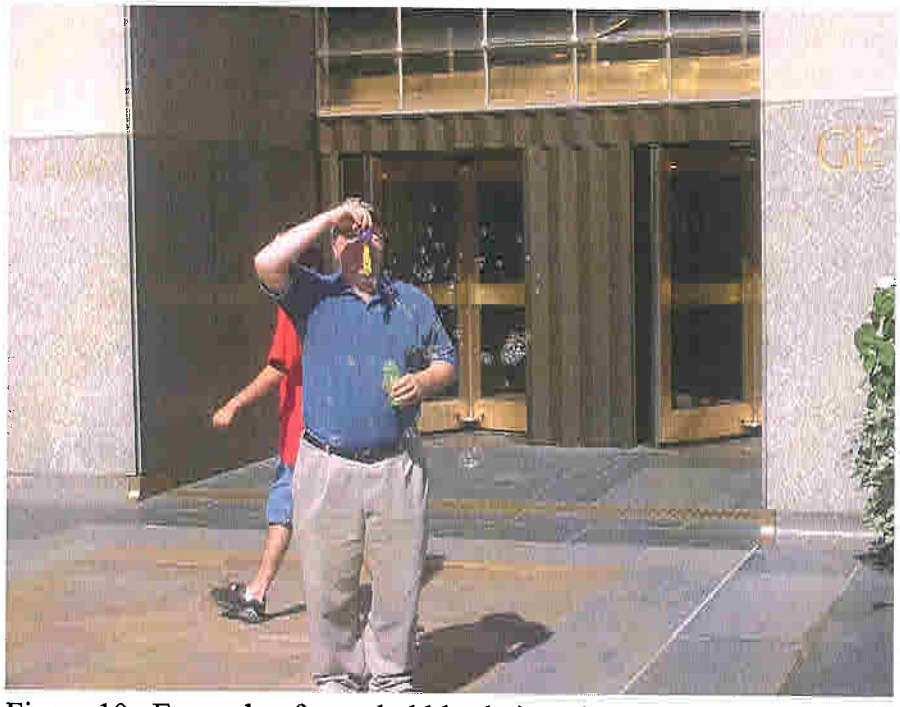

Figure 10. Example of soap bubbles being observed in front of the GE Building to study complex wind patterns in Manhattan building environments.

2.5 Multimedia Modeling and Application Studies

2.5.1 Multimedia Integrated Modeling System Spatial Allocator

The Division completed development of the Multimedia Integrated Modeling System (MIMS) Spatial Allocator[3]. The MIMS framework provides a software infrastructure to support configuring, applying, and evaluating environmental models. The spatial allocator will allow the spatial gridding, re-gridding, and projection on many geographic coordinate systems of environmental data, given input of a geographic information system shape file. During FY-2005, two versions of spatial allocator were completed: a general spatial allocation tool for any environmental data, and a more specialized version tuned to reallocate spatial surrogate data to be used for modeling air emissions, particularly with the SMOKE$^{\pm}$ modeling system. The latter version of the spatial allocator now includes the ability to grid the specialized 1-km resolution vegetation data (Biogenic Emission Land Data, or BELD3) needed for modeling of biogenic emissions.

Both MIMS and the spatial allocator have been adopted by EPA ~~s~~ OAQPS for use in their new Emission Modeling Framework (EMF), a multi-user, multi-tool database that assists in the preparation and analysis of emission modeling inventories. SMOKE$^{\pm}$ prepares the inventories for use in such chemical transport air quality model as CMAQ. OAQPS uses the MIMS framework as the basis for EMF to tie together the many files and software tools, including SMOKE$^{\pm}$ and the spatial allocator. In addition, a graphical user interface (the Surrogate Tool) and refinements for the spatial allocator have been developed for OAQPS for installing in EMF. Both MIMS and the spatial allocator are being used by the science community as starting points for further community-contributed improvements.

2.5.2 Improving Dry Deposition Models

During FY-2003, EPA initiated an interagency agreement (IAG) with NASA to develop an approach for modeling the bidirectional flux of ammonia. The IAG brought together the land-surface modeling expertise and remote sensing databases of NASA, the ammonia modeling expertise of the University of Maryland-Baltimore County, and the air quality modeling expertise of the Division. The IAG has also stimulated collaboration between the Division and EPA—s National Risk Management Research Laboratory (NRMRL), where researchers are conducting field studies to better understand the processes involved in the surface exchange of ammonia. Reduced nitrogen, in the form of ammonia, is increasingly being recognized as an important contributor to the overall nitrogen budget of ecosystems. Improved modeling techniques are critical to our attempts to predict the effects of changes in emissions on loadings to the

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[3]Developed by the Carolina Environmental Program at the University of North Carolina at Chapel Hill, the Spatial Allocator is a free tool for generating spatial surrogates for emissions and performing other spatial allocation without requiring a geographic information system.

ecosystems. The initial algorithm development has been done within the context of the Multi-Layer Biochemical Model (MLBC) (Wu *et* al., 2003a; 2003b). The MLBC model was selected because it provides a detailed model of plant processes including photosynthesis that drive uptake and emission of pollutants from the plants. Ammonia deposition/emission is driven by the relationship between ambient concentrations and the compensation point. Deposition occurs when the ambient concentration exceeds the compensation point. Conversely, emission occurs when the ambient concentration is below the compensation point. A parameterization for the ammonia compensation point was added to the MLBC model. Initial testing of the model against field study data shows promising results. A key feature of the model is the allowance for a dynamic compensation point rather than a fixed value. Further studies during FY-2006 will focus on the possible emission of ammonia from the dew-wetted surfaces of leaves as they dry.

CASTNet is operated by EPA's Clean Air Markets Division (CAMD) and the National Park Service to monitor concentration and dry deposition at sites across the country to assess long-term trends in air quality and environmental protection resulting from regulatory policies and emission reductions required under the Clean Air Act. CASTNet estimates dry deposition flux by combining measured concentrations of pollutants with modeled deposition velocities. Currently, CASTNet uses the MultiLayer Model (MLM) (Meyers *et al*, 1998) to calculate dry deposition velocities. CAMD is interested in using the MLBC model as an alternative. During FY-2004–2005, MLBC was modified for use with network meteorology and plant types. During FY-2006, the Division will be working with CAMD to implement MLBC for the CASTNet sites.

2.5.3 Chesapeake Bay 2007 Re-Evaluation

The Division 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 source of reduced and oxidized nitrogen through deposition. Chesapeake Bay is a leader in using multi-media modeling approaches. Two major Chesapeake Bay re-evaluations or assessments of required nitrogen load reductions to the Bay have already occurred.

Chesapeake Bay has been placed on EPA's list of impaired waters. The Chesapeake 2000 agreement calls for pre-empting the need for a Total Maximum Daily Load plan by cleaning up the Bay by 2010. The Bay 2007 re-evaluation is a critical step in this process towards the 2010 cleanup and ASMD is participating in the re-evaluation. The best science is desired for the re-evaluations, and during the period between major re-evaluations, the Division moved its multi-media modeling of nitrogen from the Extended Regional Acid Deposition Model (RADM) to CMAQ. The CMAQ dry deposition algorithms were revised during FY-2003, improving deposition parameterizations for NH_3, HNO_3 and other nitrogen containing species. CMAQ has been sufficiently evaluated for deposition to show that it is an improvement over the Extended RADM. A newly designed aggregation data set for CMAQ with 40 cases that could directly estimate seasonal deposition was developed in FY-2003 and adapted to the aggregation method in FY-2004. However, inconsistencies in the aggregation results were noted. Because

the 2004 version of CMAQ ran faster, it became feasible to accelerate the transition to direct simulation instead of using the 40-case CMAQ aggregation set. The transition, always a goal, took place in FY-2005. Direct simulation has many advantages, including direct time and space pairing for model evaluation and data fusion, and the ability to estimate deposition over the coastal ocean out to the continental shelf. The new climatological approach uses three full years of meteorological data to estimate average deposition over the eastern United States. The three years incorporating a wet (2003), normal (2002) and dry (2001) year over the Mid-Atlantic and northeastern region of the United States were selected. The CMAQ performance with the new three-year climatological approach was better in almost all possible comparisons than the Extended RADM performance with the older 30-case aggregation approach. Issues with summer wet deposition sharpened. The SO_2 and total sulfur comparisons were exceptionally good and better than seen before. A new 2001 base case and futures cases for the 2010 NO_x SIP and 2010 CAIR were run with CMAQ to estimate the impact on nitrogen deposition (oxidized-N and reduced-N) of the anticipated new controls on emissions. Exploration of these preliminary results was presented to the Chesapeake Bay Modeling Subcommittee. With the CMAQv4.5, dry deposition increased for both oxidized N (more species accounted for) and reduced N (higher NH_3 deposition velocity). Interesting nonlinearities between sulfate reductions and ammonia dry deposition were evident. The success of the preliminary, multi-year results opens up new possibilities for better linking the CMAQ atmospheric deposition with the Chesapeake Bay Watershed Model and other ecosystem models. That linkage is now under discussion.

2.5.4 Ammonia Budgets for Coastal Systems

An important fraction of atmospheric nitrogen deposition is reduced nitrogen (ammonia/ammonium). 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 within ten years. 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 with the Multiscale Air Quality Simulation Platform, a development predecessor to CMAQ, 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, shows that only 5 percent to10 percent of the NH_x budget dry-deposits locally, while most of the ammonia emissions are involved in long-range transport, contrary to conventional wisdom. The model results are consistent with spatial and temporal trends in the ammonia wet deposition data.

Simulations were carried out at 32-km and 8-km grid-cell sizes with the CMAQv4.3 with the updated M3Dry deposition algorithms for the 1999 summer period. For the 8-km simulation, process analysis was turned on in CMAQ. Preliminary comparisons showed very reasonable

agreement between modeled and measured NH_x levels at Clinton, North Carolina, and Atlanta, Georgia. However, with the updated M3Dry deposition algorithms, the process analysis now shows that dry deposition of ammonia in CMAQ is four to five times higher than previously estimated. The new estimates may be too high because the bi-directional air-surface exchange of ammonia is ignored. Two new simulation periods were selected, summer 2002 and summer 2004, during which dry deposition measurements in North Carolina were taken to better assess and bound the model results. The CMAQ simulations were at 12-km grid-cell size and process analysis was turned on for all model layers. With process analysis results for all layers, it is possible to estimate the fraction of the budget that goes into the free troposphere for ultimate long-range transport. The dry deposition surface budget in CMAQ for summer 2002 is very similar to that for summer 1999. A sensitivity study with lower M3Dry ammonia deposition that is consistent with surface measurements of ammonia deposition will be defined and run in FY-2006. The goal now is to develop a complete ammonia budget and provide an upper and lower bound on the ammonia budget calculations.

2.5.5 Tampa Bay Study

The Tampa Bay Estuary Program and the Florida Department of Environment asked EPA and NOAA to enter into a partnership to apply CMAQ to 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. The Division 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 involving coarse particles and sea salt. 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 aerosol module in FY-2006. Prior to any Tampa Bay assessment, it was agreed that CMAQ needs to be evaluated against high-quality local data.

The Tampa Bay study needs to have an annual average deposition as its basis to be able to be used by the Tampa Bay National Estuary Program. The use of the aggregation was contemplated. Because the sea breeze has an important influence on transport over Tampa Bay, a wind hodogram analysis was conducted to ascertain whether the aggregation set, with five-day long sequences, could support a credible analysis of transport over Tampa Bay. The conclusion was that the aggregation set would not adequately capture coastal sea breeze effects. A straight simulation of CMAQ at 32-, 8-, and 2-km cell sizes to create an annual average would be more defensible. The 2-km resolution will provide the best simulation of the chemistry in the power plant plumes and the differential in productivity due to the mandated reductions in NO_x emissions. Precipitation records for sites in and around Tampa Bay were compared against 15-year and 40-year rainfall averages. Except for December 2002, the period of April 2002 to March 2003 would have close to average rainfall on every month except June 2002, which had

50 percent higher than average rainfall. April 2002 through March 2003, excluding December and June 2002, will be used for the Tampa Bay study. The meteorology for this 10-month period at the three-grid resolutions was generated during FY-2005 while CMAQ-UCD was being evaluated.

2.5.6 Multimedia Research for CMAQ-Hg

Progress on a bi-directional flux algorithm for mercury (Hg) during FY-2005 was slowed by limited resources and other higher priority research projects. As a result, projected milestones were pushed forward by one year. In the interim, EPA/NOAA Scientist-to-Scientist meetings were held at which deposition, multimedia, and mercury research issues relevant to this task were discussed. The importance of bi-directional flux, a critical contributor to the Hg budget, is becoming more widely recognized. In addition, the ease with which atmospheric Hg and other chemicals of interest deposit to and are re-emitted from multiple-surface types that in a grid-model sense co-exist in space, suggests a new land surface-keyed spatial aggregate paradigm is needed. A mosaic approach is one potential option. Implementation of such an approach in existing deposition as well as evolving bi-directional flux models would represent a fundamental change from the current paradigm.

2.5.7 Multimedia Tool Development

Significant effort is often required to analyze observations and model results and provide them in a form required to support management decisions. Most off-the-shelf tools do not address the specialized needs or applications encountered in analyzing data from a multimedia perspective, making it more difficult to link elements of the multimedia components together. The need for specialized tools is especially pertinent to bringing atmospheric components together with watershed components for multimedia management analyses. For many air-water linkages, climatologically-averaged deposition at monthly, seasonal, or annual temporal scales is desired. This requirement can be met by the three-year simulations of a wet, dry, and average year with CMAQ. The output files can be viewed with the Package for Analysis and Visualization of Environmental[©4] data (PAVE[©]), the Models-3 visualization tool that is publically available through CMAS, and is accessible to other Models-3 tools. The ability to use PAVE[©] is very attractive and easy, and enhances the users ability to display results. Yet, the water quality modelers do not understand the outputs from the atmospheric deposition models

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[4]Effective 1/1/2004, the Package for Analysis and Visualization of Environmental data (PAVE) is hereby made available to the community by MCNC and the Carolina Environmental Program of the University of North Carolina at Chapel Hill under the terms of the GNU Public License. PAVE was originally created with the support of MCNC, EPA, and other contributors and has been made available to the environmental modeling community in the interest of the public good. MCNC--North Carolina Supercomputing Center formerly held the copyright.

and have difficulty in using them. This happens, in part, because watershed segments or components are irregular polygons and based on surface hydrology (hydrologic units, termed HUC's), requiring a special mapping.

