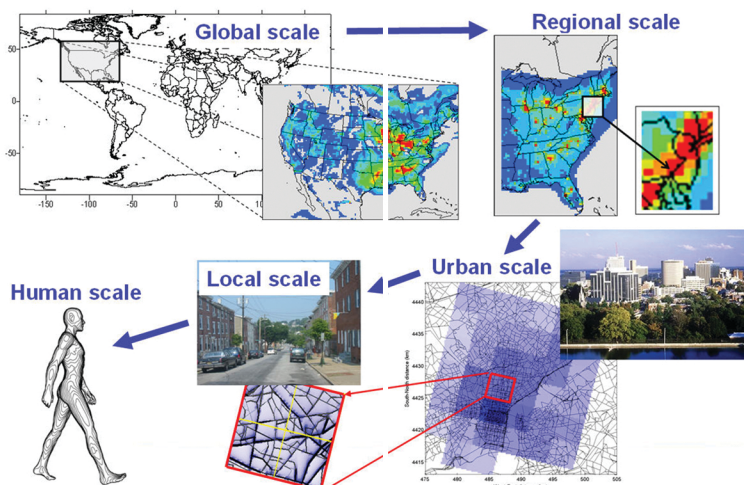


Summary Report of the Atmospheric Modeling and Analysis Division's Research Activities for 2008

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Summary Report of the Atmospheric Modeling and Analysis Division's Research Activities for 2008

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Foreword

The research presented here was performed partially under a Memorandum of Understanding and Memorandum of Agreement between the U.S. Environmental Protection Agency (EPA) and the U.S. Department of Commerce's National Oceanic and Atmospheric Administration (NOAA). These agreements were implemented through Interagency Agreements DW13938483 and DW13948634 between EPA and NOAA. Under this arrangement, most of the Division's employees were NOAA employees and worked in EPA facilities in Research Triangle Park, NC. The NOAA employees were transferred to EPA on July 1, 2008, and the Interagency Agreement ended on September 30, 2008. Under NOAA, the Division was known as the Atmospheric Sciences Modeling Division of the Air Resources Laboratory. As a division within the EPA organizational structure, it was known as the Atmospheric Modeling Division under the National Exposure Research Laboratory. In conjunction with this change in operating structure, the Division's name was changed to the Atmospheric Modeling and Analysis Division under EPA. To avoid confusion in organization structure, "the Division," usually is used in this report when referring to activities of this unique group of employees engaged in air quality modeling research.

This report summarizes the research and operational activities of the Division for calendar year 2008. A summary report of the Division's research activities has been published for many years under NOAA and/or EPA auspices. The report this year is drawn largely from the Division's Web site (www.epa.gov/amad) as of 12/31/08.

Abstract

This report summarizes the air quality modeling research activities that are associated primarily with the Community Multiscale Air Quality Model. In 2008, these activities were conducted by a division of employees associated in various capacities with the U.S. Environmental Protection Agency (EPA) and the National Oceanic and Atmospheric Administration (NOAA). The Division is responsible for providing a sound scientific and technical basis for regulatory policies to improve ambient air quality. The models developed by the Division are being used by EPA, NOAA, and the air quality community to understand and forecast the magnitude of the air pollution problem and also to develop emission control policies and regulations. This report summarizes the research and operational activities of the Division for calendar year 2008.

Acknowledgments

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CHAPTER 1

Introduction

The research presented here was performed partially under a Memorandum of Understanding and Memorandum of Agreement between the U.S. Environmental Protection Agency (EPA) and the U.S. Department of Commerce's National Oceanic and Atmospheric Administration (NOAA). These agreements are implemented through Interagency Agreements DW13938483 and DW13948634 between EPA and NOAA. Under this arrangement, most of the Division's employees were NOAA employees and worked in EPA facilities in Research Triangle Park, NC. The NOAA employees were transferred to EPA on July 1, 2008, and the Interagency Agreement ended on September 30, 2008. Under NOAA, the Division was known as the Atmospheric Sciences Modeling Division (ASMD) of the Air Resources Laboratory. As a division within the EPA organizational structure, the Division was known as the Atmospheric Modeling Division (AMD) under the National Exposure Research Laboratory (NERL). In conjunction with this change in operating structure, the Division's name was changed to the Atmospheric Modeling and Analysis Division (AMAD) under EPA. To avoid confusion in organization structure, "the Division", usually is used in this report when referring to activities of this unique group of employees engaged in air quality modeling research. This report summarizes the research and operational activities of the Division for calendar year 2008.

At the end of 2008, the Division under EPA was organized into four research branches:

(1) the Atmospheric Model Development Branch,

(2) the Emissions and Model Evaluation Branch,
(3) the Atmospheric Exposure Integration Branch, and
(4) the Applied Modeling Branch.

The appendixes to this report contain a list of Division employees (Appendix A), descriptions of the Division and its branches (Appendix B), lists of awards earned by Division personnel (Appendix C), Division publications (Appendix D), and acronyms and abbreviations used in this report (Appendix E).

The Division's role within EPA's National Exposure Research Laboratory's "Exposure Framework" and the EPA Office of Research and Development's source-to-outcome continuum is to conduct research that improves the Agency's understanding of the linkages from source to exposure (see Figure 1-1)¹. Through its research branches, the Division provides atmospheric sciences expertise, air quality forecasting support, and technical 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 [OAQPS] and regional offices), other Federal agencies, and State and local pollution control agencies.

The Division provides this technical support and expertise using an interdisciplinary approach that

¹Adapted from "A Conceptual Framework for U.S. EPA's National Exposure Research Laboratory," EPA/600/R-09/003, January 2009.

Source-to-Outcome Continuum

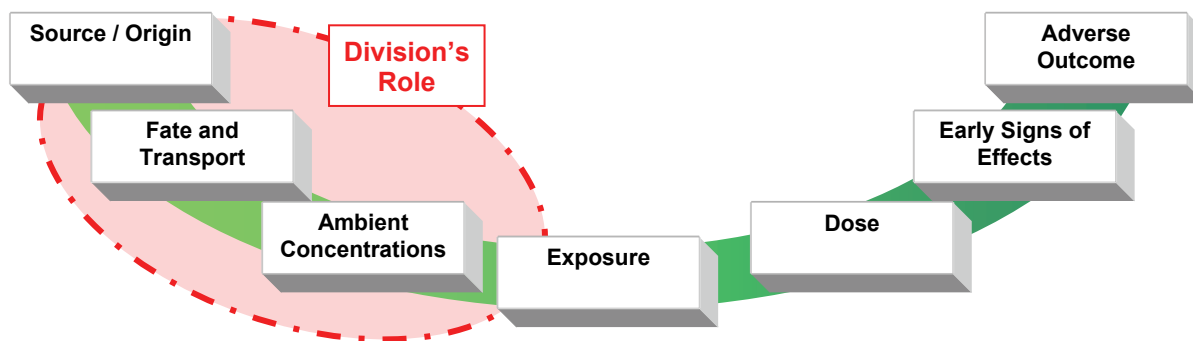


Figure 1-1. The Division's role in the source-exposure-dose-effects continuum.

emphasizes integration and partnership with EPA and public and private research communities. Specific research and development activities are conducted in-house and externally via contracts and cooperative agreements.

The Division's activities were subjected to a comprehensive peer review in January 2009. (Additional information from the peer review is available on the Division's Web site [www.epa.gov/amad.]) To present materials and programs to the peer review, the Division's activities were summarized with the focuses on five outcome-oriented theme areas:

- (1) model development and diagnostic testing,
- (2) air quality model evaluation,
- (3) climate and air quality interactions,
- (4) linking air quality to human health, and
- (5) linking air quality and ecosystem health.

Research tasks were developed within each theme area by considering the following questions.

- Over the next 2 to 3 years, who are the major clients and what are their needs?

- What research investments are needed to further the science in ways that help the clients? How will we lead or influence the science in this area?
- What personnel expertise, resources, and partners are needed to do this work?
- Does the proposed work fall within the current scope and plans of existing projects, or would personnel resources need to be shifted from other projects to make this happen?

The result is a research strategy for meeting user needs that is built around the five major theme areas and supported by the four branches of the Division, as depicted in Figure 1-2.

This report summarizes the research and operational activities of the Division for calendar year 2008. It includes descriptions of research and operational efforts in air pollution meteorology, in meteorology and air quality model development, and in model evaluation and applications. Chapters 2 through 6 of this report are organized according to the five major program themes listed above (also shown in Figure 1-2).

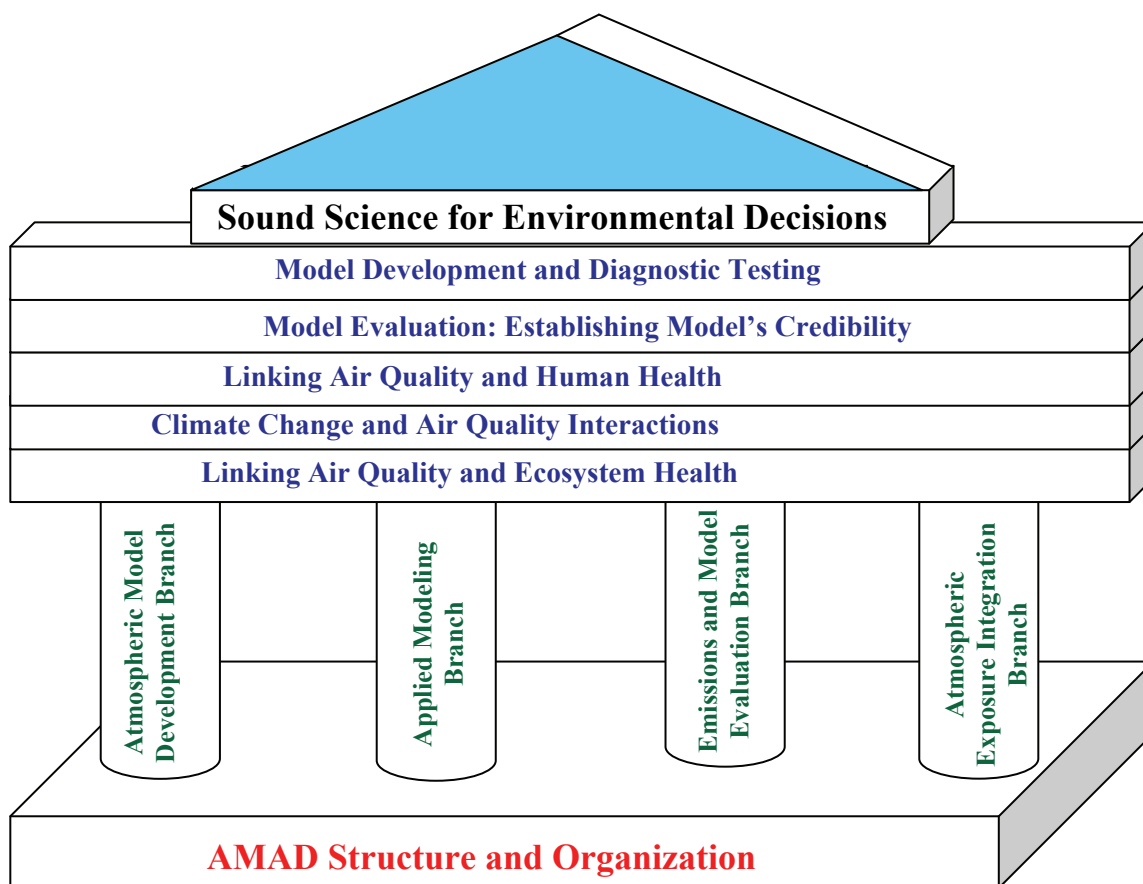


Figure 1-2. The Division's structure and organization.

CHAPTER 2

Model Development and Diagnostic Testing

2.1 Introduction

EPA and the States are responsible for implementing the National Ambient Air Quality Standards (NAAQS) for ozone (O₃) and particulate matter (PM). New standards for 8-h average ozone and daily average PM_{2.5} concentrations recently have been implemented. Air quality simulation models, such as the Community Multiscale Air Quality (CMAQ) modeling system, are central components of the air quality management process at the national, State, and local levels. The CMAQ model, used for research and regulatory applications by the EPA, States, and the scientific community, must have up-to-date science to ensure the highest level of credibility for the regulatory decisionmaking process. The research goals under the CMAQ model development and evaluation program are as follows.

- To develop, evaluate, and refine scientifically credible and computationally efficient process simulation and numerical methods for the CMAQ air quality modeling system;
- To develop the CMAQ model for a variety of spatial (urban through continental) and temporal (days to years) scales and for a multipollutant regime (ozone, PM, air toxics, visibility, and acid deposition);
- To adapt and apply the CMAQ modeling system to particular air quality/deposition/climate-related problems of interest to EPA, and use the modeling system as a numerical laboratory to study the major science process or data sensitivities and uncertainties related to the problem;
- To evaluate the CMAQ model using operational and diagnostic methods and to identify needed model improvements;
- To use CMAQ to study the interrelationships among different chemical species as well as the impact of uncertainties in meteorological predictions and emission estimates on air quality predictions;
- To collaborate with research partners to maintain the CMAQ model system; and
- To pursue computational science advancements (e.g., parallel processing techniques) to maintain the efficiency of the CMAQ model.

The National Research Council (NRC, 2004) recommended that air quality management strategies transition from a pollutant-by-pollutant approach to an integrated multipollutant strategy. In response to these recommendations, CMAQ also contains the option to simulate the atmospheric fate of mercury (Hg) compounds and 40 other hazardous air pollutants

(HAPs). The selection of HAPs included in CMAQ was based on consultation with the EPA OAQPS and includes the 33 HAPs identified under the Integrated Urban Air Toxics Strategy as posing the greatest potential public health concern in the largest number of urban areas, as well as several additional HAPs that are significant contributors to O₃ and secondary PM formation. This extended capability enables model-based air quality assessment studies to transition from the traditional pollutant-by-pollutant approach to an integrated multipollutant air quality management approach, wherein benefits/disbenefits of various control strategies can be more robustly examined.

The CMAQ model initially was released to the public by EPA in 1998. Annual updated releases to the user community and the creation of a Community Modeling and Analysis System (CMAS) center that provides user support for the CMAQ system and holds an annual CMAQ users conference have helped to create a dynamic and diverse CMAQ user community of over 1,000 users throughout the world. CMAQ has been and continues to be used extensively by EPA and the States for air quality management analyses (state implementation plans, Clean Air Interstate Rule [CAIR], Clean Air Mercury Rule, and Renewable Fuel Standard Program), by the research community for studying relevant atmospheric processes, and by the international community in a diverse set of model applications. Future research directions include development of an integrated weather research and forecasting (WRF)-CMAQ model for two-way feedbacks between meteorological and chemical processes and models and extension of the CMAQ system to hemispheric scales for global climate-air quality linkage applications and to the neighborhood scale for human exposure applications.

2.2 CMAQ Aerosol Module

Atmospheric PM is linked with acute and chronic health effects, visibility degradation, acid and nutrient deposition, and climate change. Accurate predictions of the PM mass concentration, composition, and size distribution are necessary for assessing the potential impacts of future air quality regulations and future climate on these health and environmental outcomes. The objective of this research is to improve predictions of PM mass concentrations and chemical composition, by advancing the scientific algorithms, computational efficiency, and numerical stability of the CMAQ aerosol module.

