NOAA Technical Memorandum OAR ARL-

FISCAL YEAR 2004 SUMMARY REPORT OF THE NOAA ATMOSPHERIC SCIENCES MODELING DIVISION TO THE U.S. ENVIRONMENTAL PROTECTION AGENCY

Evelyn M. Poole-Kober
Herbert J. Viebrock
(Editors)

Atmospheric Sciences Modeling Division
Research Triangle Park, North Carolina

Air Resources Laboratory
Silver Spring, Maryland
June 2005

NOAA/EPA Golden Jubilee

This year marks the 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.

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PREFACE

This year marks the 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. The relationship between the 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 and located in Cincinnati, Ohio, until it moved in 1969 to Raleigh, North Carolina, and integrated with the Public Health Service. The unit is now the NOAA Atmospheric Sciences Modeling Division (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 the Fiscal Year 2004 research and operational activities of the Division. The summary includes descriptions of research and operational efforts in air pollution meteorology, meteorology and air quality model development, evaluation and application, 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. 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 (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 2004, 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 September 2004 version of the Community Multiscale Air Quality (CMAQ) modeling system; continued development, evaluation, and improvement of CMAQ and its modules; improvement of the SMOKE© emission processing system; evaluation and improvement of the Eta-CMAQ modeling system for use in air quality forecasting; development of model evaluation tools; development of an air toxins version of CMAQ (CMAQ-AT); and the development of techniques for data analysis and interpretation.

1. INTRODUCTION

In Fiscal Year 2004, 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.

2. PROGRAM REVIEW

2.1 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 ($PM_{2.5}$), and 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 solvers development, aerosol representations in grid-based air quality models, plume-in-grid treatment 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 air quality management and NAAQS implementation tools. The CMAQ CTM includes the necessary critical science process modules for handling atmospheric transport, deposition, cloud mixing, emissions, gas- and aqueous-phase chemical transformation processes, and aerosol dynamics, and atmospheric chemistry. Research is conducted to develop and test appropriate chemical and physical mechanisms, improve the accuracy of emissions and dry deposition algorithms, and to develop and advance state-of-science meteorological models via improved process parameterizations.

By design, CMAQ is expected to be used by both scientists and policy makers for various 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 2004 release of the CMAQ modeling system.

2.1.1 Meteorological Modeling for CMAQ Applications

The Fifth-Generation Pennsylvania State University (PSU)/National Center for Atmospheric Research (NCAR) Mesoscale Model (MM5) is the primary tool for providing 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)[©1] (emissions) and CMAQ (chemistry) modules to describe the atmospheric state variables and characteristics of the planetary boundary layer.

During FY-2004, MM5 was used to apply CMAQ for an annual simulation of 2001. This year-long MM5 simulation was used to evaluate CMAQv4.4, and it provided meteorological fields for several internal development projects. Follow-on modeling with MM5 will extend the annual simulations to include 2002, 2003, and 2004. In addition, the 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.* 2004a).

Also during FY-2004, work began to transition toward using the Weather Research and Forecast (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 also attractive for air-quality modeling applications because, unlike MM5, it contains mass-conserving equations. Collaborative work has begun toward 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. 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.

2.1.2 Linking Meteorology and Chemistry Models for Research Applications

The Meteorology-Chemistry Interface Processor (MCIP) creates the off-line linkage between meteorological models and CMAQ 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-2004, MCIP was upgraded to version 2.3 and included several new features. MCIP can now

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process polar stereographic and Mercator projected meteorological data. Several new fields are now available in the MCIP output, including graupel, 10-m wind speed and direction, full-level Jacobian, and latitude and longitude coordinates for the CMAQ lateral boundaries, the latter for downscaling global simulations for CMAQ application. MCIP will now only generate certain hydrometeor species and fields associated with the PX LSM if those fields are available in the MM5 output. Several other features and code adjustments were also made. The details pertaining to the code changes can be found in Otte (2004).

2.1.3 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 meteorological models and those used in air quality models are often quite different. Part of the reason for this is simply different model development histories, but the kind of scheme that works well in meteorological models have not worked so well in air quality models or 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 other higher order terms such 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 also 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 year, we have been experimenting with various PBL formulations as well as continuing development of new PBL schemes. Most notably, a new more advanced version of the Asymmetric Convective Model (ACM) has been developed and is currently being tested and evaluated. The new model (ACM2) is a combination of local- and non-local closure.

Specifically, ACM2 is a combination of the original ACM (Pleim and Chang, 1992) and eddy diffusion. The challenge 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 so that the resultant flux is identical to that produced by either scheme running alone.

The ACM2 has been implemented in MM5 and CMAQ. Evaluation is proceeding along two tracks. A series of MM5 and CMAQ simulations has been made for the summer of 2004. Operational evaluations of these runs have shown preliminary statistics for temperature, humidity, and winds, that are similar to previous MM5 simulations using ACM. Preliminary evaluation of CMAQ runs show improved simulation of ozone compared to the 2004 air quality forecasts. A more rigorous evaluation of the PBL model will be made involving comparisons of PBL heights and profiles of meteorological and chemical parameters to ICARTT (International Consortium for Atmospheric Research on Transport and Transformation) 2004 field measurements. The other evaluation track involves idealized case study simulations for various stability and wind conditions. Profiles of temperature, winds, and chemical tracers as well as their flux profiles are being compared to large eddy simulation results for identical conditions. The goal of this effort is to develop, test, and evaluate a PBL model that accurately simulates the vertical mixing of both meteorological and chemical parameters at the ground and throughout the PBL.

The data-assimilation scheme for the Pleim Xiu Land Surface Model (PX-LSM) was analyzed and evaluated against Southern Oxidant Study (SOS) 1999 field experiment data. This scheme involves Newtonian nudging of surface and root-zone soil moisture according to model biases in 2-m air temperature and relative humidity. Sensitivity tests confirm the value of this scheme in improving temperature and surface flux simulations (Pleim and Xiu, 2003). The PX-LSM has been an available option in the MM5 for several years. Efforts are underway to implement the PX-LSM in the WRF model.

2.1.4 High-Resolution Sea Surface Temperature Initialization for Meteorological Models

The initial version of a sea surface temperature (SST) processing utility for MM5 was developed in FY-2003. The main rationale behind this development is that MM5 typically uses coarse (32 km or greater) gridded SST data interpolated from larger scale models. Within coastal areas, the sea temperature is one of the most dominating factors that influence the boundary-layer meteorology; thus, it is important to resolve SST to the horizontal grid scale of the model. The first MM5 simulation that used the high resolution SST information was focused over Tampa Bay, Florida (April 20–June 7, 2002). Initial evaluation results indicate that the sea surface temperature did improve the timing of the spring Florida sea-breeze, and resulting temperature variations. This project has expanded to consider not only the spring season, but also the summer and fall of 2002. High resolution SST grids have been prepared for the simulation of these other seasons. A similar approach has been applied to a 4-km and 1-km scale simulation over the Houston area. An advancement of the technique was developed in FY-2004 for these simulations because the Galveston Bay diurnal water temperature varied by as much as 5-10°C,

and the prior method did not have the temporal data resolution to replicate this diurnal variation. The procedure involved finding the minimum (at night) and maximum (middle of day) daily temperature at each grid point and fitting a sine curve to match the amplitude and phase. Hourly SST files were generated using this approach, and ingested into a 10 day simulation (August 2000). Once these simulations have been completed, a thorough evaluation on the benefit of the SST to the simulation accuracy will be documented and published.

2.1.5 Anthropogenic Emissions

During FY-2004, the Sparse Matrix Operator Kernel Emission (SMOKE)© modeling system (www.cep.unc.edu/empd/products/smoke/index.shtml) was enhanced to version 2.1. The Division initiated development of SMOKE©, which has evolved into a key emission processing tool for air quality management modeling. SMOKE©v2.1 allows humidity data to be extracted along with temperature data for use in modeling mobile source emissions. Both temperature and humidity data may be averaged over time, rather than using hourly data, to increase model execution speed. The mobile source model in SMOKE© was upgraded to MOBILE6.2.0.3. The biogenic emission model within SMOKE© was upgraded from the Biogenic Emission Inventory System (BEIS) version 3.09 to version 3.12. BEIS3.12 contains updated biogenic emission factors and allows use of the Biogenic Emissions Land cover Database version 3 (BELD3) 1-km resolution gridded land-use data set. SMOKE© will also model emissions using the polar stereographic projection as well as Lambert conformal projections. In addition, a variety of software bugs were fixed. Development of SMOKE© is continuing with the gradual development by the Division of an episodic biomass burning emission algorithm (based on the U.S. Forest Service's BlueSky model). The Spatial Allocator tool of the Multimedia Integrated Modeling System (MIMS) is being upgraded to provided the capability to grid input files needed by SMOKE©. It is expected to be completed by fall 2005. The Spatial Allocator requires only grid definitions and (for spatial surrogates) GIS (Geographic Information System) shape files.

As part of NOAA's air quality forecasting program, an efficient method of estimating mobile source emissions was developed and implemented for real-time forecasting. A nonlinear least-squares approach was used to create a relationship between Eta-modeled temperature and emission rates for each species from SMOKE©/MOBILE6 for each grid cell and for each hour of the week. This relationship was used to create mobile source emissions in real time using forecast temperatures to make forecast emission estimates. As shown in Figure 1, the nonlinear least squares approximation compared to the actual SMOKE©/MOBILE6 estimate is nearly identical for the 12 Universal Time Coordinate (UTC) forecast of July 19, 2004, for NO_x (nitrogen dioxide and nitric oxide).

2.1.6 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-2004, BEIS version 3.12 (Pierce *et al.*, 2003) was tested further. BEIS3.12 includes emission factors for 34 chemical species, including 14 specific monoterpenes, methanol, and methyl-butenol. BEIS3.12 was included as part of SMOKE©v2.1 release.

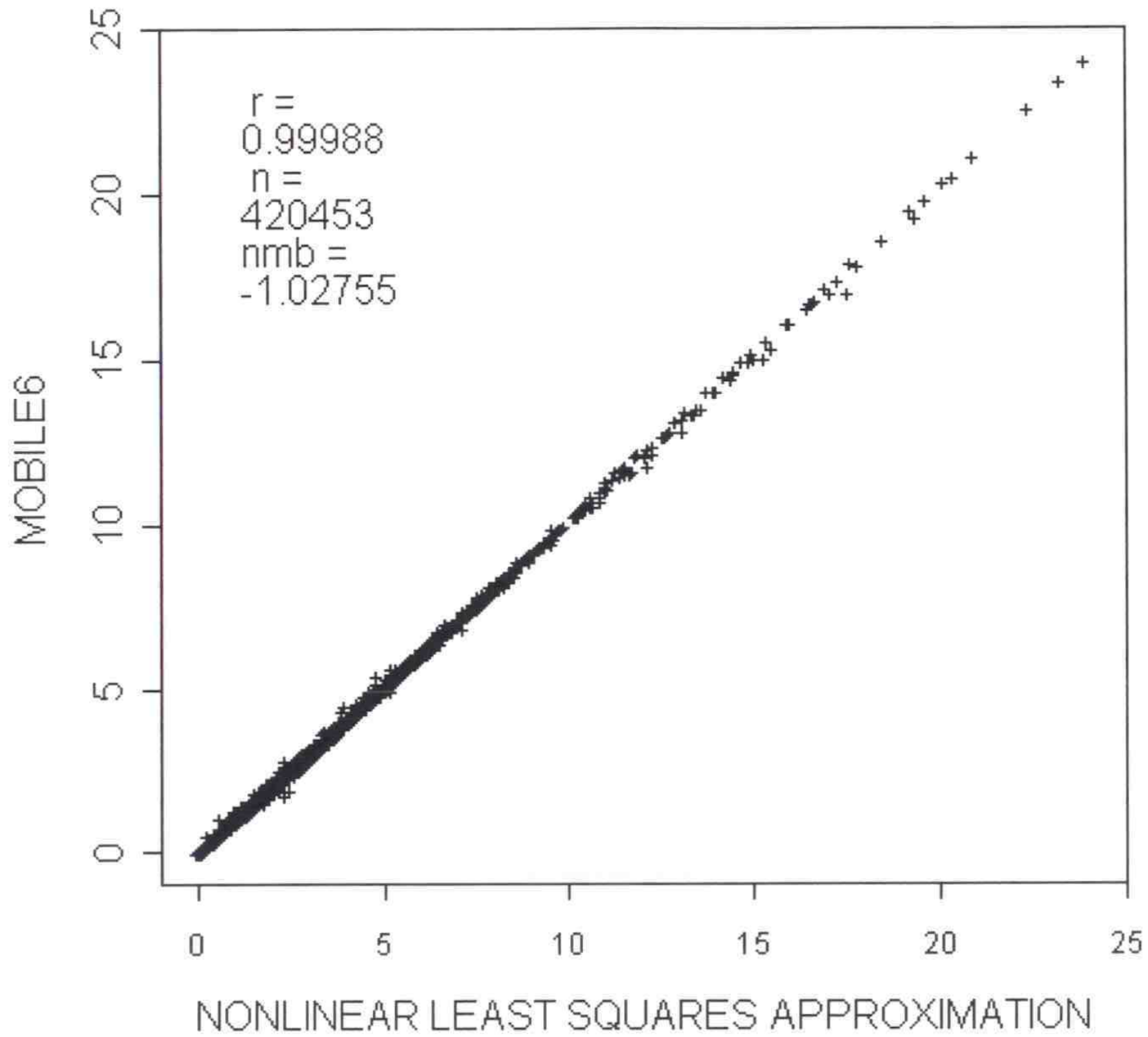

Figure 1. Comparison of NO_X emissions estimated using the nonlinear least squares approximation in the Eta-CMAQ air quality forecast system with actual SMOKE©/MOBILE6 model results for the 12 UTC forecast of July 19, 2004.

2.1.7 Modeling Smoke Emissions from Fires

In the past, emission inventories of forest fires, agricultural burning, and range fires were estimated crudely, at the county-level on a monthly basis. The Division has begun to assimilate research to improve spatial and temporal descriptions of biomass burning. The U.S. Forest Service has developed a tool known as BlueSky to predict air quality impacts of smoke from forest, agricultural, and range fires. The BlueSky modeling framework combines state-of-the-art emissions, meteorology, and dispersion models. A prototype to combine BlueSky's emission

processing algorithm with the SMOKE© emission processing system was completed during FY-2004. The combination of these tools will allow a more accurate characterization of fuel loading, temporal and spatial distribution of fire emissions, and a more accurate representation of plume rise and vertical distribution. During FY-2005, the Division will continue to improve on this new approach to distribute emissions from forest fires to specific grid cells on an hourly basis, and the Division will begin to evaluate the effectiveness of this approach in improving aerosol predictions in CMAQ.

2.1.8 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 CMAQ. Accurate representation of gas-phase chemistry is also vital for the simulation of such other important atmospheric processes as the formation of aerosols, the chemical transformations taking place in the liquid phase, and the deposition of air contaminants to land and water surfaces. Commensurate with the need for an accurate chemistry representation is the need for gas-phase chemistry solution techniques that are both highly accurate and computationally efficient. Since numerical solution techniques that have been used historically consume about 50 to 75 percent of the computer time required for model simulations, any substantial computational efficiencies that can be gained will significantly lower the computational 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/operational modeling applications by lowering the computational burden.

During FY-2004, two new gas-phase chemistry solvers were added to the array of solvers available in the CMAQ modeling system. One new solver, ROS3, is a particular version of the Rosenbrock class of solvers (Sandu *et al.*, 1997). It is a general solver and, hence, does not require any modifications when an existing chemical mechanism is changed or when a new mechanism is introduced. The ROS3 solver can achieve high accuracy at a relatively low computational cost and is the fastest of the existing CMAQ generalized solvers. The other new solver addition to CMAQ is an Euler Backward Iterative (EBI) solver (Hertel *et al.*, 1993) developed specifically for the SAPRC99 chemical mechanism (an EBI solver for the CMAQ

Carbon-Bond-IV (CB-IV) mechanism was developed in the previous year). Unlike ROS3, EBI solvers are not generalized and must be adapted to individual mechanisms. Although they are somewhat less accurate than several of the generalized solvers, they are the fastest of all the solvers available in CMAQ. Both EBI and ROS3 are also very robust and relatively easy to use, making them particularly well-suited for solving the set of stiff ordinary differential equations that arise when simulating the chemical transformations of trace gases in the atmosphere. Both solvers were included in the latest public release of CMAQ, and are, thus, available for use by the CMAQ modeling community.

During FY-2004, the existing gas-phase CB-IV mechanism in the CMAQ model was extended to include atmospheric chlorine chemistry developed at the University of Texas at Austin (Chang *at el*, 2002; Tanaka *et al*, 2003). The resulting gas-phase mechanism were incorporated into the CMAQ model and tested with the following three gas-phase chemistry solvers: Euler Backward Iterative solver, Rosenbrock solver, and Sparse-Matrix Vectorized Gear solver. The combined mechanism was used to evaluate the effect of chlorine emissions on atmospheric ozone in the continental United States. The study included anthropogenic molecular chlorine emissions, natural molecular chlorine released from sea-salt aerosol, and anthropogenic hypochlorous acid emissions from cooling towers and swimming pools. When molecular chlorine emissions were included in the model, the only significant impact occurred near the Great Salt Lake in Utah. Morning and evening ozone levels at that location increased by a maximum of 14 parts per billion by volume (ppbv) and 4 ppbv, respectively; but the impact on the daily peak ozone mixing ratios was not substantial. When both molecular chlorine and hypochlorous acid emissions were included in the model, the impacts were evident at several areas, including the Great Salt Lake and the Houston area. Ozone mixing ratios in the Great Salt Lake did not change compared to the case with molecular chlorine emissions. The morning and the daily peak ozone mixing ratios in the Houston area increased by a maximum of 10 and 7 ppbv, respectively, for the days simulated. In contrast to hydroxyl radicals, chlorine radical mixing ratios peaked in the morning and reached up to 15 and 4 percent of the corresponding hydroxyl radical mixing ratios at the Great Salt Lake and the Houston area, respectively. Chlorine emissions appeared to increase the hydroxyl radical mixing ratios compared to the case without any chlorine emissions. The increases in ozone mixing ratios were accompanied by decreases in volatile organic compounds mixing ratios.

2.1.9 Aerosol Mechanism Improvements in CMAQ

The CMAQ aerosol module was revised to improve computational efficiency, numerical stability, and the in-line code documentation. Testing of the 2003 CMAQ release revealed that 47 percent of the aerosol module computational time is spent on calculating coagulation coefficients and 13 percent on partitioning secondary organic aerosol (SOA) material between the gas and aerosol phases. A new subroutine was developed to calculate coagulation coefficients in a more efficient manner than the approach used previously. In the new subroutine, coagulation coefficients for particle number and aerosol third moment are calculated from analytical expressions reported by Binkowski and Shankar (1995), and the second moment

coagulation coefficients are calculated using a combination of analytical expressions and correction factors similar to the approach outlined by Whitby *et al.* (1991). The coagulation coefficients obtained using the new subroutine are within one percent of the results from the previous model version, but the computational efficiency of the new routine is 60 times faster. The SOA partitioning calculation involves the iterative solution of a system of quadratic equations. In the revised aerosol module, the initial guess for this iterative solution was revised to incorporate information on SOA concentrations from the previous time step. This reduces the number of iterations required for convergence, and hence, the computational time, by approximately 60 percent. The net effect of both improvements is a factor of two increase in the computational efficiency of the CMAQ aerosol module.

During developmental testing of previous CMAQ versions, small numerical perturbations caused by the use of different Fortran compilers were found to produce large (~10 $\mu g\ m^{-3}$) transient impacts on aerosol-phase nitrate concentrations over the arid southwestern United States. These effects were attributed to numerical instabilities in the ISORROPIA thermodynamics module. In collaboration with the developer of ISORROPIA at Georgia Institute of Technology, two problems were identified and corrected in the thermodynamics module. As a result, the large numerical instabilities observed in previous CMAQ versions are now removed. Recently, a second family of numerical instabilities was identified in the ISORROPIA module, which results in small (~1 $\mu g\ m^{-3}$) transient impacts on aerosol-phase nitrate concentrations in low-humidity environments. A solution to this numerical error is under investigation, with an anticipated release in FY-2005. A significant effort was made to strengthen the in-line documentation in the CMAQ aerosol code. Every major scientific formula in the aerosol chemistry and dynamics routines was annotated with comments that permit users to trace the formula back to an equation in a journal article or published report where it is described thoroughly. These in-line documentation enhancements should aid the CMAQ users seeking to modify scientific algorithms within the model. The above revisions are described in Bhave *et al.* (2004b) and are incorporated into the 2004 CMAQ public release.

In addition to the aerosol module revisions for the 2004 public release, a set of diagnostic tools are under development that will enable users to probe the sources of emissions for the modeled aerosol concentrations. With one tool, the ambient sulfate concentrations formed via different pathways can be determined quantitatively. For example, Figure 2 illustrates model calculations of the fractions of ground-level aerosol sulfate produced by aqueous-phase oxidation and gas-phase oxidation, when averaged over January 2001. 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. An example of the results obtained using this tool are shown in Figure 3, where the modeled concentrations of primary carbon originating from biomass combustion and food cooking are calculated and averaged over the June 15–August 31, 1999, time period. Both of these diagnostic tools are anticipated for the CMAQ release in FY-2005.

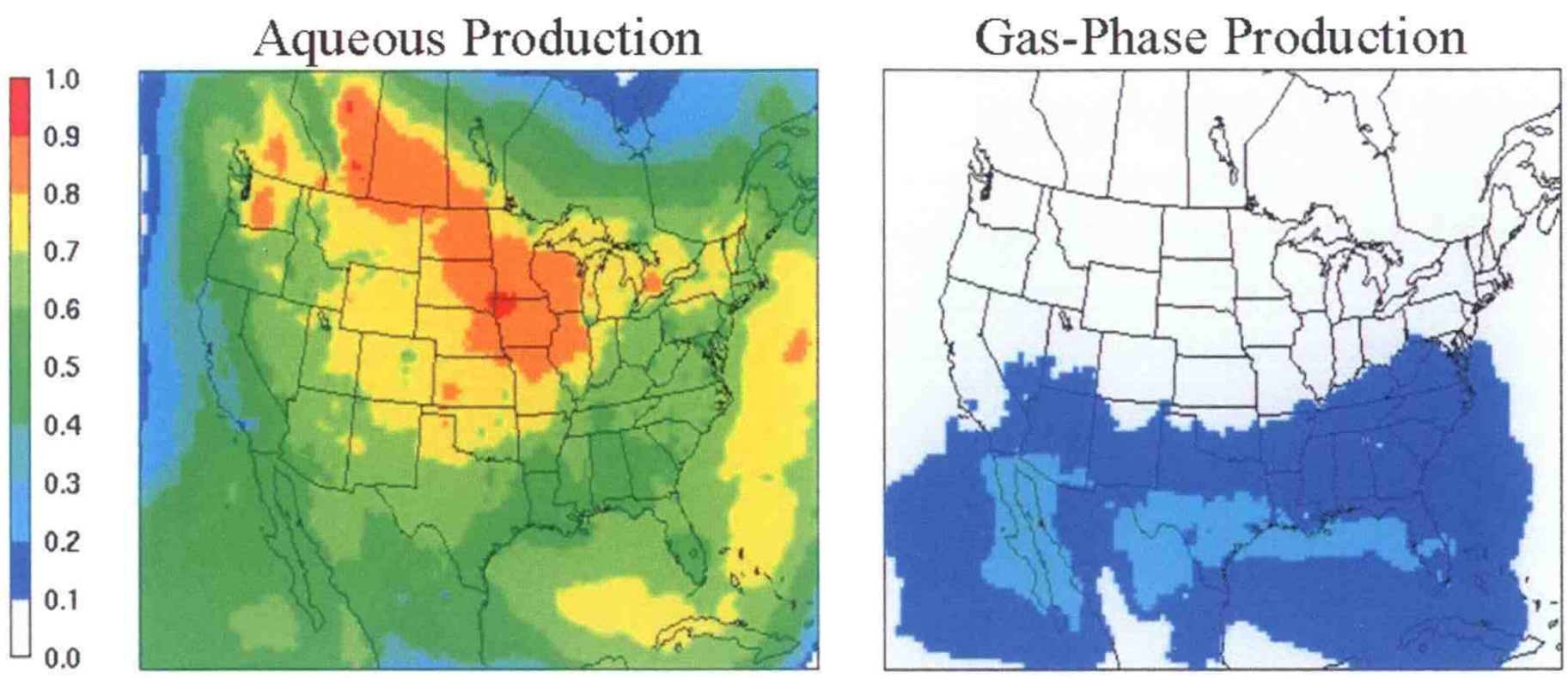

Figure 2. Fractions of ground-level aerosol sulfate produced via aqueous-phase oxidation (left) and via gas-phase oxidation (right) during January 2001, as calculated using the CMAQ sulfate-tracking diagnostic tool.

2.1.10 Plume-in-Grid Modeling

The plume-in-grid (PinG) technique provides a subgrid scale treatment of the dynamic and chemical processes governing gas-phase and aerosol species concentrations in isolated, major point-source plumes within the CMAQ Eulerian grid modeling system. The CMAQ/PinG applies a Lagrangian approach and simulates plume growth in a gradual, real-world manner due to turbulence and wind shear processes. This treatment is in contrast to the traditional Eulerian grid modeling method which is instantaneous dilution of point-source emissions into an entire grid cell volume. The overdilution effect becomes more pronounced with increasing horizontal grid sizes generally specified in regional- or continental-scale modeling domains. The key algorithms are a plume dynamics model (PDM) processor and a Lagrangian reactive plume model (PinG module), which are designed to simulate the relevant plume processes at the proper spatial and temporal scales for CMAQ model domains with grid cell sizes greater than 10 km. The PinG treatment is able to simulate plumes from multiple point sources. 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 a set of attached plume cells. The PinG module is fully integrated into the CMAQ grid model. It is exercised concurrently during a CMAQ chemical transport model (CTM) simulation and takes advantage of grid cell concentrations as boundary conditions for 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).

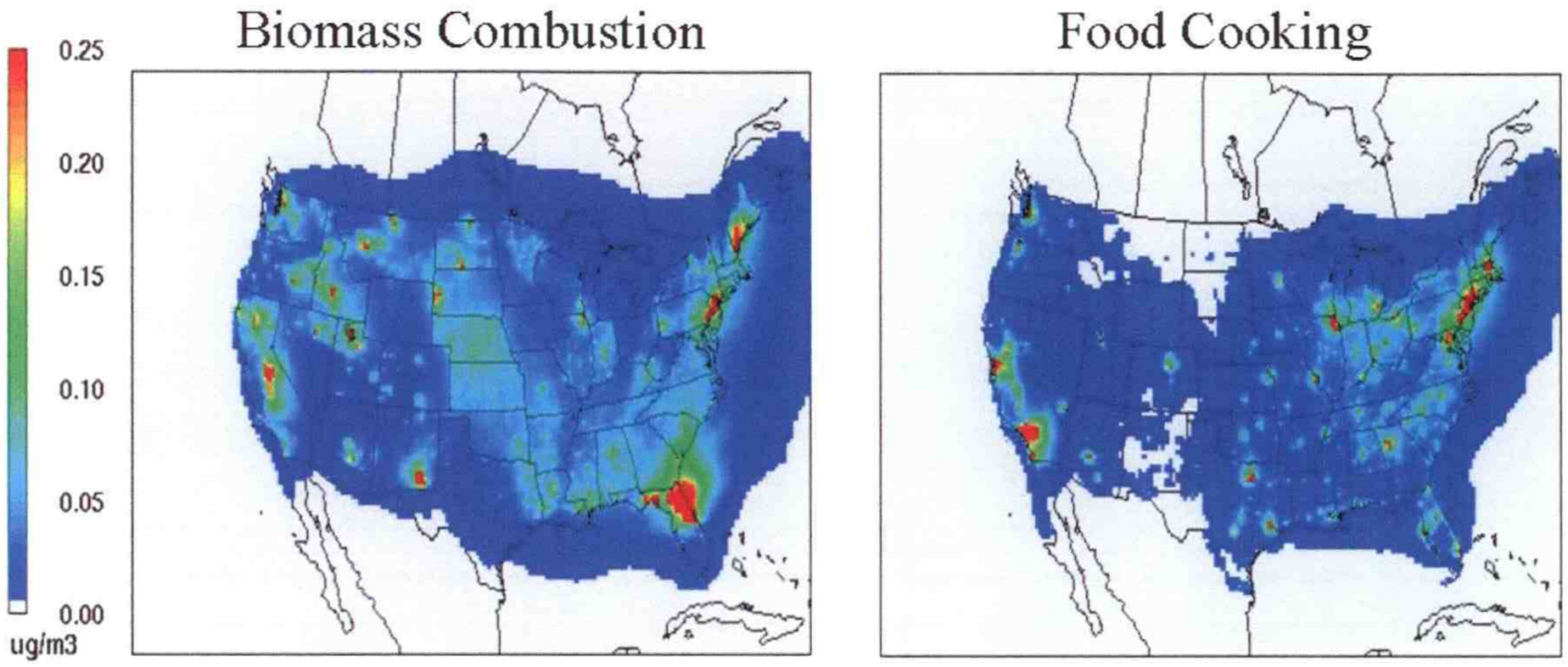

Figure 3. Ambient concentration of primary carbon originating from biomass combustion (left) and food cooking operations (right) during the June 15–August 31, 1999, time period, as calculated using the CMAQ carbon-apportionment diagnostic tool.

The updated aerosol algorithm version 3 (AE3) employed in the CMAQ /CTM was also incorporated and successfully tested in the PinG module. The 2004 public release of the CMAQ modeling system contained the PinG module with the capability to perform aerosol formation in subgrid plumes. Therefore, PinG currently simulates aerosol species and $PM_{2.5}$ along with gas-phase photochemistry in the subgrid plumes. CMAQ/PinG test simulations were successfully completed on various computational platforms with a single processor and multi-processors in a parallel processing mode. 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 plumes exhibiting a lower NO_x emission rate. These PinG results appeared to be supported by recent experimental aerosol data obtained in plumes. Additionally, CMAQ model simulations were conducted with the PinG approach and without it using existing emissions and meteorology data sets from a summer 2001 period for 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 simulated with the PinG approach. Comparisons of modeled gaseous and aerosol species against surface monitoring

network data were underway. So far, analyses of peak and hourly ozone concentrations for the days modeled reveal that the CTM/PinG results displayed better agreement and less bias than the CTM/NoPinG results, particularly in areas where numerous large point sources exist. Additional model runs are planned for a winter period and another summer experimental period in order for a comparison of model results against observed plume data collected by various airborne platforms. Further sensitivity test runs will be performed to assess computational times and to investigate the impact on oxidant and aerosol species concentrations with different chemical mechanisms (*e.g.*, CB-IV, SAPRC) and different chemistry solvers (*e.g.*, Gear or Rosenbrock solver) available in the CMAQ modeling system.