The goal of this project is to make the climatological deposition outputs from CMAQ available to the wider water quality community through an easy- to-use software tool. To meet the goal, a Deposition Mapping Tool is being developed. The objectives of the Watershed Deposition Tool are (1) to read CMAQ files in Models-3 Input/Output Applications Programming Interface format and overlay the gridded deposition values onto a selected set of watershed segment polygons (HUCs); (2) to calculate a weighted average deposition for each HUC; and, (3) to calculate a weighted average absolute or percentage change in deposition between two different sets of CMAQ simulations. During FY-2005, it was found that experienced GIS (Geographic Information System) users wanted simply to be able to export the CMAQ output files in a format easily read by GIS programs. The capability to export GIS shape files is being added to the test version of the Watershed Deposition Tool. In response to comments by less experienced users, general features of the tool are being simplified and more tutorial help will be provided. Thus, to have the greatest effectiveness, two different groups of users are being targeted.

2.6 Climate Change Impacts on Regional Air Quality

The Climate Impacts Change on Regional Air Quality (CIRAQ) project was initiated in FY-2002 and contributes 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 air quality on a national domain under current and future climate conditions. 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. Current and future (2050) 10-year regional climate simulations were developed during FY-2003–2004. During FY-2004, a Quality Assurance Project Plan was developed and approved for CIRAQ and base case model-ready meteorology and emissions files were processed. During FY-2005, future model-ready meteorology was processed and analyzed. Base case and future emission files were processed and a preliminary base case analysis was performed. During FY-2006–2007, base case and future meteorology and emissions scenarios will be used to generate CMAQ air quality simulations. The primary goal of these simulations is to develop future air quality modeling scenarios to compare against current conditions to test the sensitivity of air quality to potential climate change.

2.6.1 Model-Ready Regional Climate Scenarios

To support this project and ultimately the air quality assessment, the EPA GCRP funded the Department of Energy's Pacific Northwest National Laboratory (PNNL) to develop current and future regional climate simulations. These simulations rely on MM5 with initial and

boundary conditions from global climate model (GCM) simulations, and the future GCM simulations rely on Intergovernmental Panel on Climate Change future greenhouse gas scenarios. During FY-2004, PNNL completed two 10-year MM5 simulations with boundary condition links to the NASA Goddard Institute for Space Studies (GISS) GCM. Ten years of MM5-GISS simulations were completed for climate conditions similar to that of 2000 (*i.e.*, base case) and 10 years representing climate conditions around 2050. During FY-2005, the downscaled climate scenarios were evaluated using the CIRAQ automated quality assurance tool (Poole-Kober and Viebrock, 2005) and processed to CMAQ model-ready format using MCIP. These scenarios were carefully evaluated and subsequently used as input to meteorologically sensitive biogenic and mobile source emission models.

2.6.2 Exploration of the Regional Climate Scenarios

An initial exploration of the regional climate model (RCM) scenarios was completed and an internal draft report was produced (Cooter *et al.*, 2005). Temporal and spatial analysis methods developed during FY-2004 were applied to representative observed and RCM scenario data. Results of the study, which included extensive comparison of RCM base case to observations as well as RCM base case to RCM future scenarios, identified areas of geographic and seasonal scenario strengths and uncertainties with implications for the CMAQ analysis to come. Results of the study will be presented at a climate workshop and published in a journal article in FY-2006.

2.6.3 Chemical Emissions Processing

Chemical emissions processing through SMOKE© was completed for five base case and five future climate data years. Previous results reported by collaborators at Harvard University suggest that five years of hourly CMAQ results may be adequate to capture the most important seasonal and interannual signals of air quality variability and change. The base inventory used is the EPA 2001 modeling inventory projected from the 1999 National Emission Inventory version 3. Biogenic emission test cases completed using BEIS3.12 during FY-2004 were re-processed using BEIS3.13. The Mobile6 emissions model is used to capture climate-sensitive aspects of that emission sector. Preliminary results indicate successful processing and expected levels of regional emission response to climate variability. Preliminary findings were presented at the *14th International Emission Inventory Conference: Transforming Emission Inventories—Meeting Future Challenges Today, in Las Vegas, Nevada, held April 11–14, 2005.*

Emission processing for the remaining base case and future climate time periods was completed during FY-2005. The same EPA 2001 modeling inventory was used with the future climate scenarios for input to the 2007 air quality assessment product. Collaboration is ongoing with EPA's NRMRL regarding the development of emission inventories that could be used in future (2010) analysis products. Analysis of seasonal and interannual variability of biogenic and mobile emissions will follow the overall design defined by the RCM analysis, which emphasizes

the comparison of base case model results to observations as well as to future model results. During FY-2005, a workplan was developed to supplement data from field observations of biogenic and mobile emissions on temporal and spatial scales with additional SMOKE± scenarios derived from existing observation-nudged meteorological input data files.

2.6.4 Preparation for CMAQ Program Execution

During FY-2003 and 2004, global climate and chemical transport model simulations were completed and analyzed by colleagues at Harvard University under direct project support. A second series of global CTM simulations has been acquired from Carnegie Mellon University (CMU) that includes aerosols. While the CMU simulations are driven by the same global climate model, full consistency between the global climate and global chemistry drivers cannot be guaranteed. During FY-2005, the code to link CTM output to CMAQ through boundary conditions was obtained from the University of Houston and modified as needed for this application. Short-duration CMAQ test runs were conducted to identify a hardware configuration (which machines, how many processors) sufficient to complete the required simulations in an acceptable time frame. Production of the CMAQ/CIRAQ scenarios has been initiated and completion of base case and future scenarios is anticipated during late spring of 2006. The results will undergo analysis during FY-2006 for summary during FY-2007.

2.7 Client Support

2.7.1 The Community Modeling and Analysis System

FY-2005 was the final year of the cooperative agreement between the Division and the University of North Carolina at Chapel Hill Carolina Environmental Program. Under this agreement, the Community Modeling and Analysis System (CMAS) Center was established for support and dissemination of ASMD air quality modeling products, particularly the Community Multiscale Air Quality (CMAQ) modeling system. Future ASMD interactions with CMAS will be through a multi-year contract that was issued in mid-FY-2005. The CMAS Center is intended to leverage the modeling community—s knowledge of air quality modeling and analyses to support policy-maker decisions on air pollution control and regulations. To achieve its mission, CMAS helps foster the growth of the user community and model developers, serves as an education hub for those who need to learn about models and their uses, and serves as a bridge between various segments of the community by fostering dialogue and exchange of information, needs, and ideas.

During FY-2005, the primary focus of the applications support function of CMAS was the continued support of the Models-3 user and development community. Internet listservs and a detailed website were improved as key components of the support (http://www.cmascenter.org). There were approximately 3700 software downloads from the website during FY-2005. This continues the expanding use of CMAS as a portal for CMAQ-related products (Figure 11). CMAS tested and released CMAQv 4.5, MCIPv3.0, and SMOKE v2.2 in September 2005. A

port of CMAQv4.5 and MCIPv3.0 for the Apple OS X[5] operating system was also released. An operational guidance document for CMAQ was under development, including updating with information for v4.5. A central archive was established to allow the contribution and testing by other developers. As an initial contribution, an updated version of a sectional aerosol version of CMAQ (CMAQ-MADRID) was released. Model improvements to CMAQ were completed by CMAS, including a more efficient radiative transfer calculation for photolysis, and updated aerosol model computations, including computation of sea salt aerosols.

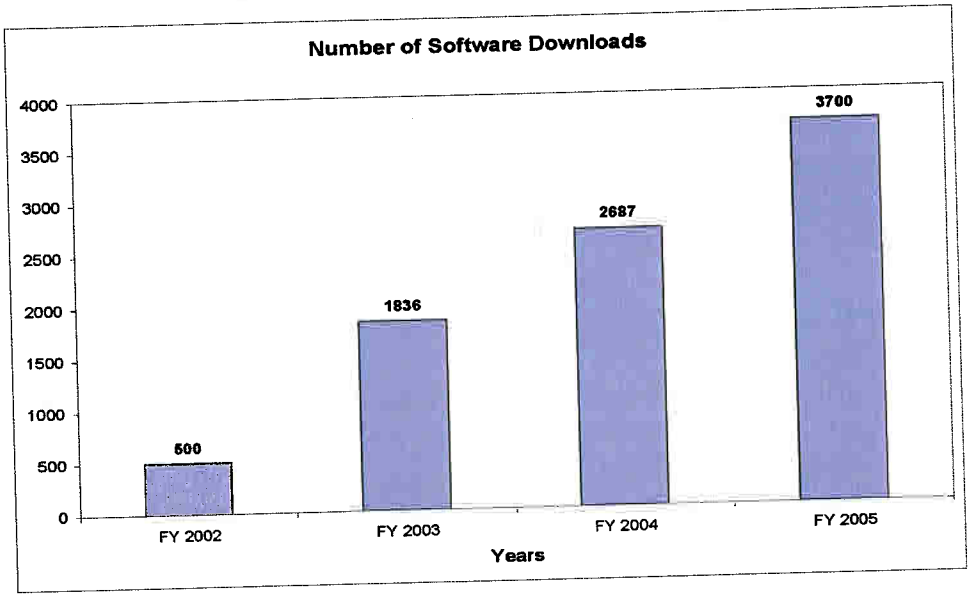

Figure 11. Increase in Internet downloads of CMAQ-related model products at CMAS

[5]Registered trademark of Apple Computer Inc.

CMAS continued its outreach program by conducting training and holding the 4th Annual CMAS User's Conference at UNC's Friday Center in Chapel Hill, North Carolina, September 24–26, 2005. Training sessions for CMAQ, SMOKE©, and the Multimedia Integrated Modeling System (MIMS) were held in the spring and in September in conjunction with the user's conference. Approximately 55 scientists were trained, a number comparable with the two previous years (Figure 12). The conference was attended by 205 participants, with a total of 120 paper and poster presentations. Model development papers based on the presentations were solicited for a special issue of the *Journal of Applied Meteorology and Climatology*, in conjunction with papers presented at the *NOAA/EPA Golden Jubilee Symposium on Air Quality Modeling and Its Applications* in September 2005. The conference demonstrated continuing growth in attendance and representation (Figure 13). Thirteen countries were represented in 2005, an increase from six countries in the previous year.

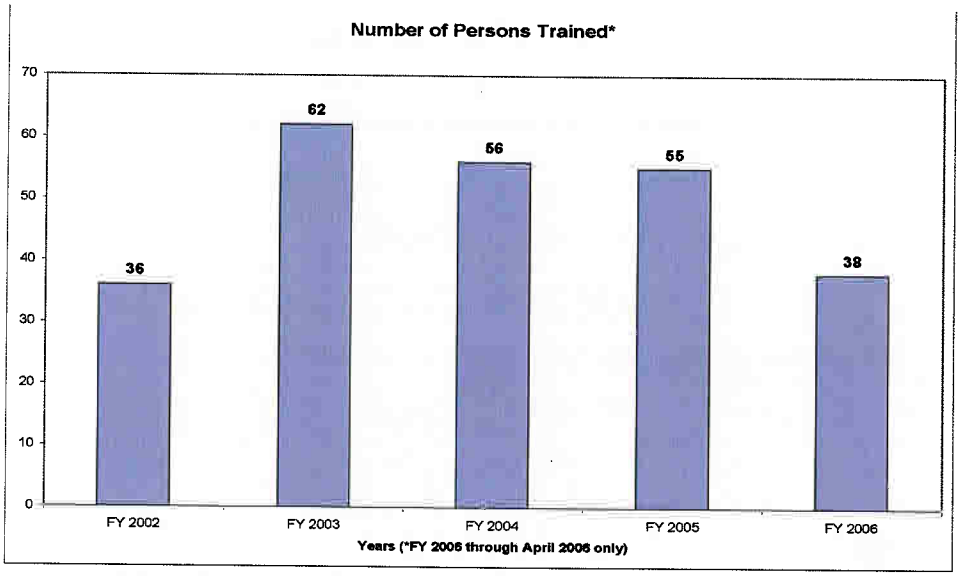

Figure 12. Persons trained in the use of CMAQ-related software by CMAS

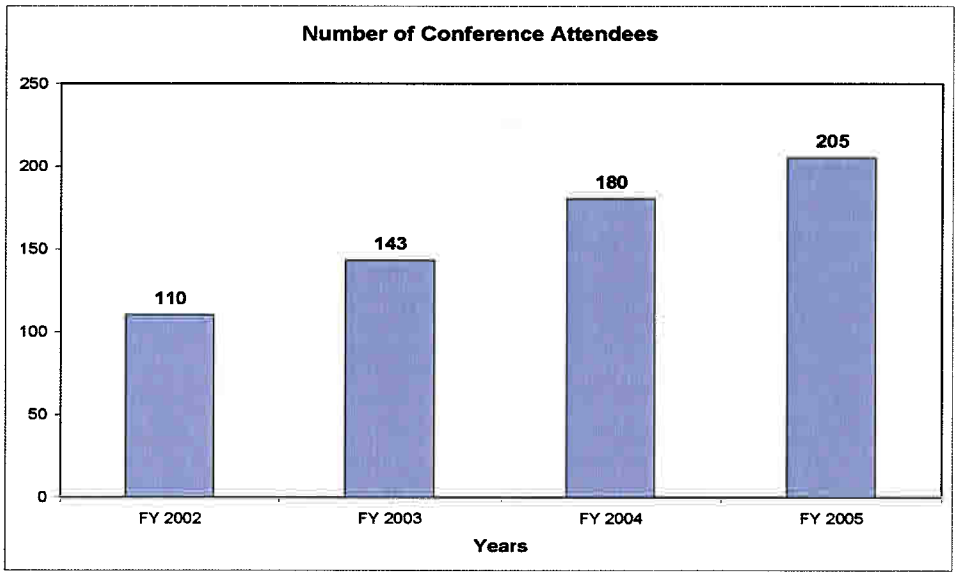

Figure 13. Growth in attendance at annual CMAQ User's Conference

CMAS provided additional service to the user community by sponsoring a peer review of recent improvements to CMAQ in May 2005. The findings of the peer review were complimentary to the program and provide guidance for additional improvements (http://www.cmascenter.org/PDF/CMAQ_Scd_Peer_Rev_July_5.pdf).