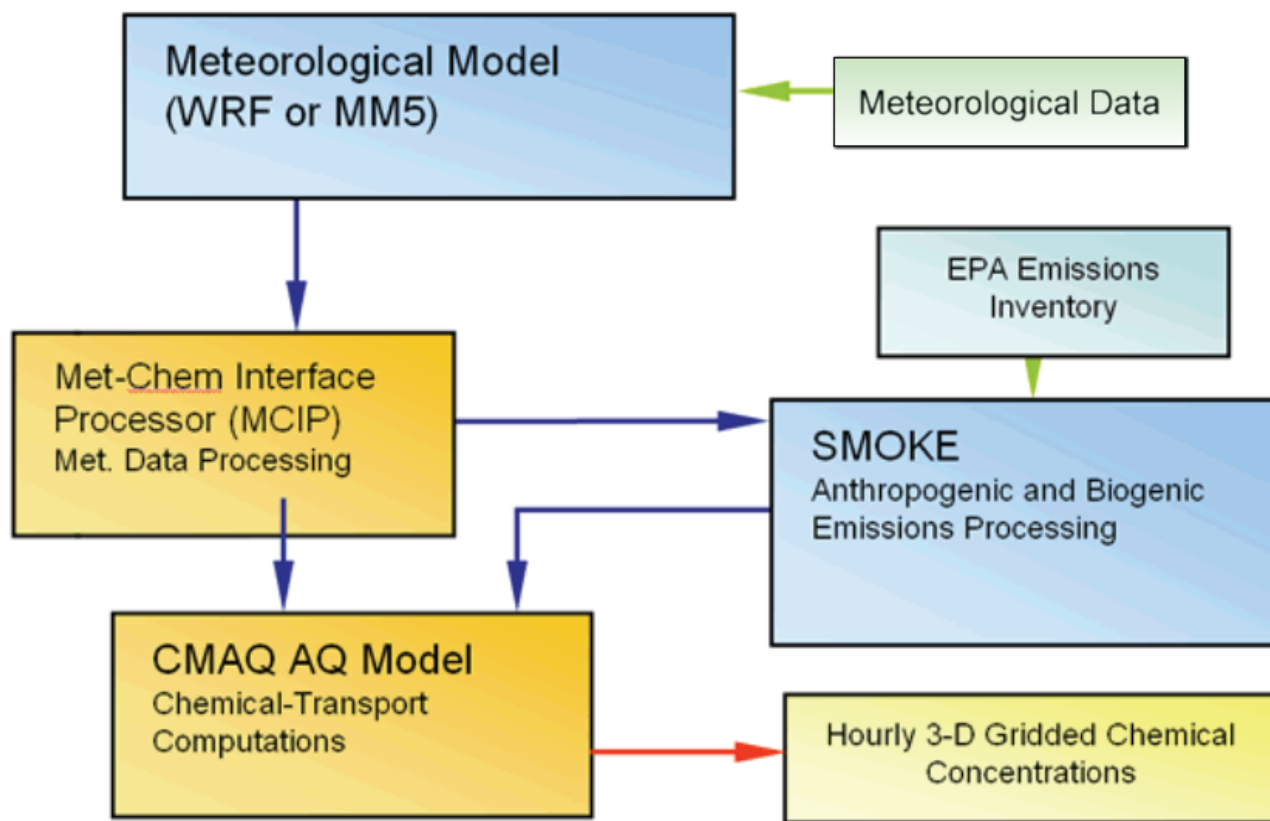


Figure 2-1. A flowchart that outlines the various components of the CMAQ modeling system.

To achieve this objective, we have focused efforts on five areas in which previous versions of the CMAQ aerosol module were deficient. First, we doubled the computational efficiency of the aerosol module by improving the computations of coagulation coefficients and secondary organic aerosol (SOA) partitioning. Second, we worked with the developer of ISORROPIA, CMAQ's thermodynamic partitioning module for inorganic species, to smooth out discontinuities. Third, we developed a new parameterization of the heterogeneous hydrolysis of nitrogen pentoxide (N_2O_5) as part of a larger effort to mitigate model overpredictions of wintertime nitrate aerosol concentrations. Fourth, we vastly improved the treatment of SOA by incorporating several new SOA precursors and formation pathways. Fifth, we implemented an efficient scheme to treat the dynamic interactions between inorganic gases and the coarse PM mode.

As a result of this research, the CMAQ aerosol module has been enhanced greatly over the past 5 years. During that time, the aerosol module has been used for regulatory and forecasting applications (e.g., EPA-CAIR, NOAA-NCEP) because it is scientifically credible, computationally efficient, and numerically stable. With the recent scientific enhancements, our

clients have increased confidence in the utility of CMAQ predictions of PM for future regulatory applications (e.g., Renewable Fuel Standards rulemaking). Meanwhile, the community of CMAQ users outside EPA continues to grow rapidly.

2.3 CMAQ Chemistry Mechanisms

An accurate characterization of atmospheric chemistry is essential for developing reliable predictions of the response of air pollutants to emissions changes, to predict spatial and temporal concentrations, and to quantify pollutant deposition. In the past, air quality modelers have focused largely on single-pollutant issues, but it has since become clear that it is more appropriate to treat chemistry in an integrated, multiphase, multipollutant manner (NRC, 2004). For example, both inorganic and organic aqueous-phase chemistry can influence formation of SOA through cloud processing (Carlton et al., 2006, 2007). High- NO_x versus low- NO_x conditions influence both O_3 and SOA formation (Ng et al., 2007). In the past 5 years, our requirements for air quality modeling also have changed: the new NAAQS for O_3 and fine PM ($\text{PM}_{2.5}$) have shifted our focus from urban-scale ozone episodes (~7 days) to regional/continental-scale simulations over longer time

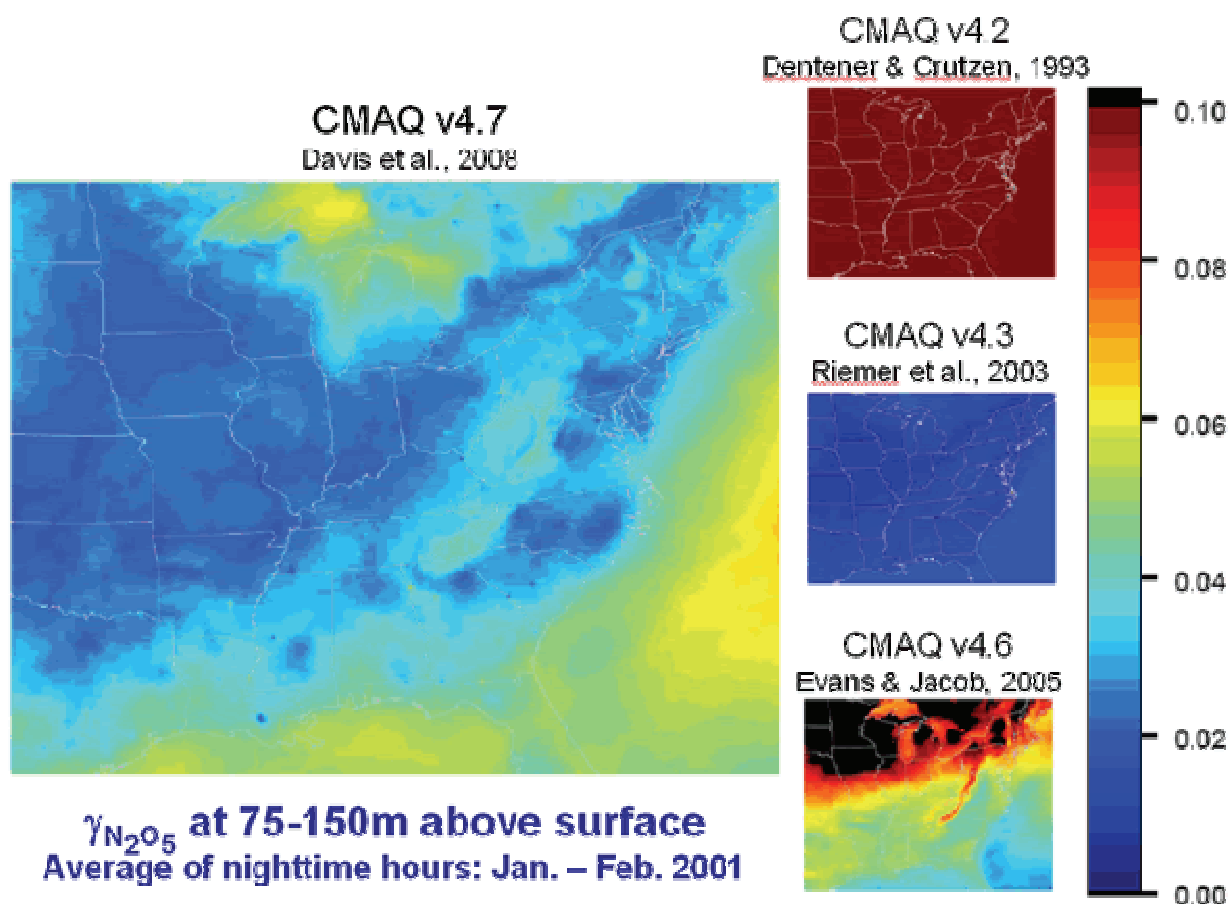


Figure 2-2. Since 2002, efforts focused on reducing model overpredictions of total nitrate (gas-phase HNO_3 plus particulate NO_3). Recently, a new parameterization of the heterogeneous reaction probability of N_2O_5 was developed in house.

periods (1 mo to 1 year). In addition, our chemical mechanisms must adapt quickly to address emerging issues of high importance, such as changing climatic conditions and the growing interest in biofuels.

The goal of our research in this area is to develop, refine, and implement state-of-the-science chemical mechanisms for use in the CMAQ model to

- ensure that CMAQ and other models that are used for regulatory and research purposes have scientifically justifiable chemical representations, are appropriate for the application being studied, and are consistent with our most up-to-date knowledge of atmospheric chemistry;
- ensure that interactions between gas-, aqueous-, and particle-phase chemistries are adequately accounted for, so that we can predict accurately multimedia chemical effects of emissions changes; and
- develop techniques, tools, and strategies so that we are able to efficiently expand current mechanisms to predict additional atmospheric pollutants that will become important in the future.

Our efforts to improve the chemical mechanisms in CMAQ have resulted in more complete and up-to-date descriptions of the important chemical pathways that influence concentrations of the criteria pollutants O_3 and PM. The inclusion of chlorine reactions and the explicit chemistry for 43 HAPs has helped to expand the applications for which CMAQ can be used. The inclusion of additional chemical detail in the aqueous and aerosol modules is providing pathways for more complete descriptions of secondary organic aerosol formation and decay.

2.4 Air Toxics Modeling

The Clean Air Act (CAA) of 1990 identified 188 individual compounds or mixtures of compounds as HAPs that have the potential for causing adverse health effects, such as cancer, reproductive and neurological effects, immune system damage, and birth defects. Toxins released into the atmosphere can disperse across the country and be inhaled or be deposited on the earth's surface, where they may be ingested directly

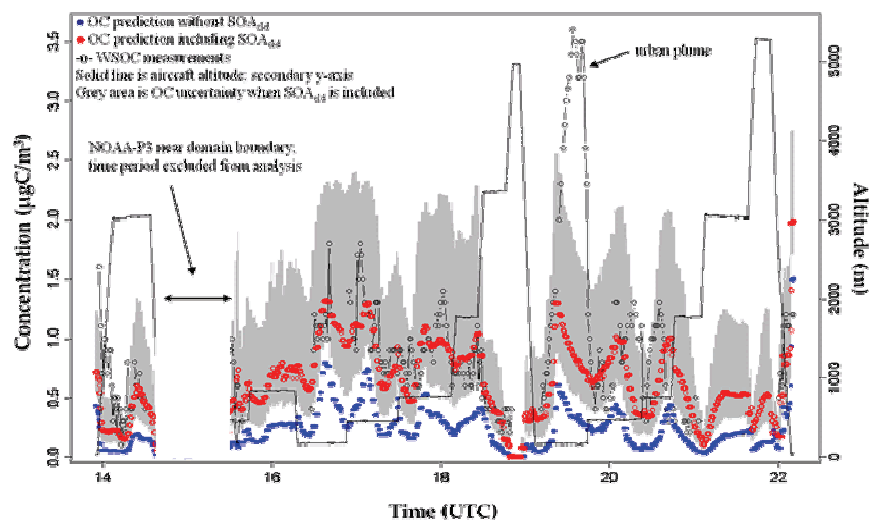


Figure 2-3. CMAQ organic carbon (OC) predictions that include cloud-produced SOA agree better with water soluble OC measurements made during ICARTT (Carlton et al., 2008). Although uncertainties still remain, inclusion of these processes in CMAQ account for some missing SOA.

by humans or taken up by plants or animals that are then consumed by humans and animals.

Air quality models that can predict ambient concentrations and deposition of these toxic compounds are needed so that we can assess the degree to which humans and ecosystems are exposed to these compounds. To obtain accurate estimates of the ambient concentrations of these compounds, the important processes that control their fate must be properly accounted for. Because each compound or mixture of compounds has unique and physical chemical properties that affect the relative importance of those processes, each compound must be considered individually. The objective of this work is to develop models that can describe the chemical and physical processes affecting concentrations of toxic air pollutants in the atmosphere, at spatial scales, ranging from 1 to 36 km. In this task, we are extending the capabilities of EPA's CMAQ model and applying this model to study high-priority issues related to toxic air pollutants. With these improvements, CMAQ will be able to handle a wide variety of processes to which toxic air pollutants are subjected, including gas and aqueous phase photochemistry, heterogeneous chemistry, transport, deposition, and reemission from the surface.

One area of research performed under this task includes the extension of chemical mechanisms so that CMAQ can be used to predict the concentrations of toxic chemicals that are not available in standard chemical mechanisms, and the application of these models at both national and urban scales, with concentration information provided to human exposure models.

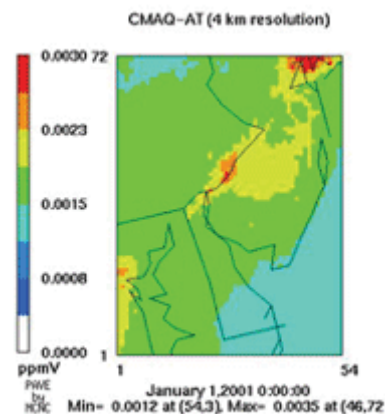


Figure 2-4. Air quality modeling in the Philadelphia area in collaboration with Region 3.

The second critical area of this research is the development of methods that can be used to apply these models at more finely resolved scales, so that we can predict hot spots in toxic concentrations and the environmental variability of potential exposure to air toxics. A near-term project involves investigating ways that we can incorporate information from Gaussian plume models with Eulerian models in a hybrid modeling approach. Longer term research work is being performed to improve the prediction of toxic air pollutant concentrations at very fine, "neighborhood" scales, accounting for the effects of urban canopies, as well as for subgrid-scale concentrations within the CMAQ model in a mass-consistent manner.

More background information on EPA's air toxics program can be found at <http://www.epa.gov/ttn/atw/>.

2.5 Mercury Modeling

ASMD has been working on the development of atmospheric Hg models since the early 1990s when the Regional Lagrangian Model of Air Pollution (RELMAP) was adapted to simulate Hg in support of EPA's Mercury Study Report to Congress. As the scientific understanding of atmospheric Hg continued to develop in the late 1990s, it became apparent that Lagrangian-type models, also known as "puff" models, would have difficulties simulating the complex chemical and physical interactions of Hg with other pollutants that were being discovered. Thus, the AMAD's focus for atmospheric Hg model development was moved to CMAQ. CMAQ simulates atmospheric processes within a three-dimensional array of predefined finite volume elements and can model complex interactions among all of the pollutants that might exist within each volume element. CMAQ previously was developed to simulate photochemical oxidants, acidic and nutrient pollutants, and PM, all of which have been shown to interact with Hg in air and cloud water and influence deposition to sensitive aquatic ecosystems. The "multipollutant" approach of CMAQ, where all pollutants are simulated together just as they exist in the real atmosphere, is applied in atmospheric Hg modeling.

A number of modifications were made to the standard CMAQ model to allow it to simulate atmospheric Hg; these are described in detail in Bullock and Brehme (2002). Because new information about chemical and physical processes affecting atmospheric Hg continually is being published, refinement of the model code is an ongoing process. The FORTRAN subroutine for the CMAQ aqueous chemistry mechanism is periodically optimized to efficiently calculate Hg chemistry in concert with the standard CMAQ cloud chemistry mechanism. Further modification of the CMAQ chemical mechanisms for mercury in both the gaseous and aqueous phases is expected as additional chemical reactions are identified and studied. The latest public release of CMAQ provides the ability to simulate atmospheric Hg in the "multipollutant" version of the model. We found this to be the most efficient way to maintain and disseminate the Hg version of CMAQ because of the increasing number of pollutants with which Hg is known to react.

AMAD has participated in two major model intercomparison studies for atmospheric Hg. The first was the *Intercomparison of Numerical Models for Long-Range Atmospheric Transport of Mercury*, sponsored by the European Monitoring and Evaluation Programme (EMEP) and organized by EMEP's Meteorological Synthesizing Center-East in Moscow, Russia. The first phase of this EMEP study involved the simulation of Hg

chemistry in a closed cloud volume given a variety of initial conditions. Results obtained from the CMAQ Hg model and the other participating models from Russia, Germany, Sweden, and the United States were compared to identify key scientific and modeling uncertainties (Ryaboshapko et al., 2002). This study led to some significant changes in some of the participating models, including CMAQ. The second phase of the EMEP study involved full-scale model simulations of the emission, transport, transformation, and deposition of Hg over Europe for two short periods (10 to 14 days). Model simulations were compared to field measurements of elemental Hg gas, reactive gaseous Hg, and particulate Hg in air. The "phase 2" results were reported in Ryaboshapko et al. (2007a). The third and final phase of the EMEP intercomparison involved model simulations for longer periods of time (up to 1 year) and comparisons with observations of the wet deposition of Hg. Results from "phase 3" of the EMEP study are reported in Ryaboshapko et al. (2007b).