2.1.11 CMAQ Mercury Model Refinements and Evaluation

During FY-2004, the third and final phase of a European intercomparison study of numerical models for long-range atmospheric transport of mercury was completed. This study was organized by the Cooperative Programme for Monitoring and Evaluation of the Long-Range Transmission of Air Pollutants in Europe, previously known as the European Monitoring and Evaluation Programme (EMEP). Operational organization of the study was provided by EMEP's Meteorological Synthesizing Center - East in Moscow, Russia. The first two phases of the intercomparison involved rather simple simulations of mercury chemistry in a hypothetical cloud volume and full-scale model simulations of the emission, transport, transformation, and deposition of mercury over Europe during two short episodes in 1995 and 1999. Comparisons were made of the full-scale modeling results to field measurements of elemental mercury gas, reactive gaseous mercury, and particulate mercury in air. The third and final phase of the intercomparison study involved full-scale simulations over Europe spanning longer time periods followed by comparisons to observations of both air concentrations and wet deposition fluxes of mercury. While some models simulated the entire calendar year of 1999, the CMAQ mercury model could only simulate the months of February and August as these were the only time periods for which MM5-derived meteorological inputs were available for the European test domain because of limited resources available for this European study.

During FY-2004, the CMAQ mercury model was updated to simulate atmospheric mercury based on CMAQv4.3 with additional corrections and enhancements conforming to version 06FEB04 as defined by the EPA Office of Air Quality Planning and Standards (OAQPS) for regulatory applications. In cooperation with OAQPS, the CMAQ mercury model was used to perform a number of simulations of the entire calendar year of 2001 over most of North America to test a number of mercury chemistry sub-model configurations. Figures 4 and 5 display some example results of these simulations. All of the full-year 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). Further CMAQ mercury model testing will continue into FY-2005.

During FY-2004, organization and planning for a mercury model intercomparison study for North America continued. As described above, atmospheric mercury model developers have begun to use model inter-comparison studies to investigate differences regarding 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 many locations in North America through the Mercury Deposition Network (MDN). While the 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. Modeling assessments conducted by the EPA and by the Electric Power Research Institute regarding the importance of mercury emissions outside of the United States to the deposition of mercury within its boundaries have led to very different conclusions. This model inter-comparison study over North America would help explain these conflicting results.

2.1.12 CMAQ Code Integration and 2004 Release

Several computational efficiency improvements were incorporated into the 2004 release of CMAQ (version 4.4). In collaboration with the Department of Energy's Sandia National Laboratory, a known bottleneck in the parallel I/O implementation was removed, which provided a significant reduction in model runtimes on Linux computer clusters. Efficiencies were also incorporated into the aerosol module of CMAQ, including a new method for calculating coagulation coefficients and updates to the gas-particle equilibrium solver for SOA. Also, a fast chemical solver, known as the Euler Backward Iterative (EBI) scheme, was developed for the SAPRC99 mechanism.

In addition to efficiency improvements, other updates in CMAQv4.4 include: (1) aerosol treatment in the plume-in-grid module (PinG); (2) a new generalized chemical solver (Rosenbrock); (3) in-line documentation; (4) code structure simplifications; (5) removal of outdated modules; and (6) several bug fixes. Note that another component of the CMAQ system, MCIP (version 2.3), was also revised and released in conjunction with the FY-2004 CMAQ release. CMAQv4.4 is publicly available from the internet site of the Community Modeling and Analysis System center at www.cmascenter.org.

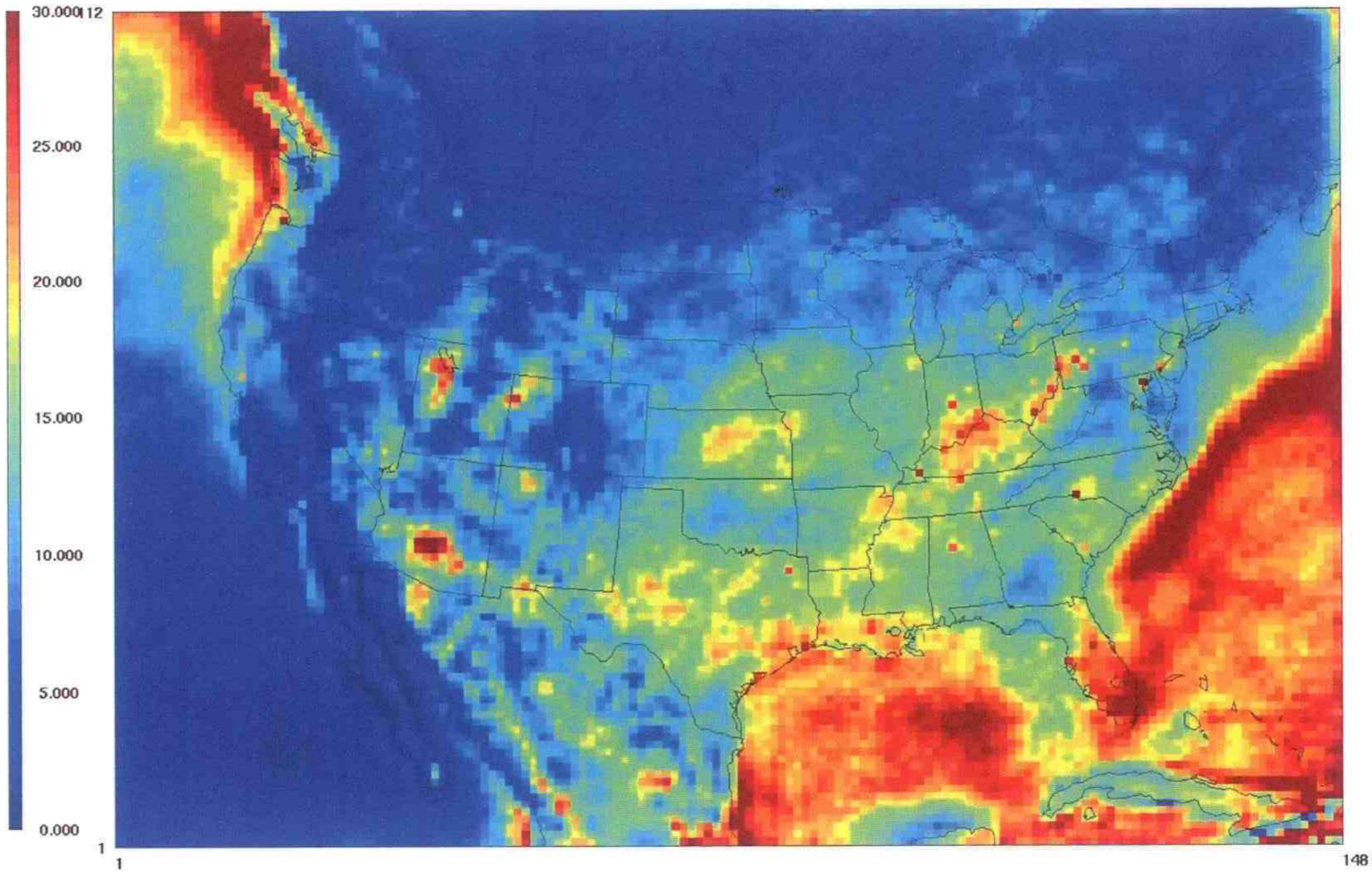

Figure 4. Total mercury wet deposition for 2001 ($\mu g/m^2$) as simulated by the CMAQ mercury model.

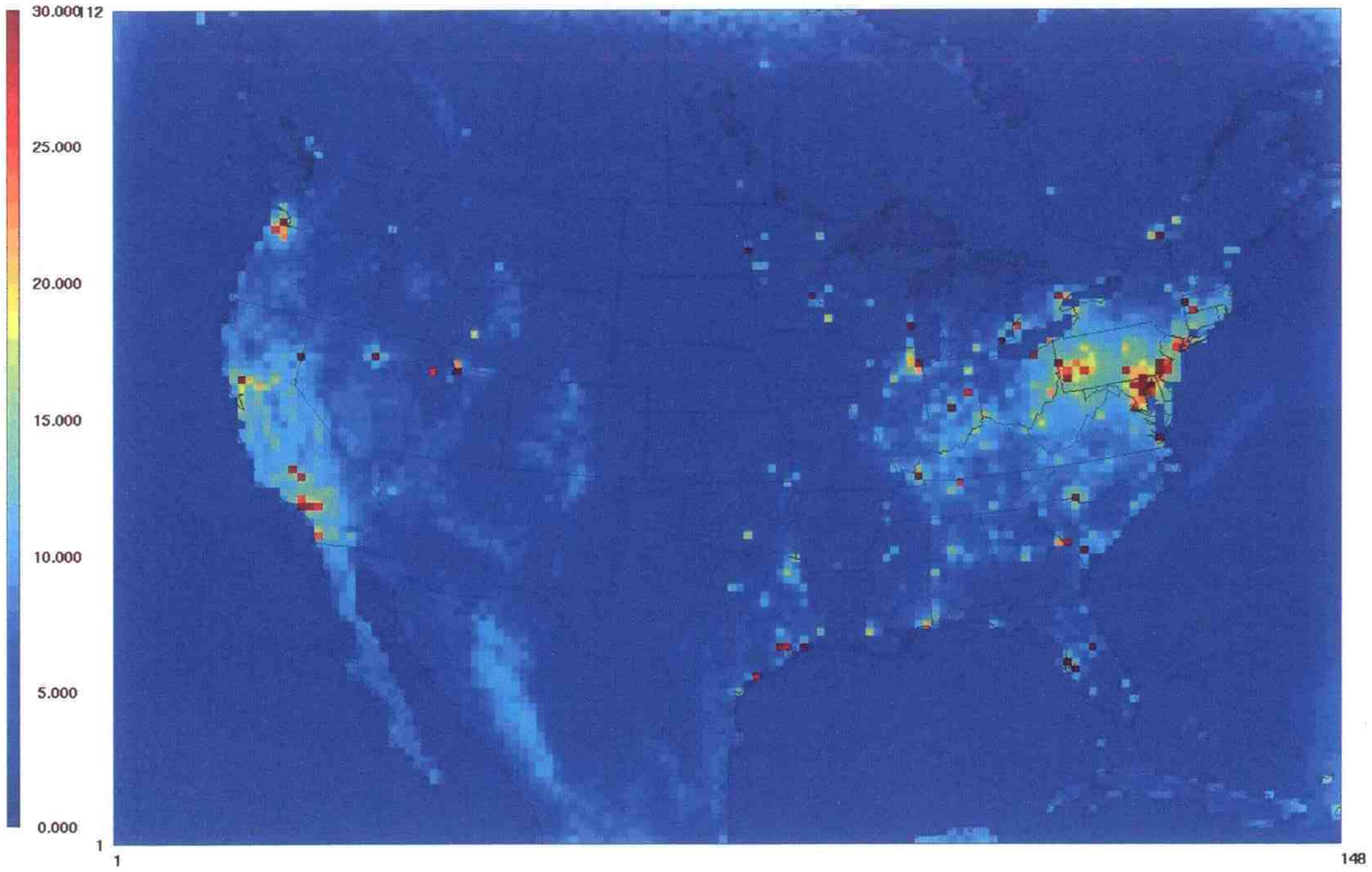

Figure 5. Total mercury dry deposition for 2001 ($\mu g/m^2$) as simulated by the CMAQ mercury model.

2.1.13 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 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. 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 2004, the air quality forecast (AQF) system was exercised in three streams: (1) experimental production of O_3 forecasts over the northeast United States. (1x domain) for dissemination to the general public; (2) developmental forecasts of O_3 over an expanded eastern U.S. domain (3x domain) for dissemination to a focus group of forecasters; and (3) 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 two applications, aerosols were not simulated by CMAQ. In all applications, the CB-IV 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 2004 forecast period. NO_x emissions from point sources were projected to 2004 (relative to a 2001 base inventory) using estimates derived from the annual energy outlook by the Department of Energy. Area source emissions were based on the 2001 National Emissions Inventory, version 3, 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.

The turbulent mixing scheme in CMAQ was enhanced to allow the minimum value of the surface layer vertical-eddy diffusivity (Kz) to vary spatially depending on the fraction of urban area in each grid cell. The approach allows for Kz 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. Two approaches for specifying lateral boundary conditions (LBCs) to CMAQ were investigated based on typical "clean" tropospheric background values; and based on seasonal averages derived from prior CMAQ simulations over the continental United States for the summer of 2001. The default clean profiles were used for the 1x domain, while the seasonal LBC profiles were used in the developmental 3x forecast applications. To improve the representation of O_3 in the free troposphere, additional modifications of the O_3 LBCs using forecast results from the National Centers for Environmental Prediction's (NCEP) Global Forecast System (GFS) were explored. In the GFS, O_3 is initialized using the Solar Backscatter Ultra Violet (SBUV-2) satellite observations. The evolution of the 3-dimensional O_3 fields in the GFS is then simulated by its transport schemes and a zonally averaged production and depletion scheme.

2.1.14 Linking the Eta Model with CMAQ for Air Quality Forecasting

A key ingredient in the linkage between the NCEP's Eta model and CMAQ is a new pre-processor for CMAQ (PREMAQ) 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.* (2004b).

In FY-2004, PREMAQ underwent several key modifications for the 2004 ozone forecasting season. PREMAQ was modified to process the vertical eddy diffusivity field directly from the Eta model for experimental simulations to improve the coupling between the Eta model and CMAQ. Ozone analyses from NCEP's GFS were also added to PREMAQ and used at heights greater than 6 km to provide time-varying chemical boundary conditions. PREMAQ was modified to process hourly precipitation increments allowing for the Eta model's accumulation "bucket" to periodically empty, as is typically done during the operational forecasts, which corrected the wet deposition calculations in CMAQ and the precipitation-based soil moisture calculations in the biogenic emissions. PREMAQ was further modified to define its input fields, which are post-processed from the Eta model on scalar points rather than dot points, which eliminates an interpolation step and ensures a more precise alignment of the meteorological fields. PREMAQ now processes percentage of urban land use, which is obtained from the emissions system and used by CMAQ to improve the nighttime vertical mixing in urban areas. Finally, PREMAQ outputs the 10-m wind speed and direction from the Eta model for assistance in model verification activities.

The linkage of the Eta model and CMAQ in the national air quality forecasting system was declared operational in September 2004. A manuscript describes the process and software components that were used to link the Eta Model and CMAQ, 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 (Otte *et al.*, accepted for publication).

2.1.15 Evaluation of Eta-CMAQ Forecast Predictions for Summer 2004

NOAA, in partnership with the EPA, has been developing an operational, nationwide air quality forecasting (AQF) system. An experimental phase of the AQF program, which couples the Eta meteorological model with CMAQ, began operations in June of 2004 and is providing forecasts of ozone (O_3) concentrations over the northeastern United States. These forecasts were first made public via NOAA's website in September 2004.

An important component of the AQF system was the development and implementation of an evaluation protocol. Accordingly, a suite of statistical metrics that facilitates 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 results reveal that the AQF system performed reasonably well in this inaugural season (mean domain wide correlation coefficient = 0.59), despite anomalously cool and wet meteorological conditions that were not conducive to the formation of O_3 (mean, domain-wide peak 8-hour concentrations = 44.6 ppb). Due in part to these anomalous conditions, the AQF system overpredicted concentrations (mean, domain-wide forecast peak 8-hour O_3 = 54.8 ppb) resulting in a mean bias of +10.2 ppb (normalized mean bias = +22.8 percent). In terms of error, the domain-wide root mean square error averaged 15.7 ppb (normalized mean error = 28.1 percent) for the season. The systematic overprediction was also evident from a categorical perspective, as most of these metrics (*i.e.* false alarm rates) indicated an excessive number of exceedances during the four-month period.

A closer 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. Figure 6 illustrates regional distributions of model forecasts for surface O_3 on two typical days characterized by high and low O_3 levels, respectively. The model performed very well during periods when anticyclones, characterized by clear skies, dominated the domain (*e.g.*, left panel of Figure 6). Conversely, periods characterized by extensive cloud associated with fronts and/or cyclones resulted in poor model performance (*e.g.*, right panel of Figure 6). Subsequent analysis revealed two main factors contributing to this overprediction. The first involved the excessive downward transport of O_3 rich air via CMAQ's convective cloud scheme in conjunction with O_3 profiles derived from the GFS model. 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. Changes to CMAQ's cloud schemes are underway that are expected to significantly improve the AQF system's performance.

2.1.16 Assessment of the Real-Time Application of CMAQ

In collaboration with NOAA and EPA, the New York State Department of Environmental Conservation (NYSDEC) has begun to perform near real-time simulations of O_3 and $PM_{2.5}$ over the northeastern United States. This pilot project builds upon the operational air quality forecasting program of National Weather Service (NWS), NOAA, and EPA by utilizing the same Eta/PREMAQ/CMAQ modeling system and the same meteorological and emission inputs.

The pilot study is aimed at assessing the feasibility of applying the CMAQ modeling system in a near real-time mode for prototyping continuous $PM_{2.5}$ modeling. The pollutants of interest are ozone, $PM_{2.5}$ total mass, and $PM_{2.5}$ species composition in New York State with a particular emphasis on the greater New York City Metropolitan Area. The study examines both

operational aspects such as data transfers, computing power, and data storage as well as scientific questions such as determining CMAQ performance for the prediction of speciated $PM_{2.5}$ over New York State and assessing the merits of CMAQ based forecasts compared to traditional forecasting approaches. The collaboration with EPA and NOAA includes NYSDEC's participation in the beta-testing of future CMAQ releases. Throughout the duration of the project, periods of model simulations alternate with phases of model evaluation, analysis, and possible refinements to the modeling setup. Finally, NYSDEC will apply and evaluate tools to combine CMAQ model outputs with observations in an attempt to better characterize ambient air quality over New York. Such combined fields may be of value when studying linkages between air pollution and public health.

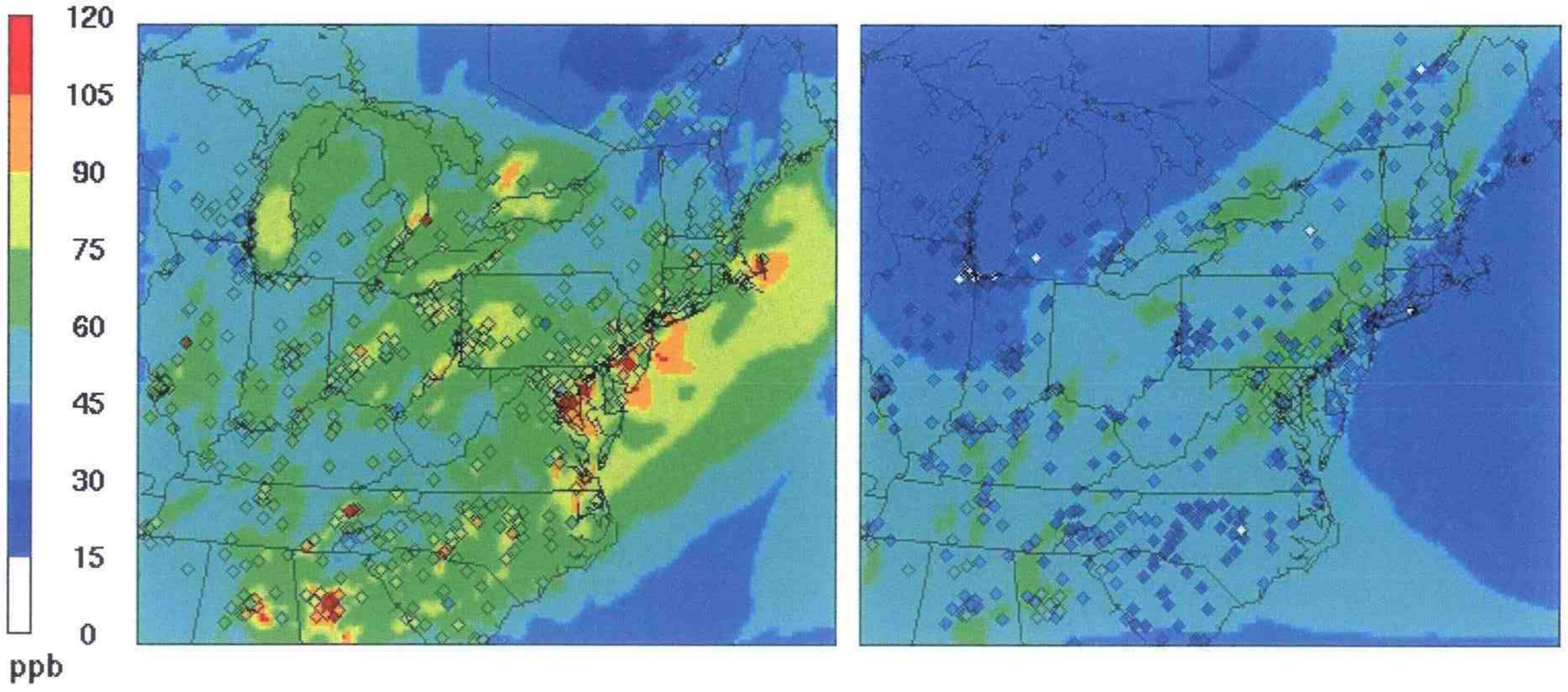

Figure 6. Forecast surface level O_3 distributions at 2000 GMT over the 1x domain on July 21, 2004 (left) and August 12, 2004 (right). Color-coded diamonds indicate observed values.

2.2 Atmospheric Model Evaluation and Application Activities

2.2.1 Meteorological Model Evaluation

Air quality modeling simulations are strongly dependent on the meteorology. Thus, the performance of meteorological simulations must be assessed in conjunction with the chemical-transport predictions. Traditional verification methods do not take advantage of the increasing amounts of non-standard meteorological observations (*e.g.*, wind profilers, aircraft, satellite winds, gridded radar derived precipitation, etc.). During FY-2003, the initial development on a meteorological evaluation system was performed. In FY-2004, the tool was

used for several evaluations that served as a test bed to improve the performance/speed, find and eliminate bugs in the system, develop new analysis options, and an interactive web-based interface. The evaluation system was also packaged for easier portability to other platforms.

Several major evaluation efforts were conducted using the meteorological evaluation tool. The main evaluation was an annual (2001) MM5 simulation 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. 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 also used in several other experiments, including an 8-km and 2-km meteorological simulation (MM5) for the Bay and Regional Atmospheric Chemistry Experiment (BRACE), a 12-km WRF and 12-km NCEP Eta model comparison during the summer of 2004, and a 12-km MM5 simulation during the summer of 2004 to aid in the development of a more accurate boundary-layer parameterization.

Promising experiments were conducted to directly link errors in the meteorology with those of the air quality model within the framework of the evaluation tool. In one particular experiment, observed and simulated aerosol-nitrate data was loaded into the model evaluation database. Observation-model (both meteorology and air quality data) pairs were extracted from the database for situation where the relative humidity was overpredicted and for times when the relative humidity was underpredicted. Model performance metrics were calculated for these two data sets. Statistics indicated that the aerosol nitrate was overpredicted by an average of 50 percent when the relative humidity is overpredicted, and there was little to no over or underprediction when the relative humidity was either accurately simulated or underestimated. This approach is actively being applied to other simulations and chemical species. The meteorological evaluation tool is being improved to suit air quality applications.

2.2.2 Diagnostic Metrics for Ozone and Inorganic Particulate Matter

Diagnostic metrics enable the examination of the process side of a model to better study the degree of reliability of control strategy predictions. Diagnostic metrics require a special set of non-routine measurements, because they typically involve ratios of species involved in photochemical production or aerosol equilibrium processes. Earlier work (Tonnesen and Dennis, 2000a; 2000b) had identified a set of metrics designed to assess the 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 (VOC) or nitrogen oxide (NO_X) emissions. The metrics are based on measurement of O_3, NO+true $NO_2 = NO_X$, NO_Y, and NO_Y-$NO_X = NO_Z$. Diagnostic tests using these metrics were applied to CMAQ for Nashville, Tennessee, for the 1995 SOS field measurements (Arnold *et al.*, 2003). The need for true-NO_2 and NO_Y measurements was passed to EPA, spawning instrument development and additional guidance within its monitoring strategy.

Examination of the metrics is underway for use in assessing 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 gas ratio (GR) defined by Ansari and Pandis (1998) was identified as the leading inorganic aerosol metric to support diagnostic testing. The GR is equal to the free ammonia divided by total-nitrate, where free ammonia is defined as the moles of gaseous ammonia plus aerosol-phase ammonium minus twice the moles of aerosol-sulfate, and total-nitrate equals gas- + aerosol-nitrate.

The GR is being assessed for its ability to provide insight into the nonlinear responses of the inorganic fine aerosols in CMAQ predictions. 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 value of the GR. For GR values much greater than 1 (*i.e.*, ammonia-rich regime), the decrease in 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), the increase in PM is expected to be proportional to the sulfate reduction because two moles of nitrate will replace each mole of sulfate that is removed. At GR values close to 1, the PM-mass response to a sulfate reduction is expected to be nonlinear.

Preliminary results indicate that in a full 3-D model like CMAQ, the nonlinear transitions are less well-defined than in the thermodynamic equilibrium box models. Nonetheless, it appears the GR provides valuable insights into the nonlinear responses in CMAQ. Examination of the CMAQ results for winter 2002 suggest that almost the entire eastern United States will be affected by these nonlinearities in the inorganic aerosol system. Several inorganic aerosol sensitivity studies are underway.

2.2.3 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 (OCpri), which is emitted directly to the atmosphere in particulate form, and secondary organic carbon (OCsec), 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 OCpri and OCsec 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-2004, Yu *et al*. (2004) devised a method to estimate the ambient concentrations of OCpri and OCsec using routine OC and EC measurements in combination with model calculations of the primary OC to EC concentration ratio. This methodology was applied to data spanning the June 15–

August 31, 1999, time period. Results indicate that during summer months, the fractional contribution of OCsec to total OC ranges from 48 percent in the western United States to 77 percent in the Northeast. In FY-2005, the methodology will be extended to a full year of data to assess the seasonal cycle of OCpri and OCsec across the continental United States.

In the southeastern United States, carbonaceous aerosol is the largest component of fine particulate mass (Hansen *et al.*, 2003) and a significant portion of it is OCpri (Zheng *et al.*, 2002). OCpri is emitted from numerous sources, including motor vehicle exhaust, residential wood combustion, coal combustion, forest fires, agricultural burning, solid waste incineration, food cooking operations, and road dust.

A diagnostic tool was developed within the CMAQ modeling framework that allows users to calculate the contributions from individual emission source categories to the ambient primary carbonaceous aerosol burden. This tool was exercised in a CMAQ simulation of the 1999 summer season. The model results were converted into concentrations of individual organic compounds and evaluated against organic-tracer measurements collected in July 1999 at eight monitoring sites across the southeastern United States, as shown in Figure 7.

Modeled-to-observed concentration ratios are displayed along the vertical axis. Seventeen organic tracers along with bulk EC and OC are arranged in groups along the horizontal axis, separated by vertical dashed lines that delineate conserved tracers emitted from different source categories. Model results for total OC are in reasonable agreement with observations at the Atlanta, Georgia, site, but are low by a factor of three at the remaining sites. This indicates that total OC is underestimated across the southeastern United States, but it is impossible to determine which source contributions have been underestimated based on bulk OC and EC measurements alone. By evaluating model results against the individual organic tracer measurements, it is found that modeled OCpri contributions from motor vehicle exhaust and natural gas combustion are reasonably accurate whereas the contributions from biomass combustion and food cooking are underestimated by a factor of 4 or more. Complete details of this evaluation are reported by Bhave *et al.* (2004a).

2.2.4 CMAQ Model Evaluation to Assess Model Readiness for Application

An operational evaluation of the 2004 release of the CMAQv4.4 was performed that compares an annual simulation (2001) covering the contiguous United States against monitored data from four nationwide networks. This effort represents one of the most spatially and temporally comprehensive performance evaluations of CMAQ, and reveals a continuation of improvement in the model's ability to accurately simulate ambient air concentrations of critical gas and particulate matter species.