2.7.2 Wind Tunnel Modeling of Urban Neighborhoods

To improve the understanding of airflow patterns and the dispersal of pollutants in urban areas, Division scientists at the Fluid Modeling Facility (FMF), in collaboration with scientists at EPA's National Homeland Security Center, modeled the flow and dispersion in a "typical" urban neighborhood based in Brooklyn, New York. This wind tunnel study complements a 2005 field study that focused on releases from traffic-related sources along a four-lane expressway passing through a neighborhood. The field study was designed to examine routine traffic emissions and simulated "malicious" releases. The goals of the wind tunnel study were twofold: (1) to aid in the interpretation of the field study results; and, (2) to improve our ability to model flow and dispersion in urban areas. The wind tunnel and field measurements are being compared to a

computational fluid dynamics (CFD) code (the commercial code, FLUENT[6]) and QUIC (Quick Urban and Industrial Complex), a fast-processing, semi-empirical flow and dispersion model being developed by Los Alamos National Laboratory and the University of Utah (Pardyjak and Brown 2001, 2002; Williams *et al.*, 2004; Bowker *et al.*, in press).

The wind tunnel study used a 1:100 scale model for the urban neighborhood. Flow and dispersion patterns were characterized in great detail for the case of a regular array of city blocks with one large tower as part of one of the blocks. Each of the city blocks was 96 cm long and 48 cm wide, with a courtyard in the middle (48 cm by 16 cm) representing the adjoining backyards of row houses forming the perimeter of each block. The model array consisted of 30 buildings (city blocks) arranged in an array five rows long (in the direction of the wind) and six rows laterally. The tower was located on the leeward end of one of the buildings in the second row from the leading edge of the array and had a total height equal to four times the height of the other buildings in the array (Figure 14).

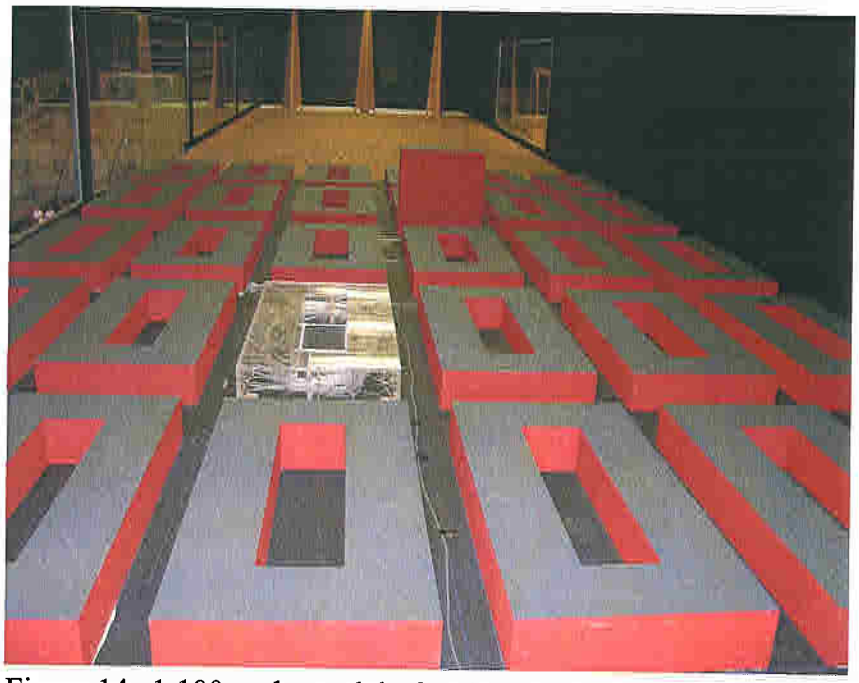

Figure 14. 1:100 scale model of an idealized urban neighborhood in the meteorological wind tunnel. Flow is towards the observer. Tower building is in the second row. The ported building, made of plexiglass, is in the fourth row.

[6]Trademark of Fluent Inc.

Flow visualizations using neutrally-buoyant theatrical smoke were performed with the smoke source positioned to simulate a line segment source with a length of 60 cm. The source was located in the second lateral street canyon downwind of the leading edge of the array. The flow visualizations were documented with still and video photography and enhanced by using a laser light sheet. Figure 15 shows the effect of the tall tower on the dispersion from the street level release, with lifting of the plume to the top of the tower on the leeward side of the building. The velocity and turbulence fields throughout the simulated urban neighborhood were quantified using Laser Doppler Velocimetry.

A computer simulation of a 4 by 4 block array (including the tower) was made with the QUIC model (at 2 m resolution), assuming the same boundary layer as simulated in the tunnel. Figure 16 shows wind tunnel velocity vectors and the QUIC model-predicted vectors in a longitudinal plane centered on the tower. Mean tracer (pure ethane) concentration patterns were sampled on and around the building employing a bank of six hydrocarbon analyzers connected to a moveable sampling rake. In Figure 17, the concentration contours are shown to be pulled laterally away from the source into the wake region behind the tower. Figure 18 shows measured velocity vectors indicating the lateral motion responsible for the distortion of the plume.

Concentrations and building surface pressures were measured through 152 sampling ports mounted on a plexiglass building representative of a test building during the field study (Figure 14). Building surface pressure measurements were obtained with a bank of five Baratron samplers. The flow, pressure, and concentration fields around the ported plexiglass building will be used to better understand the building infiltration measurements taken during the field study. Analyses and comparisons of the field and laboratory data are in progress with publication of results expected in FY-2006.

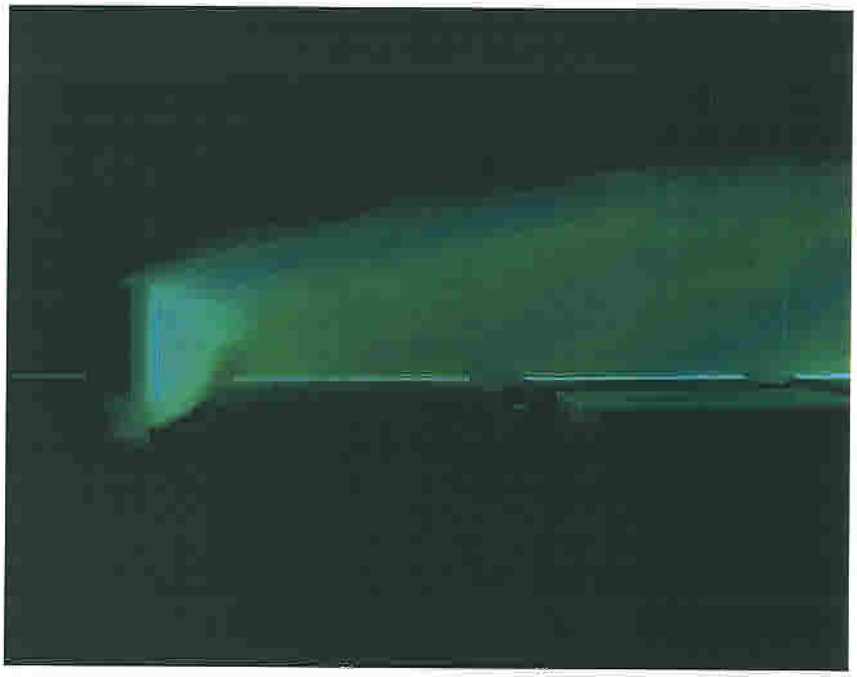

Figure 15. Flow visualization enhanced with a laser sheet. The laser sheet is oriented in a vertical plane aligned with the stream wise direction. This highlights the elevation of the plume by the tall building. Flow is from left to right.

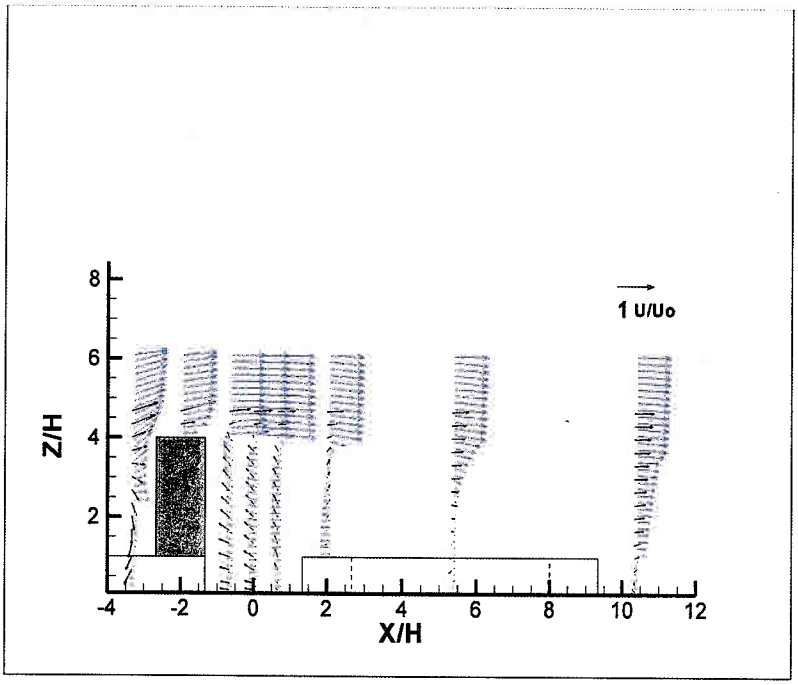

Figure 16. A longitudinal cross-section showing velocity vectors along the plane of the tower building. Wind tunnel measurements are in black and the QUIC model results are in blue.

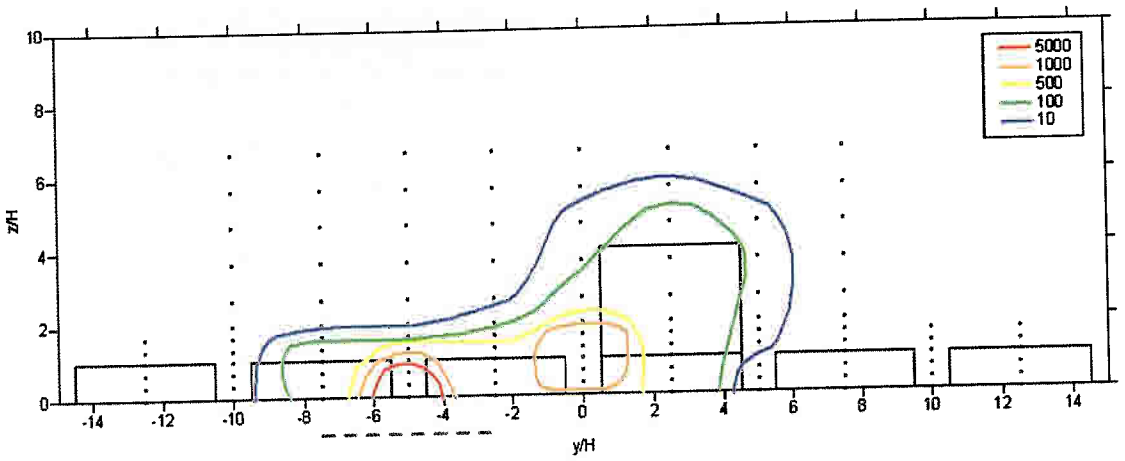

Figure 17. Concentration contours in the source street canyon. The dashed line indicates the lateral location and length of the line segment source. The flow is towards the reader.

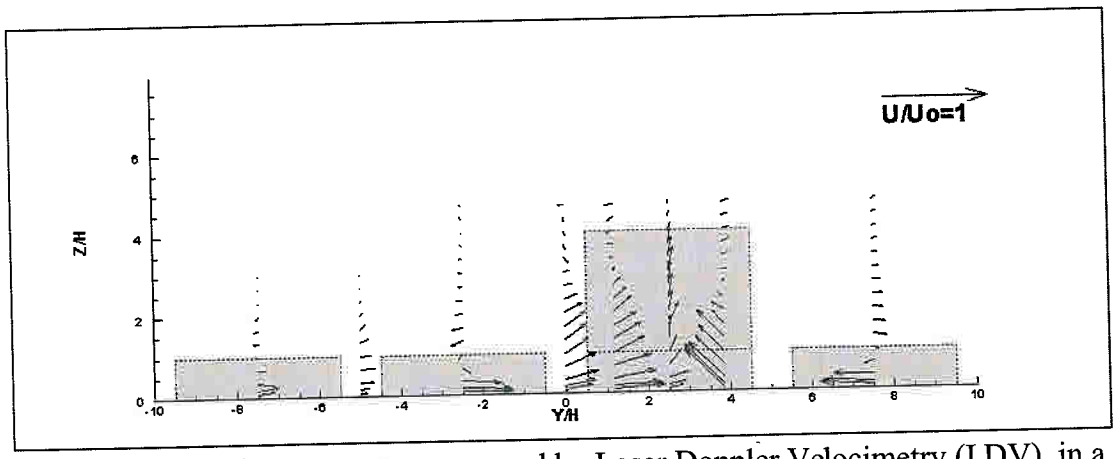

Figure 18. Velocity vectors, as measured by Laser Doppler Velocimetry (LDV), in a lateral cross-section in the source street canyon, directly behind the tower building. Approach flow is towards the reader.