2.6 Multiscale Meteorological Modeling for Air Quality

Air quality models require accurate representations of air flow and dispersion, cloud properties, radiative fluxes, temperature and humidity fields, boundary layer evolution and mixing, and surface fluxes of both meteorological quantities (heat, moisture, and momentum) and chemical species (dry deposition and evasion). Thus, meteorological models are critical components of the air quality modeling system that evolve with the state of science. Because of this evolution, there is a need to frequently challenge our established models and configurations; this includes examining not only new physics schemes but also data assimilation strategies, which serve to lower uncertainty in model output. It is also necessary to develop and refine physical process components in the models to address new and emerging research issues. Each of these research objectives has the overarching goal to improve meteorological model simulations to ultimately reduce uncertainty in air quality simulations. Our meteorology modeling research program involves several key projects that have led to improved meteorological fields. The first is the transition from the National Center for Atmospheric Research's (NCAR's) mesoscale model (MM5) system to the (WRF) model that represents the current state of science. Part of this effort was to implement in WRF land-surface (Pleim-Xiu [PX]), surface-layer (Pleim), and planetary boundary layer (PBL; Asymmetric Convective Model version 2 [ACM2]) schemes that had been used in MM5 and are designed for retrospective air quality simulations as outlined by Pleim and Gilliam (in press) and Gilliam and Pleim (2009). Part of this effort included improving the PX land-surface physics that included a deep soil

Figure 2-5a

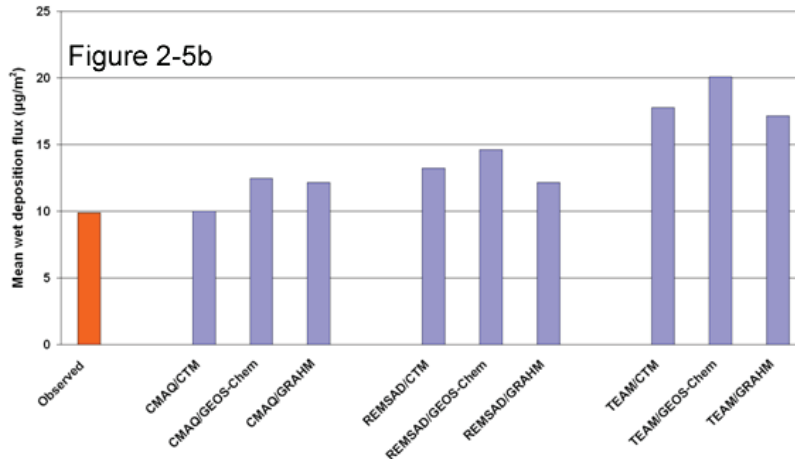
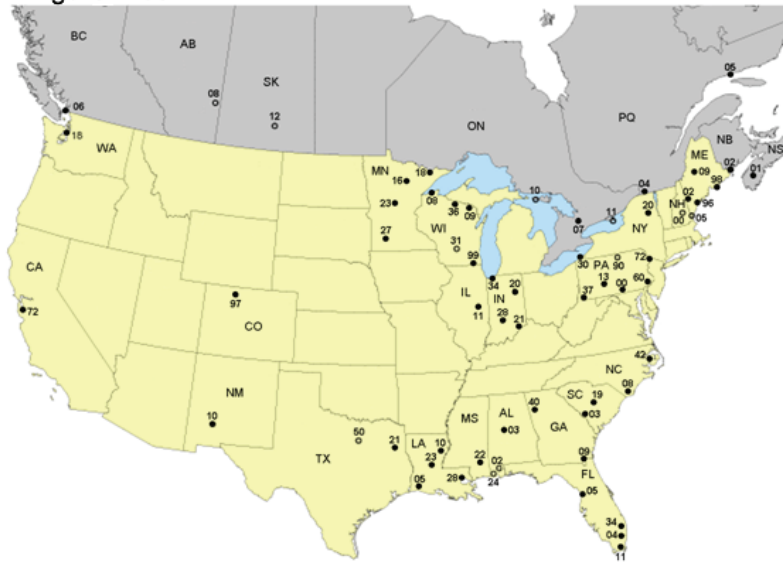


Figure 2-5a. As the EMEP study was nearing completion, AMAD organized a second Hg model intercomparison study, this time with a focus on North America. The North American Mercury Model Intercomparison Study (NAMMIS) took advantage of standardized weekly wet deposition samples taken by the Mercury Deposition Network (MDN) as described in Vermette et al. (1995) and separate event-based precipitation samples taken at Underhill, VT (Keeler et al., 2005). In addition to CMAQ, two other regional models were tested in NAMMIS; the Regional Modeling System for Aerosols and Deposition (REMSAD) and the Trace Element Analysis Model (TEAM). All three models were applied to simulate the entire year of 2001 three times, each time using a different initial condition and boundary condition (IC/BC) datasets developed from one of three global models. NAMMIS provided a comparison between regional atmospheric Hg models and also a measure of the sensitivity of each regional model to uncertainties regarding intercontinental transport. NAMMIS evaluated each regional model for its agreement to observations of wet deposition of Hg at 63 locations in the United States and Canada (Figure 2-5a). Analysis of each model's average annual wet deposition (Figure 2-5b) found CMAQ to be in best agreement with observations. Various other statistical comparisons were performed against annual, seasonal and weekly observations. In nearly every case, CMAQ showed better performance than other models considered in this study. NAMMIS results regarding model-to-model comparisons are reported in Bullock et al. (2008) and Bullock et al. (2009).

Figure 2-5b. CMAQ Hg modeling capabilities have been applied to support the development of EPA's Clean Air Mercury Rule. They also have been used to provide information regarding Hg deposition from global background concentrations to tribal, State, and regional environmental authorities in the development of their water quality protection strategies. AMAD plans to maintain and develop atmospheric Hg simulation capabilities in CMAQ to support ongoing environmental assessment and future regulatory action.

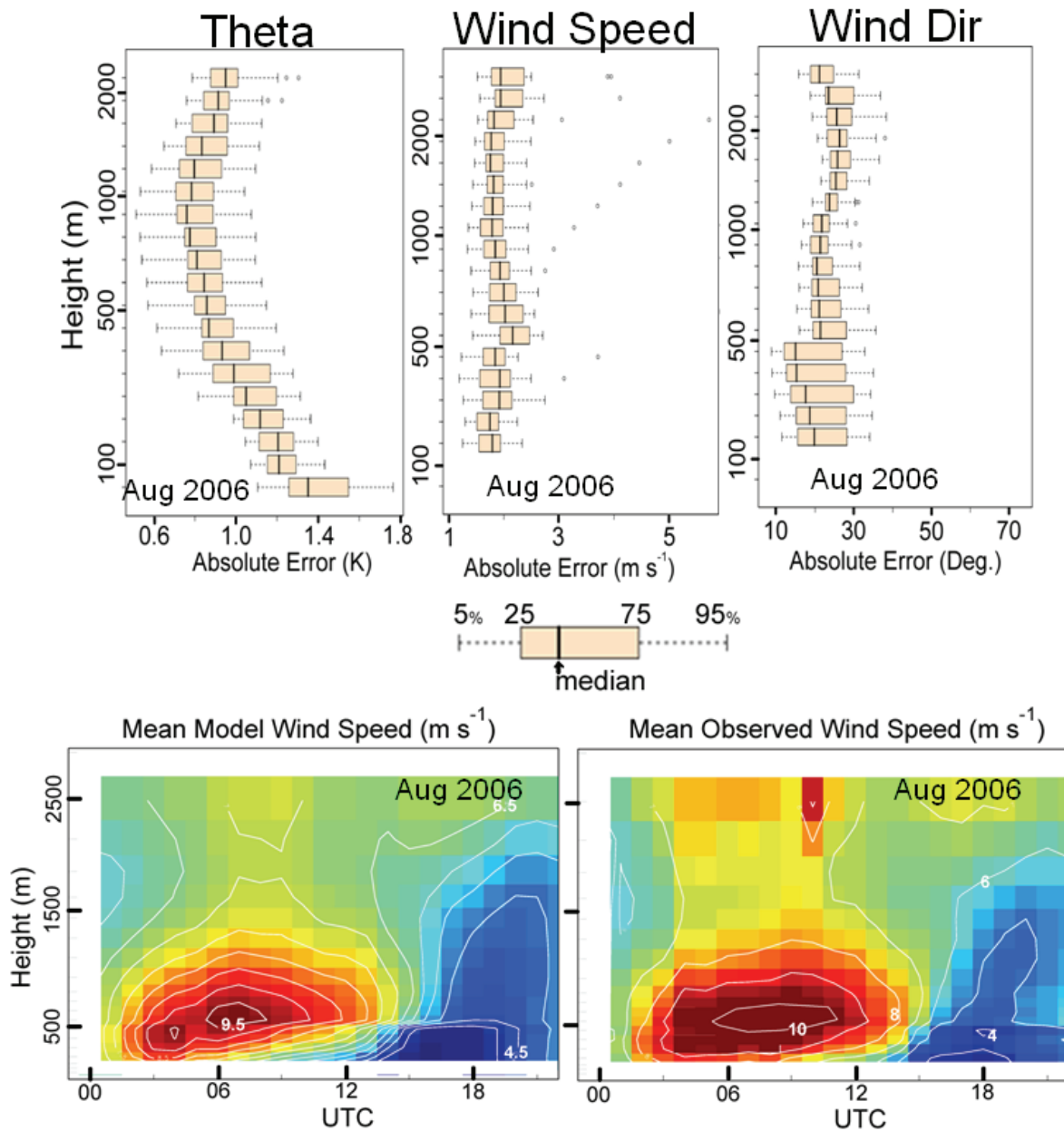


Figure 2-6. Above are the box plot distributions of absolute error (model compared to aircraft and wind profiler observations hourly for August 2006) as a function of model vertical level for potential temperature (K), wind speed (m/s) and wind direction (degrees). Also provided is the mean wind speed profile from the model and observations (wind profiler). Temperature is simulated with low error throughout the PBL. This error is close to the 2-m temperature error near the surface (~ 1.5 K), but much lower in the middle part of the PBL. Wind speed errors are between 1.0 and 2.0 m s^{-1} throughout the PBL, and wind direction errors are between 15 and 30 degrees, which is generally the same as at 10 m.

nudging algorithm and snow cover physics that dramatically improved temperature estimations in the winter simulations and in areas with less vegetation coverage. An additional effort was to work toward implementing in WRF the nudging-based four-dimensional data assimilation (FDDA) capability that had

been available in MM5. Another effort has been a reexamination of FDDA techniques, including the use of a developmental analysis package for WRF (OBSGRID) to lower the error of analyses that are used to nudge the model toward the observed state of the atmosphere.

Current results of the implementation of new physics in WRF show that our configuration is comparable to or exceeds the level of MM5 in terms of uncertainty or error in near-surface variables like 2-m temperature, 2-m moisture, and 10-m wind. This is true only when the new analysis package is used to improve analyses used for FDDA and soil moisture and temperature nudging in WRF. A new evaluation method that utilizes both wind profiler and aircraft profile measurements provides a routine method to examine not only the uncertainty of simulated wind in the planetary boundary layer but also the less examined temperature structure. The WRF model has low error in temperature (median absolute error of 1.0 to 1.5 K) in the planetary boundary layer, which is generally less than the error near the surface. The model also simulates the evolution of the wind structure, including features like nocturnal jets and the convective mixed layer, with low error ($<2.0 \text{ m s}^{-1}$). Our current configuration of WRF has met the requirements for the transition from MM5.

2.7 Planetary Boundary Layer Modeling for Meteorology and Air Quality

Air quality modeling systems are essential tools for air quality regulation and research. These systems are based on Eulerian grid models for both meteorology and atmospheric chemistry and transport. They are used for a range of scales from continental to urban. A key process in both meteorology and air quality models is

the treatment of subgrid-scale turbulent vertical transport and mixing of meteorological and chemical species. The most turbulent part of the atmosphere is the PBL, which extends from the ground up to 1 to 3 km during the daytime but is only a few tens or hundreds of meters deep at night.

The modeling of the atmospheric boundary layer, particularly during convective conditions, has long been a major source of uncertainty in numerical modeling of meteorology and air quality. Much of the difficulty stems from the large range of turbulent scales that are effective in the convective boundary layer (CBL). Both small-scale turbulence that is subgrid-scale in most mesoscale grid models and large-scale turbulence extending to the depth of the CBL are important for vertical transport of atmospheric properties and chemical species. Eddy diffusion schemes assume that all of the turbulence is subgrid-scale and, therefore, realistically cannot simulate convective conditions. Simple nonlocal-closure PBL models, such as the Blackadar convective model that has been a mainstay PBL option in MM5 for many years, and the original ACM, also an option in MM5, represent large-scale transport driven by convective plumes but neglect small-scale, subgrid-scale turbulent mixing. A new version of the ACM (ACM2) has been developed that includes the nonlocal scheme of the original ACM combined with an eddy diffusion scheme. Thus, the ACM2 can represent both the supergrid-scale and subgrid-scale components of turbulent transport in the convective boundary layer. Testing the ACM2 in

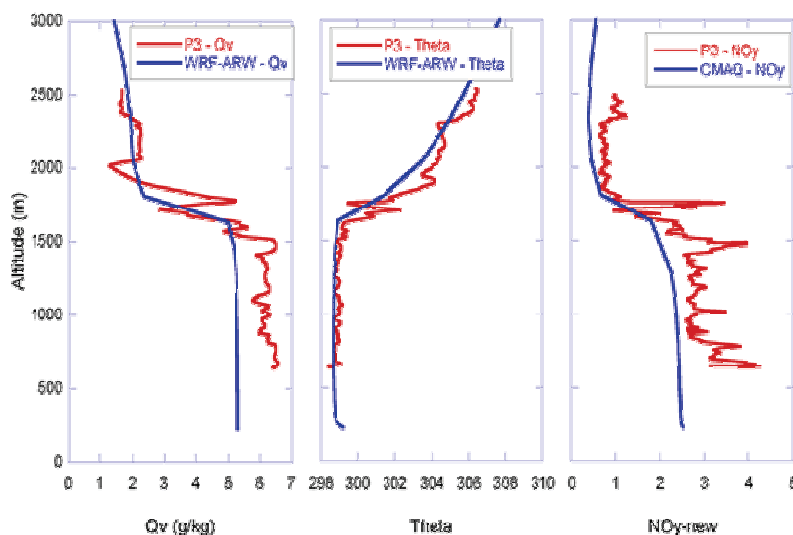


Figure 2-7. The most direct measure of success for a PBL model for both meteorology and air quality is its ability to accurately simulate the vertical structure of both meteorological and chemical species. Figure 2-7 shows an example of WRF and CMAQ profiles (both use the ACM2 scheme) compared with aircraft measurements. The top of the PBL mixed layer is well defined and modeled for both meteorology variables (water vapor mixing ratio Q_v and potential temperature θ) and chemical variables (total reactive oxides of nitrogen NO_y). Although such simultaneous measurements of vertical profiles of meteorology and chemistry are very rare, these limited results are encouraging.