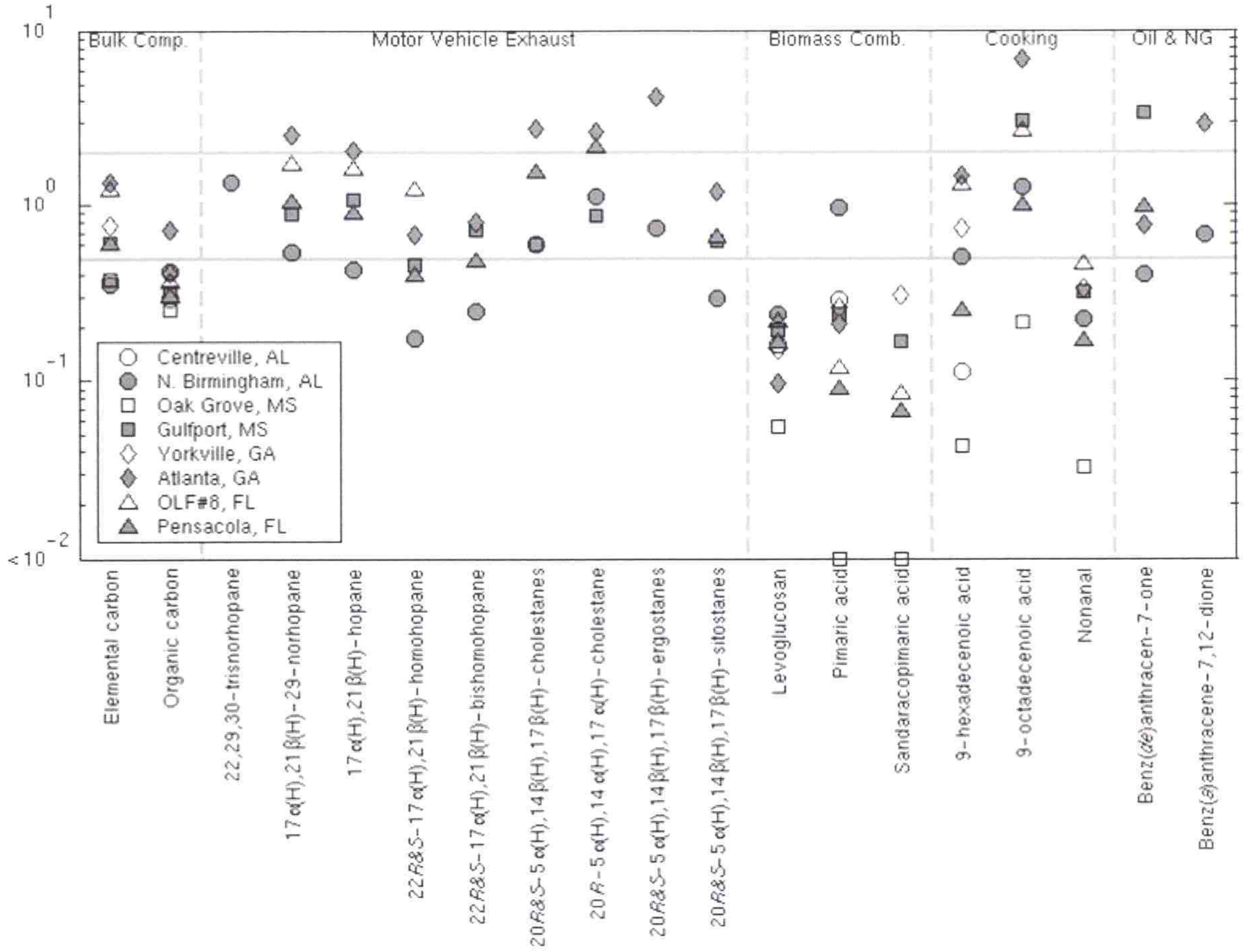

Figure 7. Ratios of CMAQ model results to ambient measurements of EC, OC, and individual organic compounds at eight southeastern United States sites in July 1999. Horizontal lines bound the region in which model-observation agreement is within a factor of two. Vertical dashed lines distinguish molecular markers specific to different source categories.

Simulations of the peak 1- and 8-hour O_3 concentrations during the "O_3 season" (April through September) were good (r = 0.68, 0.69; Normalized Mean Bias (NMB) = 4.0 percent, 8.1 percent; and Normalized Mean error (NME) = 18.3 percent, 19.6 percent), respectively. The NMB statistics associated with the peak 1-hour O_3 concentrations are better because the peak 8-hour concentrations usually include evening hours that CMAQ, historically, has overpredicted due to difficulties simulating the collapse of the boundary layer. CMAQ did display a tendency to overpredict (NMB often > 30 percent) along coastal regions, which may be tied to poor characterization of coastal boundary layers and their interaction with land/sea breezes in the 36-hour grid-cell size used for the annual simulation.

The annual simulations of SO_4^{2-} were also good ($0.77 \leq r \leq 0.92$, depending upon network) though slightly negatively biased (-2.0 percent $\leq$ NMB $\leq$ -10.0 percent) with relatively small error

(25.0 percent ≤ NME ≤ 42.0 percent). Spatially, CMAQ's performance was better over the eastern half of the United States than in the western region, while temporally, the performance was somewhat degraded during the winter months.

The performance of CMAQ's NO_3^- simulations, though still lagging that of O_3 and SO_4^{2-}, has shown marked improvement over previous releases. The correlations reflect this progress ($0.37 \leq r \leq 0.62$, depending upon network) as do the measures of error (80.0 percent ≤ NME ≤ 94.0 percent) and measures of bias (-16.0 percent ≤ NMB ≤ 4.0 percent), which have shown the largest, though somewhat misleading, improvement. Misleading in that when examined over space and time, the NO_3^- simulations exhibit large, though often compensating NMBs, which are thought to be attributable to an incomplete understanding of ammonia emissions. The quality of NH_4^+ simulations is similar to, though somewhat better than that for NO_3^-. Correlations range from 0.56 to 0.79, depending on the network. The model produces relatively modest amounts of error (35.0 percent ≤ NME ≤ 63.0 percent) and even less, though once again somewhat misleading (for the same reason as seen with NO_3^-), (bias -4.0 percent ≤ NMB ≤ 14.0 percent). The evaluation of CMAQ's performance in simulating NO_3^- is influenced both by the large uncertainties associated with characterization of ammonia emissions and also with the current scientific state of uncertainty surrounding the heterogeneous N_20_5 production pathway for HNO_3 formation.

The quality of simulations of EC and OC, while similar, are both fairly poor, which is not surprising given the level of uncertainties associate with emissions and the current state-of-the-science. Correlations range from 0.35 (OC) to 0.47 (EC). The model produces fairly large, though not unreasonable amounts of error (NME = 68.0 percent for OC, 58.0 percent for EC) and encouragingly small amounts of bias (NMB = -6.0 percent for EC and 12 percent for OC). The quality of CMAQ simulations of $PM_{2.5}$, much like $PM_{2.5}$ itself, represents a compilation of the quality of all of the simulated particulate species. Overall, the performance of this release signifies a marked improvement over the earlier version of CMAQ as correlations range from 0.51 to 0.70, depending on the network. The annual bias is very small and identical for each network (NMB = -3.0 percent) and the error, though still considerable (NME ≈ 45 percent for both networks), is greatly improved.

Potential areas of research into the sources of the deficiencies identified in this evaluation include uncertainties in the emissions inventories (especially the temporal allocation of NH_3 emissions and emissions associated with the carbonaceous species), imperfect representation of the meteorological fields, because of coarse-grid simulations as well as an incomplete understanding of the aerosol dynamics.

2.2.5 Spectral Analysis of the Observed and Predicted Meteorology and Air Quality

Evaluation of regulatory simulations of fine particulate matter ($PM_{2.5}$) is complex because simulations need to be performed for an entire annual cycle while taking into account the chemical speciation of $PM_{2.5}$ to identify its origin and develop meaningful air quality management

strategies. Moreover, annual simulations with air quality modeling systems were performed only fairly recently, making the investigation of methodologies to evaluate such extended simulations a topic of increasing interest. In this study, we applied temporal scale analysis as a technique to evaluate an annual simulation of $PM_{2.5}$ and its chemical components over the eastern United States. The concept of scale analysis is widely used for research in physical sciences, including meteorology, climatology, and air pollution, and also was applied for several air quality model evaluation studies during the past several years. The technique was applied to identify the temporal scales that are the largest contributors to the temporal variability in general and to periods of elevated $PM_{2.5}$ concentrations in particular. Next, the ability of two air quality models (CMAQ and REMSAD) to reproduce the variability and temporal evolution of total and speciated $PM_{2.5}$ fluctuations on different time scales extracted from observations was evaluated.

The spectral decomposition of total $PM_{2.5}$ mass from hourly observations and CMAQ and REMSAD (Regional Modeling System for Aerosols and Deposition) model predictions revealed that on days of high $PM_{2.5,}$ concentrations are generally characterized by positive forcings from fluctuations having periods equal to or greater than a day (*i.e.,* the diurnal, synoptic, and longer-term components), while the magnitude of intra-day fluctuations showed only small differences between average and episodic conditions. Furthermore, both modeling systems did not capture most of the variability of the high-frequency variations (*i.e.*,, intra-day component) for all variables for which hourly measurements were available (Figure 8). It was also illustrated through the use of correlation analysis that correlations were insignificant on the intra-day time scale for all variables, suggesting that these models in the setup used for this study were not skillful in simulating the higher-frequency variations in meteorological variables and concentrations of all pollutants. The models exhibited greatest skills at capturing longer-term (seasonal) fluctuations for temperature, wind speed, O_3, sulfate, and nitrate. Correlations for total $PM_{2.5}$, ammonium, elemental carbon, organic carbon and crustal $PM_{2.5}$ correlations were highest for the synoptic time scale implying problems with factors other than meteorology, such as emissions or boundary conditions, in capturing the baseline fluctuations. This indicates that capturing the meteorological fluctuations on all scales is a necessary, but not sufficient, prerequisite for capturing pollutant fluctuations on all time scales, especially for the simulation of $PM_{2.5}$.

2.2.6 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.

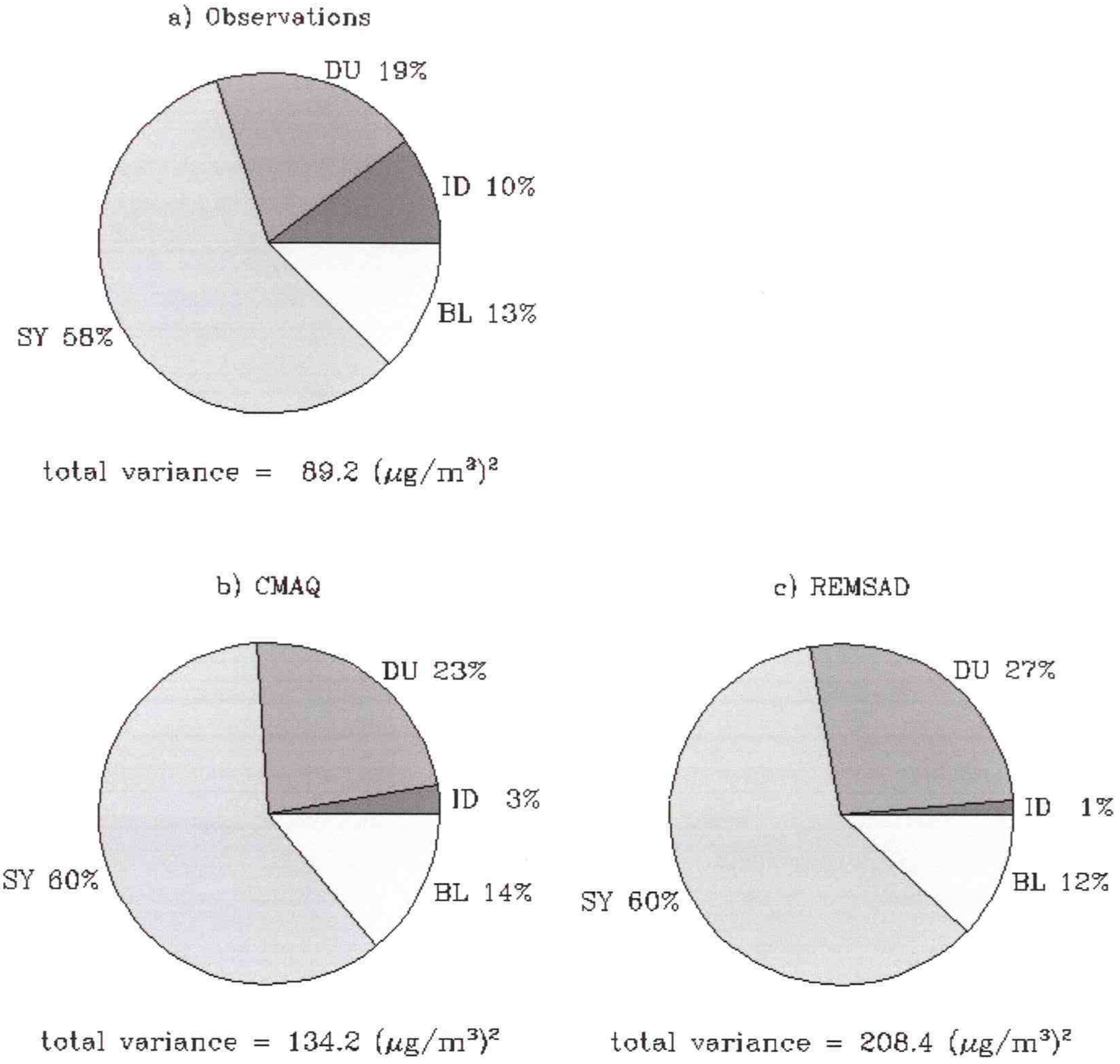

Figure 8. Pie chart showing the relative contributions of the different temporal components to the total variance of hourly $PM_{2.5}$ concentrations, averaged over all AQS monitors in the analysis domain. a) Observations from TEOM monitors, b) CMAQ predictions, and c) REMSAD predictions. ID stands for the intra-day component, DU the diurnal component, SY the synoptic component, and BL the baseline (longer-term) component.

Advanced statistical methods can be used to account for the spatial correlation structure inherent in the atmospheric process. For instance, 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 then be compared with the actual simulated values provided by CMAQ. If the difference between an estimated grid cell value and the value simulated by CMAQ is substantially larger than the error associated with the statistical estimate, then that grid cell is identified for further inspection.

In conjunction with the 2001 CMAQ evaluation, this method was used to assess CMAQ's ability to simulate aerosol sulfate in a portion of the southeastern United States during selected time periods. A pictorial summary of results for the period January 2–January 29, 2001, is contained in Figures 9–12; all sulfate values are given in units of micrograms per cubic meter μg/m3). Figure 9 displays the average sulfate observed during this period at monitoring stations in the southeastern United States. The CMAQ study area is outlined in gray. Note that observed values from outside the study region's borders are incorporated into the statistical model to improve the sulfate estimates at the edges of the region of interest. Figure 10 displays statistical estimates of the sulfate concentrations for each grid cells, based on this observed data.

Figure 11 reveals the average sulfate values as they were actually simulated by CMAQ. A comparison of Figures 10 and 11 reveals that the differences lie mainly in the northern and western portions of the region, with an additional smaller area in North Carolina. It is important to take the likely errors of the statistical estimates into account when identifying grid cells for further study. Figure 12 shows only the differences (CMAQ less statistical estimates) for which the respective CMAQ simulated values are outside the 95 percent credible intervals associated with the respective statistical estimates. From Figure 12, primary candidate areas for further investigation include the southern Indiana-Kentucky, southwestern Tennessee, and northern Virginia regions. Further development and applications of Bayesian statistical techniques for spatially-correlated processes are continuing.

2.2.7 Temporal Signatures of Model Output and Observations

Time series decomposition methods were applied to meteorological and air quality data and their numerical model estimates. Decomposition techniques express a time series as the sum of a small number of independent modes which hypothetically represent identifiable forcings, thereby helping to untangle complex processes. The objectives were to (1) compare the performance of decomposition techniques in characterizing time scales in meteorological and air quality variables, (2) use these methods to identify temporal characteristics of observations and model outputs, and (3) compare outputs expressed as temporal modes from two different modeling systems operated under nearly identical conditions. The results of this effort are briefly summarized here.

The decomposition methods included empirical orthogonal functions (EOF), empirical mode decomposition (EMD), and wavelet filters (WF). EOF, a linear method designed for stationary time series, is principal component analysis (PCA) applied to time-lagged copies of a given time series. EMD is a relatively new nonlinear method that operates locally in time and is suitable for nonstationary and nonlinear processes. Wavelet filters are linear and band-width guided with the number of modes set by the analyst.

The time series for these studies included modeled and observed temperature, $PM_{2.5}$, and ozone. Temperature should represent a relatively easy test for the decomposition methods as compared to the air quality variables. Since modeled estimates of temperature are forced to

closely track observations from a dense observation network, temporal modes of observations and model temperature time series should, therefore, be in close agreement. Comparison of modeled and observed ozone and $PM_{2.5}$, on the other hand, are more difficult tests for the decomposition techniques.

The aims of observation and model output comparisons involving temporal modes are slightly less ambitious than those of signal detection. For example, metrics can be created from modal amplitudes and periodograms without speculation about possible forcings. It is planned to continue these analyses using observed and modeled ozone. The abilities of the meteorological model (MCIP) and air quality models REMSAD and CMAQ to capture time scales of temperature and ozone were also compared. It was found that models and observations differed in the number of significant time scales present (with observations containing one to two more modes than model outputs). Individual modes differ greatly between observation and model until modes, occupying similar frequency bands are added together. As been reported elsewhere, there was a tendency for model performance to improve as mode frequency decreased. With respect to model development, displays of temporal modes may be more informative than raw outputs or correlation-like summary statistics. Literature studies of this nature used much larger signal/noise ratios than encountered in the hourly $PM_{2.5}$ observations that were analyzed. One should also attempt to identify forcings by analyzing nearby observations and climatological time series effected by similar forcings.

2.2.8 Reduction of the Space-Time Domain Dimensionality for Evaluation of Model Performance

Depending on the spatial extent of the domain, the grid cell size and the length of the period modeled, models generate enormous amounts of information. Such is the case for the annual (year 2001) model simulations using CMAQ and the REMSAD photochemical recently executed by the EPA. Although the huge amount of information generated by the models is valuable for evaluating their performance, failure to organize this information properly may lead to confusion and hamper the evaluation procedure. Therefore, the challenge is to identify a technique that, utilizing all relevant data available, indicates, in a clear and concise manner, which spatial and temporal features of the observations are well simulated and which other ones are blurred or not captured by the model.

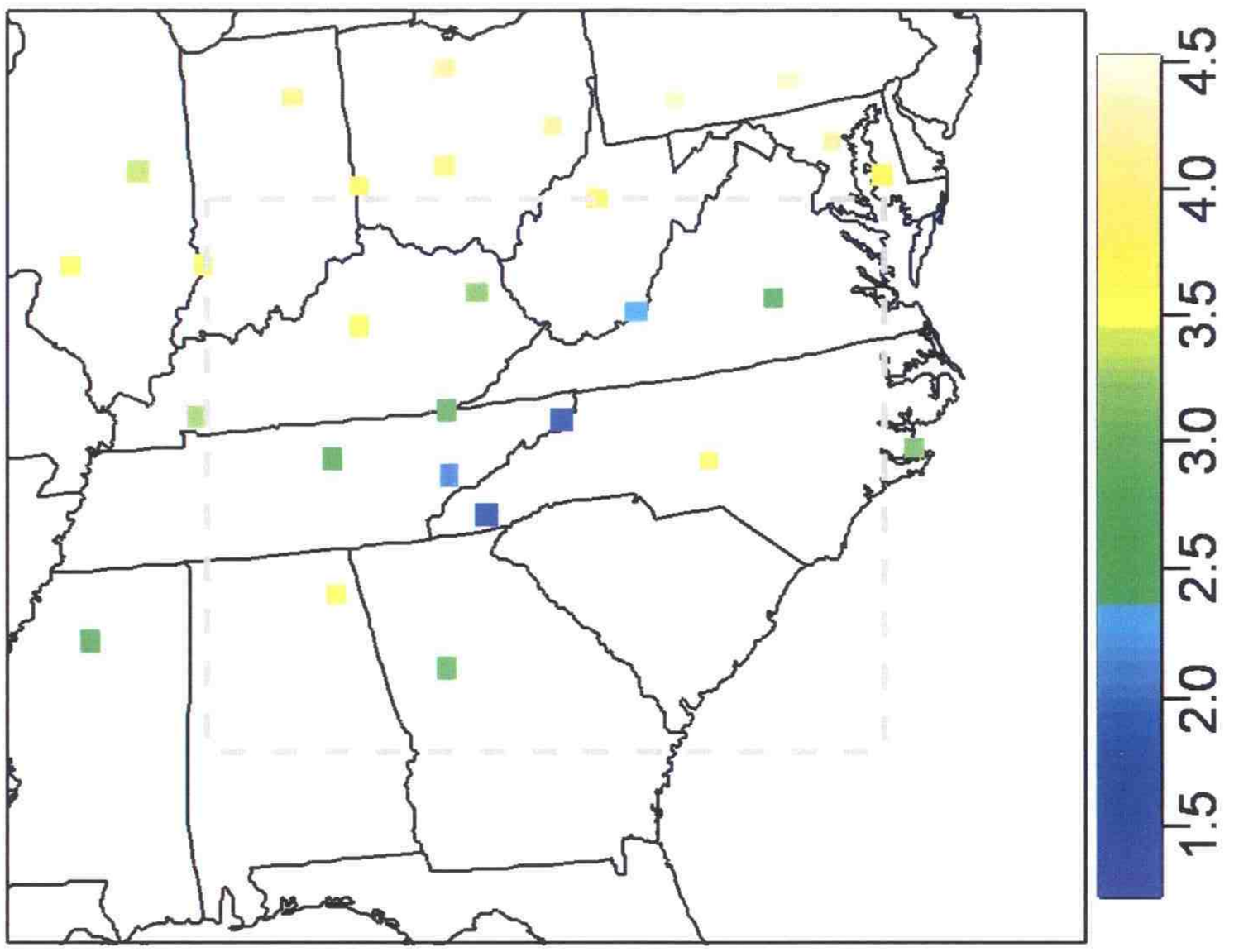

Figure 9. Average observed sulfate.

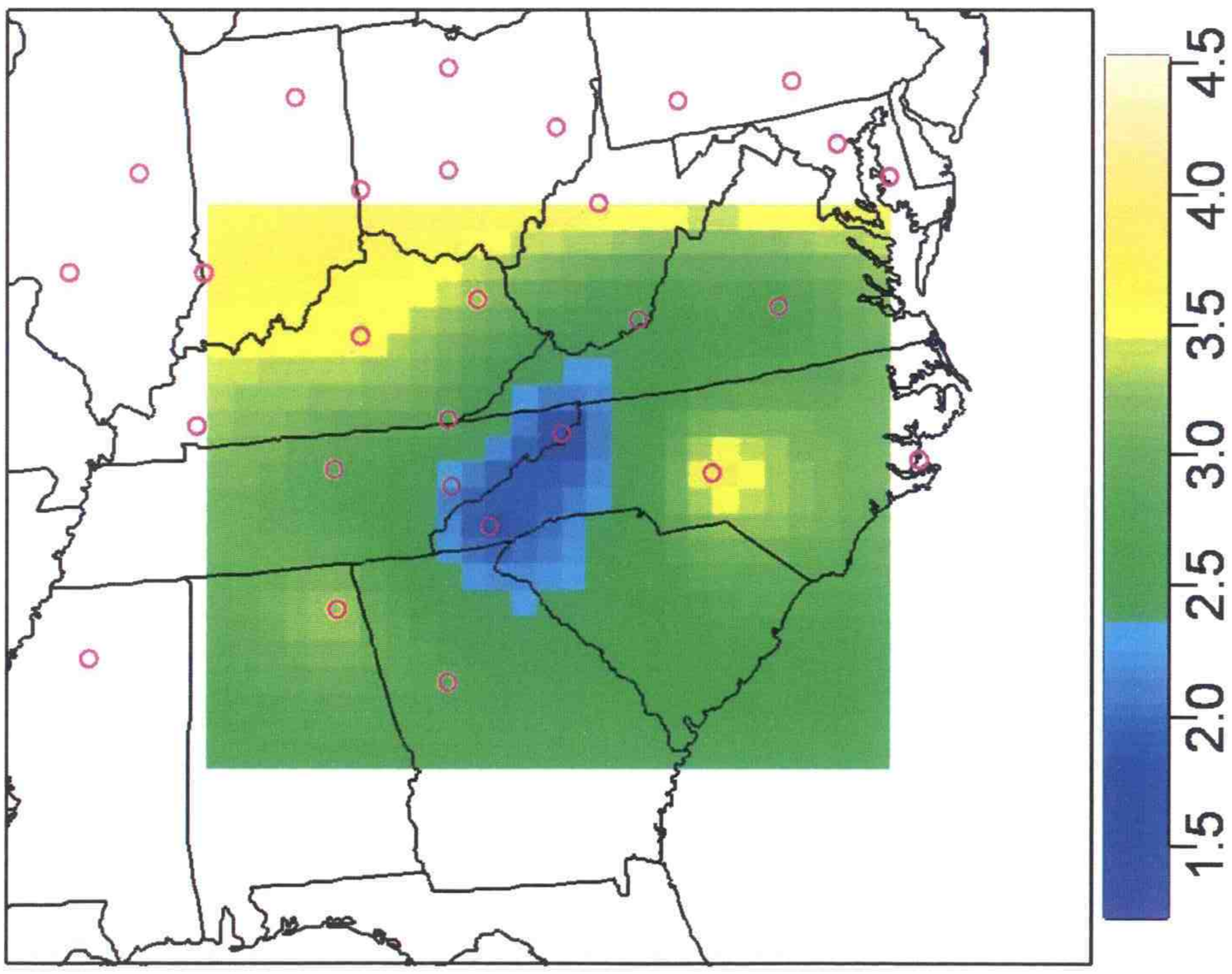

Figure 10. Statistical estimates based on monitoring data.

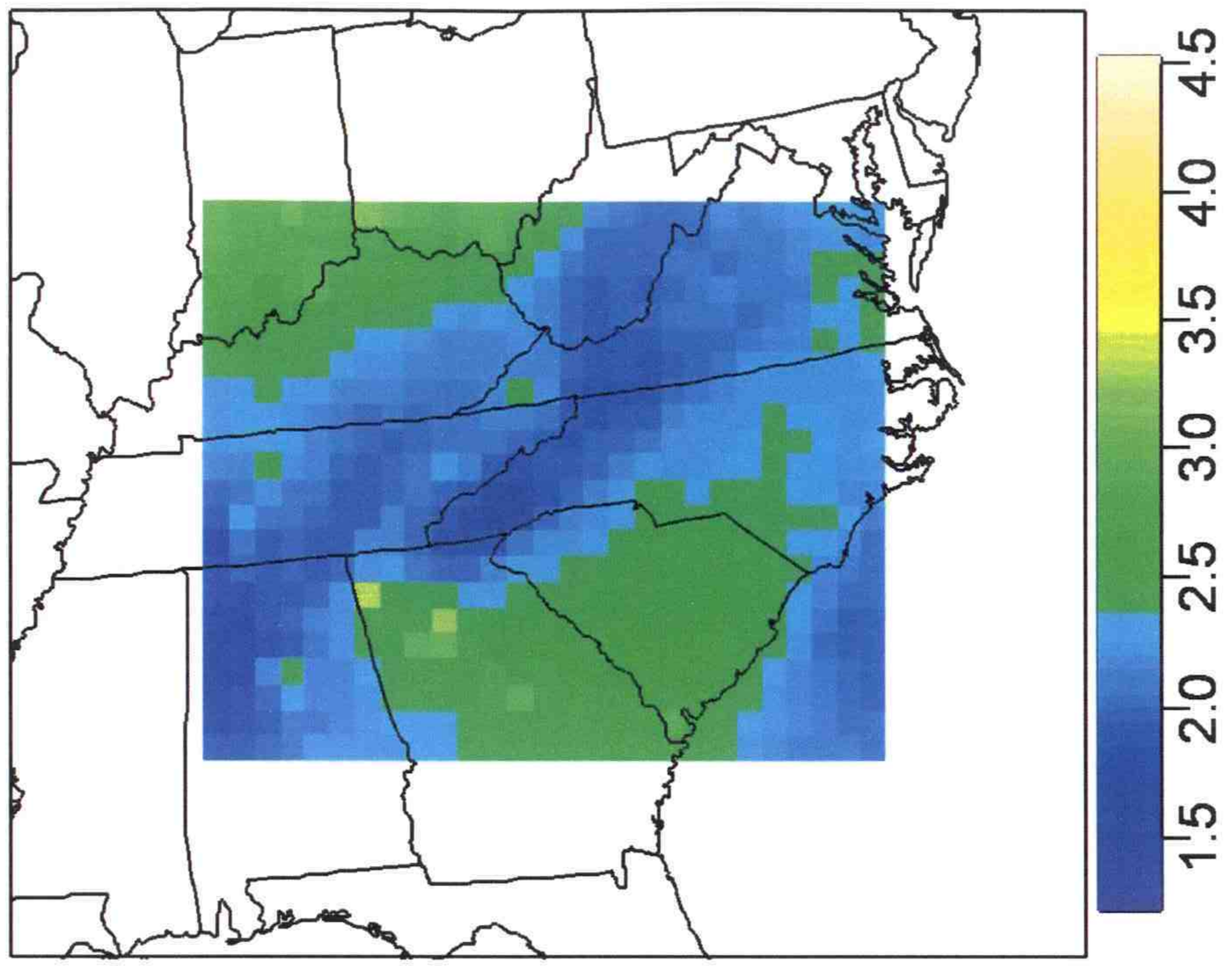

Figure 11. Average sulfate simulated by CMAQ.

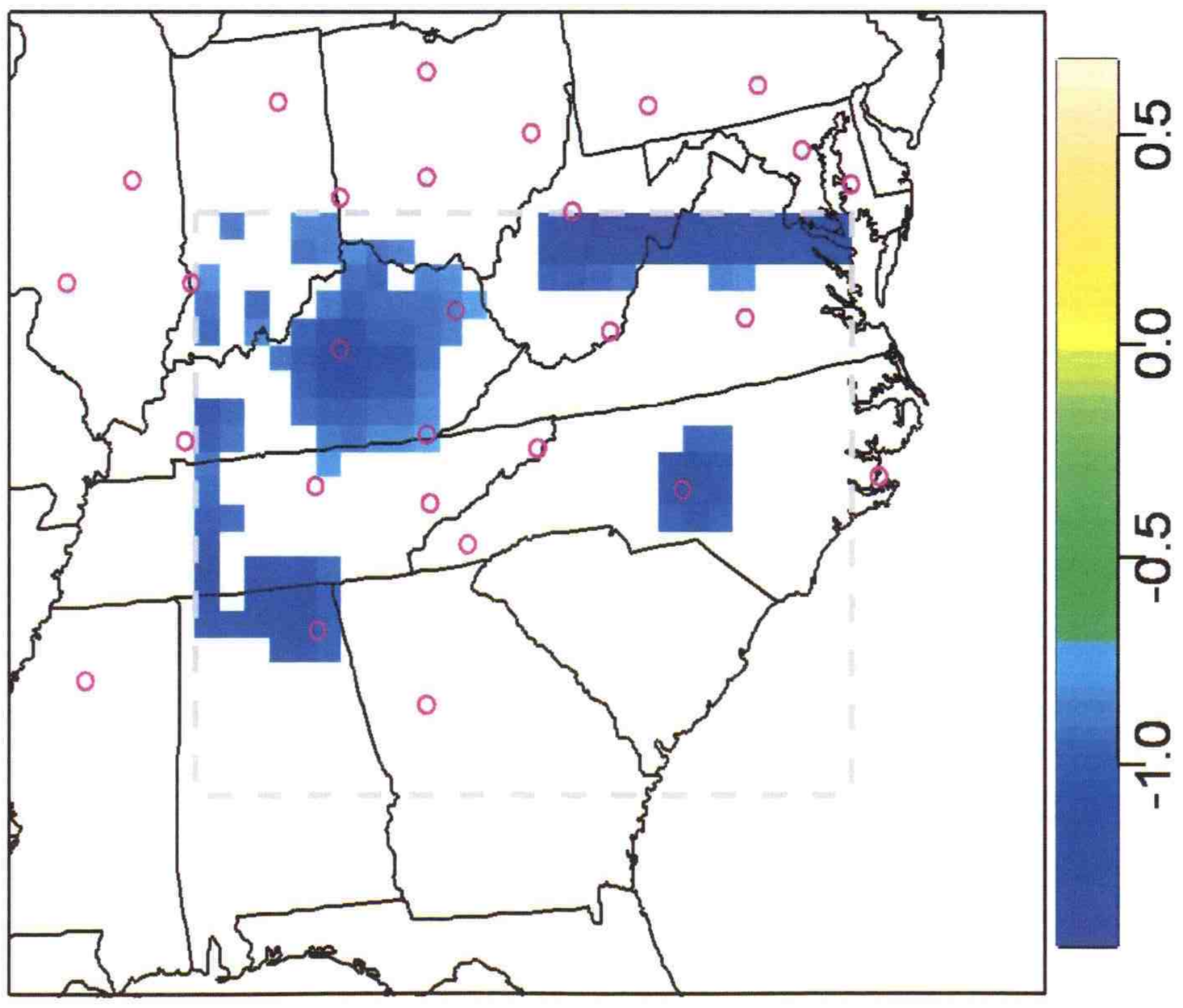

Figure 12. Significant differences (CMAQ - statistical estimates).