2.7.3 Wind-Blown Dust Emissions

The northern Chihuahuan Desert in New Mexico is a rugged region, populated by mesquite bushes, mesquite coppice dunes, and bare open patches with sandstorms occurring frequently. By studying airflow patterns, soil erosion, soil transport, and soil deposition in this region, there is an improved understanding of desert formation and the production of particulate dust aerosol. Dust production from deserts is a major contributor to the global aerosol dust budget, and global aerosol dust may affect planetary albedo and global climate.

Gillette and Pitchford (2004) showed that the largest source of dust in the northern Chihuahuan desert comes from mesquite (*Prosopis glandulosa*) ecosystems, which were established in the early 1900's and which have evolved into coppice dune-lands. Gillette and Pitchford noted further that most of the sand transport in the mesquite-vegetated sandy soils occur over elongated bare-soil areas that are oriented in the direction of the strongest winds. These areas, referred to as "streets," have only been observed in mesquite ecosystems.

For the past two years, the Division has participated in a study designed to provide a high-resolution measurement database suitable for model development and evaluation. The field study sought to measure wind at several closely-spaced sites in a mesquite-dominated ecosystem and to relate these measurements to measurements collected at a centrally-located micrometeorological tower. This included derived frictional velocities, which is a key variable for parameterizing wind-blown dust emission algorithms. A schematic of the field study site is shown in Figure 19.

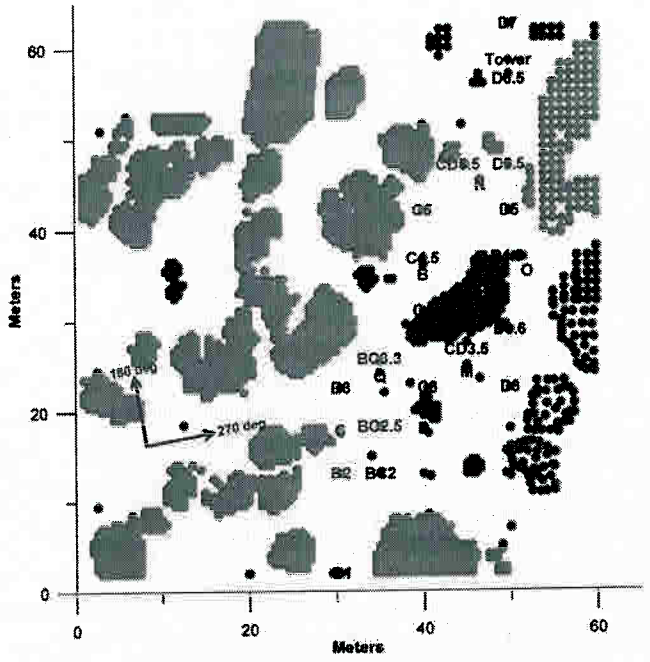

Figure 19. Map of locations of dunes and instrumentation for the northern Chihuahuan field study. Mesquite coppice dunes are shown by shading. Sand flux collectors are labeled with letters and numbers. The eight 3-m wind masts are denoted as *B, C, D, M, N, O, P,* and *Q*. The 15-m micrometeorological tower is labeled "tower." Wind directions are shown as 180° (from the south) and 270° (from the west).

Because soil erosion and dust production depend on the pattern, strength, and gradients in the wind field at an extremely fine scale, efforts to simulate these effects can be supported with fine-scale high resolution numerical models. For this study, QUIC v3.5, a semi-empirical mass-consistent diagnostic wind-field model, was tested. Wind velocities and directions measured at six study locations were found to correlate well with the model, and QUIC seems to have the ability to handle the variability in wind direction and speed across the study region as influenced by vegetation. Generally, QUIC successfully identified location of the high-wind velocities, which were predominately along "streets" that were aligned with the driving wind. The model also realistically simulated the wake flows downwind of bushes as seen in Figure 20.

This work has been extended to compare simulation with measurements of sediment transport along the streets and around the dunes. The wind velocities from QUIC were coupled with a simple sand-flux parameterization for comparison with field measurements. Modeled sand fluxes were usually within 50 percent of measured values. The good agreement between

measurements from a real-time sand-flux instrument and predictions from QUIC, for the same location and time, suggests that QUIC can be a useful tool for predicting the spatial and temporal variability of sand flux across the study domain.

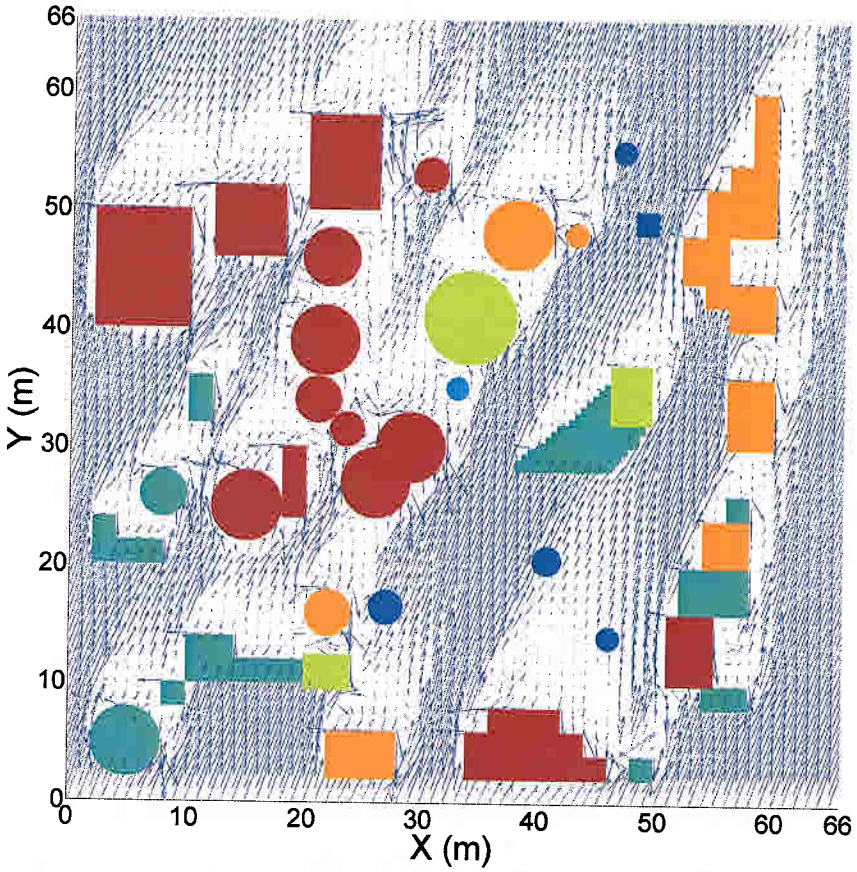

Figure 20. Velocity vectors simulated by QUIC showing the heterogeneity of the wind flow patterns in the study region. Obstacles (representing mesquite bushes and coppice dunes) are shown as colored rectangles and cylinders with the color proportion to their height.

2.7.4 Analysis of Exceptional Meteorological Events

When EPA promulgates a National Ambient Air Quality Standard (NAAQS), the Agency also promulgates rules on the measurement of air quality to determine compliance with the NAAQS. Specifically, the NAAQS for $PM_{2.5}$ contains guidance on use of data from air quality monitors known as Federal Reference Method monitors. This guidance also covers occasions in which data may be inappropriate to compare to the NAAQS and should be excluded. The $PM_{2.5}$

NAAQS provides for the exclusion of data from such monitors for a given day when the data is strongly influenced by impacts from an "exceptional event". An exceptional event is defined as a natural event—or one caused by human activity—that is unlikely to recur at a particular location, that affects air quality, and that is not reasonably controllable or preventable. One example would be wildfires producing considerable smoke. An exceptional event must be determined by EPA through the process established in the rule. This process involves rigorous examination of the atmospheric condition as a cause or contributing factor to the event. Branch meteorologists conduct these examinations and report on their significance to the cause or contribution of the event.

NOAA evaluated several petitions for determination of exceptional event days by running the HYSPLIT model. Back trajectories were run for the exceptional event days for a 72 hour period. The trajectories were used to help determine if smoke from distant fires may have had an impact on the exceptional event locations and days. After consideration, it was determined that the events were sometimes caused by such complicated conditions as local or nearby smoke from fires, smoke from distant fires, and from nearby and distant sulfate emissions. Trajectories were only one of many methods used to help determine the validity of exceptional events. After gathering and assessing all of the available data, including surface measurements, satellite photographs, and back trajectories, the evaluations conclude with determination on the likelihood of the case being an exceptional event as defined by regulation. That determination informs the regulatory decisions to grant or deny the petitions.

2.7.5 Development of a Metamodeling Response Surface Technique for Ozone

A new modeling technique called metamodeling was developed, evaluated, and applied to enable air quality planners to rapidly assess the most effective control strategies in lowering future concentrations of ozone. This was done via the development of an ozone response surface based on more than 150 individual CAMx[7],[8] modeling simulations of a 2015 future case over the eastern United States. This metamodeling technique is a "model of the model" and can be shown to reproduce the results from any individual modeling simulation with little bias or error. This approach, which allows for the rapid assessment of air quality impacts of different combinations of emission reductions, has been used to project the effects of the less-evaporative portable gasoline containers as well as to determine what additional emission controls may be needed to attain the 8-hour ozone NAAQS by 2015.

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[7]Comprehensive Air Quality model with extensions

[8]A publicly available open-source Eulerian photochemical dispersion model that allows for the integrated "one-atmosphere" assessment of gaseous and particulate air pollution (ENVIRON Holdings, Inc.).

To maximize the information obtained for use in comparing relative efficacy of different emissions control strategies, an experimental design was established consisting of a carefully selected set of air quality modeling runs. For this analysis, an experimental design was selected that covered three key areas: type of precursor emission (NO_x or VOC), emission source type (*i.e.*, onroad vehicles, nonroad vehicles, area sources, electrical generating utility (EGU) sources, and non-utility point sources), and location within or outside of a 2015 model-projected residual ozone nonattainment area. Cross-validation and out-of-sample performance statistics for the projected 2015 ozone design value metric indicated that the metamodel produces very accurate and generally non-biased predictions of the CAMx model response. The mean of the spatially averaged error across all 140 non-evaluation runs is only 0.28 ppb, or less than half a percent in relative terms. This indicates that the metamodel replicates the CAMx response to emissions changes very well for most emissions combinations and in most locations.

2.7.6 Model Analyses of Leading Contributors to Future Ozone Nonattainment

The Comprehensive Air quality Model with extensions (CAMx) contains a source apportionment tool that can be used to estimate how emissions from individual source areas and regions impact modeled ozone concentrations. Three future base years were modeled in this analysis: 2010, 2015, and 2020. An eastern United States domain was modeled using a two-way nested grid with 36- and 12-km grid-cell sizes. Contributions to exceedance-level ozone were calculated by State and by major emission source sectors: electrical generating units (EGU), non-EGU point sources, area sources, wildfire emissions, on-road mobile sources, and non-road mobile sources. The non-road sources were further broken out into individual sectors (*e.g.*, marine sources, locomotives, aircraft, diesel engines, *etc.*). The modeling determined which sources are projected to most contribute to future ozone nonattainment over 16 major metropolitan areas across the eastern United States.

The analysis showed that non-EGU point sources are projected to become an increasingly large contributor to residual ozone nonattainment. In Chicago, emissions from this sector are estimated to be the cause for 21 percent of the exceedance-level ozone in 2010. By 2020, the contribution are estimated to increase to 31 percent. The modeling indicated that mobile sources are expected to continue to play a large role in residual ozone nonattainment over the eastern United States despite significant reductions in emissions over the period due to recent Federal control programs. The contribution from non-road sources is expected to nearly equal that of on-road mobile sources by 2020. The most significant non-road category in 2020 tended to be heavy-duty diesel engines, though it varies by area. Marine sources were large contributors (*i.e.*, greater than 10 percent) to high 8-hour ozone in several locations near major ports and waterways.

2.7.7 Support Center for Regulatory Air Models

The SCRAM (Support Center for Regulatory Air Models) website continued to be a focal point for several milestones within the air dispersion modeling community. Numerous incremental updates were made to AERMOD (AMS EPA Regulatory MODel) and its modeling system. Materials from the 8th Conference on Air Quality Modeling, held September 22–23, 2005, will be provided on SCRAM during the post-workshop period. In addition, SCRAM was fully restructured during FY-2005. In general, the goal of the new SCRAM is to provide more information on the topic areas for the novice user, provide a more logical flow with explanations along the way, and provide information on regional-scale modeling that supports. In the past, the regional-scale modeling has had little recognition on SCRAM. The sidebars were changed to provide all of the major SCRAM topics at a simple glance. Once selected, each topic area opens a main topic page that provides an extensive description of the topic and lists all sub-topic areas. Two new areas were added to SCRAM: Conferences and Workshops, and Reports and Journal Articles. The meteorological data area was enhanced with information on both point-observational data (National Weather Service), and gridded-meteorological data, with extensive links to meteorological data.

2.7.8 National Air Toxics Assessment Explorer

The National Air Toxics Assessment (NATA) Explorer was developed to gain a better understanding of the relationships between model estimated cancer and non-cancer risks and emissions from an air toxics inventory. The NATA Explorer is a GIS-based visualization tool that can determine the most likely sources of emissions responsible for elevated model-estimated concentrations and associated risks. The tool shows many levels of air quality data including ambient monitoring data for air toxics.