Case 1: Eastern U.S., August 2-11, 2006, 12 km resolution

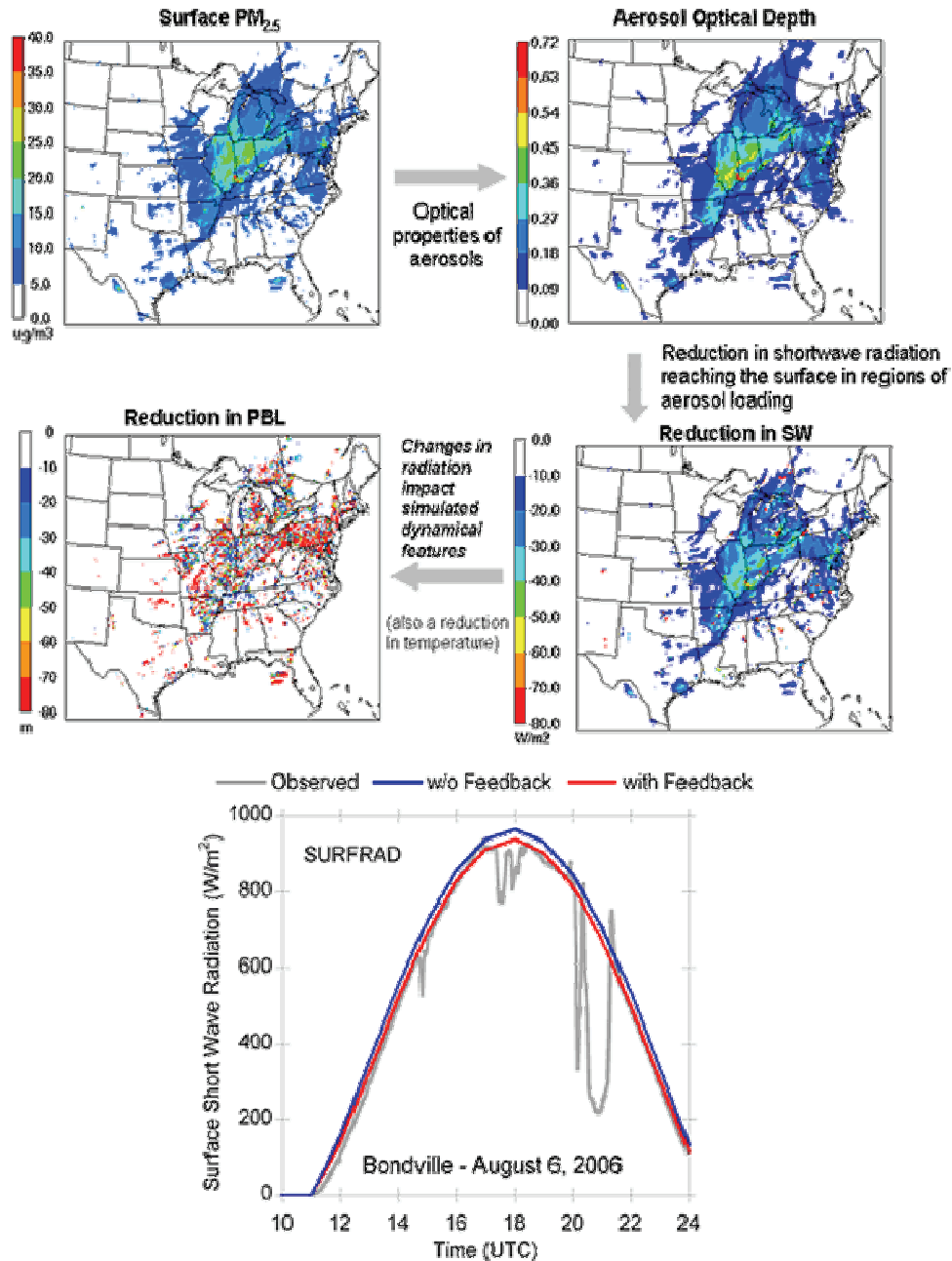


Figure 2-8. Two sets of initial simulations have been conducted to test the evolving coupled WRF-CMAQ modeling system and to systematically assess the impacts of coupling and feedbacks. Key questions in application of the coupled modeling system for assessment of air quality-climate interactions are, can aerosol radiative effects be detected in available measurements, and can such measurements be used to verify the directionality and magnitude of simulated effects? The upper panels in the figure above demonstrate the impact that aerosols estimated by CMAQ have on the meteorological models estimates of PBL height and downward shortwave radiation. The lower panel of the figure above is verification that the simulation, which includes these feedbacks, agrees better with the observed shortwave radiation.

one-dimensional form and comparing to large-eddy simulations (LES) and field data from the second and third GEWEX Atmospheric Boundary Layer Study, known as the GABLS2 (CASES-99) and GABLS3

(Cabauw, NL) experiments demonstrates that the new scheme accurately simulates PBL heights, profiles of fluxes and mean quantities, and surface-level values. The ACM2 performs equally well for both meteorological

parameters (e.g., potential temperature, moisture variables, winds) and trace chemical concentrations, which is an advantage over eddy diffusion models that include a nonlocal term in the form of a gradient adjustment (Pleim 2007a, Pleim 2007b). Comparisons to data from the TexAQS II field experiment show good agreement with PBL heights derived from radar wind profilers and vertical profiles of both meteorological and chemical quantities measured by aircraft spirals. ACM2 is in the latest releases of the WRF model and CMAQ model and now is used extensively by the air quality and research communities.

2.8 Coupled WRF-CMAQ Modeling System

Although the role of long-lived greenhouse gases in modulating the Earth's radiative budget has long been recognized, it now is acknowledged widely that the increased tropospheric loading of aerosols also can affect climate in multiple ways. Aerosols can provide a cooling effect by enhancing reflection of solar radiation, both directly (by scattering light in clear air) and indirectly (by increasing the reflectivity of clouds). On the other hand, organic aerosols and soot absorb radiation, thus warming the atmosphere. Current estimates of aerosol radiative forcing are quite uncertain. The major sources of this uncertainty are related to the characterization of atmospheric loading of aerosols, the chemical composition and source attribution of which are highly variable both spatially and temporally. Unlike greenhouse gases, the aerosol radiative forcing is spatially heterogeneous and estimated to play a significant role in regional climate trends. The accurate regional characterization of the aerosol composition and size distribution is critical for estimating their optical and radiative properties and, thus, for quantifying their impacts on radiation budgets of the Earth-atmosphere system.

Traditionally, atmospheric chemistry-transport and meteorology models have been applied in an offline paradigm, in which archived output describing the atmosphere's dynamical state as simulated by the meteorology model is used to drive the transport and chemistry calculations of the atmospheric chemistry-transport model. A modeling framework that facilitates coupled online calculations is desirable because it (1) provides consistent treatment of dynamical processes and reduces redundant calculations; (2) provides the ability to couple dynamical and chemical calculations at finer time steps, facilitating consistent use of data; (3) reduces the disk-storage requirements typically associated with offline applications; and (4) provides opportunities to represent and assess the potentially important radiative effects of pollutant loading on simulated dynamical features. To address the needs of emerging assessments for air quality-climate interactions and for finer scale air quality applications, AMAD recently began developing a coupled atmospheric

dynamics-chemistry model, the two-way coupled WRF-CMAQ modeling system. In the prototype of this system, careful consideration has been given to its structural attributes to ensure that it can evolve to address the increasingly complex problems facing the Agency. The system design is flexible regarding the frequency of data communication between the two models and can accommodate both coupled and uncoupled modeling paradigms. This approach also mitigates the need to maintain separate versions of the models for online and offline modeling (i.e., with and without direct radiative feedbacks that result from aerosols).

In the prototype coupled WRF-CMAQ system, the simulated aerosol composition and size distribution are used to estimate the optical properties of aerosols, which are then used in the WRF radiation calculations. Thus, the direct radiative effects of absorbing and scattering tropospheric aerosols estimated from the spatially and temporally varying simulated aerosol distribution can be fed back to the WRF radiation calculations; this results in a "two-way" coupling between the atmospheric dynamical and chemical modeling components. This extended capability provides unique opportunities to systematically investigate how atmospheric loading of radiatively important trace species affects the Earth's radiation budget. Consequently, this modeling system is expected to play a critical role in the Agency's evolving research and regulatory applications exploring air quality-climate interactions.

2.9 Computational Science

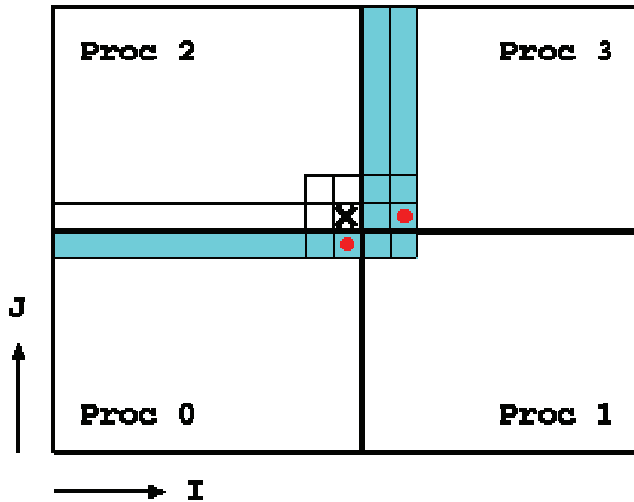
Distributed or so-called massively parallel processing enables the efficient computation of problems with very large domain sizes. However, programming for effective distributed processing requires careful code design and structuring. The basic principle of parallel computing is divide-and-conquer. This principle renders lower overall computational time and potentially reduced local memory utilization (storage) and is achieved by decomposing the problem space into many smaller problems that are solved concurrently.

In most applications, a processor must access data that reside in the memory of other processors.

The following is an example to illustrate this.

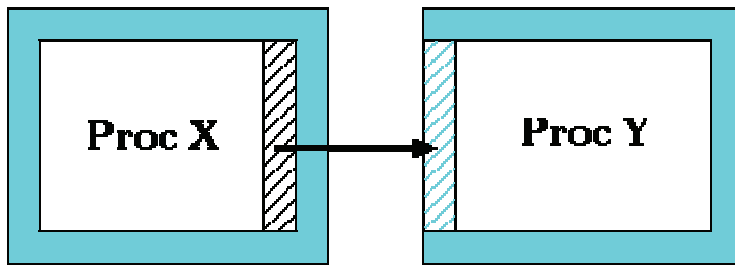
```
DO J = 1, N
DO I = 1, M
DATA(I,J) = A(I+2,J) * A(I, J-1)
END DO
END DO
```

Depending on the platform, there are two main data access paradigms: (1) message passing and (2) shared memory and, in some cases, a combination of both.

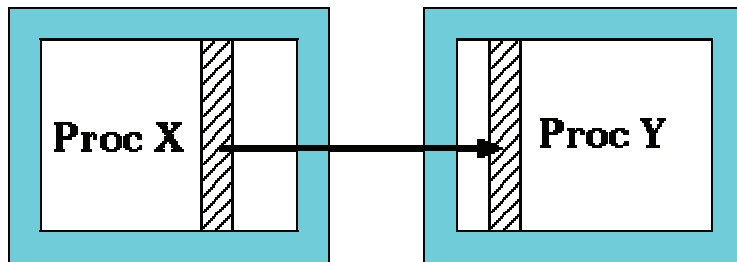


Each paradigm has its pros and cons. It might be convenient, for example, for programmers to see a global memory model on a distributed processor system. However, interprocessor communication bandwidth might become a serious performance issue. For the platforms we envision that will run the CMAQ models, message passing seems the best choice, and, consequently, we have developed some of the major codes, in particular the CMAQ Chemistry-Transport Model (CCTM), to use this paradigm.

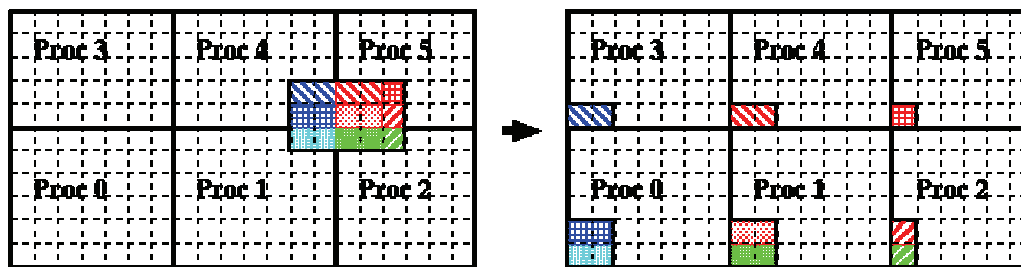
The backbone of the interprocessor communication within CMAQ is the Stencil Exchange (STENEX) library, which was developed in house and based on Message Passing Interface (MPI). STENEX library handles domain decomposition details, as well as various types of intercommunication schemes, for example, (a) interior to ghost region, where the ghost region is indicated in light blue; (b) interior to interior; (c) subsection data redistribution; and (d) selective data collection.



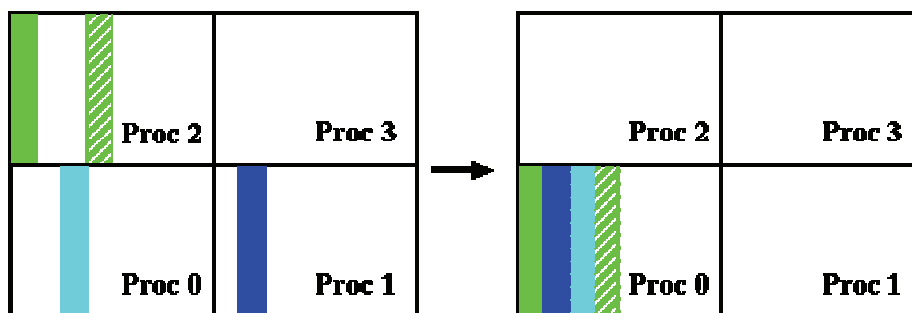
(a) interior to ghost region



(b) interior to interior



(c) redistribution of a subsection of data



(d) selective data collection

Figure 2-9. A flowchart that outlines the various components of the CMAQ modeling system.

CHAPTER 3

Air Quality Model Evaluation

3.1 Introduction

AMAD's model evaluation research program has been designed to assess CMAQ model performance for specific time periods and for specific uses of the model, and to develop innovative model evaluation techniques. Further, it has been a priority to identify improvements needed in model processes or inputs and better characterize and reduce model uncertainty. The Division has developed a framework (Figure 3-1) to describe these different aspects of model evaluation under four categories, as outlined and illustrated below.

- (1) *Operational evaluation*, as defined here, is a comparison of model-predicted and routinely measured concentrations of the end point

pollutant(s) of interest in an overall sense. This is the first phase of any model evaluation study.

- (2) *Diagnostic evaluation* investigates the atmospheric processes and input drivers that affect model performance to guide CMAQ development and improvements needed in emissions and meteorological data.
- (3) *Dynamic evaluation* assesses a model's air quality response to changes in meteorology or emissions, which is a principal use of an air quality model for air quality management.
- (4) *Probabilistic evaluation* strives to characterize uncertainty in CMAQ model predictions for model applications such as predicted concentration changes in response to emission reductions.

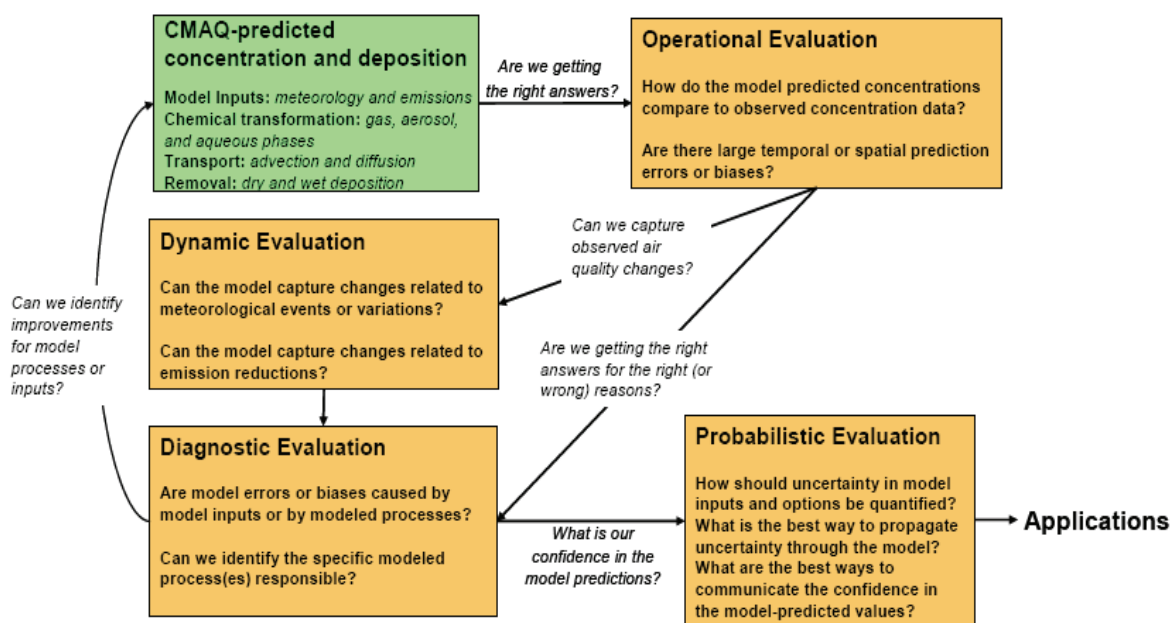


Figure 3-1. Scatter AMAD model evaluation framework.