This challenge was addressed by organizing the spatial and temporal observational domain into a limited number of spatially and temporally homogeneous categories and assessing model performance in each category. The technique utilized to compartmentalize the domain is rotated principal component analysis (RPCA). The procedure was applied to the observed time series of the variable evaluated at multiple observation sites, leading to delineation of regions responding to distinct modes of variations. RPCA was also applied to maps of daily mean sea level pressure, leading to identification of the numbers of distinct synoptic patterns observed during the simulated period and the classification of each simulated day in the relevant synoptic pattern. An illustration of the use of the technique is being published in FY-2005. The modeled variable utilized for the purpose is the 10 m wind speed estimated for the eastern United States (East of the Rocky mountains) by MCIPv 2.2 applied to MM5 fields. These models generated the meteorological inputs utilized in the annual CMAQ and REMSAD runs previously mentioned.

In summary, the quality of daily mean wind speed estimates was not even throughout the domain, as significantly different evaluation metrics were calculated for the various regions identified by RPCA. More specifically, wind speed was generally underestimated (negative bias) in the western portion of the domain (from the Dakotas southward to Texas), overestimated along the Atlantic Ocean shores (from New England to Florida), and apparently adequately simulated in the center of the domain. For the 2001 simulation considered in this study, neither the seasonal nor the synoptic-based temporal classification allowed detection of time periods with systematic weaknesses in wind speed estimates. It is speculated that the data assimilation scheme used to nudge MM5 (and, therefore, MCIP) fields towards existing observations may be the reason for this absence of contrast.

2.2.9 Objective Comparison of CMAQ and REMSAD Performances

Two of the most prominent photochemical air quality modeling systems that can be used to assess the impact of emission reduction strategies are CMAQ and REMSAD. To promote model-to-model comparison of these two modeling systems, the EPA performed simulations of air quality over the contiguous United States during year 2001 (horizontal grid cell size of 36 x 36 km) with CMAQ and REMSAD driven by identical emission and meteorological fields. The results of these simulations were used to compare the abilities of CMAQ and REMSAD to reproduce measured aerosol nitrate and sulfate concentrations. Model estimates were compared to observations reported by the Interagency Monitoring of PROtected Visual Environment (IMPROVE) and Clean Air Status and Trend Network (CASTNet) networks. Root mean squared errors (RMSEs) were calculated for simulation-observation pairs within 10 geographic regions and for 12 seasons (months). The Wilcoxon matched-pair signed rank test was used to assess the significance of the differences between corresponding RMSEs characterizing CMAQ and REMSAD skills, respectively. These conclusions were reached:

- CMAQ is more skillful than REMSAD for simulations of aerosol sulfate. The model was shown better at reproducing months of high concentrations when compared with CASTNet data. CMAQ superiority was not as prevalent although existent when assessed

with IMPROVE observations, leading us to speculate that the strength of the CMAQ model does not reside in its ability to simulate the shorter term (one day to the next), but on the longer-term (weekly and longer-term) fluctuations.

- CMAQ and REMSAD performances could seldom be differentiated for nitrate. In the rare cases where differentiation was possible, REMSAD and CMAQ were alternatively found more appropriate. As a result, the only fair statement is that both models seem to perform about equally.

2.2.10 Sensitivity of CMAQ Control Strategy Predictions to Model Input Uncertainties

Sensitivity analyses are important adjuncts to model-data comparisons. The prediction of the effects of emission controls on air concentrations is a key use of the air quality models, which are used in the State Implementation Plan (SIP) process to assess impacts of potential emissions reduction strategies for the criteria pollutants, in particular ozone and $PM_{2.5}$. These predictions can be affected by model input uncertainties, model parameter uncertainties, and structure of the model itself. One area of concern addressed in FY-2003 is the choice of vertical mixing algorithms because they alter the species concentration mixing histories and, hence, the photochemical processing, potentially altering the control strategy response from CMAQ. The area of concern for a chemistry-sensitivity analysis in FY-2004 is the chemical mechanism choices in CMAQ relative to ozone control strategy predictions. Chemical mechanisms in Eulerian models are uncertain approximations of variables and reactions in the mixed layer; hence, their mathematical implementations are varied. Differing implementation of these uncertainties in different chemical mechanisms affect photochemical dynamics. Newer chemical mechanisms that have better scientific justification can sometimes degrade the chemical transport model's performance against observed O_3. Such degraded performance against observations under current conditions lowers confidence in the control cases using the new science. Sensitivities were designed to test the performance of O_3 base case predictions and also the change in O_3 due to emissions reductions for the three photochemical mechanisms implemented in CMAQ.

CMAQ was run to simulate urban and regional tropospheric conditions in the southeastern United States over 14 days in July 1999 at 32-km, 8-km, and 2-km grid spacing. Runs were completed with either of the two older mechanisms, CB-IV and RADM2, and with the more recent and complete SAPRC99. The sensitivity matrix included the base case and separate 50 percent spatially uniform reductions for anthropogenic emissions of nitrogen oxides (NO_X) and volatile organic compounds (VOC). Comparisons to observations for the base case were performed for the grid cells containing the SOS Cornelia Fort Airpark (CFA) site downwind of Nashville, Tennessee, and the Southeastern Aerosol Research and Characterization Study (SEARCH) site at Jefferson Street (JST) in Atlanta, Georgia. Nashville (CFA) represents a small-to-moderate sized city and Atlanta (JST) represents a moderately large urban area.

For the base case, SAPRC99 predicted higher O_3 than either CB-IV or RADM2 at JST and CFA, especially for afternoon maxima. The 8-km simulation was better than the 32-km grid resolution at JST, but the performance for O_3 at the 2-km grid resolution was not better than the 8 km at either site. This is a result found quite often for O_3, performance at the finest resolution is not better, and often worse, than at intermediate resolutions of 8 or 12 km.

For the emission reduction cases, the differential O_3 response to the emission reductions showed differences among the mechanisms, most interestingly at JST. For the 50 percent VOC emission reduction cases, the range of O_3 response at JST is smaller than that for NO_X reductions, and the O_3 benefits are mostly smaller from CB-IV than from SAPRC99. RADM2 benefits were more similar to SAPRC99. For the 50 percent NO_X emission reductions, both O_3 benefits and non-benefits were predicted at JST by all photochemical mechanisms at all grid spacings though there are differences. At JST, CB-IV and RADM2 predict less O_3 benefit and more non-benefit than SAPRC99, as well as non-benefits during some hours when SAPRC99 predicts benefits. Thus, there are differences between O_3 responses to emission reductions from CB-IV vs. SAPRC99 for the days simulated. The differential sensitivity varied by more than ±15 percent with CB-IV and by more than ±10 percent with RADM2 for some hours during the days simulated.

2.2.11 Inverse Modeling for Ammonia: A New Emission Inventory and an Annual Simulation

In a previous study by Gilliland *et al.* (2003), a top-down inverse modeling method was used to estimate seasonally-varying ammonia (NH_3) emissions. As the first published estimates of seasonal NH_3 emissions, the results were heavily relied upon in air quality modeling applications; however, uncertainties are inherent because of model prediction errors for meteorology and air quality and because of interannual variability in agricultural practices and meteorological conditions, both of which can influence the strategies of seasonal forcing in the of NH_3 emissions.

In the newest series of 2001 annual air quality simulations using the Community Multiscale Air Quality (CMAQ) model, prior estimates of seasonal NH_3 emissions were produced based on the seasonal estimates from Gilliland *et al.* (2003) and newer bottom-up NH_3 inventory estimates for dairy cattle and fertilizer (Pinder *et al.*, 2004; Goebes *et al.*, 2003). An inverse modeling study was conducted to evaluate the confidence in the prior use of NH_3 emission estimates for 2001. Advantages to this analysis over the previous study include having a full annual simulation including all months and more speciated aerosol data than in the previous study that focused on the year 1990. Disadvantages include having no total ammonium (NH_3+NH_4) air concentration data available as a cross-check to the inverse modeling results using NH_4 precipitation chemistry. Several refinements were made to the inverse modeling application in Gilliland *et al* (2003) that were used in this study including the incorporation of precipitation chemistry uncertainty and removal of uncertainty biases at monitors with extremely low wet deposition or concentration values. Since CMAQ simulations are more computationally efficient

than in the past, inverse modeling results were produced using both NH_4 wet deposition and wet concentration data as the optimizing indicators for the inverse modeling application.

Inverse modeling results suggest that the summertime emissions should be higher and wintertime emissions should be lower than those originally estimated. While increasing the overall amplitude of the seasonality in this way, the results do not suggest any bias in the annual total emission inventory for NH_3. This is a notable result because a high bias was detected in previous versions of the NH_3 inventory where the annual total NH_3 emissions were approximately 25 to 30 percent too high. This new inverse modeling study suggests that corrections to the inventory have been successful in correcting that bias.

2.2.12 Bay Regional Atmospheric Chemistry Experiment Model Evaluation

The Tampa Bay Estuary Program and the Florida Department of Environment asked the 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. 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, in part because CMAQ will incorporate sea salt in its aerosol module in FY-2005 and a sectional model incorporating sea salt, CMAQ-University of California, Davis, was under development. Prior to any Tampa Bay assessment, it was agreed that CMAQ, starting with CMAQ-UCD, needs to be evaluated against high-quality local data and that the nitrogen budget around Tampa Bay needs to be more carefully characterized.

The Bay Regional Air Chemistry Experiment (BRACE), designed for the above two purposes, was conducted during May 2002. ASMD scientists, along with ARL colleagues, were involved in the planning of BRACE. ASMD scientists worked on deployment of true-NO_2 monitors and with Hillsborough and Pinellas Counties' air quality professionals on deployment of NO_Y instruments. NOAA scientists took the lead on siting three wind profilers around the Bay, and helped define the complete chemistry package of instruments for the NOAA Twin Otter aircraft flown by ARL. Analysis of the May 2002 data showed a large discrepancy in the measurement of HNO_3. Hence, ASMD scientists took the lead in organizing and conducting a HNO_3 intercomparison study during October 2003. The preliminary analyses from intercomparison showed that indeed there was most likely an inlet problem during May 2002, and the October 2003 results will provide the modelers with crucial guidance in how best to create a best estimate of the nitrogen budget for comparisons against CMAQ.

The Wexler sectional aerosol model, Aerosol Inorganic Model (AIM), was adapted to incorporate sea salt in its calculations. During FY-2004, this sectional model was implemented into the 2004 release version of CMAQ, named CMAQ-UCD. CMAQ-UCD was tested and successfully adapted to run on multiple IBM eServer CPU's (EPA's supercomputer). Calculations for the period of August 1-14,1999, and comparisons to sectional data from Tampa

Bay allowed the sea salt emissions algorithm to be tested and improved. The MM5 simulations for the May 2002 period at 8-km and 2-km resolutions were evaluated. The stratification of days with strong, weak, and no sea breeze was accurately replicated by MM5. The fidelity of MM5's simulation of the sea breeze swings appeared to be quite good. This was gratifying because modelers in Houston, Texas, had problems accurately replicating the sea breeze. However, there was little difference in the quality of the MM5 simulations between the 8-km and 2-km resolutions. At the close of FY-2004, the MM5 simulations were deemed to have passed this phase of the evaluation, allowing the CMAQ-UCD simulations to proceed.

2.2.13 Model Evaluation Tool Development

Significant effort is often required to compare observations and model results. Most off-the-shelf tools do not address the specialized needs encountered in model evaluation. The R Model Evaluation Toolkit, RMET, was commissioned and developed at the prototype level in the R statistical system to address Division and broader modeling community needs. The statistical routines and graphics use R, an open source statistical package that is free. A preliminary version of the RMET tool was delivered in December 2003. RMET provides model evaluation capability for working with CMAQ simulations and measurement data, particularly graphical displays of the comparisons. The tool handles CMAQ output in Models-3 I/O-API format. Division-wide training on R and on the RMET tool will take place in October 2004. RMET will be extended to incorporate more advanced model and data comparison capabilities.

2.2.14 Evaluating the Effect of NO_x Reductions

This is the first phase of a long-term project aimed at identifying scientific methodologies that will lead to the development of innovative analytical tools to evaluation the effectiveness of the emission control strategies implemented in achieving the intended benefits, namely, accountability. Significant reductions in NO_x emissions from stationary sources have occurred in the eastern United States, and additional reductions are anticipated in the future. These emission control programs have been required to reduce the tropospheric ozone levels based primarily on computer modeling. The NO_x Reasonable Available Control Technology rule in the NorthEast Ozone Transport Region, CAAA Title IV, NO_x SIP call, and Section 126 rule all require NO_x emission reductions throughout the eastern United States from major sources. In addition, significant future reductions are expected from mobile sources, diesel engine rules, and the Clean Air Interstate Rule. Given the significant costs associated with these emission control measures, it is important to demonstrate the effectiveness of these rules through analysis of model outputs and observations and to track progress on improving air quality.

The conceptual framework of accountability is based on measuring environmental outcomes using an integrated environmental assessment model that enables assessing and documenting relationships between emissions, air quality, atmospheric deposition, and effects to public health and ecosystems. This initiative will begin by reviewing:

1. Emission reductions observed in ambient air and atmospheric deposition. Since the 1990 Clean Air Act Amendments, a greater number of stationary sources of SO_2 and NO_x emissions have installed continuous emission monitoring systems. Improved systems for tracking emission from mobile sources have also been developed. At this level, an accountability framework provides a bridge between measured emission reductions and changes in the ambient environment. Resources under this initiative would be applied to analyze specific primary and transformed emission products in ambient air and in atmospheric deposition (*e.g.*, nitrogen oxide, particle nitrate) over relevant geographic areas.

2. Predicted air quality and atmospheric deposition improvements. Resources would be applied to enhance the predictive capability to address whether emission reductions have resulted in the expected improvements in air quality and deposition, for example:

   - Reduced ozone, $PM_{2.5}$ concentrations;
   - Reduced deposition of NO_x transformations (*e.g.*, wet and dry deposition of nitrate); and
   - Diagnostic species (*e.g.*, peroxides, nitric acid, ammonia) useful for model evaluations and interpreting dynamic-changes in the atmosphere associated emission reductions.

In addition to assessing whether the ozone improvements have occurred, this would also entail assessing whether these improvements can be attributed to specific emission control strategies that have been implemented. The objective is to research and develop analytical tools that will quantify the effect of regional NO_x emission reductions on ambient ozone air quality, thus providing a measure of control strategy accountability. The Division is coordinating and sharing research plans and products with the EPA Office of Air Quality Planning and Standards and the Office of Atmospheric Programs.

2.3 Toxic Air Pollutant Modeling

The Clean Air Act Amendments (CAAA) of 1990 identified almost 200 individual compounds or mixtures of compounds as toxic air pollutants or hazardous air pollutants (HAPs) with the potential for causing adverse health effects. Air quality models for predicting ambient concentrations of these toxic compounds are needed to provide human exposure estimates for both risk assessment and risk management. To obtain accurate estimates of the ambient concentrations of these compounds, there must be a proper accounting of the important processes that control their fate. Since each compound, or mixture of compounds, has unique physical and chemical properties that affect the relative importance of those processes, each compound must be considered individually. The objective of this work is to develop the capability to model toxic compounds at urban and regional scales using CMAQ, and at finer scales using both probabilistic, with probability distributions embedded within CMAQ, and deterministic, using computational fluid dynamics models approaches. These models are used to develop spatially and temporally

variable estimates of concentrations of important air toxins 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 modeling system, improvements in chemical and physical characterization of air toxins, and the measurement of ambient air toxics concentrations.

2.3.1. Extending CMAQ to New Species of Air Toxics

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. An efficient and perhaps 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 to assess risks to human health reported in the National Air Toxics Assessment (NATA). An EPA Science Advisory Board concluded that the NATA's modeling approach inaccurately predicted effects from long-range transport of less reactive HAPs and atmospheric photochemistry, because its Gaussian model was unable to account for complex chemical reactions and long-range (>50 km) transport. This neglect can cause significant errors in predictions, despite corrections that added "background" concentrations to model output. The corrections seemed inappropriate, because the background value sometimes accounted for most of the total risk. The resultant predictions also did not provide a good way to assess contributors to HAP concentrations or to develop control strategies. In response to these problems, CMAQ was modified and applied to simulate HAP concentrations across the continental United States.

During FY-2004, applications were completed that simulated 20 HAPs within the CMAQ (Table 1). The CB-IV mechanism and the Statewide Air Policy Research Center (SAPRC99) mechanism were modified and tested to determine whether the choice of mechanism affects the predictions. A version of the fast numerical solver, the Euler Backward Iterative (EBI) solver, was developed for both. Four HAPs– formaldehyde, acetaldehyde, 1,3-butadiene and acrolein– were included within the EBI solver because they affect key compounds in such atmospheric photochemistry as ozone and hydroxyl radical. The remaining HAPs were not included in the solver, and they undergo losses from atmospheric photochemistry based on reaction rates and air concentrations after the solver converges to a solution. This treatment was rewritten into a generalized algorithm to easily incorporate additional HAPs into CMAQ. Reactive tracers were included to track the emissions of formaldehyde, acetaldehyde, and acrolein. The tracers allow the determination of how production from photochemistry determines the overall concentrations, a key question in developing HAPs control strategies. The modified mechanism maintains computational efficiency and does not compromise accuracy in predicted HAP concentrations. For these applications, HAP concentrations across the continental United States during 2001 were simulated, and the results were evaluated against observations. The CMAQ output for HAP concentrations were processed into a format that supports the risk assessment model used in NATA.

Table 1. Toxic air pollutant species modeled explicitly in CMAQ during FY-2004.

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

Also in FY-2004, the modified CB-IV mechanism was used to evaluate the role of biogenic sources in the concentrations of formaldehyde and acetaldehyde. The results showed a large increase in the role from winter to summer conditions. The increase occurs because emitted volatile organic compounds (VOCs) increase and photochemically produce formaldehyde and acetaldehyde. Results indicate the type of VOCs that contribute to most of the photochemical production based on location and time of year.

2.3.2. Comprehensive Version of CMAQ for the National Air Toxics Assessment

NATA is designed to help EPA, state, local and tribal governments, and the public better understand the air toxics problem in the United States. The 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 NATA is to provide an estimate of the outdoor air toxin concentrations that includes an accurate, state-of-the-science description of all relevant chemical and physical processes that can affect the concentrations of toxic pollutants. Model simulations were completed of air toxin concentrations during 2001 over the continental United States. The species simulated included 20 gas phase toxins. Using CMAQ, spatially and temporally variable estimates of concentrations of important air toxins were developed, and the model predictions were evaluated against observations. With these resolved concentration fields, several observations were made about the continental-scale characteristics of HAPs in the atmosphere. Figure 13 shows an example of the formaldehyde concentrations predicted by CMAQ for 2001 in summer and Figure 14 shows the concentrations in winter.

The results have been compared with observations taken during the 2001 air toxins pilot study, which consists of 35 monitors in 8 cities (San Jacinto, California; Grand Junction, Colorado; Tampa, Florida; Cedar Rapids, Iowa; Detroit, Michigan; Rio Rancho, New Mexico; Providence, Rhode Island; and Seattle, Washington). This data set was collected using consistent protocols and was extensively analyzed and quality-assured. Data were taken at 1, 3, or 6 day intervals although some monitors did not start collecting data until spring of 2001. Explanation of this data set and its use is given in Luecken and Hutzell (2004). Figure 15 shows the monthly averages of formaldehyde concentrations measured at all sites in the air toxins pilot study and their predicted values from CMAQ. Figure 16 shows the same comparisons for benzene. The 1:1, 1:2 and 2:1 lines are shown. The majority of the model match the observations within a factor of 2. Figures 17 and 18 show that CMAQ also matches the temporal trends very well for formaldehyde and benzene. For both of these pollutants, the day-to-day variability is predicted with skill, although at some sites, the predicted concentrations are lower than the observations.

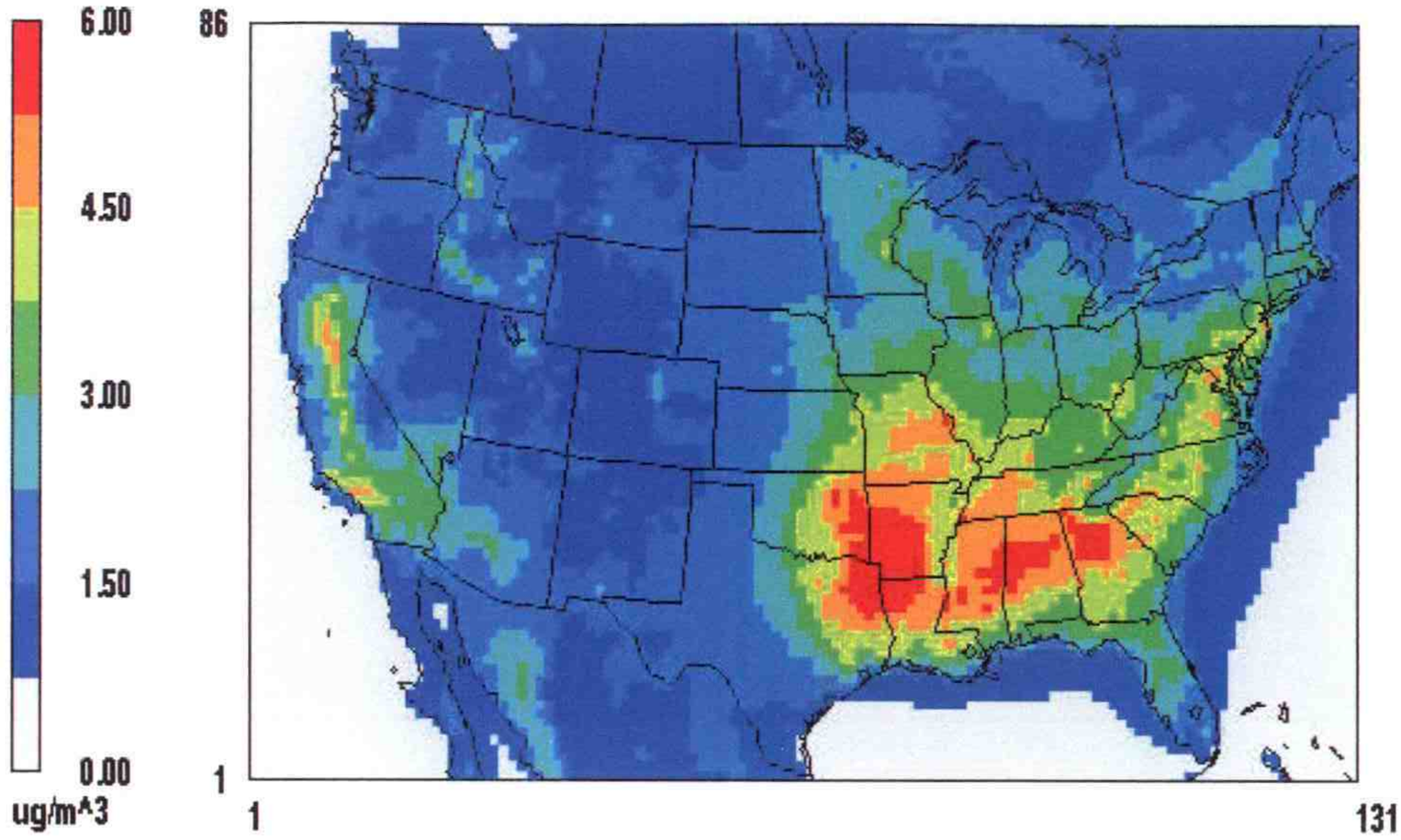

Figure 13. Summer 3-month average Formaldehyde concentrations predicted by CMAQ.

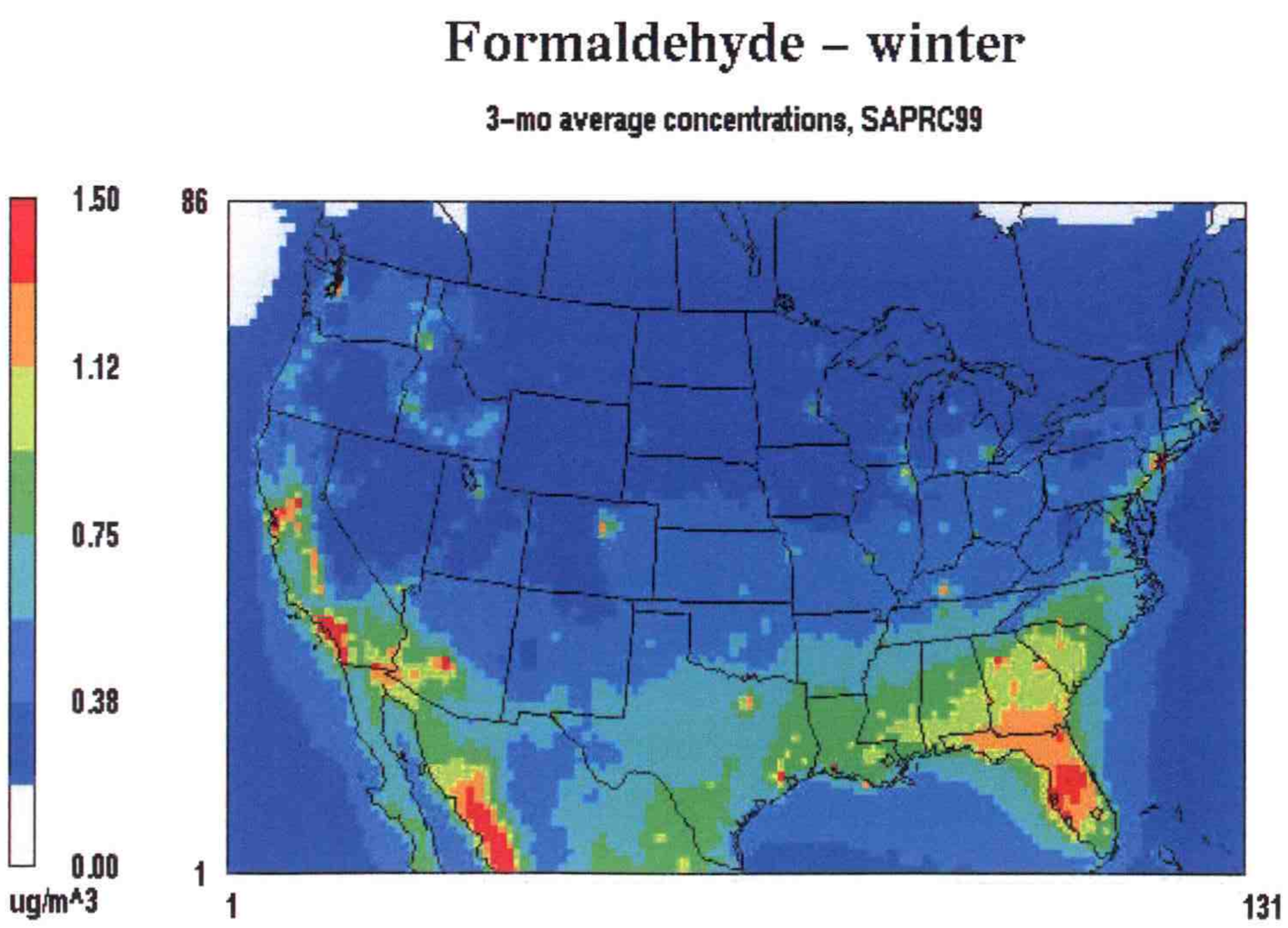

Figure 14. Winter 3-month average Formaldehyde concentrations predicted by CMAQ.