The NATA Explorer allows queries by state, county, zip code, pollutant, and source categories. The user has the ability to pan, zoom, identify census tract-level data, and overlay such data as demographics, transportation, and satellite data. This tool has proved useful by saving staff resources, where previously, data queries consumed valuable staff and contractor time.

2.6.9 NARSTO—A North American Air Quality Research Partnership

The NARSTO program is a multinational, public/private partnership of over 70 organizations sponsoring and participating in air-quality related research in North America. NOAA and EPA help coordinate communication and planning with the NARSTO membership for air quality research, science plans, and state-of-science assessments. ASMD provides a full-time associate management coordinator for the NARSTO program, whose activities include managing the infrastructure support to the NARSTO program and several related assistance agreements, and providing technical assistance and leadership to the NARSTO Quality System

Science Center, which is charged with developing and maintaining the NARSTO permanent data archive at NASA.

The most recent NARSTO activity is an assessment of current and future directions of emission inventory use in North America (NARSTO, 2005). The NARSTO Executive Steering committee has directed the management coordinators to establish workgroups and teams to formulate future NARSTO activities related to aerosol modeling on several spatial and temporal scales and to provide recommendations on regarding NARSTO assessment activities related to a multi-pollutant approach to air quality management in a accountability framework. Several NARSTO supported workshops, conferences, and meetings are anticipated.

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APPENDIX A: ACRONYMS, ABBREVIATIONS, AND DEFINITIONS

ACM	Asymmetric Convective Model
ACM2	Asymmetric Convective Model and eddy diffusion
AE3	Aerosols algorithm version 3
AER	Atmospheric and Environmental Research, Inc.
AERMOD	AMS EPA Regulatory MODel model
AER04	Aerosol module
AERONET	AErosol RObotic NETwork
AIM	Aerosol Inorganic Model
AIRNow	Air quality index data
AMET	Atmospheric Model Evaluation Tool
AOD	Aerosol Optical Depth
AQF	Air quality forecast
AQS	Air quality system
ARL	Air Resources Laboratory
ASMD	Atmospheric Sciences Modeling Division
ASPEN	Gaussian plume model
AT	Air toxins
BEIS	Biogenic Emissions Inventory System
BEIS3.13	Biogenic Emissions Inventory System version 3.13
BELD	Biogenic Emission Land Data
BRACE	Bay Regional Atmospheric Chemistry Experiment
CAA	Clean Air Act
CAAA	Clean Air Act Amendments of 1990
CAIR	Clean Air Interstate Rule
CAMD	Clean Air Markets Division
CAMx	Comprehensive Air Quality Model with extensions
CB-IV	Carbon-Bond-IV
CB05	Carbon-Bond 05 chemical mechanism
CASTNet	Clean Air Status and Trend Network
CFD	Computational fluid dynamics
CIRAQ	Climate Impact on Regional Air Quality
CAMR	Clean Air Mercury Rule
CEM	Continuous Emission Monitoring database
CMAQ	Community Multiscale Air Quality modeling system
CMAQ-AT	Air toxins version of CMAQ
CMAQ CTM	Community Multiscale Air Quality modeling system chemistry-transport model
CMAQ-Hg	Community Multiscale Air Quality - Mercury model
CMAQ-MADRID	CMAQ updated sectional aerosol version

CMAQ-UCD	The Wexler sectional aerosol model, Aerosol Inorganic Model (AIM), was adapted to incorporate sea salt in its calculations, implemented into the September 2004 release CMAQ, and named CMAQ-UCD.
CMAS	Community Modeling and Analysis System
CONUS	CONtiguous United States
CTM	Chemistry-Transport Model
CMU	Carnegie Mellon University
EBI	Euler Backward Iterative
EC	Elemental Carbon
EDATAS	Enhanced Delaware Air Toxics Assessment Study
EGU	Electric generation units
EMF	Emission Modeling Framework
EPA	Environmental Protection Agency
EPA GCRP	EPA Global Change Research Program
Eta	National Centers for Environmental Prediction mesoscale model
Extended RADM	Regional Acid Deposition Model with full dynamics of secondary inorganic fine particle formation taken from the RPM
GCM	Global Climate Models
GCRP	Global Change Research Program
GEOS-Chem	A global three-dimensional model of atmospheric composition driven by assimilated meteorological observations from the Goddard Earth Observing System
GFS	Global Forecast System
GIS	Geographic Information System
GR	Gas Ratio
HAPs	Hazardous air pollutants
HAPEM	Hazardous Air Pollutant Exposure Model
HAPEM	Hazardous Air Pollutant Exposure Model version 5
HUCs	Hydrologic units
HYSPLIT	Hybrid Single-Particle Lagrangian Integrated Trajectory model
IAG	InterAgency Agreement
ICARTT	International Consortium for Atmospheric Research on Transport and Transformation
IC/BC	Initial Condition/Boundary Condition
IMPROVE	Interagency Monitoring of PROtected Visual Environment Network
I/O API	Input/Output Applications Programming Interface
ISORROPIA	Thermodynamics module
Kz	Minimum value of the surface layer vertical-eddy diffusivity
M3Dry	Models-3 Dry Deposition Scheme
MAQSIP	Multiscale Air Quality Simulation Platform
MCIP	Meteorology-Chemistry Interface Processor
MDN	Mercury Deposition Network

MIMS	Multimedia Integrated Modeling System
MLBC	MultiLayer Biochemical Model
MM5	Mesoscale Model - version 5
Mobile6	Mobile Source Emission
MODIS	MODerate Resolution Imaging Spectroradiometer Rapid Response
MOPITT	Measurement of Pollution in the Troposphere
MySQL®	MySQL® provides a comprehensive set of open source visual database tools
NAAQS	National Ambient Air Quality Standards
NADP	National Atmospheric Deposition Program
NAM	North American Mesoscale model (currently the Eta model)
NAMMIS	North American Mercury Model Intercomparison study
NASA	National Aeronautics and Space Administration
NATA	National Air Toxics Assessment
NATA Explorer	A visualization tool for all 1999 NATA data
NCAR	National Center for Atmospheric Research
NCEP	National Centers for Environmental Prediction
NEI	National Emission Inventory
NMB	Normalized Mean Biases
NME	Normalized Mean Errors
NOAA	National Oceanic and Atmospheric Administration
OAQPS	Office of Air Quality Planning and Standards
OC	Organic Carbon
OC_{pri}	Primary Organic Carbon
OC_{sec}	Secondary Organic Carbon
ODE	Ordinary Differential Equation
PAVE©	Package for Analysis and Visualization of Environmental data
PBL	Planetary Boundary Layer
PDM	Plume Dynamics Model
PinG	Plume-in-Grid
PinG Module	Plume-in-Grid Model
PM	Particulate Matter
PNNL	Pacific Northwest National Laboratory
PREMAQ	Pre-processor for CMAQ
PSU	Pennsylvania State University
PX LSM	Pleim Xiu Land-Surface Model
QUIC	Quick Urban and Industrial Complex dispersion model
RADM	Regional Acid Deposition Model
RCM	Regional climate model
RGM	Reactive gaseous mercury
RR	Rapid response
SAPRC99	A gas-phase chemical mechanism (Statewide Air Policy Research Center)
SCRAM	Support Center for Regulatory Air Models

SGV	SubGrid variability
SIP	State Implementation Plan
SMOKE±	Sparse Matrix Operator Kernel Emission model
SSA	Single Scattering Albedo
STN	Speciated Trends Network
TMDL	Total Maximum Daily Load
UCD	University of California, Davis
UDP	Department of Homeland Security—s New York City Urban Dispersion Program
VOC	Volatile Organic Compounds
WRF	Weather Research and Forecasting
WTC	World Trade Center

APPENDIX B: PUBLICATIONS

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Zhang, Y., P. Liu, K. Wang, M. Jacobson, P. Bhave, S. Yu, S. Roselle, and K. Schere. Predicting aerosol number and size distribution with CMAQ: Homogeneous nucleation algorithms and process analysis. *4th Annual CMAS Models-3 Users' Conference, September 26--28, 2005, Chapel Hill, North Carolina*. Community Modeling and Analysis System, University of North Carolina at Chapel Hill, Chapel Hill, NC, CD-ROM 5.11 (2005).

APPENDIX C: PRESENTATIONS

Appel, K.W. An operational evaluation of the 2005 release of Models-3 CMAQ. Presentation at the 4th Annual CMAS Models-3 Users' Conference, Friday Center, UNC at Chapel Hill, Chapel Hill, NC, September 27, 2005.

Appel, K.W. The atmospheric model evaluation tool (AMET): Air quality module. Poster presentation at the 4th Annual CMAS Models-3 Users' Conference, Friday Center, UNC at Chapel Hill, Chapel Hill, NC, September 28, 2005.

Appel, K.W. An annual evaluation of the 2005 release of Models-3 CMAQ. Poster presentation at the NOAA/EPA Golden Jubilee Symposium on Air Quality Modeling and Its Applications, Research Triangle Park, NC, September 20, 2005.

Benjey, W.G. Wildfire emission modeling: Integrating BlueSky and SMOKE. Presentation at the 14th International Emission Inventory Conference: Transforming Emission Inventories—Meeting Future Challenges Today, Las Vegas, NV, April 13, 2005.

Benjey, W.G. Inter-annual and seasonal variability of meteorologically influenced emissions. Presentation at the 14th International Emission Inventory Conference: Transforming Emission Inventories—Meeting Future Challenges Today, Las Vegas, NV, April 14, 2005.

Benjey, W.G. EPA's new emissions modeling framework. Presentation at the 4th Annual CMAS Models-3 Users' Conference, Friday Center, UNC at Chapel Hill, Chapel Hill, NC, September 26, 2005.

Bhave, P.V. Recent developments in the CMAQ Modal aerosol module. Presentation at the 4th Annual CMAS Models-3 Users' Conference, Friday Center, UNC at Chapel Hill, Chapel Hill, NC, September 27, 2005.

Bhave, P.V. The Community Multiscale Air Quality (CMAQ) aerosol module development: Recent enhancements and future plans. Presentation at the 3rd Annual CMAS Models-3 Users' Conference, Friday Center, UNC at Chapel Hill, Chapel Hill, NC, October 20, 2004.

Bhave, P.V. Source apportionment of primary carbonaceous aerosol using the Community Multiscale Air Quality model. Presentation at the 27th NATO International Technical Meeting on Air Pollution Modeling and its Applications, Banff, Canada, October 26, 2004.

Bowker, G.E. Using the QUIC (Quick Urban & Industrial Complex) model to study air flow and dispersion patterns in deserts. Interagency Nuclear Safety Review Panel's Particle Resuspension Technical Interchange Meeting, Cape Canaveral, FL, March 23, 2005.

Bullock, O.R., Jr. Atmospheric mercury transport and deposition. Presentation at the 2005 Air Toxics Workshop, Research Triangle Park, NC, March 31, 2005.

Bullock, O.R., Jr. Atmospheric mercury modeling. Presentation at the NOAA/EPA Scientist-to-Scientist Meeting, Laurel, MD, June 2, 2005.

Bullock, O.R., Jr. Simulating atmospheric mercury with the Community Multiscale Air Quality (CMAQ) model. Presentation at the NOAA/EPA Golden Jubilee Symposium on Air Quality Modeling and Its Applications, Research Triangle Park, NC, September 20, 2005.

Ching, J.K.S. Overview: ORD's advanced modeling tools for air toxics assessments. 2005 Air Toxics Workshop, Research Triangle Park, NC, April 1, 2005.

Ching, J.K.S. A prospectus for bridging meso-urban scale to building-scale meteorological and dispersion modeling. 9th Annual George Mason University Conference on Atmospheric and Dispersion Modeling, Fairfax, VA, July 19, 2005.

Ching, J.K.S. Advanced urbanized meteorological modeling and air quality simulations with CMAQ at neighborhood scales. NOAA/EPA Golden Jubilee Symposium on Air Quality Modeling and Its Applications, Research Triangle Park, NC, September 20, 2005.

Ching, J.K.S. Investigation and implications of sub-grid variability of CMAQ modeled concentrations. Presentation at the 4th Annual CMAS Models-3 Users' Conference, Friday Center, UNC at Chapel Hill, Chapel Hill, NC, September 26, 2005.

Ching, J.K.S. Incorporating sub-grid variability concentration distributions with CMAQ. Presentation at the 4th Annual CMAS Models-3 Users' Conference, Friday Center, UNC at Chapel Hill, Chapel Hill, NC, September 27, 2005.

Cooter, E.J. An overview of the Climate Impact on Regional Air Quality (CIRAQ) project. Presentation at the 3rd Annual CMAS Models-3 Users' Conference, Friday Center, UNC at Chapel Hill, Chapel Hill, NC, October 20, 2004.

Dennis, R.L. Diagnostic evaluation of CMAQ response of inorganic fine particulate species to emissions changes. Poster presentation at the 3rd Annual CMAS Models-3 Users' Conference, Friday Center, UNC at Chapel Hill, Chapel Hill, NC, October 18, 2004.

Dennis, R.L. High time-resolved comparisons for in-depth probing of CMAQ fine particle and gas predictions. Presentation at the 27th NATO/CCMS International Technical Meeting, Banff, Canada, October 29, 2004.

Dennis, R.L. Investigation of the relative value of spatial and temporal data for evaluating air quality models and tracking changes for the inorganic fine-particle system. Presentation at the American Association for Aerosol Research Supersite Specialty Conference, Atlanta, GA, February 9, 2006.

Dennis, R.L. Uncertainties in CMAQ's predictions of the nonlinear effect of SO_2 reductions on aerosol nitrate, using the gas ratio as a construct to guide inquiry. Presentations at the American Association for Aerosol Research Supersite Specialty Conference, Atlanta, GA, on February 9, 2005.

Dennis, R.L. Modeling approaches for the management of multimedia pollutants. Poster presentation at the EPA Board of Scientific Counselors (BOSC) Ecological Research Subcommittee Review, Research Triangle Park, NC, March 8, 2005.