3.2 Operational Performance Evaluation of Air Quality Model Simulations

Two of the three main components of an air quality model (e.g., CMAQ) simulation are the input meteorology and the air quality model simulation itself, with the third being the input emissions. Meteorological data are provided by models, such as MM5 and WRF. The quality of the meteorological data, specifically how well the predicted values (e.g., temperature, wind speed, etc.) compare with the observed state of the

atmosphere, is critical to the performance of the air quality model, which is highly dependent on the meteorological data to accurately simulate pollutants in the atmosphere. As such, an important aspect of any air quality simulation is the evaluation of the quality of the predicted meteorological data. This is accomplished by comparing model-simulated values with observed data (Figure 3-2). This type of evaluation is referred to as operational evaluation. An example of meteorological evaluation can be found at

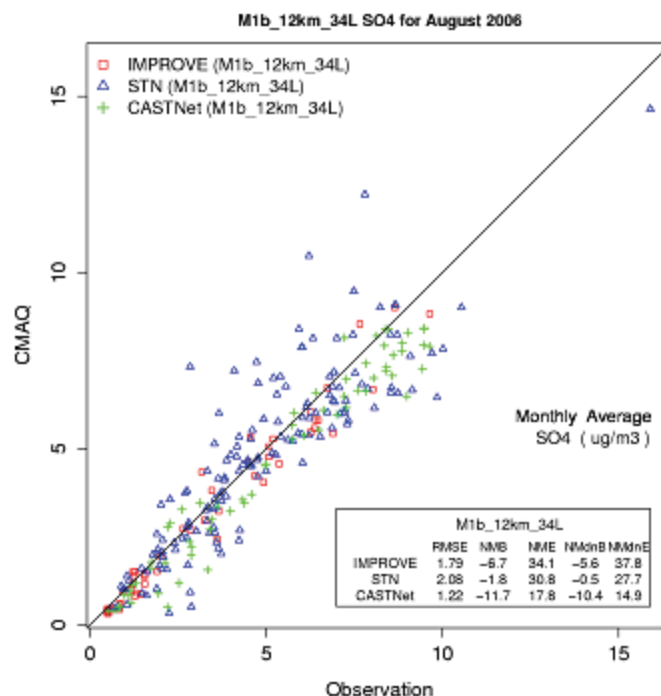


Figure 3-2. Scatter plot of observed versus CMAQ-predicted sulfate for August 2006 created by AMET.

<http://www.epa.gov/asmdnerl/ModelDevelopment/meteorologyModeling.html>. A similar evaluation of the air quality model simulation also is performed using available observed air quality measurements.

As the developers of the CMAQ model, AMAD frequently is evaluating CMAQ simulations as part of the testing process as the model evolves with state-of-the-art science. Examples of changes to the modeling system that may require testing include updates/corrections to the model code, changes in the model inputs (e.g., meteorology, emissions), and any other changes that may impact the model predictions. As computing power has increased (and continues to increase), the time required to run a simulation has decreased. Additionally, the duration of model simulations has increased from a week or several weeks to multiple months and multiple years. With this increase in the number and duration of air quality simulations comes an increase in the time required to thoroughly evaluate each simulation. To evaluate a simulation within a reasonable amount of time, AMAD developed the Atmospheric Model Evaluation Tool (AMET), which aids researchers in evaluating the operational performance of a meteorological or air quality simulation. A brief description of AMET is given below, and a link to AMET code can be found at <http://www.epa.gov/asmdnerl/tools.html>.

AMET is a combination of an open source database software (MYSQL), the R statistics software, and FORTRAN and PERL scripts that together provide an

organized and powerful system for processing meteorological and air quality model output and then evaluating the performance of model predictions. AMET uses FORTRAN and PERL scripts to pair observed meteorological and air quality data with model predictions, then populates a MYSQL relational database with the paired data, and, finally, uses R statistics scripts to create statistics and plots to show the operational model performance. Many R scripts are already available with the release version of AMET, but users familiar with R can modify existing scripts or create new scripts to suit their evaluation needs.

3.3 Diagnostic Evaluation of the Oxidized Nitrogen Budget Using Space-Based, Aircraft, and Ground Observations

Recent studies have shown that when compared with field observations, chemical transport models make significant errors in the simulated partitioning of nitrogen compounds (NO_y) between NO₂, HNO₃, and peroxyacyl nitrates (PANs). This impacts the long-range transport of ozone precursors, misrepresents the relative effectiveness of local versus regional emission control strategies, and distorts the spatial and temporal distribution of nitrogen deposition. In this research, we use a combination of modeling tools equipped with process analysis, satellite data, aircraft observations from the International Consortium for Atmospheric Research on Transport and Transformation (ICARTT),

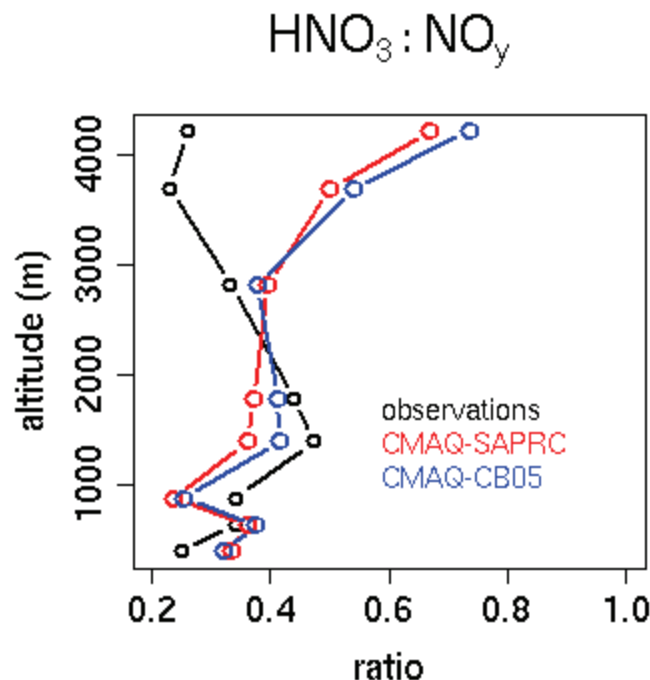


Figure 3-3. Vertical profile of the ratio of nitric acid (HNO_3) to total oxidized nitrogen (NO_y), as sampled during the August 8, 2004, ICARTT flight over the northeastern United States. When the observations are paired in time and space with the CMAQ simulations, we find that the chemical mechanisms used in CMAQ overestimate the contribution of nitric acid to total NO_y , especially in the free troposphere.

INTEX-NA, and TexAQS 2006 field campaigns, and surface observations to better understand and improve the simulated fate and transport of oxidized nitrogen species. We are applying this analysis to better quantify the relative impact of local versus regional NO_x emission control strategies, the contribution of lightning NO_x to atmospheric chemistry, and the long-range transport and deposition of NO_y to remote ecosystems.

3.4 Diagnostic Evaluation of the Carbonaceous Fine Particle System

Routine measurements of speciated $\text{PM}_{2.5}$ (e.g., IMPROVE, STN) are often insufficient to diagnose the causes of model errors in OC concentrations because they cannot distinguish the origin of OC between primary versus secondary, anthropogenic versus biogenic, or mobile sources versus area sources. Through identification of the sources and processes contributing the OC, the necessary improvements in the modeled processes or emission inputs can be identified. Current diagnostic evaluation work is listed below that will support better understanding of the carbonaceous aerosol system.

Estimating how much OC observed is secondary. Routine measurements of elemental carbon

(EC) and OC can be used in conjunction with model predictions of EC and primary OC to estimate concentrations of secondary OC (Yu et al., 2007). These estimates can be used as a preliminary assessment of model performance for secondary OC.

Primary OC predictions from different sources.

Measurements of individual organic compounds that are specific to certain primary emission sources may be used to evaluate model predictions of primary OC on a source-by-source basis. Measurements of this type at the SEARCH monitoring sites have been used to evaluate model results during the July-August 1999 period in the southeastern United States (Bhave et al., 2007).

Fossil-fuel versus modern carbon predictions.

Measurements of radiocarbon (^{14}C isotope) allow one to distinguish fossil-fuel carbon (e.g., motor vehicle exhaust, coal and oil combustion) from modern carbon (e.g., biomass combustion, biogenic SOA). Measurements of this type at Nashville in summer 1999 (Lewis et al., 2004) are being used to evaluate model predictions of these two types of carbon.

Tracers of anthropogenic and biogenic SOA.

Novel analytical techniques for quantifying individual organic compounds that are unique tracers of

anthropogenic and biogenic SOA have been developed by EPA scientists. These compounds have been measured at an RTP site throughout the 2003 calendar year (Kleindienst et al., 2007) and have been used to evaluate recent improvements to the CMAQ SOA module (Bhave et al., 2007). A copy of the presentation

is located at <http://iccpa.lbl.gov/presentations/iccpa-08-bhave.pdf>.

Many of these exploratory projects are in collaboration with scientists in the NERL Human Exposure and Atmospheric Sciences Division (HEASD). The web address is <http://www.epa.gov/heasd/>.

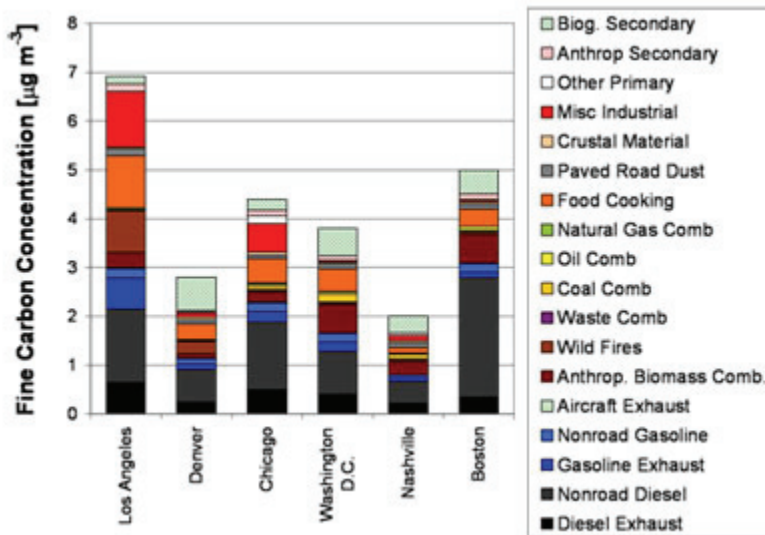


Figure 3-4. Source contributions to the modeled concentrations of fine-particulate carbon in six U.S. cities.

3.5 Diagnostic Evaluation Using Inverse Modeling To Improve Emission Estimates

Although continuously updated and improved, emission inventories still are considered to be one of the largest sources of uncertainty in air quality modeling. It is often difficult to measure either the emission factors, activity information, or both for various emitting processes, such as forest fires, animal husbandry practices, and motor vehicles. Therefore, bottom-up inventories for such processes often are based on estimates and averages.

To complement, evaluate, and better inform bottom-up emission inventories, we develop and apply inverse modeling methods. These types of “top-down” approaches employ observational data from continuously operating pollutant measurement networks, intensive field campaigns, and remote sensing technologies to infer emission inventories based on current state-of-the-science understanding of physical and chemical processes in the atmosphere. In one specific application, we use the satellite-derived NO₂ column density to attempt to identify any possible bias in the NO_x emission inventories over several regions in the southeastern United States. Figure 3-5 shows a model comparison of satellite observations (from scanning imaging absorption spectrometer for

atmospheric cartography [SCIAMACHY] retrieval) and CMAQ prediction. This application relies on the adaptive-iterative Kalman filter as an inverse method and decoupled direct method in 3D (DDM-3D) as a way to quantify the relationship between emission rates of NO_x and atmospheric concentrations of NO₂. We find that urban emissions in Atlanta and Birmingham are likely to be overestimated; more rural concentrations of NO₂ are likely to be low because of missing emissions and chemical processes aloft in the CMAQ model.

3.6 Dynamic Evaluation of a Regional Air Quality Model

A dynamic evaluation approach explicitly focuses on the model-predicted pollutant responses stemming from changes in emissions or meteorology. However, the emergence of the dynamic evaluation approach introduces new challenges. In particular, retrospective case studies are needed that provide observable changes in air quality that can be related closely to known changes in emissions or meteorology. The NO_x SIP call has offered a very strong initial case study to test model responses via dynamic evaluation.

The most direct example of a dynamic evaluation study is described in Gilliland et al. (2008), where air

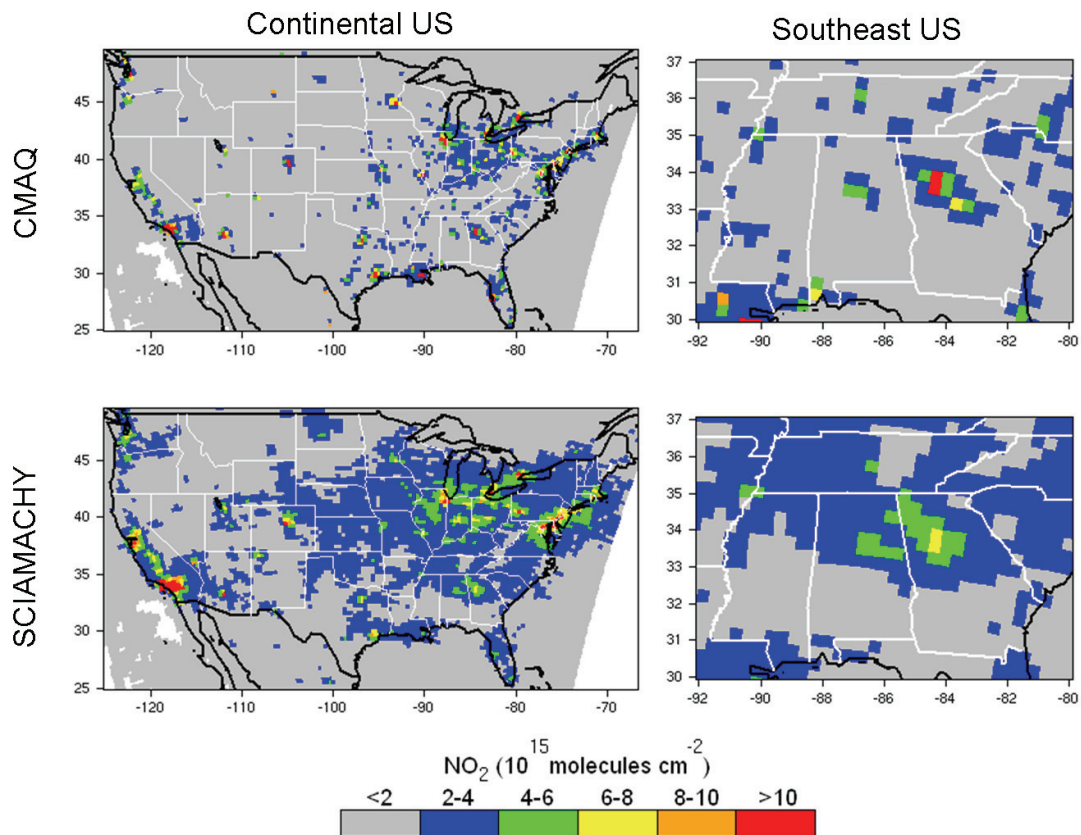


Figure 3-5. Comparison of modeled and observed NO₂ column concentrations.

quality model simulation results with the CMAQ model were evaluated before and after major reductions in NO_x emissions. EPA's NO_x SIP call required substantial reductions in NO_x emissions from power plants in the eastern United States during summer O₃ seasons with the emission controls being implemented during 2003 through May 31, 2004. G  go et al. (2007) and USEPA (2007) show examples of how observed O₃ levels have decreased noticeably after the NO_x SIP call was implemented. Because air quality models are applied to estimate how ambient concentrations will change because of possible emission control strategies, the NO_x SIP call was identified as an excellent opportunity to evaluate a model's ability to simulate O₃ response to known and quantifiable observed O₃ changes. Figure 3-6 provides an example from this prototype modeling study where changes in maximum 8-h O₃ are compared between the summer 2005 after the NO_x controls and the summer 2002 before these controls. The spatial patterns of percentage decreases in O₃ derived from observations and the model exhibit strong similarities.

However, these results also revealed model underestimation of O₃ decreases as compared with observations, especially in northeastern states at extended downwind distances from the Ohio River Valley source region. This may be attributed to an underestimation of NO_x emission reductions or a dampened chemical response in the model to those emission changes or to other factors. Analysis methods, such as the e-folding distances (Gilliland et al., 2008, Godowitch et al., 2008), have been used to show that NO_x emissions in these simulations are not impacting O₃ levels as far downwind as observations suggest, which could be a factor here. Next steps must involve further diagnostic evaluation to identify what chemical, physical, or emission estimation uncertainties are contributing to these initial results from the model. Findings from additional analysis of this case study ultimately can lead to model improvements that are directly relevant to the way air quality models are used for regulatory decisions.