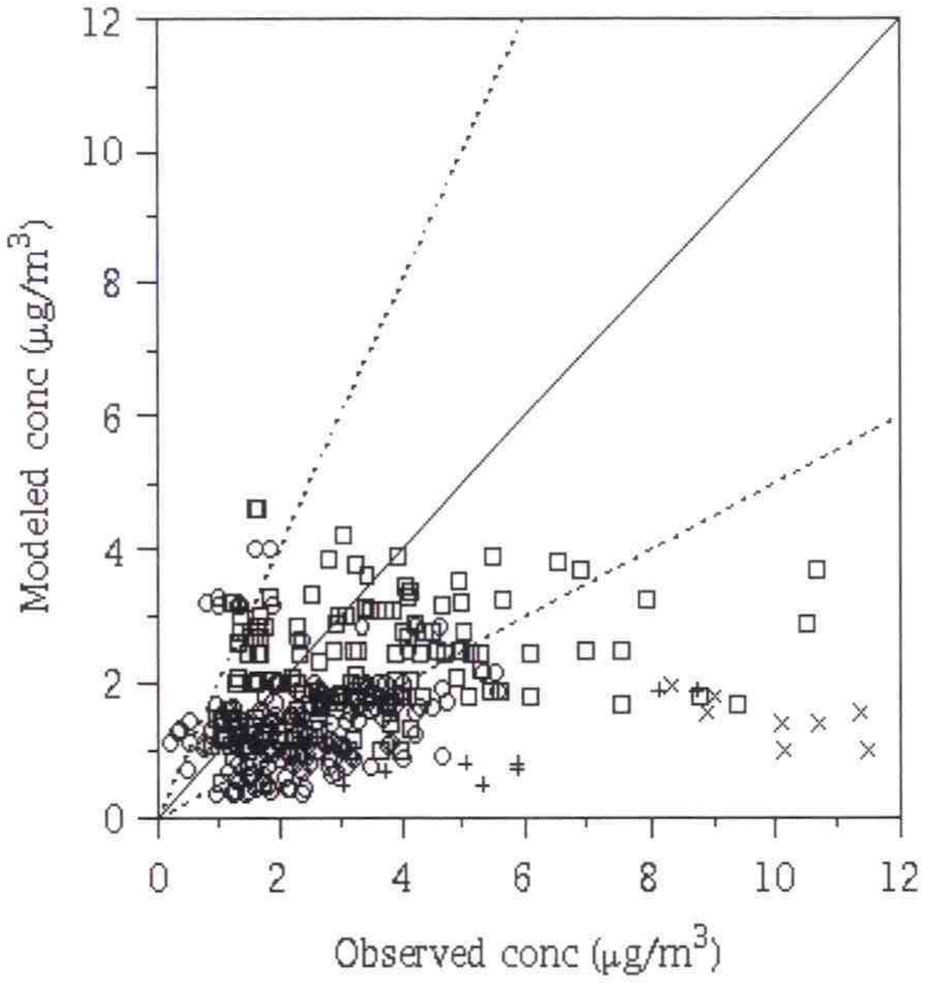

Figure 15. Comparison of monthly-averaged observed concentrations with model predictions for formaldehyde.

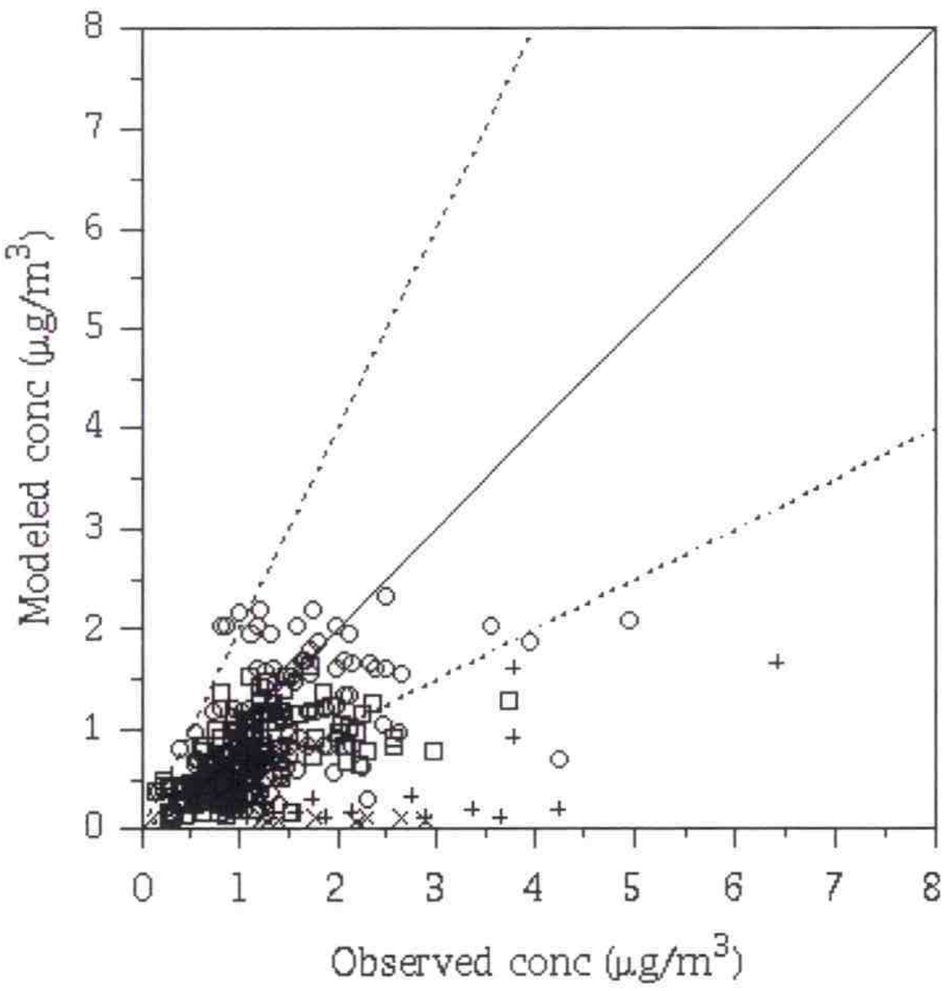

Figure 16. Comparison of monthly-averaged observed concentrations with model predictions for benzene.

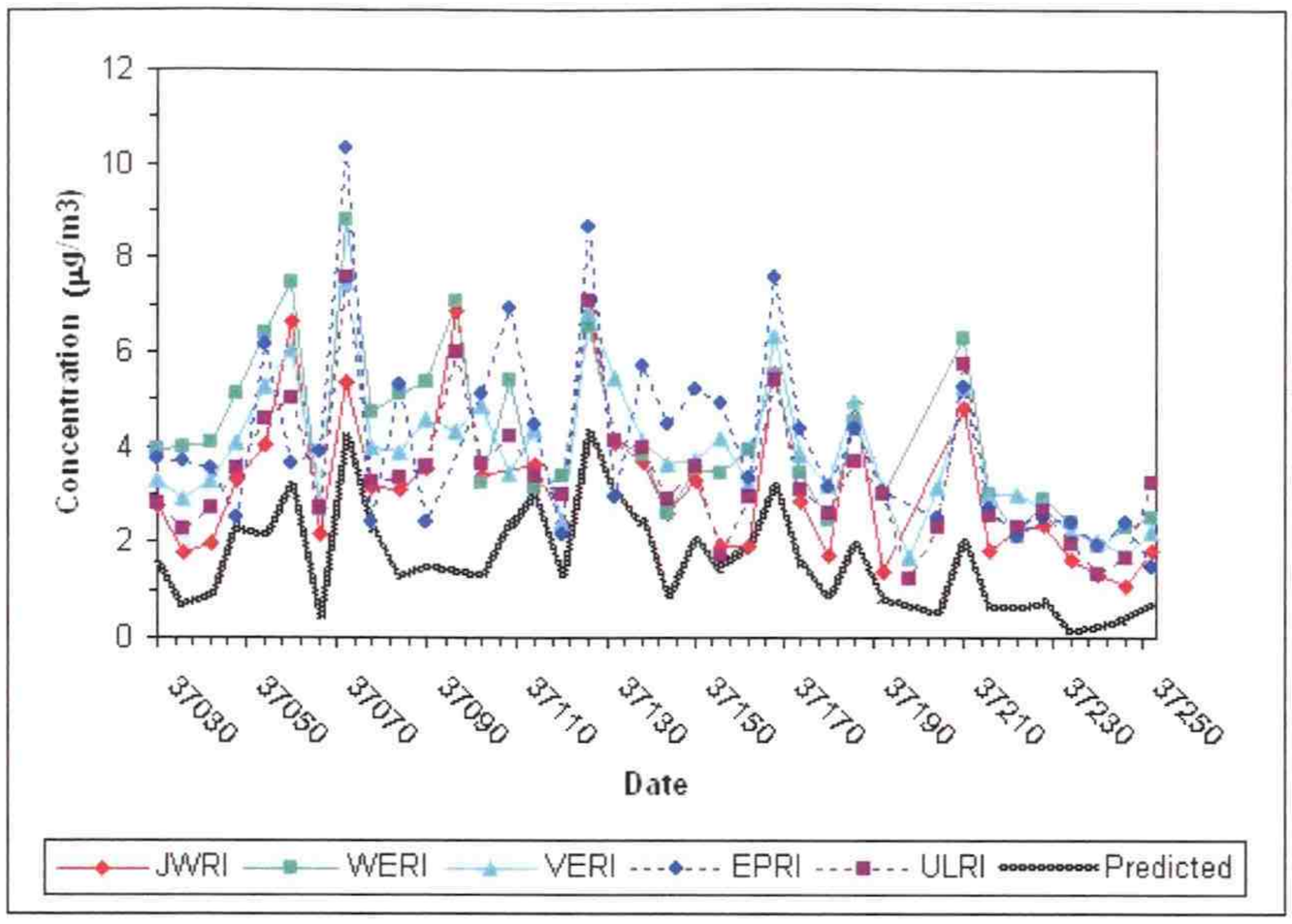

Figure 17. Time series of 24-hr averaged formaldehyde concentrations measured at the Providence, Rhode Island site for all monitors falling within the single CMAQ grid cell (135,72) and the model predictions at this grid cell.

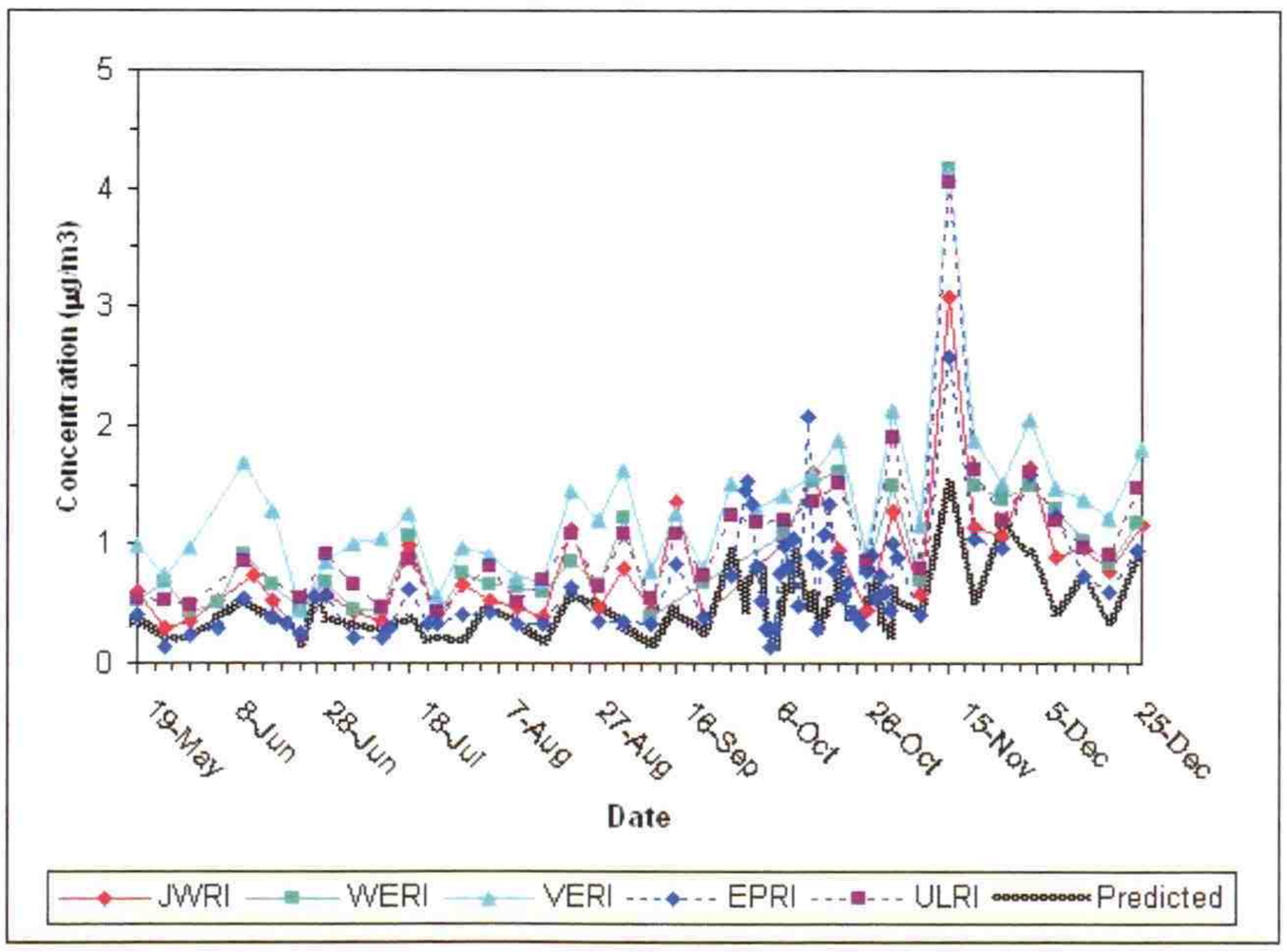

Figure 18. Time series of 24-hr averaged benzene concentrations measured at the Providence, Rhode Island site for all monitors falling within the single CMAQ grid cell (135,72) and the model predictions at this grid cell.

The CMAQ model results were compared with predictions from the Gaussian plume model, ASPEN, used to support NATA. It was found that CMAQ produced the same values for the general statistics used to compare the ASPEN model to observations, although with slightly more of a bias. The results were post-processed into a format that supports the risk assessment model used in the NATA. Hourly values for acrolein were extracted and delivered to other EPA laboratories for consideration of the diurnal variation of acrolein in an upcoming mobile source rule. This work has demonstrated that a numerical chemical transport model, CMAQ-CTM, is a useful and appropriate tool for predicting concentrations of HAPs across the United States for a year-long period. Overall, key findings from this analysis include the following:

- Formaldehyde concentrations are largest in the Southeast and central California, due mainly to reaction products of biogenic isoprene.

- There is a large degree of seasonal, daily, and hourly variability in the concentrations. Formaldehyde, for example, can vary by a factor of six from winter to summer, and a factor of two from mid-morning to noon within a typical day.

- Atmospheric chemical formation plays a critical role in the concentrations of some HAPs. Formaldehyde and acetaldehyde, for example, are mostly chemically-formed in the atmosphere, with only a small portion due to direct emissions.

- A comparison of the modeled concentrations with a limited set of observations shows that CMAQ is generally able to reproduce the temporal variability in the data.

- CMAQ concentrations can differ substantially from ASPEN predictions for species whose concentration depends substantially on atmospheric chemistry.

To follow up this work, plans for the 2002 NATA include improving on the previous analysis by including additional toxic species and developing ways to account for local "hot spots" of high concentration.

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

The Division completed a FY-2004 pilot study to develop the capability to provide advanced photochemical grid-model air-toxic concentrations to a human exposure model. The pilot study also began to assess whether a grid-based chemical transport model could successfully replace and/or augment traditional Gaussian plume modeling approaches to providing annual ambient concentration estimates of air toxics for human exposure assessments in urban settings.

The study consisted of: (1) extending an air toxics version of the CMAQ modeling system to a modeling domain centered over Philadelphia at 12- and 4-km grid meshes; (2) performing model simulations for the year 2001; (3) comparing the modeling results limited with observational data collected at Camden, New Jersey, under the Urban Air Toxics Monitoring

Program www.epa.gov/ttn/amtic/files/ambient/airtox/main-2a.pdf; (4) reformatting the modeling results into the 3-hour annual averages needed for input to HAPEM5; 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 an useful tool to simulate the air toxic concentration fields needed to drive a human exposure model. A comparison of the modeled concentrations with a limited set of observations suggests that the CMAQ model was able to reproduce the temporal features embedded in the data. 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 the HAPEM5. Based on these results, CMAQ is being considered for application for the EPA's NATA program.

The next phase of this research effort will focus on extending the CMAQ modeling system for simulating air toxics with finer grid cell sizes (~1 km) and to examine the practicality of intermingling Gaussian dispersion model estimates with CMAQ results. 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 2000 Air Quality Study that can be used for extensive model evaluation.

2.3.4 Parameterizing the Urban Canopy

The difficulty of predicting air pollutant dispersion at high spatial resolution is exacerbated by the need for high quality, high definition of the meteorological fields that govern transport and turbulence in urban areas. Air quality fields are now being modeled at finer spatial resolution to reveal "pollutant hot spots" in urban areas. These fine resolution mesh simulations will need to be driven by meteorology at commensurate mesh sizes. Since most of the primary atmospheric pollutants are emitted inside the roughness sub-layer (RSL), and consequently, the first chemical reactions and dispersion occur in this layer, it is necessary to generate detailed meteorological fields inside the RSL to perform air quality modeling at high-spatial resolutions.

At neighborhood scale (on order of 1-km horizontal grid spacing), the meteorological fields are strongly influenced by the presence of the vegetation and building morphology of varying complexity, which requires developing more detailed treatment of the influence of canopy structures in the models and using additional morphological databases as input. The assumptions of the roughness approach, used by most of the mesoscale models, are unsatisfactory at this scale. Hence, a detailed urban and rural canopy parameterization (Dupont *et al.*, 2004), called DA-SM2-U, was developed and incorporated inside MM5 to simulate the meteorological fields within and above the urban and rural canopies. DA-SM2-U uses the drag-force approach to represent the dynamic and turbulent effects of the buildings and vegetation, and a modified version of the soil model SM2-U (Dupont *et al.*, a and b accepted for publication), called

SM2-U(3D), to represent the thermodynamic effects (e.g.,estimates the heat and humidity fluxes) of the canopy elements at different levels within the canopy.

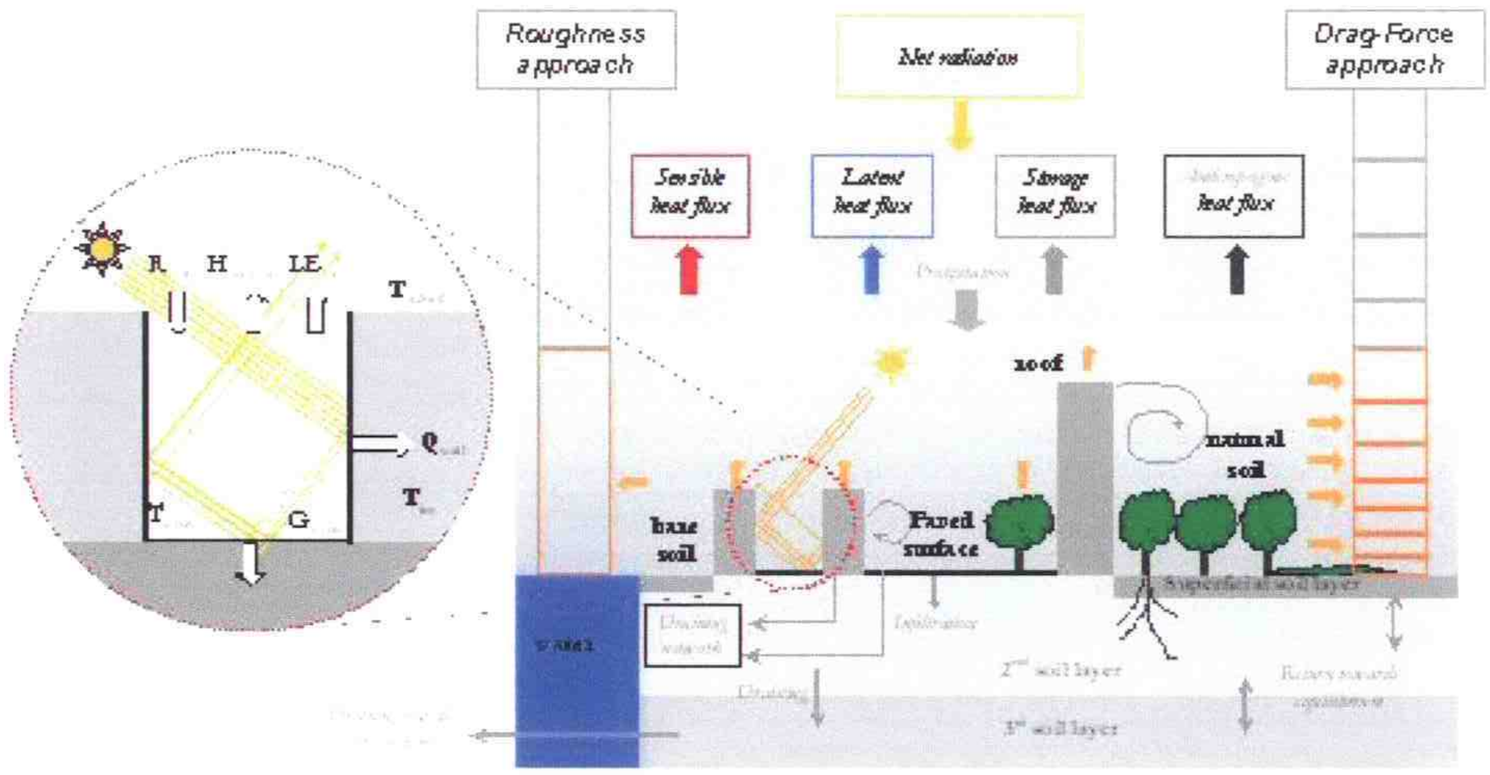

Figure 19. Scheme of the new MM5 canopy parameterization, DA-SM2-U, using the drag-force approach with the soil model SM2-U(3D), compared with the roughness approach.

The drag-force approach transmits directly to the atmosphere the dynamic, thermodynamic and turbulent effects of the canopy elements (vegetation and buildings) by changing the conservation equations of the mesoscale model. The lower level of the computational domain corresponds to the real level of the ground, and additional vertical layers are included within the canopy to allow more detailed meteorological fields within the RSL (Figure 19). Inside the canopy, the effects of buildings and vegetation are represented by adding in the dynamic equation a friction force induced by horizontal surfaces of buildings, and a pressure and viscous drag force induced by the presence of buildings and vegetation. In the temperature equation, the sensible heat fluxes due to buildings and vegetation, and the anthropogenic heat flux parameterization followed Taha (1999). In the specific humidity equation, the humidity sources coming from the evapotranspiration of the vegetation and the evaporation of the water intercepted by buildings were included. A shear production term induced by horizontal surfaces of buildings, turbulent kinetic energy sources induced by the presence of buildings and vegetation, and buoyant production terms from the sensible heat fluxes emitted by buildings and vegetation were included in the turbulent kinetic energy equation. The turbulence length scale was also modified inside the urban canopy, as proposed by Martilli *et al.* (2002). The volume of buildings is considered in each cell, whereas the volume of the vegetation is neglected. The turbulent transport in the vertical is also modified to consider the real volume of air in the cell.

DA-SM2-U is thus a multi-layer canopy and soil model with few layers of a couple meters within the canopy depending on the mesh of the mesoscale model domain, and three layers within the ground; a surface soil layer for the natural surfaces, a root zone layer, and a deep soil layer. A first evaluation of DA-SM2-U on the City of Philadelphia (Dupont *et al.*, 2004) with a simple urban morphology representation showed that the model is capable of simulating the important features observed in the urban and rural areas.

In FY-2004, an effort was undertaken to apply the DA-SM2-U version of MM5 to Houston, Texas. A detailed GIS database of urban canopy parameters (UCP) gridded at 1 km was created for the entire MM5 computational domain. To provide the most accurate representation of the morphological parameters for the entire MM5 computational domain on Houston, a GIS urban database was created (Burian *et al.*, 2004). This database includes multiple surface topography and surface cover digital data sets, including land use, bare earth elevation, full-feature digital elevation model, and roadway locations. The parameters were then correlated to the underlying land-use type using area-weighted averages. The average values for each parameter for each land use type were then extrapolated to each 1-km grid cell in the MM5 modeling domain using an area-weighting scheme based on land use fraction with the grid cell. Table 2 lists the 23 different UCPs that were developed for this project.

Table 2. Urban Canopy Parameters (UCP) for Houston, Texas.

Canopy UCPs:	Building UCPs:	Vegetation, Other UCPs:
Mean Canopy Height Canopy plan area density Canopy top area density Canopy frontal area density Roughness length Displacement height Sky view factor	Mean building height Standard deviation of building height Building height histograms Building wall-to-plan area ratio Building height-to-width ratio Building plan area density Building rooftop area density Building frontal area density	Mean vegetation height Vegetation plan area density Vegetation top area density Vegetation frontal area density Mean orientation of streets Plan area fraction surface covers Percent directly connected impervious area Building material fraction

This effort provides the first implementation of this detailed set of gridded UCPs into the DA-SM2-U/MM5 system. A case study for August 30, 2000, was selected for a domain encompassing the greater Houston-Galveston area (Ching *et al.*, 2004a). The period of interest also corresponds to the Texas 2000 Air Quality Study. Simulations were made at 36-, 12-, and 4-km grid sizes using 30 sigma layers in the vertical.

Sensitivity studies of work in progress have indicated a need for accurate input boundary conditions of flow fields from the coarser 4-km grid mesh influenced by the mesoscale circulation induced by Gulf of Mexico and Galveston Bay. The inclusion of high resolution, diurnally varying sea surface temperatures, was necessary for accurate fine scale flow simulations and was applied in the comparative results for Figures 20 and 21, which display significant differences in predicted dispersion parameters between standard MM5 (using Reynolds averaging) and the urbanized version of MM5 (using DA-SM2-U-UCP) at a 1 km grid mesh.

The DA-SM2-U/MM5 system was successfully implemented using a sophisticated set of gridded UCPs based on high resolution building and vegetation data. Modeling tools to help resolve physically, flows in urban areas that are impacted by the presence of canopy features at 1-km grid sizes were developed. This method reduces the problems or uncertainties associated with simple interpolation schemes that cannot be expected to accurately represent the flow in urban areas. Thus, the combination of UCP-driven meteorology for fine scale modeling and more-accurately modeled lake-land breeze circulations will provide stronger scientific basis for advancing the simulations of the flow and air quality for Houston and other urban areas with similar climatic features.

A city-specific database of urban morphological data and UCP daughter products are needed for running these advanced UCP for all urban areas. Initial discussions are underway to explore the creation of such a database (Williams and Ching, 2004). If such a database can be achieved, the utility of advanced approaches as described in this section may become attractive.

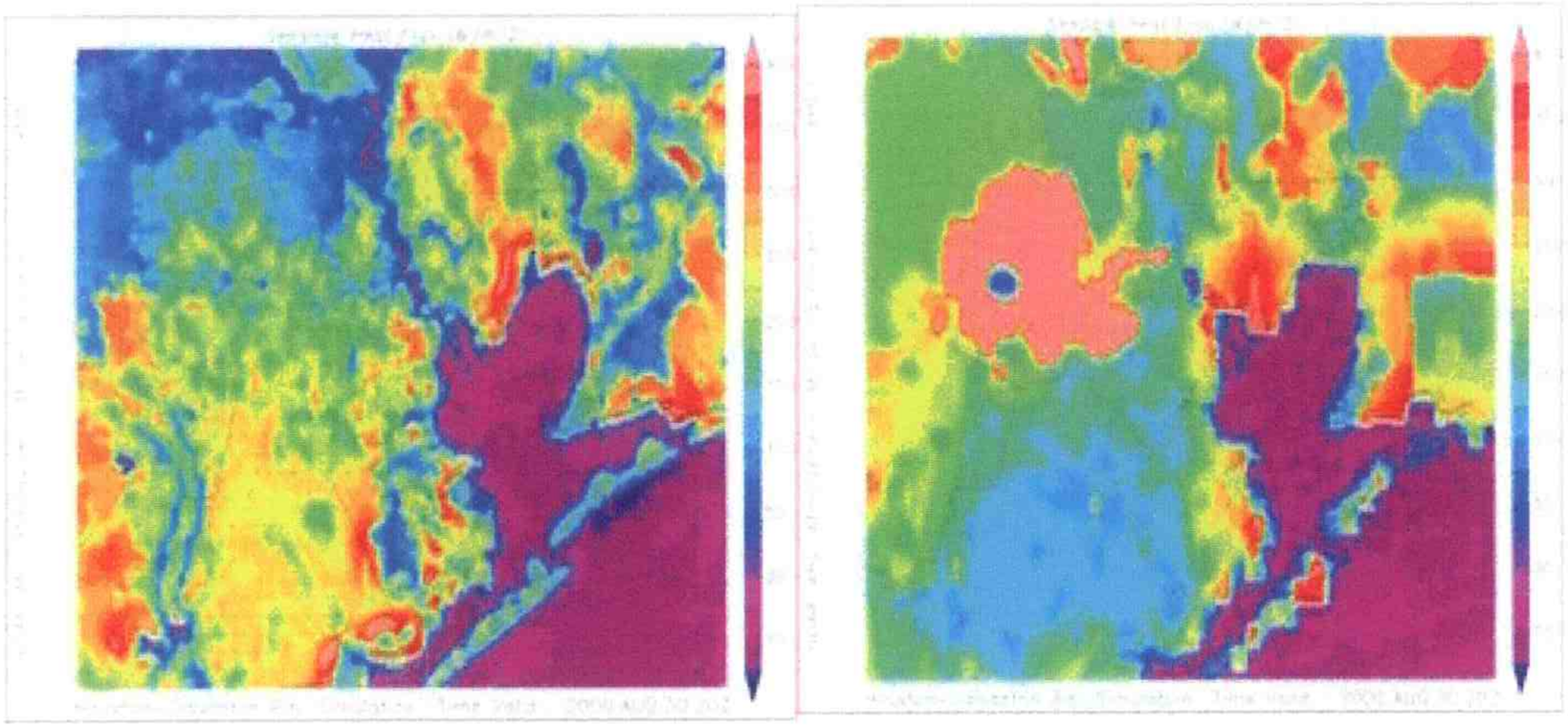

Figure 20. Sensible heat flux (20 UTC, August 2000) DA-SM2-U (left hand side); Standard roughness approach (right hand side).