Dennis, R.L. The nonlinear response of nitrate replacement that mitigates sulfate reductions: Gas Ratio as an indicator and sensitivity to errors in total ammonia and total nitrate. Poster presentation, NOAA/EPA Golden Jubilee Symposium on Air Quality Modeling and Its Applications, Research Triangle Park, NC, September 20, 2005.

Dennis, R.L. The nonlinear response of nitrate replacement that mitigates sulfate reductions: Gas Ratio as an indicator and sensitivity to errors in total ammonia and total nitrate. Poster presentation at the 4th Annual CMAS Models-3 Users' Conference, Friday Center, UNC-Chapel Hill, Chapel Hill, NC, September 27, 2005.

Eder, B.K. An evaluation of the 2004 release of CMAQ. Presentation at the 27th NATO/CCMS International Technical Meeting on Air Pollution Modelling and its Application, Banff, Alberta, Canada, October 29, 2004.

Eder, B.K. An operational evaluation of the Eta-CMAQ air quality forecast model. Presentation at the 3rd Annual CMAS Models-3 Users' Conference, Chapel Hill, NC, October 20, 2004.

Eder, B.K. The Eta-CMAQ air quality forecast model: background, operation and evaluation. Invited presentation to the Central North Carolina Chapter-American Meteorological Society, Raleigh, NC, January 20, 2005.

Eder, B.K. An evaluation of the Eta-CMAQ air quality forecast model. Presentation at EPA's 2005 National Air Quality Conference, San Francisco, CA, February 15, 2005.

Eder, B.K. A performance evaluation of the Eta-CMAQ air quality forecast model for the summer of 2005. Presentation at the NOAA/EPA Golden Jubilee Symposium on Air Quality Modeling and Its Applications, Research Triangle Park, NC, September 20, 2005.

Eder, B.K. A performance evaluation of the 2004 release of Models-3 3rd. Presentation at the 3rd Annual CMAS Models-3 Users' Conference, Friday Center, UNC at Chapel Hill, Chapel Hill, NC, October 18, 2004.

Eder, B.K. An evaluation of the Eta-CMAQ air quality forecast model for July 2005. Presentation at the 4th Annual CMAS Models-3 Users' Conference, Friday Center, UNC at Chapel Hill, Chapel Hill, NC, September 28, 2005.

Eder, B.K. An evaluation of the 2005 release Models-3 CMAQ. Presentation at the NOAA/EPA Golden Jubilee Symposium on Air Quality Modeling and Its Applications, Research Triangle Park, NC, September 21, 2005.

Gillette, D.A. Resuspension of particles from grass: Comparison of aerodynamic and mechanical mechanisms. Interagency Nuclear Safety Review Panel's Particle Resuspension Technical Interchange Meeting, Cape Canaveral, FL, March 23, 2005

Gillette, D.A. Wind velocities and sand fluxes in mesquite dune-lands in the Northern Chihuahuan desert: A comparison between field measurements and the QUIC (Quick Urban & Industrial Complex) model. NOAA/EPA Golden Jubilee Symposium on Air Quality Modeling and Its Applications, Research Triangle Park, NC, September 21, 2005.

Gillette, D.A. Dust emissions in the northern Chihuahuan desert. Western Regional Air Pollution (WRAP) Dust Forum, Las Vegas, NV, November 16, 2004.

Gilliam, R.C. The atmospheric model evaluation tool: Meteorology module. Presentation at the 4th Annual CMAS Models-3 Users' Conference, Friday Center, UNC at Chapel Hill, Chapel Hill, NC, September 27, 2005.

Gilliam, R.C. A year-long MM5 evaluation using a model evaluation toolkit. Presentation at the 3rd Annual CMAS Models-3 Users' Conference, Friday Center, UNC at Chapel Hill, Chapel Hill, NC, October 19, 2004.

Gilliland, A.B. Seasonal NH_3 emissions for an annual 2001 simulation: Inverse model estimation and evaluation. Presentation at the 3rd Annual CMAS Models-3 Users' Conference, Friday Center, UNC at Chapel Hill, Chapel Hill, NC, October 19, 2004.

Gilliland, A.B. Inverse model estimation of seasonal NH_3 emissions, American Association for Aerosol Research Supersites Conference, Atlanta, GA, February 8, 2005.

Gilliland, A.B. Seasonal NH_3 emissions: Inverse model estimation and evaluation. Invited presentation at the Department of Marine Earth & Atmospheric Sciences, North Carolina State University, Raleigh, NC, April 18, 2005.

Godowitch, J.M. Modeling photochemistry and aerosol formation in point source plumes with the CMAQ Plume-in-Grid system. Presentation at the 7th Conference on Atmospheric Chemistry, 85th AMS Annual Meeting of the American Meteorological Society, San Diego, CA, January 10, 2005.

Godowitch, J.M. Development and applications of the CMAQ Plume-in-Grid model. Presentation at the 4th Annual CMAS Models-3 Users' Conference, Friday Center, UNC at Chapel Hill, Chapel Hill, NC, September 27, 2005.

Godowitch, J.M. Community Multiscale Air Quality (CMAQ) model—Plume-in-Grid (PinG). Presentation at the 7th Conference on Atmospheric Chemistry, 85th AMS Annual Meeting of the American Meteorological Society, San Diego, CA, January 10, 2005.

Heist, D.K. Residence times in an array of buildings. PhysMod 2005, International Workshop on Physical Modeling of Flow and Dispersion Modelling, London, Ontario, Canada, August 24, 2005.

Huber, A.H. Applications of CFD simulations of pollutant transport and dispersion within ambient urban building environments: Including homeland security. Presentation at the 98th Annual Conference of the Air & Waste Management Association, Minneapolis, MN, June 23, 2005.

Hutzell, W.T. Biogenic sources of formaldehyde and acetaldehyde during summer and winter conditions. Presentation at the American Geophysical Union's 2004 Fall Meeting, San Francisco, CA, December 17, 2004.

Hutzell, W.T. Simulating urban air toxics over continental and urban scales. Presentation at the 3rd Annual CMAS Models-3 Users' Conference, Friday Center, UNC at Chapel Hill, Chapel Hill, NC, October 18, 2004.

Isakov, V. Resolving fine scale in air toxics modeling and the importance of its sub-grid variability for exposure estimates. NOAA/EPA Golden Jubilee Symposium on Air Quality Modeling and Its Applications, Research Triangle Park, NC, September 21, 2005.

Kang, D. Variations in weekday and weekend regional surface ozone levels: An analysis of observed and model forecast trends. Presentation at the NOAA/EPA Golden Jubilee Symposium on Air Quality Modeling and Its Applications, Durham, NC, September 20, 2005.

Kang, D. Development of new categorical metrics for air quality model evaluation and their application to Eta-CMAQ forecasts. Presentation at the 4th Annual CMAS Models-3 Users' Conference, Friday Center, UNC at Chapel Hill, Chapel Hill, NC, September 27, 2005.

Kang, D. Simulating atmospheric fate of ammonia in southeast U.S. using CMAQ with a 4-km resolution. Presentation at the 4th Annual CMAS Models-3 Users' Conference, Friday Center, UNC at Chapel Hill, Chapel Hill, NC, September 27, 2005.

Lin, H.-M.. Development of the off-line clear sky radiation flux by using the operational Eta code: Applications for photolysis rate calculations. Presentation at the NOAA/EPA Golden Jubilee Symposium on Air Quality Modeling and Its Applications, Durham, NC, September 20, 2005.

Luecken, D. Concentrations of toxic air pollutants in the U.S. simulated by an air quality model. Presentation at the 27th NATO International Technical Meeting on Air Pollution Modeling and its Applications, Banff, Canada, October 25, 2004.

Luecken, D. Concentrations of mobile source toxic pollutants simulated by Community Multiscale Air Quality (CMAQ) in the continental United States. Presentation at the Coordinating Research Council Workshop on Mobile Source Air Toxics, Scottsdale, AZ, December 2, 2004.

Luecken, D. Progress report on the use of CMAQ to study reactivity metrics. Presentation at the Reactivity Research Working Group, Research Triangle Park, NC, May 25, 2005.

Mathur, R. Adaptation and application of the Community Multiscale Air Quality (CMAQ) modeling system for real-time air quality forecasting during the summer of 2004 Presentation at the 3rd Annual CMAS Models-3 Users' Conference, Friday Center, UNC at Chapel Hill, Chapel Hill, NC, October 20, 2004.

Mathur, R. Verification of surface layer ozone forecasts in the NOAA/EPA air quality forecast system in different regions under different synoptic scenarios. Presentation at the 7th Conference on Atmospheric Chemistry, 85th AMS Annual Meeting of the American Meteorological Society, San Diego, CA, January 10, 2005.

Mathur, R. Assessment of Eta-CMAQ forecasts for particulate matter distributions through comparisons with surface network and specialized measurements. Presentation at the 7th Conference on Atmospheric Chemistry, 85th AMS Annual Meeting of the American Meteorological Society, San Diego, CA, January 13, 2005.

Mathur, R. Eta-CMAQ modeling system's capability to provide $PM_{2.5}$ and aerosol optical thickness forecast. Presentation at the 7th Conference on Atmospheric Chemistry, 85th AMS Annual Meeting of the American Meteorological Society, San Diego, CA, January 13, 2005.

Mathur, R. An assessment of the performance of the Eta-CMAQ air quality forecast modeling system during the ICARTT field experiment. Presentation at the International Consortium for Atmospheric Research on Transport and Transformation (ICARTT) Data Analysis Workshop, Durham, NH, August 9, 2005.

Mathur, R. Evaluation of Eta-CMAQ O_3 forecasts during the summer of 2005 over the eastern and continental US domains. Presentation at the 2005 Air Quality Focus Group Workshop, Silver Spring, MD, September 7, 2005.

Mathur, R. The Community Multiscale Air Quality (CMAQ) model: Model configuration and enhancements for 2005 air quality forecasting. Presentation at the 2005 Air Quality Focus Group Workshop, Silver Spring, MD, September 7, 2005.

Mathur, R. Particulate matter forecasts with the Eta-CMAQ modeling system: Towards development of a real-time system and assessment of model performance. Presentation at the 4th Annual CMAS Models-3 Users' Conference, Friday Center, UNC at Chapel Hill, Chapel Hill, NC, September 26, 2005.

Nolte, C.G. Evaluation of the CMAQ-AIM model against size- and chemically-resolved impactor data at a coastal urban site. Presentation at the American Association for Aerosol Research Supersites Conference, Atlanta, GA, February 9, 2005.

Nolte, C.G. Using CMAQ-AIM to evaluate the gas-particle partitioning treatment in CMAQ. Presentation at the 4th Annual CMAS Models-3 Users' Conference, Friday Center, UNC at Chapel Hill, Chapel Hill, NC, October 18, 2004.

Otte, T.L. What's new in MCIP2? Presentation at the 3rd Annual CMAS Models-3 Users' Conference, Friday Center, UNC at Chapel Hill, Chapel Hill, NC, October 20, 2004.

Otte, T.L. PREMAQ: A new pre-processor to CMAQ for air-quality forecasting. Presentation at the 3rd Annual CMAS Models-3 Users' Conference, Friday Center, UNC at Chapel Hill, Chapel Hill, NC, October 20, 2004.

Perry S.G. The NOAA/EPA Fluid Modeling Facility's contributions to the understanding of atmospheric dispersion. NOAA/EPA Golden Jubilee Symposium on Air Quality Modeling and Its Applications, Research Triangle Park, NC, September 21, 2005

Pierce, T.E. Earth, wind, and fire: Building meteorologically-sensitive biogenic and wildland fire emission estimates for air quality models. NOAA/EPA Golden Jubilee Symposium on Air Quality Modeling and Its Applications, Research Triangle Park, NC, September 21, 2005.

Pierce, T.E. Modulating emissions from electric generating units as a function of meteorological variables. Presentation at the 4th Annual CMAS Models-3 Users' Conference, Friday Center, UNC at Chapel Hill, Chapel Hill, NC, September 28, 2005.

Pierce, T.E. The use of the NOAA Hazards Mapping System (HMS) for characterizing biomass emissions in the Eta-CMAQ air quality forecast system. EastFire Conference on Wildland Fires in the eastern United States, George Mason University, Fairfax, VA, May 12, 2005.

Pleim, J.E. New developments in the Community Multiscale Air Quality (CMAQ) model. Presentation at the 3rd Annual CMAS Models-3 Users' Conference, Friday Center, UNC at Chapel Hill, Chapel Hill, NC, October 18, 2004.

Pleim, J.E. Community Multiscale Air Quality (CMAQ) model—cloud cover and radiation effects. Presentation at the 7th Conference on Atmospheric Chemistry, 85th Annual Meeting of the American Meteorological Society, San Diego, CA, January 13, 2005.

Pleim, J.E. Diagnostic evaluations, sensitivity analysis, and new developments in the Eta/CMAQ air quality forecast system. Presentation at the 7th Conference on Atmospheric Chemistry, 85th AMS Annual Meeting of the American Meteorological Society, San Diego, CA, January 13, 2005.

Pleim, J.E. Developing MCIP to process WRF-EM output. Presentation at the 2005 Ad Hoc Meteorological Modeling Workshop, Denver, CO, June 30, 2005.

Pleim, J.E. The impact of different PBL models on meteorology and air quality model results. Presentation at the NOAA/EPA Golden Jubilee Symposium on Air Quality Modeling and Its Applications, Research Triangle Park, NC, September 20, 2005.

Pleim, J.E. New developments in Community Multiscale Air Quality (CMAQ) model. Presentation at the 4th Annual CMAS Models-3 Users' Conference, Friday Center, UNC at Chapel Hill, Chapel Hill, NC, September 26, 2005.

Poole-Kober, E.M. Past and present: 50 years of air quality research and application by the Atmospheric Sciences Modeling Division in partnership with the U.S. Environmental Protection Agency. Poster presentation at the NOAA/EPA Golden Jubilee Symposium on Air Quality Modeling and Its Applications, Research Triangle Park, NC, September 19, 2005.