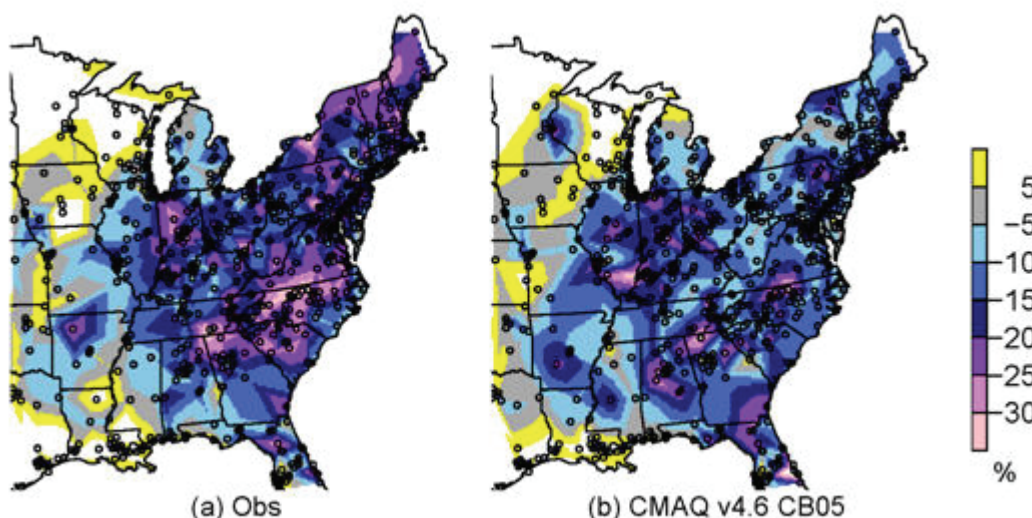


Figure 3-6. Example of dynamic evaluation showing (a) observed and (b) air quality model-predicted changes (%) from differences between summer 2005 and summer 2002 ozone concentrations from Gilliland et al. (2008). The results illustrate the relative change in ozone when comparing the 95th percent daily 8-h maximum levels between the two summers.

3.7 Probabilistic Model Evaluation

When weighing the societal benefits of different air quality management strategies, policymakers need quantitative information about the relative risks and likelihood of success of different options to guide their decisions. A key component in such a decision support system is an air quality model that can estimate not only a single “best-estimate” but also a credible range of values to reflect uncertainty in the model predictions. Probabilistic evaluation of CMAQ seeks to answer the following questions.

- How do we quantify our uncertainty in model inputs and parameterizations?
- How do we propagate this uncertainty to the predicted model outputs?
- How do we communicate our level of confidence in the model-predicted values in a way that is valuable and useful to decisionmakers?

To address these questions, we’ve deployed a combination of deterministic air quality models and statistical methods to derive probabilistic estimates of air quality. For example, an ensemble of deterministic simulations frequently is used to account for different sources of uncertainty in the modeling system (e.g., emissions or meteorological inputs, boundary conditions, parameterization of chemical or physical processes). A challenge with ensemble approaches is that chemical transport models require significant input data and computational resources to complete a single simulation. We have applied the CMAQ-DDM-3D to generate large member ensembles avoiding the major computational cost of running the regional air quality model multiple times. We also have used statistical methods to

postprocess the ensemble of model runs based on observed pollutant levels. Maximum likelihood estimation is used to fit a finite mixture statistical model to simulated and observed pollutant concentrations. The final predictive distribution is a weighted average of probability densities, and the estimated weights can be used to judge the performance of individual ensemble members, relative to the observations.

These approaches provide an estimated probability distribution of pollutant concentration at any given location and time. The full probability distribution can be used in several ways, such as estimating a range of likely, or “highly probable,” concentration values or estimating the probability of exceeding a given threshold value of a particular pollutant. For example, Figure 3-7 shows the estimated probability of exceeding an ozone threshold concentration of 60 ppb over the southeastern United States for current conditions (top) and with a 50% reduction in NO_x emissions (bottom). Compared to the single-base CMAQ simulation (far left), the spatial gradients provided by the ensemble-based estimates (middle and right) more accurately reflect the observed exceedances under current conditions.

3.8 Statistical Methodology for Model Evaluation

Model evaluation efforts often include graphical comparisons of monitoring data paired with the output for the model grid cells in which the monitors lie and statistical summaries of the differences that exist. If certain differences or regions are of particular interest, the investigator may narrow the evaluation’s focus to a limited area and time period. Advanced statistical

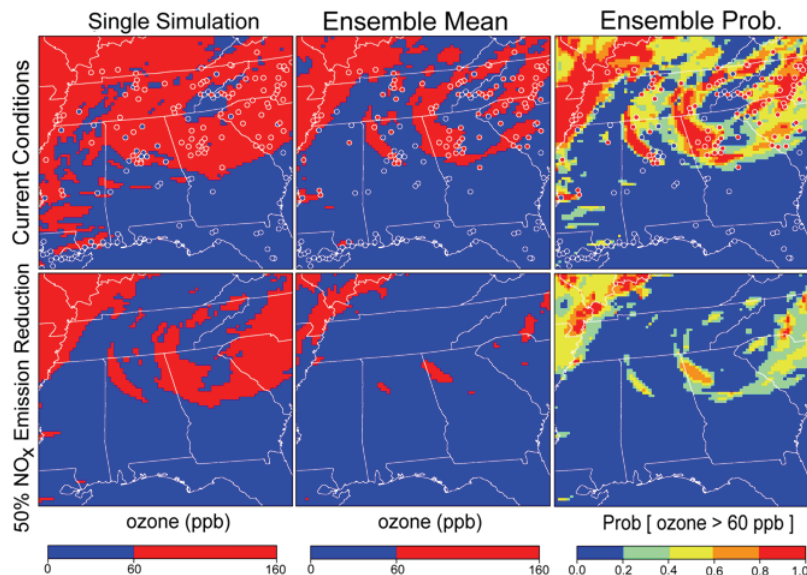
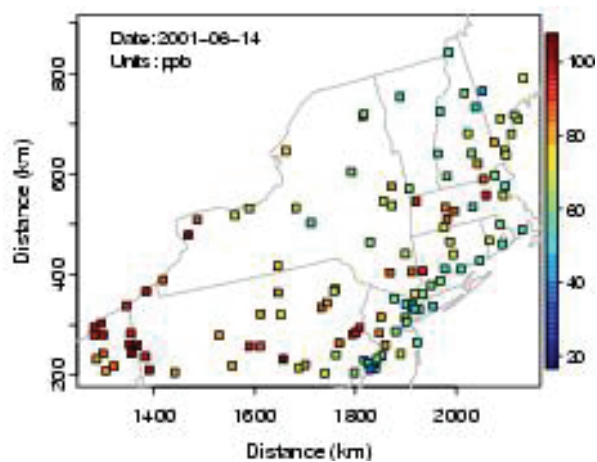


Figure 3-7. Spatial plots of ozone and probability of exceeding the threshold concentration for July 8, 2002, at 5 p.m. EDT. Observations are shown in white circles.

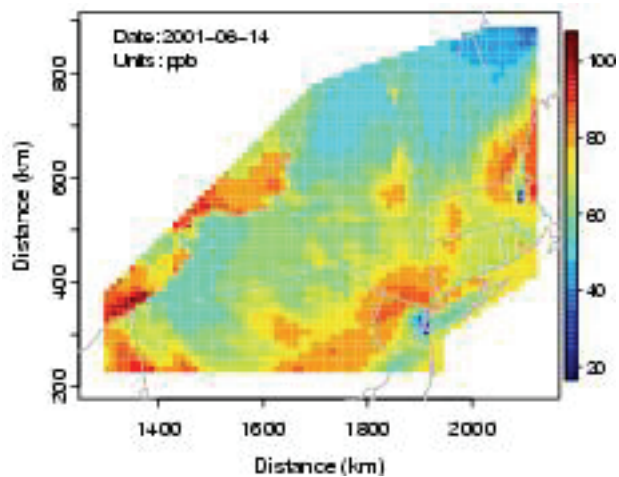
methods can aid the evaluator by making the best use of the limited monitoring data available, accounting for the differences between point-based measurements (monitors) and grid cell averages (model output), and assessing the model output for grid cells in which no monitors are located.

Although a variety of approaches could reasonably be utilized, we have focused on methods that allow us to better understand and utilize the spatial correlation of

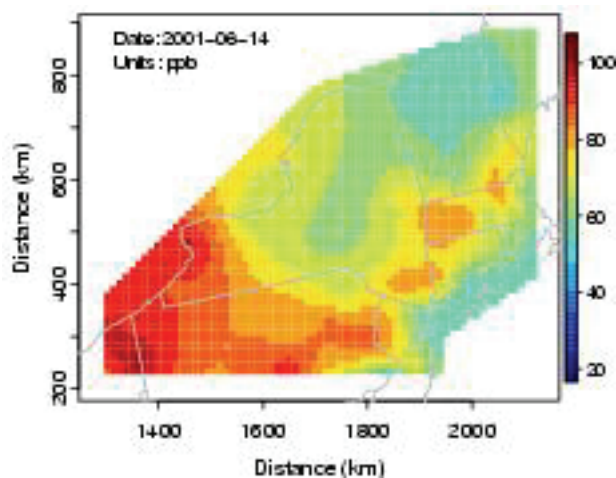
pollutant fields, such as kriging-based methods. For example, we have used Bayesian kriging to investigate the relationship between ammonium wet deposition and precipitation and kriging with adjustments for anisotropy to better understand O_3 and $PM_{2.5}$ concentrations in the northeastern U.S. In addition, recent work has explored the impact on model evaluation of incommensurability (i.e., the mismatch between point-based measurements and areal averages [model output]).



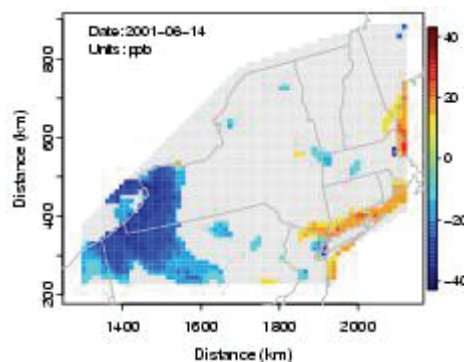
(a) Observed concentrations



(b) Modeled concentrations



(c) Block kriging estimates based on observations



(d) Grid cells of interest for further investigation

Figure 3-8. Assessment of CMAQ's performance in estimating maximum 8-h ozone in the northeastern United States on June 14, 2001.

CHAPTER 4

Climate and Air Quality Interactions

4.1 Introduction

Air quality is determined both by emissions of pollutants, including volatile organic compounds, NO_x , sulfur dioxide (SO_2), carbon monoxide, and Hg, and by meteorological conditions, including temperature, wind flow patterns, and the frequency of precipitation and stagnation events. For air quality management applications, regional-scale models are used to assess whether various emission control strategies will result in attainment of the NAAQS. These modeling applications typically assume present meteorological conditions, which means that potential changes in climate are not included in the assessment. Because emission controls are designed to be effective for several decades, future climate trends could impact their adequacy in meeting the NAAQS.

The first phase of the Climate Impact on Regional Air Quality (CIRAQ) pilot study on the effect of climate change on air quality has been completed. Future work is proceeding in the following three broad areas.

- (1) Developing methods to generate a range of future regional-scale climate scenarios by downscaling outputs from global climate models.
- (2) Developing alternative scenarios for future U.S. emissions of O_3 precursors and species that form atmospheric PM, taking into account current regulations, technological change, and population growth, and analyzing the impact of these emission changes on air quality.
- (3) Using the coupled WRF-CMAQ meteorology and chemistry model to investigate feedbacks of future emission scenarios on radiative budget.

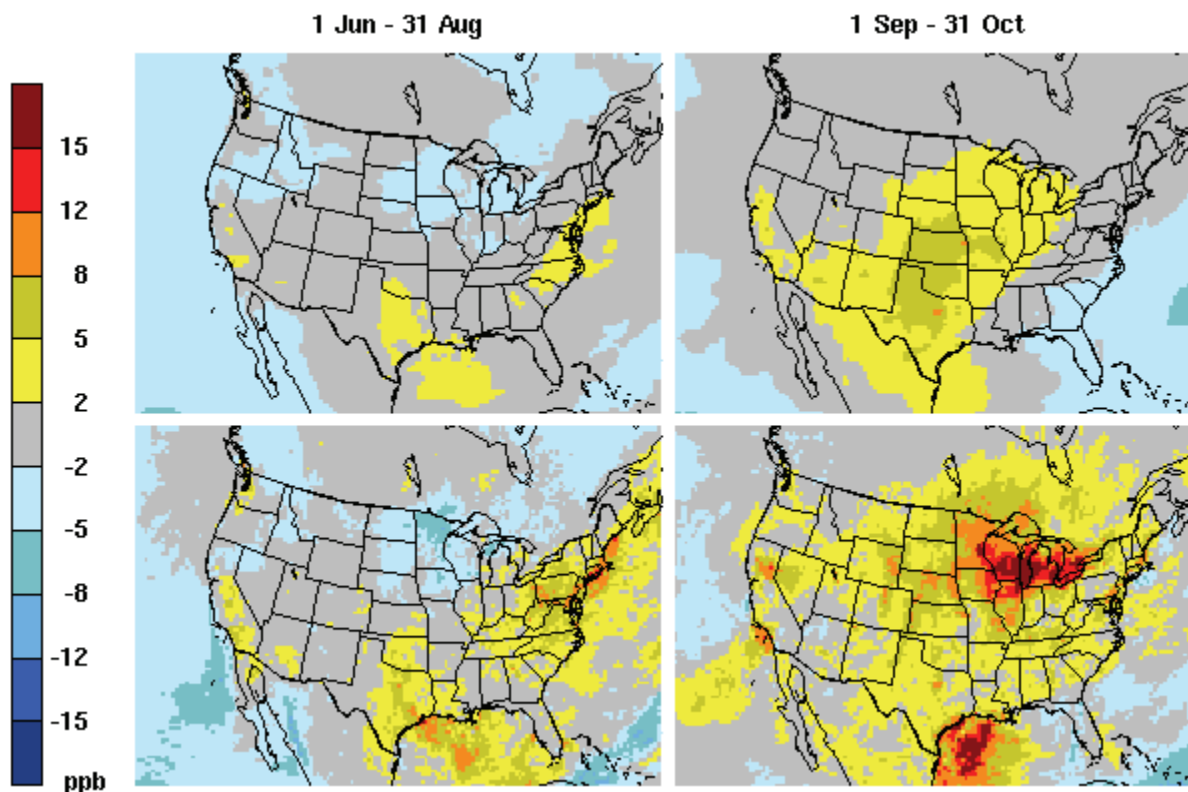


Figure 4-1. Differences in mean (top) and 95th percentile (bottom) maximum daily 8-h average (MDA8) ozone concentrations. Results show summertime increases of 2 to 5 ppb in mean MDA8 concentrations in Texas and parts of the eastern United States and even larger increases in 95th percentile concentrations, suggesting increased severity of ozone episodes. Still larger increases are predicted for the September-October time period, suggesting a lengthening of the ozone season (Nolte et al., 2008).

4.2 CIRAQ Pilot Study

AMAD initiated the CIRAQ project in 2002 to develop a pilot modeling study to incorporate regional-scale climate effects into air quality modeling. It involved collaboration across multiple Federal agencies and with academic groups with global-scale modeling expertise, who were supported through the EPA Science to Achieve Results grant program.

The Goddard Institute for Space Studies global climate model (GCM) version 2' was used to simulate the period from 1950 to 2055 at 4° latitude × 5° longitude resolution. Estimated historical values for greenhouse gases (as carbon dioxide equivalents) were used for 1950 to 2000, with future greenhouse gas forcing following the Intergovernmental Panel on Climate Change's A1B (Special Report on Emissions Scenarios [Nakicenovic et al., 2000]) scenario. Colleagues at the Pacific Northwest National Laboratory downscaled the GCM outputs using the Penn State/NCAR MM5 model to simulate meteorology over the continental United States at 36-km resolution for two 10-year periods centered on 2000 and 2050.