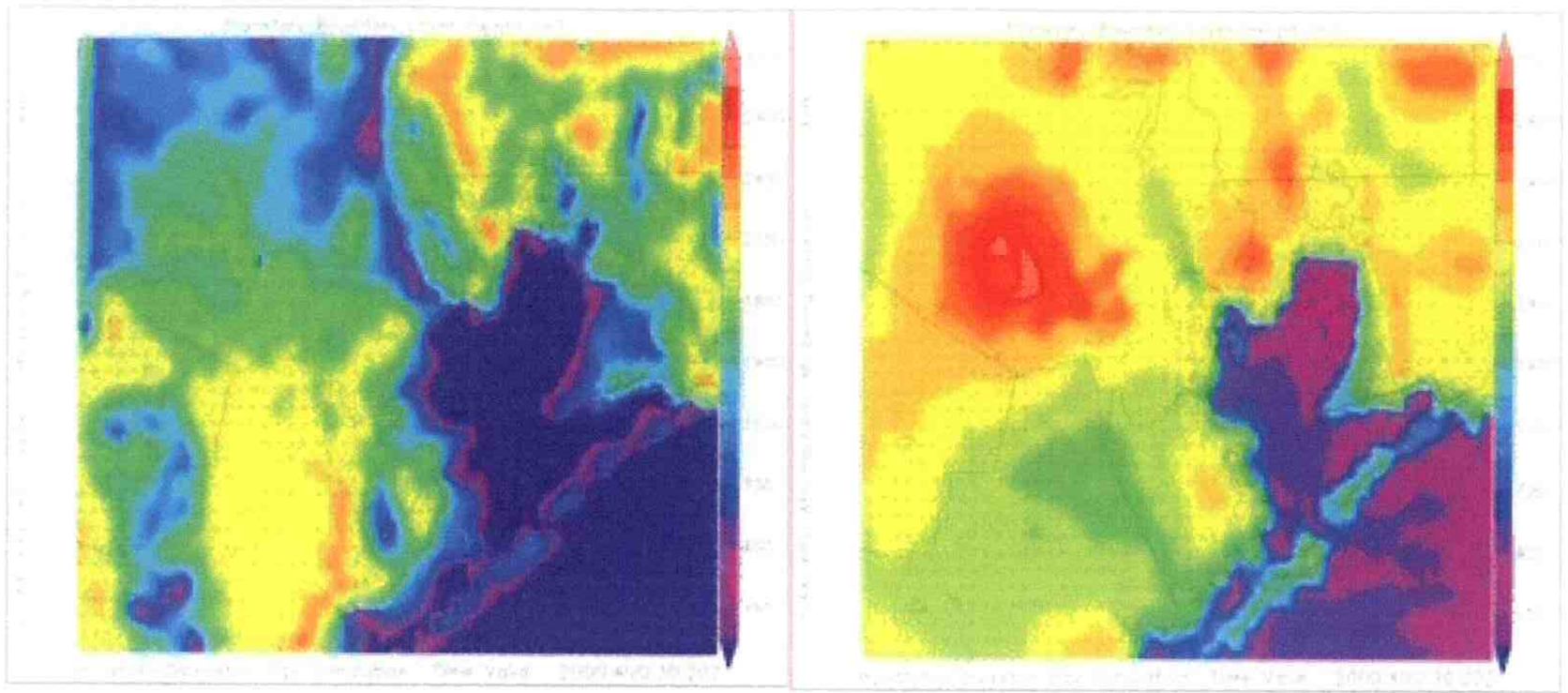

Figure 21. PBL height (m) (20 UTC, August 2000) DA-SM2-U (left hand side); Standard roughness approach (right hand side).

2.3.5 Advancing the Neighborhood-Scale Version of CMAQ

Air quality simulation models need a more advanced capability for application at finer scales and to serve as tools for performing exposure and risk assessments in urban areas (Ching *et al.*, 2004a; 2004b; 2004c). Also, air pollutants need to be modeled at relatively-fine spatial resolutions to reveal "hot spots" in urban areas. Fine resolution mesh simulations require that emissions and meteorology be characterized at commensurate mesh sizes and that a suitable database be available to evaluate the model results. One of the challenges in extending CMAQ to a relatively fine mesh is to account for the presence of urban streets and tree canopies. Preliminary results by Ching *et al.* (2003) at 1.3 km mesh size, using a simplified set of urban canopy parameters for Philadelphia based on surveys of urban building geometries (Otte *et al.*, 2004), have shown that the resulting MM5 and CMAQ fields are significantly impacted by the introduction of urban canopy parameters (UCPs) of buildings. To examine the impact of a finer grid mesh, the use of a more sophisticated urban canopy parameterization (Dupont *et al.*, 2004) with a detailed urban morphology data set, and an improved depiction of the nearby water temperatures, the CMAQ system is being tested over the Houston, Texas, area.

Before embarking on a comprehensive suite of model simulations and evaluations, the sensitivity of the CMAQ system was examined using a one-day test case on August 30, 2000. For this case, sensitivity tests were designed to examine the differences in concentration fields resulting from the urbanized MM5 system and the standard version of MM5 run at 1-km resolution. Before setting up the 1-km simulations, 4-km grid-mesh simulations were improved using high-resolution sea-surface temperature (SST) observations taken from the Polar-orbiting Operational Environmental Satellites Advanced Very-High Resolution Radiometer. The use of

the SST observations in MM5 improved the accuracy of the near-surface land-bay breeze circulation simulations, by clearly reproducing the observed wind directions and the wind shift at the time of the Bay breeze passage not captured in the control run. Subsequently, it was decided to adopt the use of the more accurate temporally-resolved SSTs for Galveston Bay in the Houston study.

The sensitivity of CMAQ to different grid meshes is shown in Figure 22. The left panel shows a one-hour snapshot of formaldehyde from the 1-km grid simulations driven by the DA-SM2-U version of MM5, and the center panel shows results from the 4-km standard version of CMAQ. While the general pattern is similar for the two panels, "hot spots" with the 1-km version of the model are clearly visible. The right most panel illustrates the sub-grid variability associated with the 4-km resolution concentration variations that are possible using the 1-km predictions. Variability in this panel is indicated by computing in each 4-km grid the ratio of the range of the 1-km results by the mean of the 1-km results. These results were obtained by sampling the 16 1-km grid values in each 4 km cell. Areas with large normalized range-to-mean values are visible throughout the model domain.

During FY-2005, additional studies are planned to examine the use of the UCP for 1-km CMAQ simulations over Houston. Working in collaboration with scientists from the University of Houston, the Division plans to simulate several weeks of the Texas 2000 air quality study period and to evaluate model results with observations collected during the study. The combination of UCP-driven meteorology for fine-scale modeling and more accurately modeled lake-land breeze circulations may in the future improve the simulations of atmospheric flow and air toxic concentrations for Houston and other urban areas with similar climatic features.

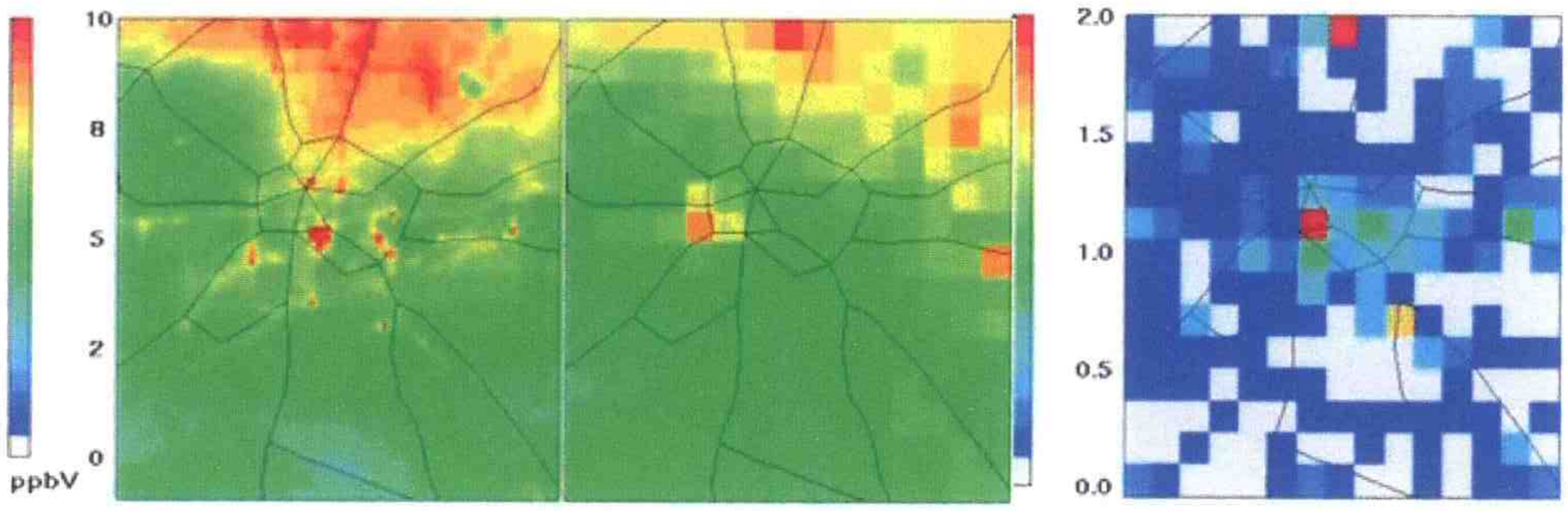

Figure 22. Formaldehyde (ppb) simulations for August 30, 2000 at 2100 GMT. Left panel is the 1 km simulation (with UCP), middle panel is native 4 km grid size. Right panel is range of values of the individual 16 1-km cells in each 4 km grid normalized by the 4 km aggregated cell mean.

2.3.6 Modeling Subgrid Concentration Variability

When air quality (AQ) models are used for human exposure and risk assessments they need to provide detailed information on the location and magnitude of hazardous air pollutant, or air toxics, concentrations, with particular interest in capturing extreme values, or hot spots. Regional-scale AQ models are typically limited to relatively coarse resolutions when simulating mean pollutant concentrations for each grid cell volume. Computational fluid dynamics and coupled large-eddy simulation with photochemistry techniques allow AQ simulations with much finer grid spacings, but these types of simulations are impractical for long-time integrations or operational use. Thus, procedures are needed for representing the subgrid pollutant concentration extremes in regional models without requiring concurrent fine resolution simulations.

During FY-2004, an initial effort to formulate distribution functions to represent subgrid variability (SGV) fields was begun by the Division and the ARL Atmospheric Turbulence and Diffusion Division, Oak Ridge, Tennessee. Initial description and results are provided in Herwehe *et al.* (2004). The approach is to improve air quality simulation capability for human exposure and risk assessment modeling tools in urban settings by providing within-grid concentration variability distribution functions in the form of probability density functions (pdf) as a complement to regional or urban scale grid simulations (Ching and Byun, 1999). This effort continues an exploratory phase begun in FY-2003, using results from a CMAQ simulation for Philadelphia at 1.3-km grid size to determine the pollutant pdf characteristics and parameters representing the subgrid scale variability for 4-km and 12-km grid meshes. Preliminary analyses indicate that the within-grid spatial variability in concentration fields arising from the distribution of sources in each grid can be very important, and in many instances, perhaps even as or more important than the grid resolved fields for exposure analyses. Further refinements will be possible when modeling results from the source distributions and from subgrid chemistry become available.

Work continues to describe and characterize properties of distribution functions in terms of their shape, location and scale parameters as a means to derive parametric fields of SGV functions. The Dataplot command script under development for research was named Concentration Distribution Functionware, or CDFware. Desired CDFware improvements include the ability to detect multi-modal, particularly the relatively common bimodal, data and to fit such mixed multiple distributions as a mixture of two Weibull distributions in the bimodal case to the data set. CDFware will also be applied to higher resolution outputs from neighborhood-scale models in order to determine whether more coherent parameter fields can be detected at the finer resolutions.

2.3.7 Developing and Applying CFD 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. 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 RANS (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. Progress has been made on CFD development of wide ranging atmospheric boundary layers (Huber *et al.,* 2004a).

While setting up a working model of the extremely complex building environment for Lower Manhattan was a challenging exercise, there were many lessons learned that should make it easier to set up similarly complex urban environments in the future. An overview was published on numerical modeling done in support of the studies following the event of September 11, 2001, in Lower Manhattan (Huber *et al.*, 2004b). A CFD simulation for the Lower Manhattan building model has not been done. Cooperation from other agency is being arranged to support a full simulation during FY-2005. Nonetheless, the current results are valid for winds from the West (negative x direction) since all upwind buildings to the Hudson River are included. Figure 23 presents a comparison with a vertical profile of measurements from the EPA wind tunnel model. Figures 24 and 25 show an example of the flow field details for a vertical and horizontal slice. Figures 26 and 27 show example flow and concentration detail surrounding an emissions source in the "ground zero" area. 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, 2004).

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 could 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). Preliminary results supporting this program are presented in Figures 28 and 29. 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.

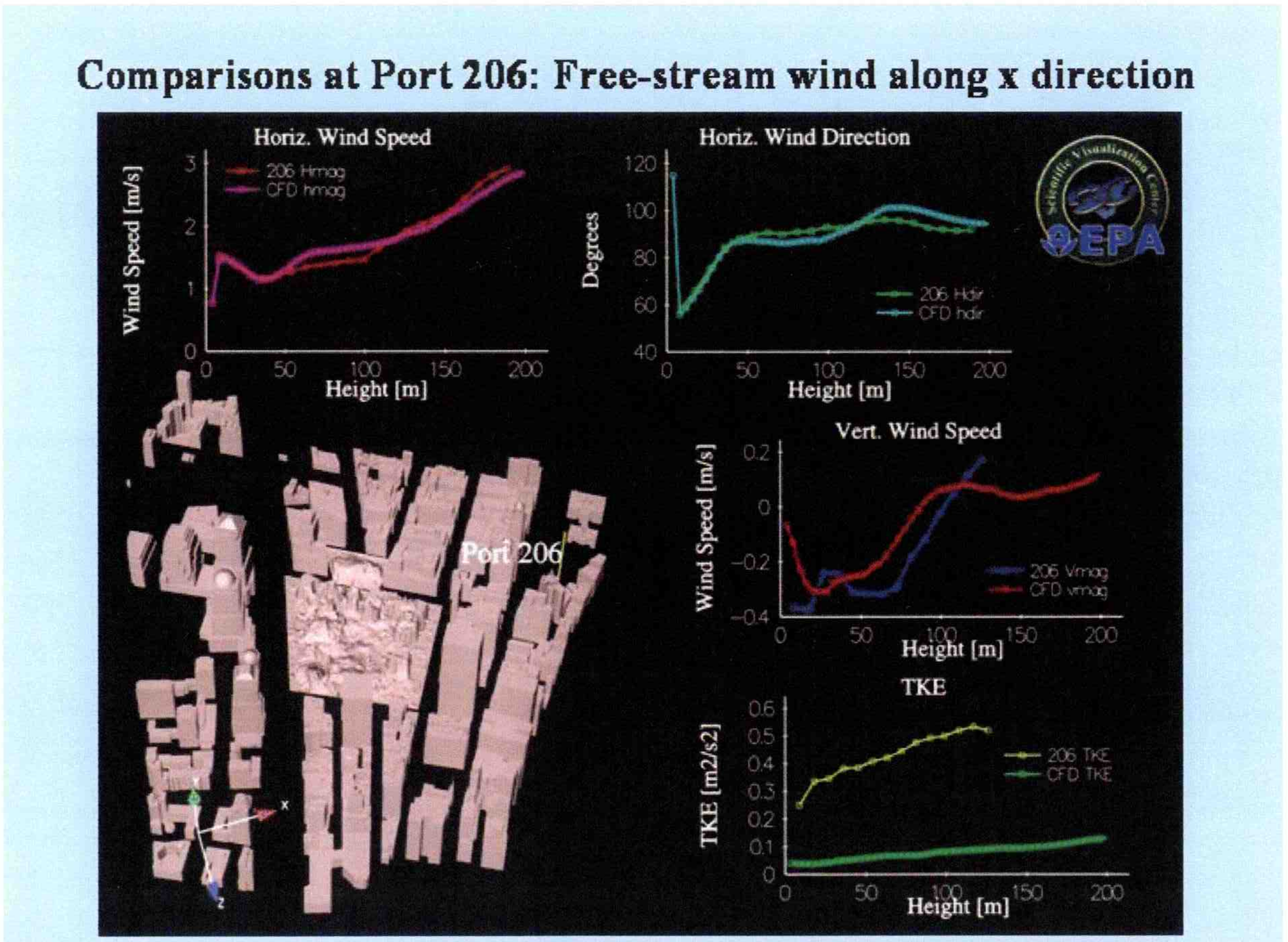

Figure 23. Comparison between vertical profile measurements of wind speed, wind direction, and TKE (Turbulent Kinetic Energy) made in the EPA wind tunnel model of lower Manhattan, and the corresponding CFD predictions.

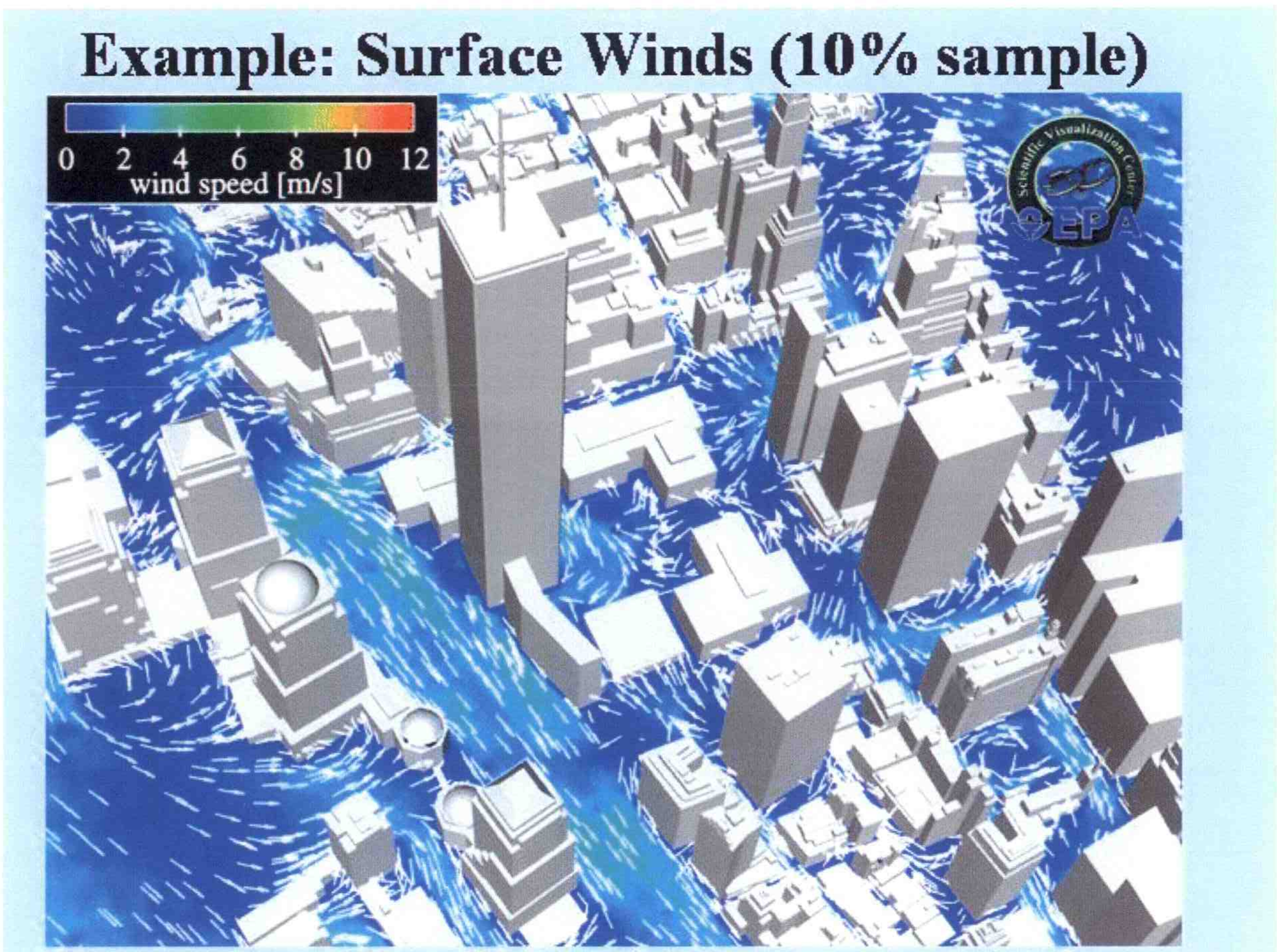

Figure 24. Predicted wind speed (m/sec). Flow field details for a horizontal slice at the surface.

Example: Winds of Vertical Plane (10% sample)

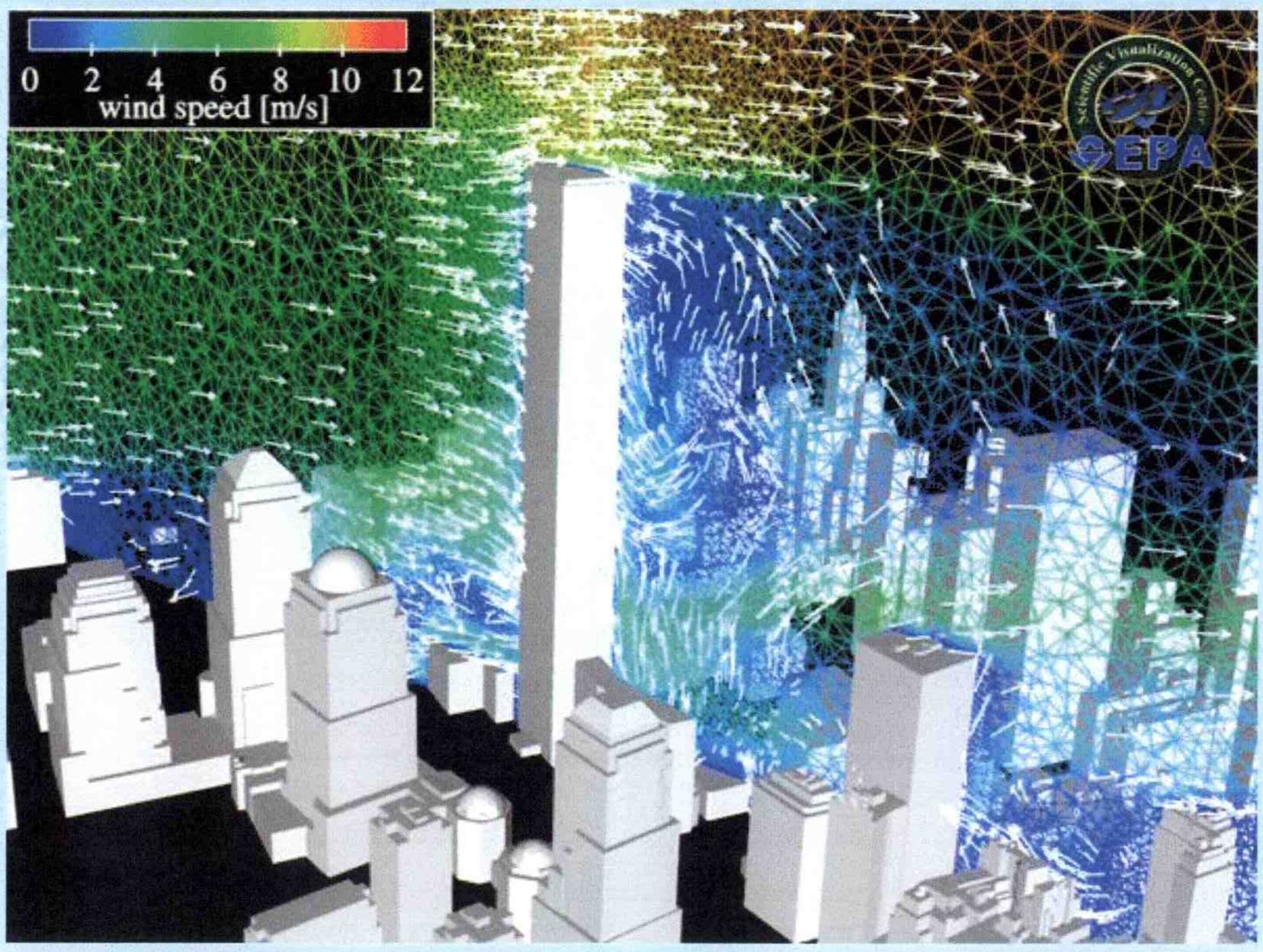

Figure 25. Predicted wind speed (m/sec). Flow field details for a vertical slice.

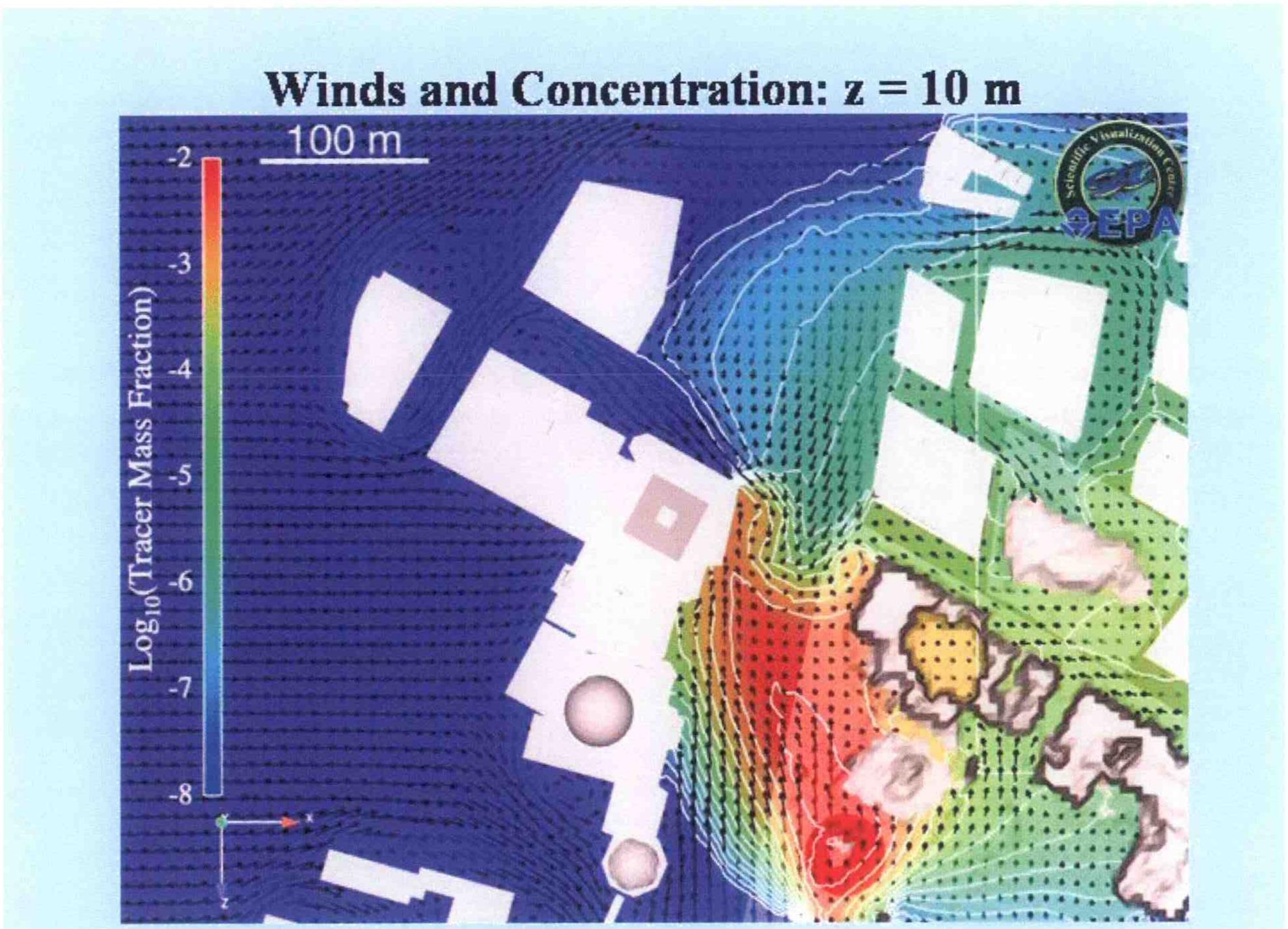

Figure 26. Wind vectors and concentration contours surrounding an emissions source in the "ground zero" area.

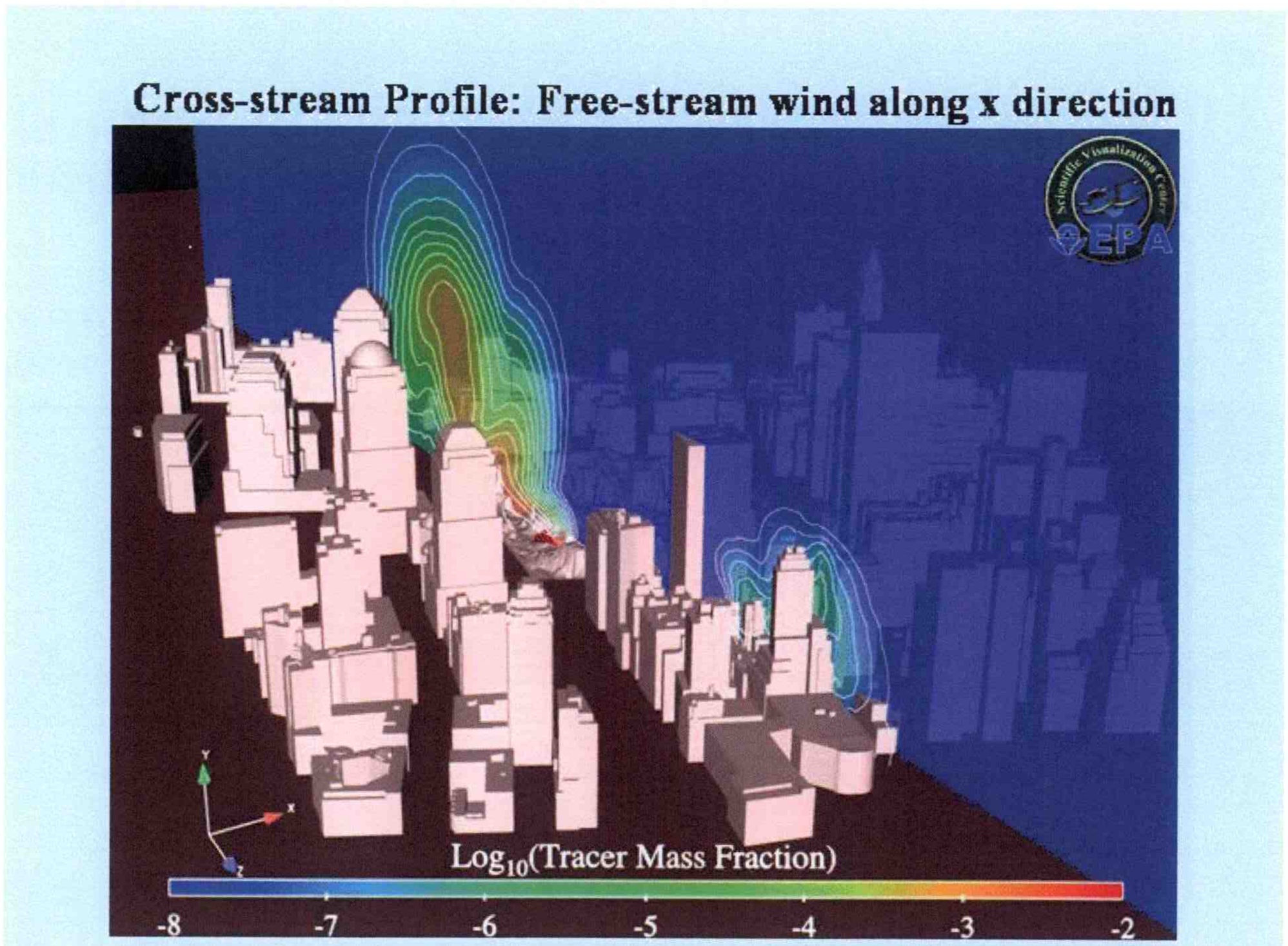

Figure 27. Vertical concentration profiles surrounding an emissions source in the "ground zero" area.