Pouliot, G.A. Wildland fire emissions modeling for CMAQ: An update. Presentation at the 4th Annual CMAS Models-3 Users' Conference, Friday Center, UNC at Chapel Hill, Chapel Hill, NC, September 28, 2005.

Pouliot, G.A. The emissions processing system for the Eta/CMAQ air quality forecast system. 7th Conference on Atmospheric Chemistry, San Diego, CA, January 12, 2005.

Rao, S.T. An overview of CMAQ research program at U.S. EPA. Presentation at the University of Waterloo Board Meeting, Waterloo, Ontario, Canada, October 15, 2004.

Rao, S.T. Using urban models in designing emission control plans. Presentation at the US-India Workshop on Urban Air Pollution, Pune, India, March 14, 2005.

Rao, S.T. Role of models in air quality management. Presentation at the Indian Institute of Tropical Meteorology, Pune, India, March 17, 2005.

Rao, S.T. Linking air quality and human health. Presentation at the International Conference on Atmospheric Sciences and Air Quality, San Francisco, CA, April 28, 2005.

Rao, S.T. EPA data sets. Presentation at the Working Group for Environmental Support to Homeland Security's Recovery of Existing Atmospheric Transport and Diffusion Data Meeting, Silver Spring, MD, May 10, 2005.

Rao, S.T. Highlights of 2005 version of CMAQ. Presentation at the Auto/Oil Industry's Coordinated Research Council's Atmospheric Impacts Committee Meeting, Detroit, MI, July 26, 2005.

Rao, S.T. Integrating air quality data to inform human health decisions. Presentation at the EPA-NIEHS Workshop, Research Triangle Park, NC, August 1, 2005.

Roy, B. Comparison of modeled aerosol optical depth with satellite columns and sensitivity to wildfire emissions. Guest lecture at the Department of Marine Earth & Atmospheric Sciences, North Carolina State University, Raleigh, NC, April 28, 2005.

Sarwar, G. Modeling the effect of chlorine emissions on atmospheric ozone and secondary organic aerosol across the United States. Presentation at the NOAA/EPA Golden Jubilee Symposium on Air Quality Modeling and Its Applications, Durham, NC, September 20, 2005.

Sarwar, G. Implementing an updated carbon bond mechanism into the Community Multiscale Air Quality model. Presentation at the 4th Annual CMAS Models-3 Users' Conference, Friday Center, UNC at Chapel Hill, Chapel Hill, NC, September 26, 2005.

Sarwar, G. The effect of chlorine emissions on tropospheric ozone in the United States. Presentation at the 98th Annual Conference of the Air & Waste Management Association, Minneapolis, MN, June 24, 2005.

Schere, K.L. Operational and diagnostic evaluations of the ozone forecasts by the Eta-CMAQ Model Suite during the 2002 New England Air Quality Study. Presentation at the 4th Annual CMAS Models-3 Users' Conference, Friday Center, UNC at Chapel Hill, Chapel Hill, NC, October 20, 2004.

Schere, K.L. Air quality modeling for the Twenty-First Century. Presentation at the NOAA/EPA Golden Jubilee Symposium on Air Quality Modeling and Its Applications, Research Triangle Park, NC, September 21, 2005.

Schwede, D.B. Changes to the Biogenic Emissions Inventory System Version 3 (BEIS3). 4th Annual CMAS Models-3 Users' Conference, Friday Center, Chapel Hill, NC, September 27, 2005.

Swall, J.L. Some statistical issues in the evaluation of air quality models. Presentation at the North Carolina State University Environmental Statistics Seminar Series, Raleigh, NC, September 29, 2005.

Swall, J.L. Bayesian statistical approaches for the evaluation of CMAQ. Poster presentation at the 3rd Annual CMAS Models-3 Users' Conference, Friday Center, UNC at Chapel Hill, Chapel Hill, NC, October 19, 2004.

Tang, W. Example application of CFD simulations for short-range atmospheric dispersion over the open fields of Project Prairie Grass. Presentation at the 98th Annual Conference of the Air & Waste Management Association, Minneapolis, MN, June 23, 2005.

Walter, G.L. A pilot environmental data grid distribution system. Presentation at the EPA Science Forum 2005: Collaborative Science for Environmental Solutions, Washington DC, May 17, 2005.

Walter, G.L. Remote sensing information gateway. Presentation at the 2005 Summer Federation of Earth Science Information Partners Conference, Connections: Linking Data and Information to Decision Makers, San Diego, CA, June 4, 2005.

Walter, G.L. EPA compute and data grid. Presentation at the EPA Science Forum 2005: Collaborative Science for Environmental Solutions, Washington DC, May 17, 2005.

Young, J.O. Computational aspects of the air quality forecasting version of CMAQ (CMAQ-F). Presentation at the 3rd Annual CMAS Models-3 Users' Conference, Friday Center, UNC at Chapel Hill, Chapel Hill, NC, October 19, 2004.

Young, J.O. Layer dependent advection in CMAQ. Presentation at the 4th Annual CMAS Models-3 Users' Conference, Chapel Hill, NC, September 27, 2005.

Yu, S. A comprehensive evaluation of the Eta-CMAQ forecast model performance for 0_3, its related precursors, and meteorological parameters during the 2004 ICARTT study. Presentation at the 4th Annual CMAS Models-3 Users' Conference, Chapel Hill, NC, September 26, 2005.

Yu, S. Real-time forecasts of three ozone episodes by the Eta-CMAQ model during the 2004 New England Air Quality Study (NEAQS). Presentation at the NOAA/EPA Golden Jubilee Symposium on Air Quality Modeling and Its Applications, Research Triangle Park, NC, September 20, 2005.

Yu, S. Seasonal and regional variations of primary and secondary organic aerosols over the continental United States: Observation-based estimates and model evaluation. Presentation at the 3rd Annual CMAS Models-3 Users' Conference, Friday Center, UNC at Chapel Hill, Chapel Hill, NC, October 19, 2004.

Zhang, Y. Predicting aerosol number and size distribution with CMAQ: Homogeneous nucleation algorithms and process analysis. Presentation at the 4th Annual CMAS Models-3 Users' Conference, Chapel Hill, NC, September 26, 2005.

APPENDIX D: WORKSHOPS AND MEETINGS

American Association for Aerosol Research Conference, Atlanta, GA, October 4–8, 2004.

C.G. Nolte

Symposium on Border Air Quality at the University of Waterloo, Waterloo, Canada, October 15, 2004.

K.L. Schere

Waterloo Centre for Atmospheric Sciences Advisory Board Meeting, Waterloo, Ontario, Canada, October 15, 2004.

S.T. Rao

3rd Annual CMAS Models-3 Users' Conference, Friday Center, University of North Carolina at Chapel Hill, Chapel Hill, North Carolina, October 18–20, 2004.

W.K. Appel
P.V. Bhave
W.G. Benjey
G.E. Bowker
J.K.S. Ching
E.J. Cooter
R.L. Dennis
B.K. Eder
R.C. Gilliam
A.B. Gilliland
D.K. Heist
D.J. Luecken
R. Mathur
C.G. Nolte
T.L. Otte
S.G Perry
T.E. Pierce
J.E. Pleim
G.A. Pouliot
B. Roy
K.L. Schere
D.B. Schwede
J.L. Swall
J.O. Young
S. Yu

Second Intercontinental Transport and Climatic Effects of Air Pollutants (ICAP) Workshop, October 21–22, 2004, Chapel Hill, NC.

R. Mathur
J.E. Pleim

27th NATO/CCMS International Technical Meeting on Air Pollution Modeling and its Application, Banff, Canada, October 25–29, 2004.

P.V. Bhave
R.L. Dennis
B.K. Eder
D.J. Luecken
S.T. Rao

NOAA/EPA Scientist-to-Scientist Meeting on Climate Change and Air Quality Linkages, Boulder, CO, October 27–28, 2004.

R.L. Dennis, Co-Organizer
J.E. Pleim
K.L. Schere

NOAA-EPA Air Quality Management Committee Meeting, Silver Spring, MD, November 3, 2004.

S.T. Rao

NARSTO Reactivity Research Working Group Meeting, Research Triangle Park, North Carolina, November 3–4, 2004.

D.J. Luecken

Albemarle Pamlico National Estuary Program (APNEP) Science and Technical Advisory Committee (STAC) Meeting, Greenville, NC, November 10, 2004.

R.L. Dennis

Western Regional Air Pollution (WRAP) Dust Forum, Las Vegas, NE, November 15–16, 2004.

D.A. Gillette

Interdepartmental Committee for Meteorological Services and Supporting Research, Washington, DC, November 16, 2004.

S.T. Rao

Interagency Steering Committee on Multimedia Environmental Models Working Group 5 Meeting, Manhattan, NY, November 17–19, 2004.

A.H. Huber

Interagency Steering Committee on Multimedia Environmental Models, Manhattan, NY, November 18–19, 2004.

S.T. Rao

Federal Committee for Meteorological Services and Supporting Research Meeting, Washington, DC, December 1, 2004.

S.T. Rao

2004 Better Air Quality Workshop, Agra, India, December 6–8, 2004.

S.T. Rao

Community Multiscale Air Quality (CMAQ) Model Scientists Meeting, Houston, TX, December 15–17, 2004.

K.L. Schere

7th Conference for Atmospheric Chemistry, 85th Annual Meeting of the American Meteorological Society, San Diego, CA, January 9–13, 2005.

J.M. Godowitch
R. Mathur
J.E. Pleim
G.A. Pouliot

Chesapeake Bay Modeling Subcommittee Meeting, Annapolis, MD, January 12, 2005.

R.L. Dennis

Department of Homeland Security Model Evaluation Planning Workshop, Washington, DC, January 13, 2005.

S.T. Rao

Eighth Annual Atmospheric Science Librarians International Conference, held in conjunction with the 85th Annual Meeting of the American Meteorological Society, San Diego, CA, January 12–14, 2005.

E.M. Poole-Kober

SAMSI (Statistical & Applied Mathematical Sciences Institute) Program on Data Assimilation for Geophysical Systems, Tutorial and Workshop, Research Triangle Park, January 23–26, 2005.

T.L. Otte
J.L. Swall

Working Group for Weather Information for Surface Transportation, Silver Spring, MD, January 27, 2005.

S.T. Rao

Workgroup on Environmental Support and Homeland Security Meeting, Silver Spring, MD, February 1, 2005.

Ching, J.K.S.

Albemarle Pamlico National Estuary Program (APNEP) Science and Technical Advisory Committee (STAC) Meeting, Greenville, NC, February 2, 2005.

R.L. Dennis

American Association for Aerosol Research Supersites Conference, Atlanta, GA, February 7–11, 2005.

R.L. Dennis, Co-Chair Model Performance Evaluation II, Session 11C
A.B. Gilliland
C.G. Nolte

BRACE (Bay Regional Air Chemistry Experiment) Workshop, Tampa Bay, FL, February 23–24, 2005.

R.L. Dennis

EPA Board of Scientific Counselors (BOSC), Ecological Research Subcommittee Review, Research Triangle Park, NC, March 7–9, 2005.

R.L. Dennis

13th Expanding Your Horizons Conference, North Carolina State University, Raleigh, NC, March 8, 2005.

T.L. Otte

Interagency Nuclear Safety Review Panel's Particle Resuspension Technical Interchange Meeting, Cape Canaveral, FL, March 22–24, 2005.

G.E. Bowker
D.A. Gillette,

NOAA/EPA Scientist-to-Scientist on Atmospheric Deposition Meeting, Chesapeake Bay Office, Annapolis, MD, March 30–31, 2005.

R.L. Dennis, Co-convener
T.E. Pierce
J.E. Pleim
S.T. Rao

Air Toxics Workshop, Research Triangle Park, NC, March 30–April 1, 2005.

J.K.S. Ching

NARSTO Executive Assembly Meeting, Las Vegas, NV, April 11–12, 2005.

S.T. Rao

Department of Homeland Security (DHS) Urban Dispersion Program Planning Meeting, Manhattan, NY, April 13–15, 2005.

A.H. Huber

The 15th Annual Meeting of SAIL (Southeast Affiliate of IAMSLIC), National Aquarium in Baltimore, Baltimore, MD, April 19–22, 2005.

E.M. Poole-Kober, Chair of Meeting

Electric Power Research Institute Workshop on Interactions of Climate Change and Air Quality, Washington, DC, April 26–27, 2005.

S.T. Rao

Atmospheric Sciences and Air Quality Meeting, San Francisco, CA, April 28, 2005.

S.T. Rao

National Urban Morphological Database Meeting, Defense Threat Reduction Agency, Alexandria, VA, April 30, 2005.

J.K.S. Ching

Recovery of Existing Atmospheric Transport and Diffusion Data Meeting, Silver Spring, MD, May 10, 2005.

S.T. Rao

Joint Action Group for Atmospheric Transport and Diffusion Test Beds Meeting, Silver Spring, MD, May 11, 2005.

S.T. Rao

EastFIRE Conference on Wildland Fire Research in the Eastern United States, George Mason University, Fairfax, VA, May 11–13, 2005.

T.E. Pierce
G.A. Pouliot

EPA Science Forum—Collaborative Science for Environmental Solutions, Washington DC, May 16-18, 2005.

T.E. Pierce
R. Mathur

Community Multiscale Air Quality (CMAQ) Model-Peer Review Meeting, Research Triangle Park, NC, May 17–19, 2005.

P.V. Bhave	T.L. Otte
O.R. Bullock, Jr.	J.E. Pleim
D.J. Luecken	S.J. Roselle
C.G. Nolte	K.L. Schere

Reactivity Research Working Group, Research Triangle Park, NC, May 25–26, 2005.