For the first phase of this project, the effect of potential climate change alone was considered, without attempting to account for changes in emissions of O₃ and PM precursors. Hourly emissions were simulated using the Sparse Matrix Operator Kernel Emissions (SMOKE). Anthropogenic emissions were based on the EPA 2001 modeling inventory, projected from the 1999 National Emission Inventory version 3. Biogenic emissions were calculated using the simulated meteorology. Air quality was simulated for two 5-year periods (1999 to 2003 and 2048 to 2052) using CMAQ v4.5.

As the next step, we are investigating the combined effect of climate change together with emission changes on air quality. Emission projections for different scenarios of economic growth and technological utilization are under development by colleagues at EPA/ Office of Research and Development's (ORD's) National Risk Management Research Laboratory (NRMRL). Air quality simulations using these emissions projections and the climatological meteorology described above will be conducted using CMAQ v4.7 in 2009.

CHAPTER 5

Linking Air Quality to Human Health

5.1 Introduction

This research theme applies existing models and tools and develops new tools and approaches to link air quality to human exposure and human health. Typically, epidemiological studies rely on ambient observations from sparse monitoring networks to provide metrics of exposure. Yet, for many pollutants in urban areas, large spatial variations exist, particularly near roads and major industrial sources. Further complicating the issue, ambient concentrations do not necessarily represent actual exposures, which are influenced by the infiltration of ambient concentrations into indoor facilities (such as automobiles, homes, schools, and work places) and the activity of individuals (such as outdoor exercise, walking, commuting, etc.). Finally, populations also are impacted by the transport of pollutants. These multiple factors

affecting exposure require approaches that scale from regional to local environments and to the individuals experiencing the exposure. Thus, this research provides analytical and physical modeling approaches that provide the spatial and temporal detail of concentration surfaces needed to understand the relationships among pollutants emitted, the resulting air quality, and exposure of humans to these pollutants.

Research conducted under this theme focuses on developing analytical tools and methods based on models and observations to improve the characterization of human exposure, evaluate the effectiveness of control strategies with respect to health outcomes, and address critical exposure issues, such as exposure to multiple pollutants for multiple scales.

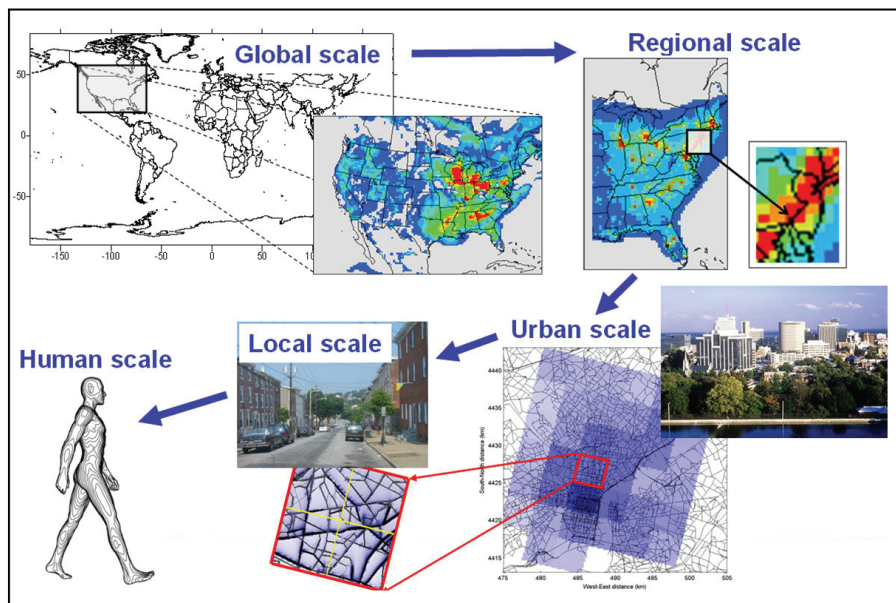


Figure 5-1. Linking local-scale and regional-scale models for exposure assessment characterizing spatial variation of air quality near roadways assessing the effectiveness of regional-scale air quality regulations (Source: Stein et al., 2007).

5.2 Characterizing Spatial Variation of Air Quality Near Roadways

Recent studies have identified increased adverse health effects in the large percentage of the population that lives, works, and attends school near some major roadways. EPA's Clean Air Research multiyear plan, therefore, emphasizes air research to better understand the linkages between traffic-pollutant sources and health outcomes. The effort described here is to further

understand the atmospheric transport and dispersion of emissions within the first few hundred meters of the roadway, a region often characterized by complex flow (e.g., sound barriers, road cuts, buildings, vegetation) and where steep gradients of concentration have been observed. Work within AMAD has focused on developing and improving various numerical modeling tools necessary for assessing potential human exposure in near-road environments.

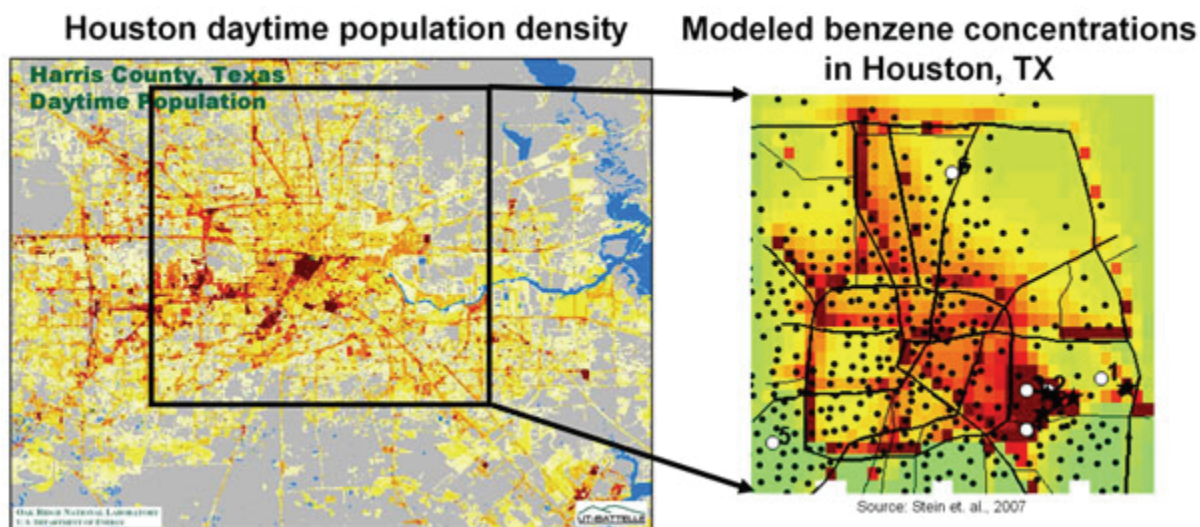


Figure 5-2. Population density and modeled benzene concentrations in Houston, TX.

Over the past decade, the Division has played a central role in developing the AERMOD near-field dispersion model, adopted by EPA as the preferred tool for urban-scale analyses. Although the model can simulate simple roadway configurations, it does not specifically account for many complexities commonly found near roads. However, after a thorough review of publicly available modeling tools, AERMOD was selected as the preferred platform on which improvements could be made for local-scale dispersion simulations of near-road applications and for inclusion in hybrid modeling (with CMAQ) for urban-scale exposure assessments. After initial wind tunnel studies, algorithms for estimating the concentration gradients downwind of roadways in the presence of noise barriers and depressed roadways have been developed. Initial evaluation of these enhancements are promising. Additional wind tunnel studies with variations in wind direction, barrier height, and surrounding surface characteristics are in progress. Computational fluid dynamics modeling of these and other scenarios is in progress and is expected to yield a significant database from which further improved parameterizations will result. Ongoing and future field campaigns and tracer studies will provide an excellent database for development and evaluation efforts.

Once improved and evaluated, the new near-road dispersion model will be used in the Air Quality Modeling Study in Atlanta as a part of a Cooperative Research Agreement between EPA/NERL and Emory University. In this project, air quality estimates will be correlated with a 10-year history of emergency room data and with the experiences of over 800 patients with Implanted Cardiac Defibrillators. Air quality estimates will be based on the hybrid approach using combined regional (CMAQ) and

local-scale (AERMOD) modeling. Various source configuration options will be tested in a sensitivity study to estimate the impact of noise barriers on air quality and exposure near roadways. Similar hybrid modeling activities will be conducted for Baltimore as a part of another cooperative agreement with the University of Washington.

Finally, related urban research in AMAD prior to the near-roadway program involved focus on homeland security. Between 2002 and 2005, the Division's Fluid Modeling Facility (FMF) examined flow and dispersion in three actual urban settings. Using the meteorological wind tunnel, AMAD provided critical modeling information for EPA's response to the tragic events in Manhattan in late 2001. As part of the Pentagon Shield Program, FMF scientists examined the flow and potential exposure to hazardous releases around the. In collaboration with EPA's National Homeland Security Research Center, wind tunnel measurements were conducted for an examination of street canyon flows in an urban neighborhood in Brooklyn, NY.

5.3 Evaluating the Effectiveness of Regional-Scale Air Quality Regulations

A core objective of the Clean Air Act is to "protect and enhance the quality of the Nation's air resources so as to promote the public health and welfare and the productive capacity of its population." To achieve this goal, billions of dollars are spent annually by the regulated community and Federal and State agencies on promulgating and implementing regulations intended to reduce air pollution and improve human and ecological health. Historically, the impact of air pollution regulations has been measured by tracking trends in emissions and ambient air concentrations. Now, however, EPA is

exploring the potential of extending the concept of measuring impact to a more complete understanding of the relationships along the entire source-to-outcome continuum. Assessing whether air quality management activities are achieving the originally anticipated results from sources through outcomes requires (1) the

development of indicators that capture changes in source emissions, ambient air concentrations, exposures, and health outcomes; and (2) the ability to characterize the processes that impact the relationships among these indicators.

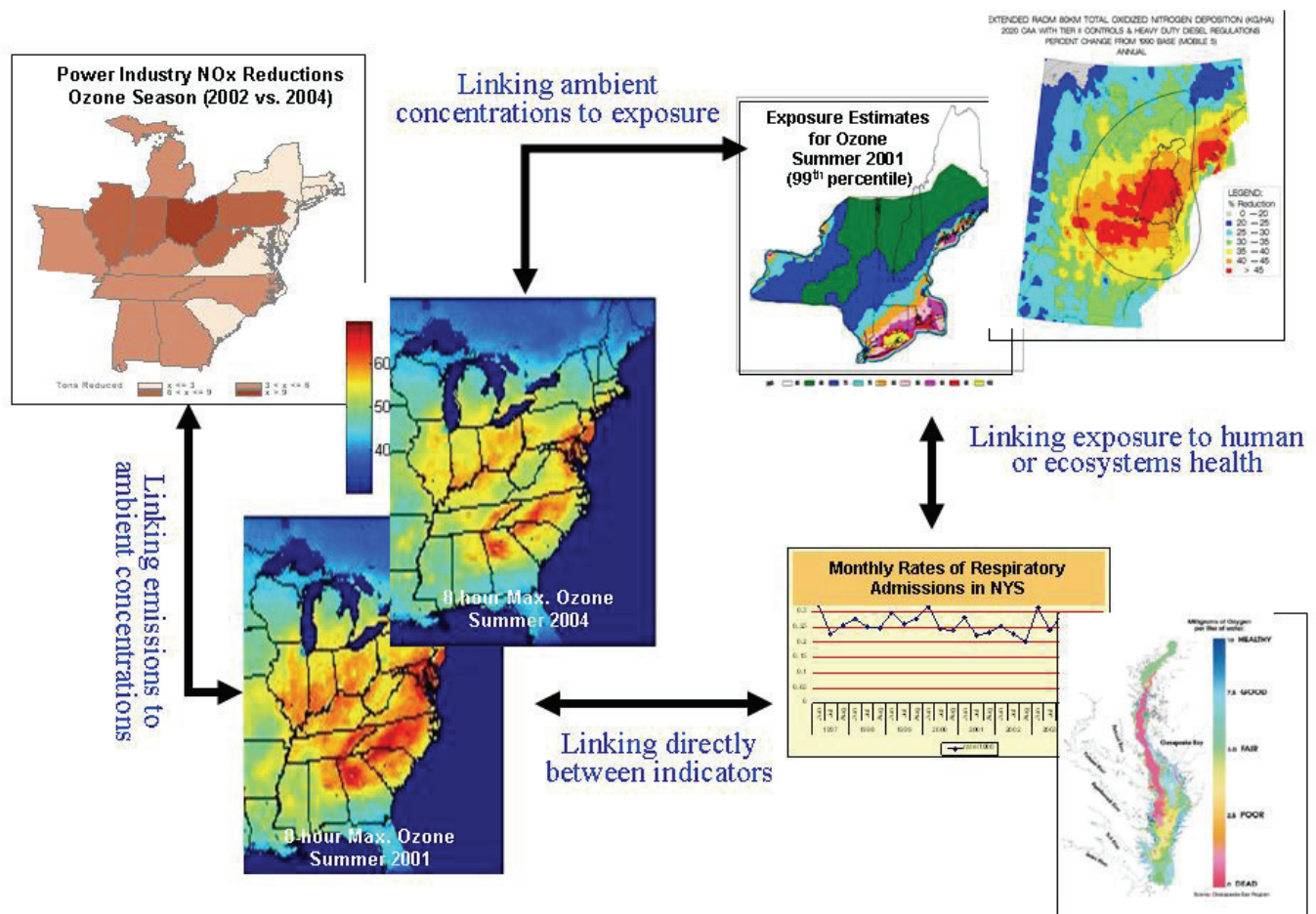


Figure 5-3. Assessing the impact of regulations on ecosystems and human health end points showing the indicators (boxes) and process linkages (arrows) associated with the NO_x Budget Trading Program. (Source: <http://www.epa.gov/asmdnerl/HumanHealth/evaluatingRegulations.html>).

The NO_x SIP call recently was implemented by EPA to reduce the emissions of NO_x, and the secondarily formed O₃, to decrease the formation and transport of O₃ across state boundaries. Over the past 3 years, AMAD's research has demonstrated reductions in observed and modeled ozone concentrations resulting from the NO_x SIP call. The CMAQ model was used to characterize air quality before and after the implementation of the NO_x SIP call and to evaluate correlations between changes in emissions and pollutant concentrations. Model simulations were used to estimate the anthropogenic contribution to total ambient concentrations and the

impact of not implementing the regulation. Methods were developed to differentiate changes attributable to emission reductions from those resulting from other factors, such as weather and annual and seasonal variations. Trajectory models were used to investigate the transport of primary and secondary pollutants from their sources to downwind regions.

We will continue to develop ways to systematically track and periodically assess progress in attaining national, State, and local air quality goals, particularly those related to criteria pollutants regulated under the NAAQS and related rules. Current research is focused

on relating NO_x emissions and ambient O₃ concentrations to human exposure and health end points. Improved air quality surfaces that combine observed and modeled data are being generated for use in exposure models, epidemiological health studies, and risk assessments. These studies will examine the benefits of using improved air quality surfaces versus central monitoring approaches and of using exposure probability factors versus ambient O₃ concentrations in health studies. In addition, these studies will evaluate changes in predicted exposure and risk assessments and actual changes in health end points (e.g., respiratory diseases) between the pre- and post-NO_x SIP call time periods. Finally, research is moving beyond the NO_x SIP call to assess upcoming regulations. An approach for evaluating a CAIR is being investigated to establish and integrate “metrics” (predictions of changes associated with the promulgation of CAIR) and “indicators” (actual

levels of the same or closely related parameters observed during the implementation of CAIR).

5.4 Linking Local-Scale and Regional-Scale Models for Exposure Assessments

Population-based human exposure models predict the distribution of personal exposures to pollutants of outdoor origin using a variety of inputs, including air pollution concentrations; human activity patterns, such as the amount of time spent outdoors versus indoors, commuting, walking, and indoors at home; microenvironmental infiltration rates; and pollutant removal rates in indoor environments. Typically, exposure models rely on ambient air concentration inputs from a sparse network of monitoring stations.