Figure 28. Preliminary predictions of wind speed for a simulation supporting the Department of Homeland Security's New York City Urban Dispersion Program.

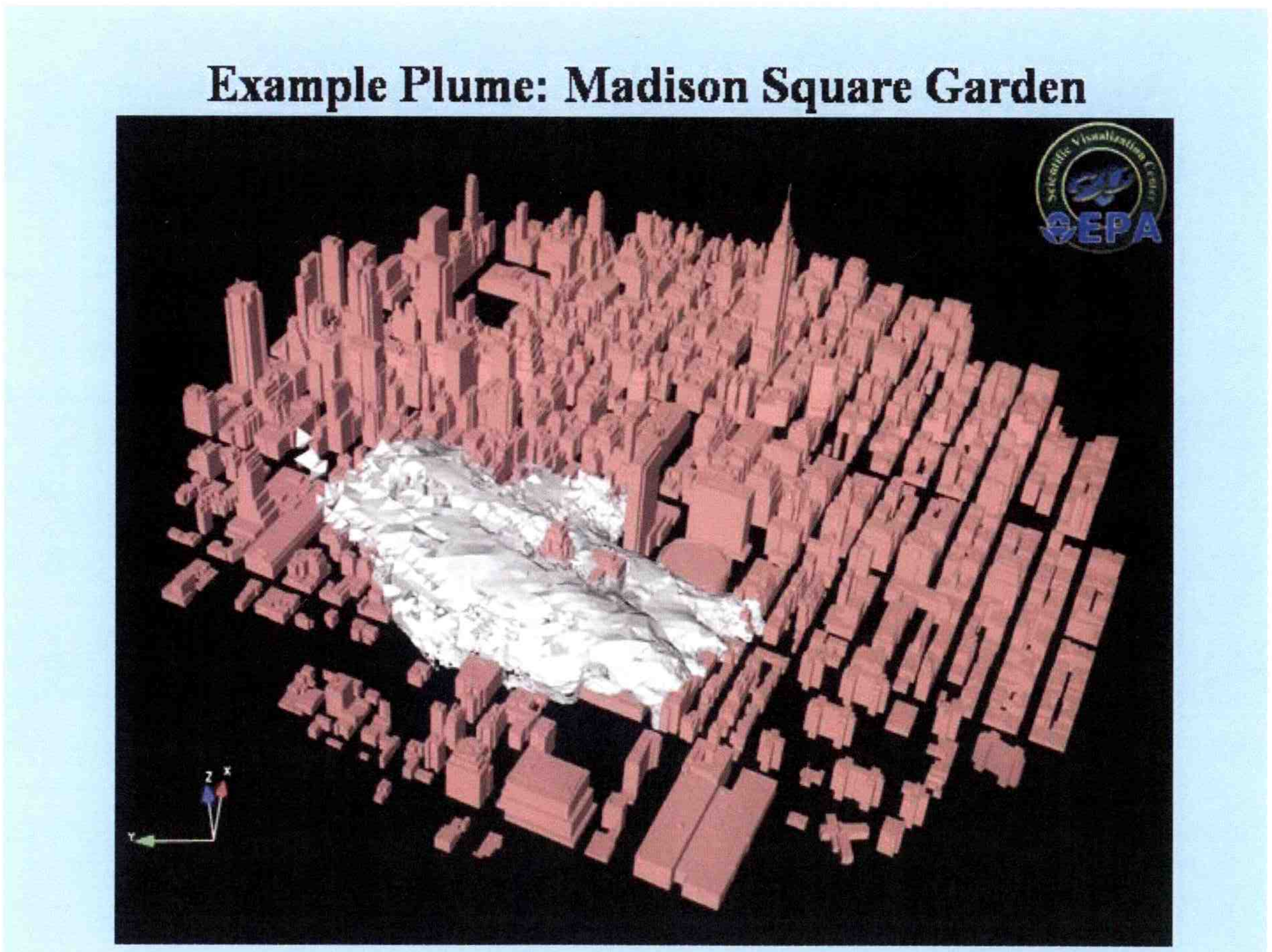

Figure 29. Example of predicted plume dispersion for a simulation supporting the Department of Homeland Security's New York City Urban Dispersion Program.

2.4 Multimedia Modeling and Application Studies

2.4.1 Multimedia Integrated Modeling System Spatial Allocator

ASMD continued development of the Multimedia Integrated Modeling System (MIMS), which includes the MIMS framework and the Spatial Allocator[2]. The MIMS framework provides a software infrastructure to support configuring, applying, and evaluating environmental models. ASMD enhanced the framework to make it easier to set up complex simulations, for instance, where models are invoked repetitively or where there are many input or output parameters. A Java scientific plotting library, based on the open source statistical package R, was also significantly enhanced. OAQPS used MIMS as the basis for a prototype decision support system. The decision support system uses nonlinear optimization to find promising alternatives that balance economic and environmental objectives. In that system, MIMS provides the infrastructure for user interaction and managing multiple model executions, which are used to explore the decision space.

The Spatial Allocator tool of MIMS is in the process of being upgraded to provide the capability to grid input files needed by SMOKE, including emission inventory data, surrogate files for spatial allocation of emission sources and land cover data needed for modeling of biogenic emissions. It is expected to be completed by fall 2005. The Spatial Allocator requires only grid definitions and for spatial surrogates GIS shape files.

2.4.2 Multi-Layer BioChemical Model for Calculating Dry Deposition

The Clean Air Status and Trends Network (CASTNet) is operated by EPA's Clean Air Markets Division 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. The Multi-Layer Biochemical Model (MLBC) (Wu *et al.*, 2003a; 2003b) is being examined for use in the network operations for predicting the deposition velocity. In its original design, MLBC treats all canopies as a mixture of the plant species. For CASTNet, the canopy at a site is treated as spatially distinct species where the deposition velocity is determined from area weighting the deposition velocities for each of the local species. MLBCv1.0 was modified to allow for this latter approach to develop a new version of the model, MLBC-AW (Area Weighted). Development of MLBC-AW is continuing to assure that the model can be run with network meteorological data. One area of focus will be determining a better

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[2]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.

approximation for the leaf temperature since this is not measured at the network sites, but is an important input to MLBC-AW.

Leaf area index (LAI) and canopy height are not routinely measured at CASTNet sites and are currently modeled using a step-function that is based on measurements made in 1991-1992, and 1997 and depend only on the day of the year. Thus, the same annual leaf-out profile is used each year, whereas actual LAI values respond to interannual variability in rainfall, temperature, radiation, etc. Given the sensitivity of deposition models to LAI, obtaining better estimates of LAI should provide more realistic estimates of deposition flux. Plant growth models offer one option for predicting the response of plants to interannual variability in meteorological conditions. There are many different approaches to plant growth modeling ranging from simple parameterizations to more complicated photosynthetically- based models. During FY-2004, the plant growth algorithm was extracted from the Erosion Productivity-Impact Calculator and embedded within MLBC-AW. This version of MLBC is denoted as MLBC-PG. In MLBC-PG, the meteorology used as input for the deposition model is also used for the plant growth algorithm. Water and temperature stress factors calculated by the deposition model for determining canopy resistance were used in the plant growth algorithm. The LAI and canopy height determined from the plant growth algorithm are used in the deposition model for determining pollutant deposition velocities. Comparisons of model derived LAI with the CASTNet step-function showed potentially important differences in LAI. However, the CASTNet sites have numerous extended periods with missing meteorological data, which make the use of the plant growth model unfeasible at this time. As a result of this modeling work, consideration is being given to having site operators routinely measure LAI for input to the deposition model.

2.4.3 Chesapeake Bay 2007 Re-Evaluation

ASMD has established a long-term relationship with the EPA and NOAA Chesapeake Bay Programs to address multi-media environmental problems where the atmosphere is an important 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 TMDL (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 delisting, and ASMD is participating in the re-evaluation process. The best science is desired for the re-evaluations, and during the period between major re-evaluations, ASMD is changing its multi-media modeling of nitrogen from the Extended RADM to its new model, CMAQ. The CMAQ dry deposition algorithms were revised in 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 with 40 cases was developed for CMAQ that can

directly address seasonal deposition. The outer, continental grid resolution is 36-km, a significant reduction over the 80-km resolution used with the Extended RADM, and now covers the entire lower 48 States. For Chesapeake Bay multi-media simulations, a 12-km nest over the Mid-Atlantic region covering most of the Chesapeake Bay airshed was developed. This inner nest better resolves the Bay surface compared to the 20-km nest used with the Extended RADM. In FY-2004, the adaptation of the aggregation method to the new aggregation data set was completed and the base year simulation was updated to use 1999 and 2001 emissions to better match the new base year of 2000 used by the water quality model. Also, a new 2010 NO_x SIP call futures case was simulated to compare the changes with previous estimates made using the Extended RADM, which used a 1990 base year. The CMAQ-predicted relative change was consistent with the Extended RADM-predicted relative. As expected, the relative change from 2001 to 2010 was smaller than the change from 1990 to 2010 because NO_x emission began trending downward after 1996. However, the absolute changes in nitrogen deposition were not consistent. Comparisons against the 2001 annual run of CMAQ also showed inconsistencies with the aggregation results. This will be investigated in FY-2005.

2.4.4 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. 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 MAQSIP (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, show that only 5 to10 percent of the NH_x budget dry-deposits locally, while most of the ammonia emissions are involved in long-range transport, contrary to conventional wisdom. The model results are consistent with spatial and temporal trends in the ammonia wet deposition data. Nonetheless, the conventional wisdom persists and distorts studies of nitrogen-cycling in coastal estuaries, introducing significant errors in them.

The 1999 summer period was chosen for the next phase of analysis due to availability of special 12-hour integrated gas and particle measurements at the Clinton site in the middle of the hog farm area in North Carolina. The ammonia inverse modeling was re-applied to July and August 1999. Simulations were carried out at 32-km and 8-km grid-cell sizes with the newer CMAQ with the new M3Dry deposition algorithms. 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 and Atlanta, Georgia. However, with the updated

M3Dry deposition algorithms, the process analysis now shows that dry deposition of ammonia in CMAQ is 4-5 times higher than previously estimated. The new estimates may be too high because the bi-directional air-surface exchange of ammonia is ignored. A new simulation period is being selected for which dry deposition measurements in North Carolina exist to better assess and bound the model results. The goal now is to provide some bounds on the ammonia budget calculations.

2.4.5 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. ASMD was asked to work with the Tampa Bay National Estuary Program to assess the atmospheric contribution of nitrogen to Tampa Bay. Tampa Bay provides an important atmospheric multi-media problem 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-2005. 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 5-day long sequences, could support a credible analysis of transport over Tampa Bay. The conclusion was no, 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. Retaining the 2-km resolution would also provide better 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 rainfall be 50 percent higher than average. April 2002 through March 2003, excluding December 2002, will be used for the Tampa Bay study. The meteorology for this period will be generated during FY-2005 while CMAQ-UCD is being evaluated.

2.4.6 Multimedia Research for CMAQ-Hg

During FY-2004, the CMAQ-Hg code as described in Bullock and Brehme (2002) was updated to the September 2004 release of CMAQ. After confirmation of correct implementation, the code was moved to an ASMD Linux machine. Proper implementation was again confirmed. Upon completion, the code was shared with OAQPS. Following initial Linux implementation, a single column version of CMAQ-Hg was defined, which will be used to test proposed CMAQ modifications to facilitate dynamic surface/atmosphere flux estimation within the CMAQ system.

2.4.7 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 than is necessary 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, multi-year averaged deposition is desired. The Aggregation method was developed and embodied in a software tool to create climatological average fields of atmospheric deposition of sulfur and nitrogen across the United States to support air-water linkages, using outputs from a regional air quality model. This method essentially uses a set of air quality modeling simulations based on an archive of atmospheric transport cases to create climatological average deposition estimates. The Aggregation method/air-water linkage was used extensively by the Chesapeake Bay Project for its nitrogen management planning, demonstrating its usefulness. However, ASMD is the only group using the Aggregation method. Wider use was limited because it was developed in SAS.

The objective of this project in Multimedia Tools Development is to make the Aggregation method available to the wider client community through an easy to use software tool. To meet the objective, the upgraded Aggregation software program was converted from SAS to R, a widely used and supported open-source statistical package. The output was converted to the Models-3/CMAQ format, an easy to understand front end to the package was developed, and documentation was written. The R package is easier to use than the SAS approach, allowing less experienced users to be able to carry out the aggregation methodology. The output files can be viewed with the Package for Analysis and Visualization of Environmental Data™[3] (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 compared to mapping the

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

results using SASGraph™[4] and enhances the users ability to display results. The R Aggregation Package, RAGG, documentation, and a test data set with inputs and the correct output answer are on EPA's anonymous ftp site for download. The ftp site can be reached from the ASMD website page on Multimedia Modeling Tools (*www.epa.gov/asmdnerl/Multimedia/software.html*) under the heading R Aggregation Tool or RAGG. A URL is also provided for the R website in case a user needs to install R.

2.5 Climate Change Impacts on Regional Air Quality

The Climate Impacts on Regional Air Quality (CIRAQ) project was initiated in FY-2002 and will directly contribute to the EPA Global Change Research Program's (EPA GCRP) assessment reports 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 change 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-2003-04. During FY-2004, a Quality Assurance Project Plan was developed and approved for CIRAQ and baseline model-ready meteorology and emissions files were processed. During FY-2005-06, these baseline scenarios will be followed by processing of model-ready future (2050) meteorology and emissions scenarios and 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.

2.5.1 Regional Climate Downscaling of Meteorology

To support this project and ultimately the air quality assessment, the EPA GCRP is funding the Department of Energy's (DOE) Pacific Northwest National Laboratory (PNNL) to develop current and future regional climate simulations. These simulations 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-2003, 10-year MM5 simulations using NCEP reanalysis fields as boundary conditions were completed (1990-2000) and transferred to ASMD for archiving. During FY-2004, PNNL completed two additional 10-year MM5 simulations with boundary condition links to the National Aeronautics and Space Administration (NASA) Goddard Institute for Space Studies (GISS) GCM. MM5-GISS simulations were performed for a reference period (*e.g.*, 2000 ± 5 years) and a future period under climate change conditions (*e.g.*, 2050 ± 5 years). As regional climate modeling simulations become available, ASMD regularly archives the data and develops the model-ready meteorology fields needed for CMAQ and the emissions processor SMOKE©.

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[4]SAS is a registered trademark of SAS Institute, Inc., Cary, NC, USA

2.5.2 Chemical Emissions Processing

This effort was formally initiated during FY-2004. Sample model-ready regional climate scenarios were processed through SMOKE© to better determine resource requirements and to identify potential quality assurance issues. The base inventory used is the EPA 2001 modeling inventory, projected from the 1999 National Emission Inventory (NEI) version 3. Preliminary results indicate successful processing and expected levels of regional emission response to climate variability. Emissions processing for the remaining reference period will be completed in early FY-2005, with future scenario processing to be completed as model-ready meteorology become available. The same EPA 2001 modeling inventory will be used with the future climate scenarios for input to the 2007 air quality assessment product. Collaboration is on-going with the EPA National Risk Management Research Laboratory regarding the development of emission inventories that could be used in future (2010) analyses products.

2.5.3 Global Climate and Chemical Transport Simulations

During FY-2003 and 2004, global climate and chemical transport simulations were completed and analyzed by collaborators at Harvard University under direct project support. Results from this study suggest that under potential future climate change conditions, an increase in stagnation events and pollution episodes would occur. These findings are particularly relevant for the ASMD portion of this study because these global climate and chemical boundary conditions are used in CIRAQ regional downscaling simulations of MM5 and CMAQ. These global chemical transport modeling results have been archived at ASMD, and software code has been developed and tested to produce CMAQ boundary conditions from these modeling results. Since this series of global simulations only included ozone chemistry, the boundary condition estimates for aerosol species is currently limited to default estimates. A second series of global CTM simulations has been offered by 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 2005, chemical boundary conditions from both sets of global CTM will be considered for the CMAQ simulations.

2.5.4 Methods Developed for Analysis and Evaluation of Regional Climate Simulations

Analysis tools were developed during FY-2004 to evaluate historical MM5 simulations against a suite of observations and to generate graphs using GrADS (Grid Analysis and Display System)[5]. A second tool was developed to extract meteorological data, corresponding to weather

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[5]Copyright 1988-2004 by Brian Doty, Center for Ocean-Land-Atmosphere Studies(COLA), Institute of Global Environment and Society, Calverton, MD. All Rights Reserved. Permission is granted for an individual or institution to use this software (in any

observation sites, from the MM5 simulation and insert into a CIRAQ database table. Additionally, the tool decodes observed meteorology and inserts it into the same database. A program was developed to extract simulated and observed meteorological variables from the database and plot distributions for comparison between model and observations. During FY-2005, these tools will be combined with time series and spatial analysis methods developed during FY-2004 to analyze, evaluate and compare present-day downscaled climate scenarios to observations.

Spatial analysis during FY-2004 focused on preliminary evaluation of two global reanalysis data sets as a method development test and as a means to estimate uncertainty in our estimates of present climate condition. A cluster analysis method was implemented in which dominant patterns of 700 mb atmospheric transport derived from *u* and *v* component wind are identified from reanalysis meteorological data. Distributions of dominant pattern frequency, a combination of event frequency and persistence, were developed and applied seasonally to 1800 UTC 700 mb reanalysis data from 1985 through 1994 across the continental United States. Results of this analysis indicate that, although the dominant 700 mb transport patterns appear very similar (very good agreement regarding direction and +/-15 percent windspeed agreement), the frequency of these patterns often occur differently within their respective data sets. During FY-2005, these estimates of baseline uncertainty will be compared with similar GISS/MM5 baseline results to construct statements regarding baseline and future model pattern similarities and differences as well as bias implications for the air quality simulations to be initiated during FY-2005.

Time series analysis methods were tested to separate out temporal variability in the regional climate modeling results. With a 10-year simulation, it will be possible to consider daily, synoptic, seasonal, and interannual variations. Use of time series analysis may help to identify differences between periodic variations and actual trends in climate. The same general methods can also be used to analyze air quality predictions once CMAQ simulations are completed.

A summary report regarding analysis and evaluation of the regional climate simulations will be produced during FY-2005. The report comprises a description of the ASMD regional climate scenario data management and quality assurance tool along with quality assurance summaries. The statistical methods that have been developed for the regional climate analysis application will be described and analysis results for point, time series and spatial analyses will be presented. Scenario evaluation for the baseline period will include comparison to surface observations and global reanalysis data sets. Such comparison will be used to identify regional climate model strengths, weakness and bias' that could potentially impact the air quality model simulations. If future climate scenario results are available, the analysis will also include comparison of baseline climate scenarios to projected future conditions. These analysis will be performed on the full 20 year (10 year baseline and 10 year future) climate simulation.

2.6 Specialized Client Support

2.6.1 European Monitoring and Evaluation Program

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

In FY-2004, the United States and Canadian representatives hosted a workshop on fine particulate matter measurement and modeling to summarize the experiences of the EPA Supersite program for the benefit of the EMEP program. The workshop was held in April 2004 in New Orleans, Louisiana. The last EMEP workshop sponsored by Canada and the United States was over a decade ago in Nova Scotia. The purposes of this workshop were to exchange information with European colleagues and arrive at a sense of the community regarding the current state of measurement and regional modeling for fine particulate matter in the atmosphere and recommend where we need advances in tools and techniques. Approximately 60 participants attended, 18 from Europe, 15 from Canada, and 28 from the United States. A United Nations UNECE (United Nations Economic Commission for Europe) EMEP summary report with key, high-level workshop conclusions is on the EMEP website in Geneva. The workshop discussions had such a wealth of information and insights of use to both EPA and Environment Canada that it was decided to produce a longer workshop report.

2.6.2 Support of the 1999 National Air Toxics Assessment

Spatial allocations were improved for aircraft emissions in support of the 1999 National Air Toxics Assessment. This improvement is implemented in an EMS-HAP (Emissions Modeling System for Hazardous Pollutants) User's Guide, Version 3 (U.S. Environmental Protection Agency, 2004). Specifically, the improved spatial allocations for aircraft involve including itinerant operations for general aviation, commercial aircraft, military, and air taxi as a basis for allocating associated county-level emissions to corresponding airport locations. This capability was added to the SMOKE© 2.0 emission processor. As a result of this work, inconsistencies in the 1999 National Emission Inventory were exposed.

Data structures for NATA involving concentration, exposure, and risk model estimates were synthesized for application within the EPA Data Warehouse. This synthesis allows greater utilization of the single data set, opens the data set to more improvement and refinement by the user community, and allows rapid implementation of last-minute program changes. This data format will be used as a base for the NATA Explorer, a visualization tool for all 1999 NATA data.

2.6.3 The Philadelphia Air Toxics Project

An extensive air toxics modeling project was conducted in Philadelphia to assist communities in reducing air toxics emissions and risk through voluntary air toxics emissions reduction efforts. This project modeled voluntary emission reduction efforts to address the air toxics contributions from diesel powered trucks, buses, and other mobile sources, which were identified through NATA as major contributors to air toxics emissions in the region.

The Air Toxics Project included modeling of emission sources in Philadelphia and the surrounding counties in Pennsylvania, New Jersey, and Delaware. Point, area, mobile, and emissions from such large sources as airports and landfills were processed through the EMS-HAP for input in the Industrial Source Complex dispersion model. The concentrations estimated by ISC were then adjusted to take into account air toxics concentrations resulting from secondary reactions in the atmosphere and from background sources. These results are a component of human exposure modeling and risk analysis. In addition to focusing on current air toxics emissions and risks, this detailed modeling study includes an assessment of expected air toxics emissions and concentrations levels in 2010. This information will assist in determining the likely effect of required control efforts.

2.6.4 Support Center for Regulatory Air Models

SCRAM (Support Center for Regulatory Air Models) website continued to be updated to reflect additions of models and data sets. Some of these changes included modifications to the 7th Modeling Conference for Air Quality Modeling (http://www.epa.gov/scram001/ttn26.htm) files specifically related to the promulgation of the AERMOD (AMS EPA Regulatory MODel) system. Modifications to AERMOD include new dry and wet deposition algorithms. The SCRAM website is currently undergoing a structural change to provide more information to users and utilize a more intuitive logic flow for navigation. Each major area of SCRAM is being analyzed: models, guidance, meteorological data, *etc*. The Model Clearinghouse area, which provides scientific and technical support to the Regional Offices, will be restructured to provide full access and search capabilities to the general public. Responsibilities and technical support of the Model Clearinghouse were provided on an on-going basis to the Regional Offices on a variety of issues related to PSD (Prevention of Significant Deterioration) and NSR (New Source Review).

2.6.5 Eta Data Assimilation System Review

Six- and seven-year EDAS (Eta Data Assimilation System) 700mb wind cluster data were analyzed to study the effects of global change. The time series output were stratified by season (3 months/season) using the SAS FASTCLUS©[6] routine to generate clusters of days with the most similar spatial patterns through the entire national domain. These preliminary clusters were then re-analyzed to compare the EDAS (1997–2002) analysis results to those presented in Cohn *et al.* (2001) for the period of 1984–1992. The resulting array of data consisted of 1,935 observations. These two output analyses were compared to see if the methodologies employed were consistent. Half of the two analyses compared very well and the other half compared moderately well, while very few of the analyses did not match.

2.6.6 Development of a Response Surface Model for Ozone

One of the most time-consuming tasks in identifying effective strategies to improve air quality is running the air quality model for all possible control options. More air quality control options can be considered by using a response surface model that accurately replicates the complex interactions of an individual air quality simulation. ASMD staff, with various EPA and non-governmental partners, applied techniques used in meteorological and other model response analyses to develop an ozone response surface based on CAMx[7] modeling that will be used to estimate the effects of a series of planned mobile source emission reductions. Over 140 CAMx runs were analyzed and interpreted to develop the surface that considered 14 separate dimensions. An additional 10 runs were analyzed for validation purposes. The "model of the model" was determined to accurately reproduce the results from an individual simulation, typically within 0.2 ppb depending upon the output metric.

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[6] Copyright 1999 by SAS Institute Inc., Cary, NC, USA. All rights reserved.

[7] Comprehensive Air Quality Model with Extensions

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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
AERMOD	Air dispersion model
AIM	Aerosol Inorganic Model
AQ	Air quality models
AQF	Air quality forecast
ARL	Air Resources Laboratory
ASMD	Atmospheric Sciences Modeling Division
ASPEN	Gaussian plume model
AT	Air toxins
AVIRIS	Airborne Visible/Infrared Imaging Spectrometer
BEIS3.12	Biogenic Emissions Inventory System version 3.12
BRACE	Bay Regional Atmospheric Chemistry Experiment
CAA	Clean Air Act
CAAA	Clean Air Act Amendments
CAMx	Comprehensive Air Quality Model with extensions
CB-IV	Carbon-Bond-IV
CASTNet	Clean Air Status and Trend Network
CDFware	Concentration Distribution Functionware
CFA	SOS Cornelia Fort Airpark
CFD	Computational fluid dynamics
CIRAQ	Climate Impact on Regional Air Quality
CLEANER	Collaborative Large-Scale Engineering Analysis Network for Environmental Research
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 PinG	Community Multiscale Air Quality modeling system Plume in Grid mod
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 plume-in-grid model
CTM	Chemistry-Transport Model
CMU	Carnegie Mellon University

DA-SM2-U	A multi-layer canopy and soil model with few layers of a couple meters within the canopy depending on the mesh of the mesoscale model domain, and three layers within the ground; a surface soil layer for the natural surfaces, a root zone layer, and a deep soil layer
DOE	Department of Energy
EBI	Euler Backward Iterative
EC	Elemental Carbon
EDAS	Eta Data Assimilation System
EMD	Empirical Mode Decomposition
EMEP	European Monitoring and Evaluation Program
EMS-HAP	Emissions Modeling System for Hazardous Pollutants
EOF	Empirical Orthogonal Functions
EPA	Environmental Protection Agency
EPA GCRP	EPA Global Change Research Program
Eta	National Center for Environmental Prediction Mesoscale Model
EtaDry	dry deposition routine
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
GISS	Goddard Institute for Space Studies
GR	Gas Ratio
GrADS	Grid Analysis and Display System
HAPEM5	Hazardous Air Pollutant Exposure Model version 5
ICARTT	International Consortium for Atmospheric Research on Transport and Transformation
IC/BC	Initial Condition/Boundary Condition
IMPROVE	Interagency Monitoring of PROtected Visual Environment Network
ISORROPIA	Thermodynamics module
JST	SOS Jefferson Street
Kz	Minimum value of the surface layer vertical-eddy diffusivity
LAI	Leaf Area Index
LBC	Lateral boundary conditions
M3Dry	Models-3 Dry Deposition Scheme
MAQSIP	Multiscale Air Quality Simulation Platform
MCIP	Meteorology-Chemistry Interface Processor

MCIP2.2	Meteorology-Chemistry Interface Processor version 2
MDN	Mercury Deposition Network
MIMS	Multimedia Integrated Modeling System
MLBC	MultiLayer Biochemical Model
MLBC-AW	MultiLayer Biochemical Model-Area Weighted
MLBC_PG	MultiLayer Biochemical Model- Calculator (EPIC) model was embedded in MLBC and denoted as MLBC-PG
MM5	Mesoscale Model - version 5
Mobile6	Mobile Source Emission
NAAQS	National Ambient Air Quality Standards
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
NMSE	Normalized Mean Square Error
NOAA	National Oceanic and Atmospheric Administration
NSR	New Source Review
NWS	National Weather Service
NYSDEC	New York State Department of Environmental Conservation
OAQPS	Office of Air Quality Planning and Standards
OC	Organic Carbon
OCpri	Primary Organic Carbon
OCsec	Secondary Organic Carbon
ODE	Ordinary Differential Equation
PAVE	Package for Analysis and Visualization of Environmental Data
PBL	Planetary Boundary Layer
PDFs	Probability Density Functions
PDM	Plume Dynamics Model
PinG	Plume-in-Grid
PinG Module	Plume-in-Grid Model
PM	Particulate Matter
PNNL	Pacific Northwest National Laboratory
ppbv	Parts per billion by volume
PREMAQ	Pre-processor for CMAQ
PSD	Prevention of Significant Deterioration
PSU	Pennsylvania State University
PX LSM	Pleim Xiu Land-Surface Model

RADM2	Regional Acid Deposition Model version 2
RANS	Reynolds-Averaged Navier-Stokes
REMSAD	Regional Modeling System for Aerosols and Deposition
RMET	The R Model Evaluation Toolkit,
RMSEs	Root mean squared errors
ROS3	A particular version of the Rosenbrock class of solvers
RSL	Roughness sub-layer
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
SIP	State Implementation Plan
SM2-U(3D)	Represents the thermodynamic effects (e.g.,estimates the heat and humidity fluxes) of the canopy elements at different levels within the canopy
SOA	Secondary Organic Aerosol
SOS	Southern Oxidants Study
SST	Sea Surface Temperature
TEOM	Tapered element oscillating microbalance
TMDL	Total Maximum Daily Loan
UCPs	Urban Canopy Parameterizations
UDP	Department of Homeland Security's New York City Urban Dispersion Program
UNECE-EMEP	United Nations Economic Commission for Europe-European Monitoring and Evaluation Program
UTC	Universal Time Coordinate
VOC	Volatile Organic Compounds
WF	Wavelet Filters
WRF	Weather Research and Forecast
WTC	World Trade Center

APPENDIX B: PUBLICATIONS

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Yu, S., R.L. Dennis, P.V. Bhave, and B.K. Eder. Primary and secondary organic aerosols over the United States: Estimates on the basis of observed organic carbon (OC) and elemental carbon (EC), and air quality modeled primary OC/EC rations. *Atmospheric Environment* 38:5257–5268 (2004).