D.J. Luecken

14th Annual Workshop on Hyperspectral Imaging, National Aeronautics and Space Administration Jet Propulsion Laboratory, Pasadena, CA, May 25–28, 2005.

J.J. Streicher

Air Toxics Workshop, New Orleans, LA, May 27, 2005.

V. Isakov.

NOAA/EPA Scientist-to-Scientist Meeting on Multimedia Aspects of Environmental Pollution in Freshwater, Coastal and Marine Environments, Patuxent Research Refuge on the National Wildlife Center, Laurel, MD, June 1–3, 2005.

O.R. Bullock, Jr.	S.T. Rao
R.L. Dennis, Co-convener	K.L. Schere

Department of Homeland Security Urban Dispersion Program Planning Meeting, Manhattan, NY, June 7–9, 2005.

A.H. Huber

Board on Atmospheric Sciences and Climate Meeting, Washington, DC, June 21, 2005.

S.T. Rao

Air & Waste Management Association 98th Annual Conference, Minneapolis, MN, June 21–24, 2005.

A.H. Huber
B. Roy

Coordinating Research Council Atmospheric Impacts Committee and Working Group Meeting, Detroit, MI, July 26, 2005.

S.T. Rao

2005 Joint WRF/MM5 User's Workshop, Boulder, CO, June 27–30, 2005.

T.L. Otte
J.E. Pleim

Journada Symposium, La Cruces, NM, July 5–17, 2005.

D.A. Gillette

International Workshop on Mercury Pollution, Madison, WI, July 13–18, 2005.

O.R. Bullock, Jr.

9th Annual George Mason University Conference on Atmospheric Transport and Dispersion Modeling, Fairfax, VA, July 18–20, 2005.

G.E. Bowker
J.K.S. Ching
D.K. Heist
V. Isakov
S.G. Perry
T.E. Pierce

Federal Managers Group on Air Quality Meeting, Silver Spring, MD, July 19, 2005.

S.T. Rao

Albemarle Pamlico National Estuary Program (APNEP) Science and Technical Advisory Committee (STAC) Workshop on Indicators, Smithfield, NC, August 3–4, 2005.

R.L. Dennis

2005 Joint Statistical Meetings: Using our Discipline to Enhance Human Welfare, Minneapolis, MN, August 7–11, 2005.

J.L. Swall

International Consortium for Atmospheric Research on Transport and Transformation (ICARTT) Data Analysis Workshop, Durham, NH, August 9–11, 2005.

R.L. Dennis
R. Mathur

International Workshop on Physical Modeling of Flow and Dispersion Phenomena (PhysMod), University of Western Ontario, Kingston, Ontario, Canada, August 24–26, 2005.

Heist, D.K.

State-of-the-Science on Organic Particulate Matter, Research Triangle Park, NC, August 31, 2005.

P.V. Bhave

European Monitoring and Evaluation Program Steering Body Meeting, Geneva, Switzerland, September 5–7, 2005.

R.L. Dennis

2005 Air Quality Focus Group Workshop, Silver Spring, MD, September 7–8, 2005.

K.L. Schere
R. Mathur

NOAA/EPA Golden Jubilee Symposium on Air Quality Modeling and Its Applications, Research Triangle Park, NC, September 20–21, 2005.

W.K. Appel	J.M. Godowitch	E.M. Poole-Kober
D.G. Atkinson	D.K. Heist	G.A Pouliot
W.G. Benjey	A.H. Huber	S.T. Rao
P.V. Bhave	V. Isakov	S.J. Roselle
G.E Bowker	D. Kang	B. Roy
O.R. Bullock, Jr.	H.-M Lin	G. Sarwar
J.K.S. Ching	R. Mathur	K.L. Schere
E.J. Cooter	C.G. Nolte	D.B. Schwede
R.L. Dennis	B.L. Orndorff	S.T. Rao
P.D. Dolwick	T.L. Otte	K.L. Schere
B.K. Eder	S.G. Perry	J.S. Touma
M.L. Evangelista	T.E. Pierce	H.J. Viebrock
R.C. Gilliam	J.E. Pleim	G.L Walter
A.B. Gilliland	E.M. Poole-Kober	S. Yu

4th Annual CMAS Models-3 Users' Conference, Chapel Hill, NC, September 26–28, 2005.

W.K. Appel	D. Kang	B. Roy
P.V. Bhave	D.J. Luecken	K.L. Schere
R.L. Dennis	R. Mathur	G. Sarwar
B.K. Eder	C.G. Nolte	J.L. Swall
R.C. Gilliam	T.L. Otte	J.O. Young
A.B. Gilliland	J.E. Pleim	S. Yu
J.M. Godowitch	S.J. Roselle	G.L. Walter

Weather Research and Forecasting (WRF) Training Workshop, Boulder, Colorado, September 26–30, 2005.

J. Herwehe

Texas Air Research Center Review Meeting, Houston, TX, September 28–29, 2005.

R.L. Dennis

APPENDIX E: VISITING SCIENTISTS

Dr. Jerry Davis
Marine, Earth, and Atmospheric Sciences Department
North Carolina State University
Raleigh, North Carolina

Dr. Davis was a visiting scientist with the Division from May 2004 until May 2005. Since May 2005, he has continued to work with the Division on several research projects.

Drs. G. Bermegetti and B. Marticorena
University of Paris
12 LISA (Laboratoire Interuniversitaire Sciences Atmospherique)
Pairs, France

Drs. Bermegetti and Marticorena visited the Division on November 3-6, 2004, and from January 28–February 5. 2005, to discuss a joint project by the National Science Foundation and the Centre National de la Recherche Scientifique on the effects of vegetation on dessert dust.

Dr. William Pennell
Department of Energy
Pacific Northwest National Laboratory
Richland, Washington

Dr. William Pennell visited the Division on November 17, 2004, to discuss research in the areas of Global Change and Aerosols.

Dr. Ted Yamada
Yamada Science and Art
Santa Fe, NM

Dr. Ted Yamada visited the Division on December 8, 2004, for discussions on using the Fluid Modeling Facility's urban databases for evaluation and development of numerical dispersion models.

Dr. Gregory Withee
Assistant Administrator for Satellite and Information Services
National Oceanic and Atmospheric Administration
Silver Spring, MD

Dr. Gregory Withee visited the Division on December 14, 2004, to discuss topics of mutual interest and tour the Fluid Modeling Facility.

Dr. Jerry Allwine
Department of Homeland Security
Washington DC

Dr Jerry Allwine visited the Division on January 20, 2005, to discuss the Fluid Modeling Facility's work on Midtown Manhattan, New York City.

Dr. Yang Zhang
North Carolina State University
Raleigh, North Carolina

Dr. Zhang visited the Division on February 16, 2005, to discuss her recent evaluation of the Community Multiscale Air Quality (CMAQ) model predictions for the July 1-10, 1999, period in the southeastern United States. Future collaborative work on modeling cloud-aerosol interactions and on comparing CMAQ predictions with aerosol number distributions was discussed.

Dr. Carlie Coats
Barons Advanced Meteorological Services
Raleigh, North Carolina

Dr. Coats visited the Division on February 24, 2005, and presented a seminar on linking the Sparse Matrix Operator Kernel Emissions (SMOKE) model to the chemistry version of the Weather Research and Forecasting model (WRF-Chem).

Drs. Uri Doron, and Boaz Doron
Doron Project,
Tel-Aviv, Israel

Drs. Uri Doron and Boaz Doron visited the division on March 1, 2005, to discuss building a fluid modeling facility in Israel.

Dr. Myoseon Jang
University of North Carolina at Chapel Hill
Chapel Hill, North Carolina

Dr. Jang visited the Division on March 2, 2005, to discuss the prospects of modeling heterogeneous production of secondary organic aerosols using the CMAQ model.

Drs . Satoro Chatani and Tazuko Morikawa
Japan Petroleum Energy Center
Tokyo, Japan

Drs. Saroto Chatani and Tazuko Morikawa visited the Division on March 10, 2005, to discuss topics of mutual interest.

Professor Simon Avliani
Russian Academy of Advanced Medical Studies
Ministry of Public Health
Moscow, Russia

Georgii Safonov
Ecological Center of Moscow
Moscow, Russia

Professor Simon Avliani and Georgii Safonov visited the Division on March 17, 2005, to discuss urban air quality models and their application to human exposure models.

Dr. Daniel Tong
Princeton University
Princeton, New Jersey

Dr. Tong visited the Division on July 29, 2005, to discuss his group's concerns about numerical instabilities in the Community Multiscale Air Quality (CMAQ) aerosol module. The Division's recent improvements to the CMAQ model were conveyed to Dr. Tong.

Dr. Masaki Ohba
Tokyo Polytechnic University
Tokyo, Japan

Dr. Ohba visited the Division on August 22, 2005, and presented a seminar entitled "COE project of wind effects on buildings and urban environments."

Katherine Snead
U.S. EPA, Interagency Modeling and Atmospheric Assessment Center
Washington, DC

Katherine Snead visited the Division, presented a seminar entitled "Introduction to the IMAAC" and toured the Fluid Modeling Facility on September 19, 2005.

Dr. Nikola Garber
NOAA Headquarters
Silver Spring MD

Dr. Garber visited the Division on September 19, 2005, and toured the Fluid Modeling Facility.

APPENDIX G: ATMOSPHERIC SCIENCES MODELING DIVISION STAFF AND AWARDS

All personnel listed are National Oceanic and Atmospheric Administration employees, 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
J. David Mobley (EPA), Environmental Engineer, Associate Director
William B. Petersen, Physical Science Administrator, Assistant Director
Patricia F. McGhee, Secretary

Program Operations Staff

Herbert J. Viebrock, Supervisory Physical Scientist, Chief
Sherry A. Brown
Linda W. Green, Administrative Specialist
Veronica Freeman-Green (Since May 1, 2005)
Evelyn M. Poole-Kober, Librarian
Jeffrey L. West, Physical Science Administrator

Atmospheric Model Development Branch

Kenneth L. Schere, Supervisory Meteorologist, Chief
Dr. Prakash V. Bhave, Physical Scientist
O. Russell Bullock, Jr., Meteorologist
Dr. Simon Clegg (Visiting Scientist), Physical Scientist
Robert C. Gilliam, Meteorologist
Gerald L. Gipson (EPA), Meteorologist (Until April 2005)
James M. Godowitch, Meteorologist
Dr. Alan H. Huber, Physical Scientist
Dr. William T. Hutzell (EPA), Physical Scientist
Deborah Luecken (EPA), Physical Scientist
Dr. Rohit Mathur, Physical Scientist
Dr. Christopher G. Nolte (EPA), Physical Scientist (Until June 11, 2005)
Tanya L. Otte, Meteorologist
Dr. Jonathan E. Pleim, Physical Scientist
Dr. Adam Reff (EPA), Physical Scientist
Shawn J. Roselle, Meteorologist

Dr. Golam Sarwar (EPA), Physical Scientist
John Streicher, Physical Scientist
Dr. Jeffrey O. Young, Mathematician
Shirley Long (SEEP), Secretary

Model Evaluation and Applications Research Branch

Dr. Alice B. Gilliland, Supervisory Physical Scientist, Chief
Wyat Appel, Physical Scientist
Dr. Jerry Davis (Visiting Scientist), Meteorologist
Dr. Robin L. Dennis, Physical Scientist
Dr. Brian K. Eder, Meteorologist
Dr. Peter L. Finkelstein, Physical Scientist (Until April 1, 2005)
Steven C. Howard, IT Specialist
Dr. Chris Nolte, Physical Scientist (Since June 12, 2005)
Dr. Rob Pinder, (ORISE August 29, 2005), Physical Scientist
Dr. Biswadev Roy (EPA), Physical Scientist
Dr. Jenise L. Swall, Statistician
Alfreida R. Torian, IT Specialist
Gary L. Walter, Computer Scientist
Carolyn Poe-Gurley (SEEP), Secretary

Air-Surface Processes Modeling Branch

Thomas E. Pierce, Supervisory Physical Scientist, Chief
Dr. William G. Benjey, Physical Scientist
Dr. George E. Bowker (EPA), Physical Scientist
Dr. Jason K.S. Ching, Meteorologist
Dr. Ellen J. Cooter, Meteorologist
Dr. Dale A. Gillette, Physical Scientist
Dr. David K. Heist, Physical Scientist
Dr. Steven G. Perry, Meteorologist
Dr. George A. Pouliot, Physical Scientist
Donna B. Schwede, Physical Scientist
John J. Streicher, Physical Scientist
Ashok Patel (SEEP), Engineer
John Rose (SEEP), Machinist/Modeler
Jane Coleman (SEEP), Secretary (Since March 2003)

Applied Modeling Branch

Mark L. Evangelista, Supervisory Meteorologist, Chief
Dennis A. Atkinson, Meteorologist
Dr. Desmond T. Bailey, Meteorologist
Patrick D. Dolwick, Physical Scientist
Richard A. Mason, Physical Scientist (Since January 2004)
Brian L. Orndorff, Meteorologist
Jawad S. Touma, Meteorologist

Awards

Bronze Medals Awarded Division's Community Multiscale Air Quality Modeling Team. The Division's Community Multiscale Air Quality (CMAQ) Modeling Team was awarded EPA Bronze Medals on August 10, 2005, for their contributions to the development and application of the Nation's premier numerical air quality simulation model at EPA/ORD award ceremonies in Cincinnati, Ohio. ASMD members honored by this award include Dennis Atkinson, Prakash Bhave, William Benjey, Russell Bullock, Jason Ching, Ellen Cooter, Robin Dennis, Patrick Dolwick, Brian Eder, Mark Evangelista, Robert Gilliam, Alice Gilliland, Jerry Gipson, James Godowitch, William Hutzell, Deborah Luecken, David Mobley, Tanya Otte, Thomas Pierce, Jonathan Pleim, George Pouliot, Shawn Roselle, Kenneth Schere, Donna Schwede, Gary Walter, and Jeffrey Young.