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Yu, S., B.K. Eder, R.L. Dennis, S. Chu, and S. Schwartz. New unbiased symmetric metrics for evaluation of the air quality model. *CMAS Models-3 Users' Workshop, One Atmosphere, One Community, One Modeling System: Models-3, October 27–29, 2003, Research Triangle Park, North Carolina.* Community Modeling and Analysis System and the UNC at Chapel Hill Carolina Environmental Program, Chapel Hill, NC, CD-ROM, (2003).

APPENDIX C: PRESENTATIONS

Benjey, W.G. An approach for a processed-based unified emission flux based modeling platform. Presentation at the 13th International Emission Inventory Conference, "Working for Clean Air in Clearwater," Clearwater, FL, June 10, 2004.

Bhave, P.V. Postprocessing of model output for comparison to ambient data. Invited presentation at the Particulate Matter Model Performance Evaluation Workshop, Chapel Hill, NC, February 10, 2004.

Bhave, P.V. Measurement needs for evaluating model calculations of carbonaceous aerosol. Presentation at the European Monitoring and Evaluation Program (EMEP) Workshop, Particulate Matter Measurement & Modeling, New Orleans, LA, April 22, 2004.

Bowker, G.E. Wind tunnel projects in EPA's Fluid Modeling Facility. Presentation at the EPA Science Forum 2004: Healthy Communities and Ecosystems, Washington, DC, June 2, 2004.

Bullock, O.R., Jr. Modeling atmospheric mercury deposition to the sounds and other water bodies. Presentation at the Mercury and CO_2 Workshop, sponsored by the North Carolina Department of Environment and Natural Resources, Raleigh, NC, April 19, 2004.

Bullock, O.R., Jr. Modeling transport and transformation of mercury and its compounds in continental air masses. Presentation at the International Workshop on Harmonization of Mercury Measurements, Methods and Models to Assess Source-Receptor Impact on Air Quality and Human Health, Maratea, Italy, May 24, 2004.

Bullock, O.R., Jr. Aqueous reduction of Hg^{2+} to Hg^0 by HO_2 in the CMAQ-Hg model. Presentation at the 7th International Conference on Mercury as a Global Pollutant, Ljubljana, Slovenia, July 1, 2004.

Bullock, O.R., Jr. Atmospheric chemistry and the relative importance of mercury sources. Presentation at the 2004 Mercury Workshop sponsored by the U.S. Geological Survey - Eastern Region, Reston, VA, August 17, 2004.

Ching, J.K.S. Community modeling with CMAQ. Presentation at the 2003 Models-3 Users' Workshop, One Atmosphere, One Modeling System: Models-3, Research Triangle Park, NC, October 27, 2004.

Cooter, E.J. Detecting effect of climate/downscaling issues (scenario development and testing). Presentation at the U.S. EPA Consequences of Global Change for Air Quality STAR Grant Progress Review Workshop, Research Triangle Park, NC, May 24, 2004.

Dennis, R.L. Air quality modeling of ammonia: A regional modeling perspective. Presentation at the NADP Ammonia Workshop, Washington, DC, October 24, 2003.

Dennis, R.L. Time-resolved & in-depth evaluation of PM and PM precursors using CMAQ. Presentation at the Particulate Matter Model Performance Workshop, Chapel Hill, NC, February 10, 2004.

Dennis, R.L. In-depth/diagnostic model evaluation. Presentation at the EPA-NOAA Air Quality Scientist-to-Scientist Meeting, Research Triangle Park, NC, March 2, 2004.

Dennis, R.L. Evaluation of 3-D regional particulate models: measurement needs for inorganic species. Presentation at the US-Canada EMEP Workshop on Monitoring and Modeling, New Orleans, LA, April 22, 2004.

Dupont, S. Application of the urbanized version of MM5 for Houston. Presentation at the 2003 Models-3 Users Workshop, Research Triangle Park, NC, October 27, 2003.

Eder, B.K. An evaluation of the 2003 release of CMAQ. Presentation at the 2003 Models-3 Users' Workshop, One Atmosphere, One Modeling System: Models-3, Research Triangle Park, NC, October 28, 2004.

Eder, B.K. An evaluation of the Eta-CMAQ air quality forecast model as part of NOAA's national program. Presentation at the 2003 Models-3 Users' Workshop, One Atmosphere, One Modeling System: Models-3, Research Triangle Park, NC, October 29, 2004.

Eder, B.K. An evaluation of the Eta-CMAQ air quality forecast model. Presentation at the EPA 2004 National Air Quality Conference: Your Forecast to Breathe By, Baltimore, MD, February 24, 2004.

Eder, B.K. An annual evaluation of Models-3 CMAQ using a 2001 simulation. Presentation at the US-Canada EMEP Workshop on Particulate Matter Measurement and Modeling, New Orleans, LA, April 21, 2004.

Eder, B.K. An operational evaluation of the Eta-CMAQ air quality forecast model for the summer of 2004. Presentation to NWS at Silver Spring, MD, September 8, 2004.

Finkelstein, P.L. Recent research at Purchase Knob, NC. Presentation at the National Park Service Meeting on Sub-Canopy Research, Great Smoky Mountains National Park, March 25, 2004.

Finkelstein, P.L. CMAQ evaluation for acid rain. Presentation at the NADP annual meeting, Halifax, NS, Canada, September 22, 2004.

Gillette, D.A. Wind characteristics during dust storms at Jornada del Muerto. Seminar given to the Department of Range Science, New Mexico State University, Las Cruces, NM, April 10, 2004.

Gilliland, A.B. The Climate Impacts on Air Quality (CIRAQ) project. Presentation to the Committee on Environment and Natural Resources (CENR) Air Quality Subcommittee via teleconference, July 17, 2004.

Huber, A.H. Development of CFD simulation applications for local-scale urban areas and potential interface with mesoscale models. Invited presentation at the American Meteorological Society Workshop on Merging Mesoscale and Computational Fluid Dynamics Modeling Capabilities, Seattle, WA, January 11, 2004.

Huber, A.H. Development, application and evaluation of CFD simulations for local-scale pollutant dispersion. Presentation at the EPA-NOAA Air Quality Scientist-to-Scientist Meeting, Research Triangle Park, NC, March 2, 2004.

Huber, A.H. Program in support of CFD simulations of micrometeorology and contaminant transport within exterior urban building environments. Presentation at the Eighth Annual George Mason University Conference on Transport and Dispersion Modeling, Fairfax, VA, July 13, 2004.

Huber, A.H. CFD simulations within complex urban building environments. Presentation at the Fifth Symposium on the Urban Environment, British Columbia, Canada, August 23, 2004.

Hutzell, W.T. A biogenic role in exposure to two toxic compounds. Poster presentation at the Fall Meeting of the American Geophysical Union, San Francisco, CA, December 8, 2003.

Luecken, D.J. Use of pilot study monitoring data to help evaluate an air quality model (CMAQ) for toxic air pollutants. Presentation at the Workshop on Air Toxics Data Analysis, Chicago, IL, June 3, 2004.

Mathur, R. The Community Multiscale Air Quality (CMAQ) model: Model configuration and enhancements for air quality forecasting. Presentation at the 2004 Air Quality Forecasting Focus Group Meeting, Silver Spring, MD, September 8, 2004.

Pierce, T.E. The importance of lightning NO for regional air quality modeling. Presentation to the Joint Action Group for Lightning Detection System, Office of the Federal Coordinator for Meteorology, Silver Spring, MD, December 3, 2004.

Pierce, T.E. Emissions modeling research in the Atmospheric Sciences Modeling Division. Presentation to representatives from the Mid-Atlantic Regional Air Management Association (MARAMA), Silver Springs, MD, February 18, 2004.

Pleim, J.E. A new non-local boundary layer model. Presentation at the WRF-MM5 User's Workshop, Boulder, CO, June 22, 2004.

Pleim, J.E. New features of the 2003 release of the CMAQ model. Presentation at the 2003 Models-3 Users' Workshop, One Atmosphere, One Modeling System: Models-3, Research Triangle Park, NC, October 27, 2004.

Pleim, J.E. NOAA's Eta-CMAQ modeling system for air quality forecasting. Lecture provided at the Air Quality Forecast Training Workshop, Environment Canada-Eastern Region Headquarters, Halifax, Nova Scotia, February 11, 2004.

Pleim, J.E. Updates and evaluation of the Community Multiscale Air Quality (CMAQ) model. Presented at the 13th Joint Conference on the Applications of Air Pollution Meteorology with the Air & Waste Management Association, Vancouver, BC, Canada, August 23, 2004

Pouliot G.A. Recent advances in the modeling of airborne substances. Presentation at the 2003 Models-3 Users' Workshop, One Atmosphere, One Modeling System: Models-3, Research Triangle Park, NC, October 27, 2003.

Rao, S.T. Using air quality models for emissions management decisions. Presentation at the NRC Committee Meeting, Washington, DC, March 18, 2004.

Rao, S.T. Integrated use of observations and model outputs in air quality management. Presentation at the 3rd Canadian Workshop on Air Quality, Quebec, Canada, March 24, 2004.

Rao, S.T. Climate-air quality interactions. Presentation at the NOAA Climate Board, Washington, DC, April 9, 2004.

Rao, S.T. Using CMAQ in air quality policy decisions: Research to applications. Presentation at the Office of Management and Budget Meeting, Washington, DC, April 21, 2004.

Rao, S.T. Role of satellite observations in understanding the link between air quality and health. Presentation at the EPA-NOAA Meeting on Satellite Data Assimilation, Washington, DC, May 4, 2004.

Rao, S.T. Federal-State partnerships for enhanced understanding of air quality and health relationships. Presentation at the EPA Science Forum 2004: Healthy Communities and Ecosystems, Washington, DC, June 3, 2004.

Rao, S.T. Role of models in air quality management. Presentation at the EPA-FACA's Science & Technology Subgroup Meeting, Research Triangle Park, NC, September 9, 2004.

Schere, K.L. NOAA's Eta-CMAQ modeling system for air quality forecasting. Lecture provided at the Air Quality Forecast Training Workshop, Environment Canada-Eastern Region Headquarters, Halifax, Nova Scotia, March 10, 2004.

Schere, K.L. Atmospheric modeling of air pollutants with the Community Multiscale Air Quality (CMAQ) model. Poster presentation at the EPA Science Forum 2004: Healthy Communities and Ecosystems, Washington, DC, June 1, 2004.

Swall, J.L. Nonstationary spatial modeling of environmental data using a process convolution approach. Presentation at the Joint Statistical Meeting 2004, Toronto, Canada, August 11, 2004.

Yu, S. Statistics Definitions and issues: Deriving "unbiased symmetric" metrics. Invited presentation at the Particulate Matter Model Performance Evaluation Workshop, Chapel Hill, NC, February 10, 2004.

APPENDIX D: WORKSHOPS AND MEETINGS

Texas Association of Regional Councils Proposal Review Panel, Houston, TX, October 4–7, 2003.

R.L. Dennis

NOAA/NCEP Air Quality Forecast Model Meeting, Camp Springs, MD, October 14–15, 2003.

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

NARSTO Emissions Inventory Workshop, Austin, TX, October 14–17, 2003.

R.L. Dennis (Session Co-Chair)
W.G. Benjey
T.E. Pierce
J.L. West

Standing Air Emissions Working Group (last meeting), San Francisco, CA, October 18, 2003.

W.G. Benjey

NADP Ammonia Workshop, Washington, DC, October 22–24, 2003.

R.L. Dennis

Office of the Federal Coordinator for Meteorology, Committee for Climate Analysis, Monitoring, and Services, Silver Springs, MD, October 24, 2003.

E.J. Cooter

American Association of Aerosol Research 21st Annual Conference, Anaheim, CA, October 20–24, 2003.

P.V. Bhave

NOAA Design Review Meeting for Air Quality Forecast Capability, Silver Spring, MD, October 23, 2003.

K.L. Schere

CMAS Models-3 Users' Workshop, One Atmosphere, One Community, One Modeling System: Models-3, Research Triangle Park, NC, October 27–29, 2003.

W.G. Benjey
P.V. Bhave
J.K.S. Ching
R.L. Dennis
B.K. Eder
P.L. Finkelstein
R.C. Gilliam
A.B. Gilliland
G.L. Gipson
J.M. Godowitch
D.J. Luecken
C.G. Nolte
T.L. Otte
T.E. Pierce
J.E. Pleim
G.A. Pouliot
S.T. Rao
S.J. Roselle
K.L. Schere
D.B. Schwede
J.O. Young
S. Yu

Meeting of External Advisory Committee of the CMAS Center, Research Triangle Park, NC, October 30, 2003.

K.L. Schere

National Exposure Research Laboratory Leadership Team Meeting, Athens, GA, November 3–6, 2003.

S.T. Rao

EPA Joint TMDL (Total Maximum Daily Loads) Coordinators' Meeting, Chicago, IL, November 3–7, 2003.

R.L. Dennis

National Science Foundation, Collaborative Large-scale Engineering Analysis Network for Environmental Research Workshop, Duke University, Durham, NC, November 10–11, 2003.

R.L. Dennis

EPA-DOE Sandia National Laboratory Scientist-to-Scientist Workshop, Albuquerque, NM, November 12–13, 2003.

J.E. Pleim
S.T. Rao
K.L. Schere

American Geophysical Union Fall Meeting, San Francisco, CA, December 8–12, 2003.

W.T. Hutzell

EPA-DOE Lawrence Livermore National Laboratory Scientist-to-Scientist Workshop, Research Triangle Park, NC, December 16–17, 2003.

E.J. Cooter

EPA Scientist-to-Scientist Air/Water Meeting on Effects of Nitrogen in Estuarine and Coastal Marine Systems, Washington, DC, December 17, 2003.

R.L. Dennis

American Meteorological Society Workshop on Merging Mesoscale and Computational Fluid Dynamics Modeling Capabilities, Seattle, WA, January 11, 2004.

A.H. Huber

84th American Meteorological Society Annual Meeting, Seattle, WA, January 11–15, 2004.

A.H. Huber
E.M. Poole-Kober

American Meteorological Society's MGA Advisory Board, Seattle,WA, January 12, 2004.

E.M. Poole-Kober

Seventh Annual Atmospheric Science Librarians International Conference, Seattle, WA, January 14–16, 2004.

E.M. Poole-Kober

Workshop on Carbonaceous Particulate Matter: The State of the Science - Part I, EPA's National Center for Environmental Assessment, Research Triangle Park, NC, January 14, 2004.

P.V. Bhave
C.G. Nolte
J.E. Pleim
K.L. Schere

7th Annual Electric Utilities Environmental Conference, Tucson, AZ, January 18–22, 2004.

S.T. Rao

Particulate Matter Model Performance Evaluation Workshop, Chapel Hill, NC, February 10–11, 2004.

P.V. Bhave
R.L. Dennis
B.K. Eder
R. Mathur
S. Yu

Air Quality Forecast Training Workshop, Environment Canada-Eastern Region Headquarters, Halifax, Nova Scotia, Canada, February 11, 2004.

J.E. Pleim

Arctic Council Action Plan Steering Group Meeting on Mercury Inventory Development, Moscow, Russia, February 17–20, 2004.

O.R. Bullock, Jr.

BRACE Data Analysis Workshop, Tampa Bay, FL, February 18–19, 2004.

R.L. Dennis

Urban Atmospheric Observatory Planning Meeting, New York, NY, February 23–24, 2004.

S.T. Rao

EPA 2004 National Air Quality Conference, Baltimore, MD, February 23–25, 2004.

B.K. Eder

EPA-NOAA Scientist-to-Scientist Meeting on Air Quality Research to Guide National Policy and Programs, Research Triangle Park, NC, March 2–3, 2004.

J.K.S. Ching
E.J. Cooter
R.L. Dennis
B.K. Eder
P.L. Finkelstein
A.B. Gilliland
A.H. Huber
D.J. Luecken
R. Mathur
C.G. Nolte
T.L. Otte
T.E. Pierce
W.B. Petersen
J.E. Pleim
S.T. Rao
K.L. Schere
J.L. Swall

Earth Observations Systems Expert Panel Workshop, Research Triangle Park, NC, March 9–10, 2004.

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

Air Quality Forecast Training Workshop, Environment Canada-Eastern Region Headquarters, Halifax, Nova Scotia, Canada, March 10, 2004.

K.L. Schere

Watershed Analysis Risk Management Framework Model Peer Review Panel Meeting convened by the Minnesota Sea Grant, Minneapolis, MN, March 10–12, 2004.

O.R. Bullock, Jr.

National Research Council Committee on Models in the Regulatory Decision Process, Washington, DC, March 18–19, 2004.

S.T. Rao

3rd Canadian Workshop on Air Quality, Quebec, Canada, March 23–25, 2004.

S.T. Rao

NASA 2004 AVIRIS (Airborne Visible/Infrared Imaging Spectrometer) Earth Science Workshop, National Aeronautics and Space Administration, Pasadena, CA, March 31–April 2, 2004.

J.J. Streicher

NOAA Climate Board Meeting, Washington, DC, April 9, 2004.

S.T. Rao

Workshop on Carbonaceous Particulate Matter: The State of the Science - Part II, EPA's National Center for Environmental Assessment, Research Triangle Park, NC, April 12, 2004.

P.V. Bhave
C.G. Nolte
J.E. Pleim
S.T. Rao
K.L. Schere

Mercury and CO_2 Workshop sponsored by the North Carolina Department of Environment and Natural Resources, Raleigh, NC, April 19–21, 2004.

O.R. Bullock, Jr.

Mercury Model Intercomparison Meeting, Meteorological Synthesizing Center-East, Moscow, Russia, April 20-25, 2004.

O.R. Bullock, Jr.

European Monitoring and Evaluation Program (EMEP) Workshop, Particulate Matter Measurement and Modeling, New Orleans, LA, April 20–23, 2004.

R.L. Dennis (Co-organizer of the workshop)
P.V. Bhave
B.K. Eder

Meeting of the ARL/RTP, NCEP AQ Forecast Team, Research Triangle Park, NC, April 23, 2004.

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

Workshop on Air Quality Applications of Satellite Data: Using Satellite Data to Monitor and Improve Air Quality Forecast, NOAA/NESDIS/Center for Satellite Applications and Research (STAR), Camp Springs, MD, May 4, 2004.

J.E. Pleim
S.T. Rao

National Wildland Fire Emissions Technical Workshop, New Orleans, LA, May 4–6, 2004.

J.M. Godowitch
T.E. Pierce

14th Annual SAIL (Southeast Affiliate of IAMSLIC Libraries) Annual Meeting, University of Texas-Marine Sciences Institute, Port Aransas, TX, May 11–14, 2004.

E.M. Poole-Kober

Air Pilot Project Group for Environmental Public Health Tracking Meeting, New York, NY, May 12, 2004.

S.T. Rao

Interdepartmental Committee for Meteorological Services and Support Research Meeting, Washington, DC, May 14, 2004.

S.T. Rao

U.S. EPA Consequences of Global Change for Air Quality Science-to-Achieve Results (STAR) Grant Progress Review Workshop, Research Triangle Park, NC, May 24–25, 2004.

E.J. Cooter

U.S. EPA Science Forum 2004: Healthy Communities and Ecosystems, Washington, DC, June 1–3, 2004.

C.G. Nolte
S.T. Rao
G. Sarwar
K.L. Schere

Workshop on Air Toxics Data Analysis, Chicago, IL, June 3, 2004.

D.J. Luecken

Annual Review of the EPA Science-to-Achieve Results (STAR) Grant Program on Carbonaceous Particulate Matter, Research Triangle Park, North Carolina, June 7–8, 2004.

P.V. Bhave
C.G. Nolte

U.S. EPA International Emission Inventory Conference, Working for Clean Air in Clearwater, Clearwater, FL, June 8–10, 2004

W.G. Benjey
T.E. Pierce

WRF/MM5 User's Workshop, Boulder, CO, June 22–25, 2004.

R.C. Gilliam
J.E. Pleim

Meeting of the External Advisory Committee to the Columbia University Project on New York Climate and Health, New York City, NY, June 25, 2004.

K.L. Schere

7th International Conference on Mercury as a Global Pollutant, Ljubljana, Slovenia, June 27–July 2, 2004.

O.R. Bullock, Jr.

Workshop on CFD Models Applied to Atmospheric Transport and Dispersion, George Mason University, Fairfax, VA, July 12, 2004.

A.H. Huber

Eight Annual George Mason University Transport and Dispersion Modeling Conference, Fairfax, VA, July 13–15, 2004.

A.H. Huber
S.T. Rao

Atmospheric Impacts Committee Meeting of the Coordinating Research Council, Detroit, MI, July 20–21, 2004.

K.L. Schere

ICARTT (International Consortium for Atmospheric Research on Transport and Transformation) Science Meeting and visit to the NOAA Ship Ronald H. Brown, Durham and Portsmouth, NH, July 23–27, 2004.

R.L. Dennis

Albemarle-Pamlico National Estuary Program, Science & Technology Advisory Committee Meeting, Greenville, NC, July 28, 2004.

R.L. Dennis

2004 Joint Statistical Meeting, Statistics as a Unified Discipline, Toronto, Ontario, Canada, August 8–12, 2004.

J.L. Swall

2004 Mercury Workshop sponsored by the U.S. Geological Survey, Eastern Region, Reston, VA, August 17–18, 2004.

O.R. Bullock

Fifth Symposium on the Urban Environment, American Meteorological Society, Vancouver, British Columbia, Canada, August 23–26, 2004.

J.K.S. Ching
G.E. Bowker
D.K. Heist
A.H. Huber
T.E. Pierce
J.E. Pleim
W. Tang

13th Joint AMS/AWMA Conference on the Applications of Air Pollution Meteorology, Vancouver, British Columbia, Canada, August 23–26, 2004.

A. H. Huber
W. Tang

U.S. EPA National Center for Environmental Research Relevancy Review Meeting on Source Apportionment of Particulate Matter, Research Triangle Park, NC, August 26, 2004.

P.V. Bhave

Texas Association of Regional Councils Proposal Review Panel, Houston, TX, September 1–2, 2004.

R.L. Dennis

European Monitoring and Evaluation Programme (EMEP) Steering Body Meeting, Geneva, Switzerland, September 6-8, 2004.

R.L. Dennis

Air Quality Forecast Focus Group Meeting, Silver Spring, MD, September 8–9, 2004.

D. Kang
H.-M. Lin
R. Mathur
T.L. Otte
J.E. Pleim
K.L. Schere
J.O. Young
S. Yu

NOAA/NCEP Air Quality Forecast Model Meeting, Silver Spring and Camp Springs, MD, September 9–10, 2004.

R. Mathur
T.L. Otte
J.E. Pleim
K.L. Schere

NASA-NOAA-EPA Workshop on Air Quality and Related Climate Change Issues, Research Triangle Park, NC, September 14–15, 2004.

W.G. Benjey
J.K.S. Ching
R. Mathur
T.E. Pierce
K.L. Schere

Office of the Federal Coordinator for Meteorology, Workshop on Urban Meteorology, Rockville, MD, September 20–23, 2004.

J.K.S. Ching
T.E. Pierce
S.T. Rao

Challenges in Urban Meteorology: A Forum for Users and Providers, Rockville, MD, September 21–23, 2004.

J.K.S. Ching
T.E. Pierce
S.T. Rao

NADP Technical Committee Meeting, Halifax, Nova Scotia, Canada, September 21–24, 2004.

P.L. Finkelstein

APPENDIX E: VISITING SCIENTISTS

Dr. Georg Grell
NOAA/Forecast Systems Laboratory
Boulder, Colorado

Dr. Grell visited the Division on January 29, 2004, to discuss the WRF/Chem model, and gave a presentation entitled, *A next generation air quality prediction model based on the Weather Research and Forecast (WRF) model.*

Dr. Mohammed Majeed
Delaware Department of Natural Resources and Environmental Control
State of Delaware
New Castle, Delaware

Dr. Majeed visited the Division on February 12, 2004, to discuss his collaboration on fine-scale MM5/CMAQ modeling.

Jeff McQueen
NOAA/NCEP
Camp Springs, Maryland

Drs. Pius Lee, and Marina Tsidulko
Scientific Applications International Corporation
NCEP
Camp Springs, Maryland

Mr. McQueen, and Drs. Lee and Tsidulko visited the Division on April 23, 2004, to participate in an Air Quality Forecast Team meeting with ASMD staff.

Dr. Michael Reynolds
Brookhaven National Laboratory
Environmental Sciences Department
Upton, New York

Dr. Petra M. Kastner-Klein
Assistant Professor
School of Meteorology
University of Oklahoma

Dr. Pablo Huq
Associate Professor
College of Marine Studies
University of Delaware
Newark, Delaware

Drs. Reynolds, Kastner-Klein, and Huq visited the Division during March 31–April 2, 2004, to discuss modeling urban pollution transport and dispersion related to potential future studies as part of the developing New York City Urban Atmospheric Observatory (UAO). Dr. Reynolds was the program manager developing the UAO, which is now the Department of Homeland Security, New York City Urban Dispersion Program (UDP). Dr. Petra M. Kastner-Klein presented a seminar entitled, *Mean flow, turbulence and dispersion characteristics in urban areas*. Dr. Huq gave a seminar entitled, *Modeling the atmospheric boundary layer and flow around buildings in a water tunnel*.

Dr. Jerry Davis
Marine, Earth, and Atmospheric Sciences Department
North Carolina State University
5134 Jordan Hall, Box 8208
Raleigh, North Carolina

Dr. Davis has been working on-site at the Division as a visiting scientist since May 2004.

Mr. Jim Tuccillo
IBM Corporation
Peachtree City, Georgia

Mr. Tuccillo visited the Division on June 28, 2004, to discuss the computational efficiency aspects of the Eta-CMAQ Air Quality Forecasting system.

Dr. Daewon Byun
Department of Geosciences
University of Houston
Houston, Texas

Dr. Byun visited the Division during July 28–29, 2004. He presented a seminar on entitled, *Simulation of Houston-Galveston Metropolitan airshed episode with CMAQ*.

APPENDIX F: POSTDOCTORAL RESEARCHERS

Dr. Daiwen Kang worked on operational model evaluations of ozone for the NOAA air quality model forecast project.

Dr. Wei Tang conducted research on computational fluid dynamics modeling and assessing the modeling techniques with field study data.

Dr. Shaocai Yu conducted research on CMAQ diagnostic model evaluation for the EPA retrospective assessment simulations and the NOAA forecast simulations.

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
Jeffrey L. West, Physical Science Administrator
Barbara R. Hinton (EPA), Secretary (Until December 2003)
Patricia F. McGhee, Secretary (Since January 2004)

Program Operations Staff

Herbert J. Viebrock, Supervisory Physical Scientist, Chief
Linda W. Green, Administrative Specialist
Evelyn M. Poole-Kober, Librarian
John H. Rudisill, III, Equipment Specialist (Until May 2004)

Atmospheric Model Development Branch

Kenneth L. Schere, Supervisory Meteorologist, Chief
Dr. Prakash V. Bhave, Physical Scientist
O. Russell Bullock, Meteorologist
Robert C. Gilliam, Meteorologist
Gerald L. Gipson (EPA), Physical Scientist
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 (Since January 2004)
Dr. Christopher G. Nolte (EPA), Physical Scientist
Tanya L. Otte, Meteorologist
Dr. Jonathan E. Pleim, Physical Scientist
Shawn J. Roselle, Meteorologist
Dr. Golam Sarwar (EPA), Physical Scientist
Dr. Jeffrey O. Young, Mathematician

Patricia F. McGhee, Secretary (Until January 2004)
Shirley Long (SEEP), Secretary

Model Evaluation and Applications Research Branch

Dr. Alice B. Gilliland, Supervisory Physical Scientist, Chief
Dr. Robin L. Dennis, Physical Scientist
Dr. Brian K. Eder, Meteorologist
Dr. Peter L. Finkelstein, Physical Scientist
Steven C. Howard, IT Specialist
Dr. Biswadev Roy (EPA), Physical Scientist (Since December 2003)
Dr. Jenise L. Swall, Statistician
Alfreida R. Torian, IT Specialist
Gary L. Walter, Computer Scientist
Sherry A Brown, Secretary

Air-Surface Processes Modeling Branch

Thomas F. 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
Bruce Pagnani (SEEP), Computer Programmer
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
John S. Irwin, Meteorologist (Until August 2004)
Richard A. Mason, Physical Scientist (Since January 2004)

Brian L. Orndorff, Meteorologist
Jawad S. Touma, Meteorologist

Awards

William B. Petersen received an EPA Gold Medal Award for his contributions as a member of the Brentwood Post Office Anthrax Crises Exception Team.

John S. Irwin received a NOAA Distinguished Career Award for his leadership in boundary-layer dynamics, transport and diffusion, and model evaluation; and for merging sound science and regulatory policy.

Dr. Robin L. Dennis and Jeffrey L. West received an EPA Bronze Medal for serving as contributing authors to the NARSTO PM Assessment document.

Dr. Alan H. Huber received an EPA Bronze Medal for the promotion of strong science in making agency decisions.

Shawn J. Roselle received an EPA Bronze Medal for his work with the Five-Year PM Accomplishment Team.