The extent of variability in spatial and temporal concentration gradients associated with large point sources and roadways shown in this research is

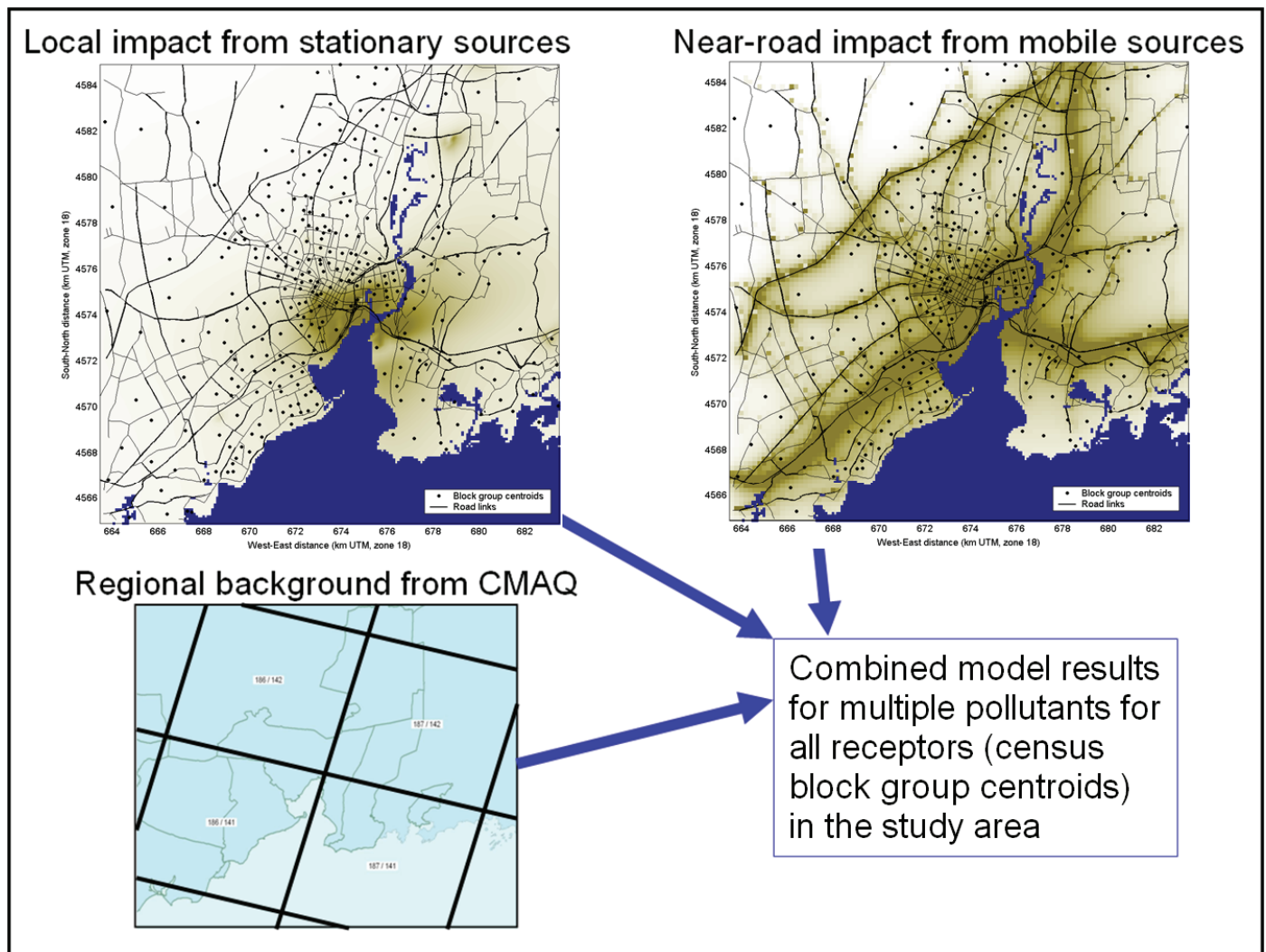


Figure 5-4. Combined model results for multiple pollutants for all receptors (Source: Isakov et al., 2009).

especially important, given the growing body of literature on the potential adverse health effects associated with elevated concentrations near such sources. A new method to enhance air quality and exposure modeling tools has been advanced to provide finer-scale air toxics concentrations to exposure models. This hybrid modeling approach combines the results from two types of regional- and local-scale air quality models (the CMAQ chemistry-transport model and the AERMOD dispersion model). The resulting hourly concentrations are used as inputs to population exposure models (the Hazardous Air Pollutant Exposure Model [HAPEM] and the Stochastic Human Exposure and Dose Simulation [SHEDS] model) to enhance estimates of urban air pollution exposures that vary temporally (annual and seasonal) and spatially (at census block group resolution). Thus, linkage between air quality and exposure modeling will help improve health assessments that include near-source impacts of multiple ambient air pollutants.

Testing and demonstration of how this linked air quality/exposure modeling approach may be used in future community-level environmental health studies is underway with an initial feasibility study providing exposure estimates for residences near large industrial facilities or major roadways in New Haven, CT. The study objective is to examine the cumulative impact of various air pollution reduction activities (at local, State, and national levels) on changes in air quality concentrations, human exposures, and potential health outcomes in the community. In conjunction with local data on emission sources, demographic and socioeconomic characteristics, and indicators of exposure and health, the methodology presented here can serve as a prototype for providing high-resolution exposure data in future community air pollution health studies. For example, the methodology can be used to provide the baseline air quality assessments of impacts of regional- or local-scale air pollution control measures. It also can be applied to estimate the likely impact of future projected air pollution control measures or urban and industrial growth on human exposures and health in the community.

This hybrid approach provides deterministic outcomes at local scales. The Division also is engaged in studies of a complementary approach in which an air quality (e.g., CMAQ) grid model's deterministically based outputs operational at regional-urban grid size scales are augmented with information on subgrid spatial variability (SGV) provided a priori and in a stochastic framework as parameterized distribution functions. In this paradigm, the SGV for each grid would be determined uniquely, and model parameterizations based on its emissions distributions and relevant ventilation factors. For this paradigm, the scope of this prototypic effort includes the step of developing linkages with exposure models.

The hybrid modeling approach combines concentrations from a grid-based chemical-transport model and a local plume dispersion model to provide the contribution from photochemical interactions and long-range (regional) transport and local-scale dispersion. In the New Haven feasibility study, we used the AERMOD dispersion model, which treats individual road links as area sources to simulate hourly concentrations of various pollutants near the road. AERMOD also simulates near-source impacts from stationary sources. Contributions to photochemical interactions were provided as background concentrations from CMAQ, a regional grid model.

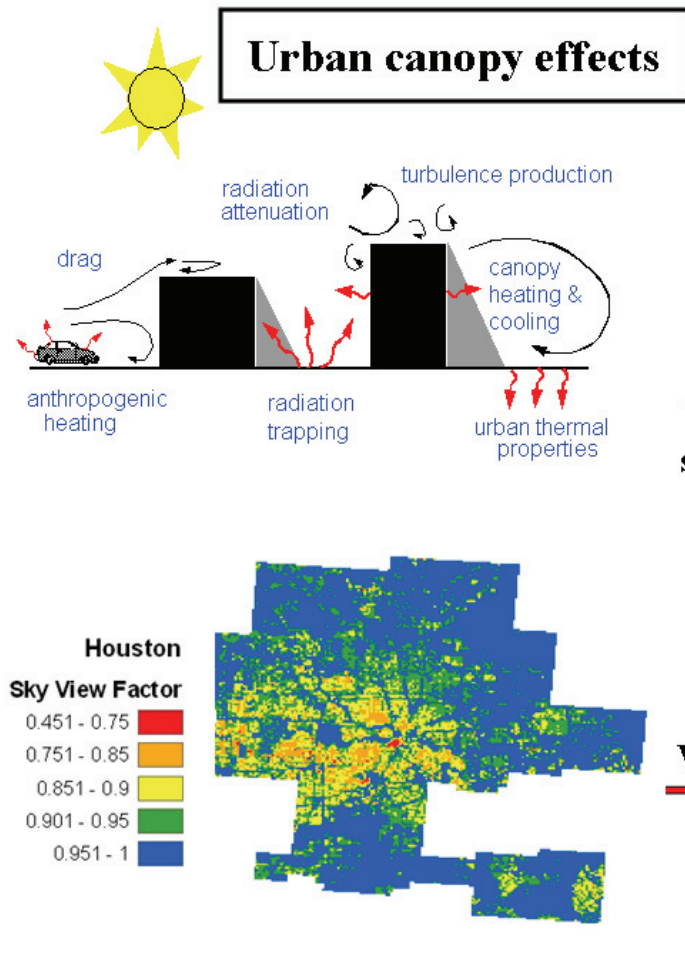
5.5 National Urban Database and Access Portal Tool

Based on the need for advanced treatments of high-resolution urban morphological features (e.g., buildings, trees) in meteorological, dispersion, air quality, and human exposure modeling systems, a new project was launched called the National Urban Database and Access Portal Tool (NUDAPT). The prototype NUDAPT was sponsored by EPA and involved collaborations and contributions from many groups, including Federal and State agencies and from private and academic institutions here and in other countries. It is designed to produce gridded fields of urban canopy parameters (UCPs) to improve urban simulations given the availability of new high-resolution data of buildings, vegetation, and land use. Urbanization schemes have been introduced into the Mesoscale Model, version 5 (MM5), the WRF, and other models and are being tested and evaluated for grid sizes on an order of 1 km or so. Additional information includes gridded anthropogenic heating and population data, incorporated to further improve urban simulations and to encourage and facilitate decision support and application linkages to human exposure models. An important core-design feature is the utilization of Web portal technology to enable NUDAPT to be a "community"-based system. This Web-based portal technology will facilitate customizing of data handling and retrievals (<http://www.nudapt.org>).

High-resolution building information is being acquired by the National Geospatial Agency (NGA; formerly the National Imagery and Mapping Agency). When completed, NGA will have obtained data from as many as 133 urban areas. Building data can be acquired by extractions from paired stereographic aerial images by photogrammetric analysis techniques or from digital terrain models (DTMs) acquired by airborne light detecting and ranging (LIDAR) data collection. LIDAR data are acquired by flying an airborne laser scanner over an urban area and collecting return signals from pairs of rapidly emitted laser pulses and processed to produce terrain elevation data products, including

full-feature digital elevation models (DEMs) and bare-earth DTMs. Subtracting the DTM from the DEM produce data on building and vegetation heights above ground level. Currently, NUDAPT has acquired datasets and hosts 33 cities in the United States with different degrees of coverage and completeness. Data are

presented in their original format, such as building heights, day and night population, vegetation data, and land-surface temperature and radiation, or in a “derived” format such as the UCPs for urban meteorology and air quality modeling applications.



Modeling Requirement

To capture the grid average effect of detailed urban features in meso-scale atmospheric models

Solution

Defined and implemented Urban canopy parameterizations such as height-to-width ratios and sky view factors into their model formulations

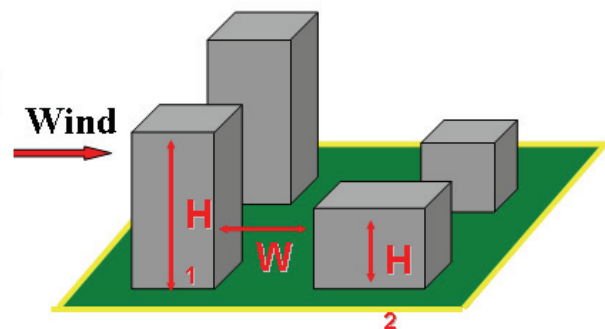


Figure 5-5. Urban canopy effects. (Source: Ching et al., 2009).

CHAPTER 6

Linking Air Quality and Ecosystems

6.1 Introduction

A long-term goal of environmental management is to achieve sustainable ecological resources. Ecological resources are exposed to atmospheric pollutants through wet and dry deposition processes (atmospheric stressors) that can impact the means by which this goal is met and maintained. Progress toward this goal rests on a foundation of science-based methods and data integrated into predictive multimedia, multidisciplinary, multistressor open architecture modeling systems. The strategic pathway described by the tasks presented here progresses from the current approach that addresses one stressor at a time to a comprehensive multimedia-multiple stressor assessment capability for current and projected ecosystem health.

The ecosystem exposure tasks in AMAD address a number of issues that arise in multimedia modeling, with an emphasis on interactions among the atmosphere and other environmental media. The interaction between the atmosphere and the underlying surface increasingly is being recognized as an important factor in ecosystem exposure and pollutant transport issues. However, differences in functional scale are a fundamental challenge to understanding and modeling these interactions. For instance, the watershed is a fundamental unit of ecosystem analysis, because primarily of its containment of the hydrologic cycle and related stresses, but the relevant atmospheric scale of modeling and analysis is regional/continental in scope, encompassing multiple States or watersheds. Targeted development, evaluation, and application of state-of-the-art, multipollutant atmospheric models of O₃, sulfur, nitrogen, and Hg to multimedia issues help determine how to further improve the one-atmosphere models and support ongoing ecological assessments by providing ecosystem exposure estimates where monitoring data are not available.

A thorough understanding of air quality model sensitivities can guide the design of field campaigns so that measurements of parameters needed for further model development are collected, model uncertainties can be reduced, and robust model evaluations can be produced, which further the understanding of the atmosphere-biosphere exchange. Software tools are needed to support the linkage of models across media and specialized multimedia data analysis applications.

Finally, this multimedia research brings the results of air pollution control, that primarily stem from addressing human health effects, into the management

purview for addressing multimedia or ecosystem problems. Humankind benefits from a multitude of resources and processes that are supplied by natural ecosystems. Collectively, these benefits are known as ecosystem services and include products like clean air and clean water. Ecosystem services are distinct from other ecosystem products and functions because there is human demand for these natural assets.

Measurement of ecosystem services is the new strategic focus for EPA's Ecological Services Research Program (ESRP). It is believed that making the evaluation of these services a routine part of decisionmaking will transform the way we understand and respond to environmental issues. The ESRP's mission is to conduct innovative ecological research that provides the information and methods needed by decisionmakers to assess the benefits of ecosystem services to human well-being and, in turn, to shape policy and management actions at multiple spatial and temporal scales.

6.2 Research Description

The ecosystem research team has identified several key research areas that have the potential to reduce model uncertainties in deposition, to assess model credibility, and to link the CMAQ model to multimedia ecosystem exposure models.

Specific research tasks have been grouped under the following more general research program elements.

- Linking air quality to aquatic and terrestrial ecosystems
- Linking air quality to ecosystem services
- Improvements to CMAQ dry deposition algorithms
- CMAQ ecosystem exposure studies
- Multimedia tool development

Through the *linking air quality to aquatic and terrestrial ecosystems* program element, the Division develops and enhances dry deposition algorithms for land cover specific subgrid cell ecological receptors to facilitate improved interactions with ecosystem and water quality models and to provide more relevant information to ecosystem managers. Ecosystem exposure occurs when stressors and receptors occur at the same time and place. To model the exposure, models for different media (e.g., air, water, land) must be linked together. Linkages between models for air, water, and land can occur through the use of consistent input data, such as land use and meteorology, and through the appropriate exchange of data at relevant spatial and temporal scales.

At present, mesoscale meteorological inputs (e.g., MM5) and CMAQ v4.7 rely on 1992 National Land Cover Dataset (NLCD) classes to identify the location of general land cover types (e.g., urban, row agriculture, etc.). Most ESRP research employs more recent 2001 NLCD and 2001 to 2006 NOAA Coastal Change Analysis Program (C-CAP) databases that also provide higher resolution information. Meteorological and CMAQ models are being updated to make use of these more recent landcover databases. Vegetation species detail currently is accessed by CMAQ only for the calculation of bioemissions and is based on the Biogenic Emissions Landcover Database, version 3 (BELD3). Agricultural species distributions in BELD3 reflect 1995 U.S. Department of Agriculture (USDA) National Agricultural Statistics Service (NASS) surveys. To maintain consistency with the 2001 NLCD vegetation classes, these estimates are being updated to reflect 2001 crop distributions. We anticipate more extensive use of the updated BELD information in the estimation of ecosystem-specific exposure to atmospheric nitrogen and Hg deposition.

Watershed models are calibrated to multiple years of observed hydrology and precipitation. Chemical simulations are generated using the same inputs as well as drawing on current monitored deposition fields from the National Acid Deposition Program (NADP). Scenarios of changes in deposition, however, are drawn from CMAQ simulations (Sullivan et al., 2008). Unfortunately, temporal and spatial agreement between the modeled meteorological data used to drive CMAQ deposition estimates and observed precipitation used to drive the water quantity and quality simulations can be poor, so that the base case and the futures case are not consistent.

Focus areas of the linking air quality to aquatic and terrestrial ecosystem program element include

- developing landcover-specific dry deposition algorithms as opposed to a single grid value blended across all landcover types;
- updating the current CMAQ landcover database with more recent higher resolution databases;
- updating the BELD3 crop distributions based on more recent USDA crop data; and
- developing a methodology to rectify the differences in CMAQ model input and output fields and water quality model input fields.

Through the *linking to ecosystem services* program element, the Division develops modeling tools, scenarios and multidisciplinary collaborations to assess the impact of air quality on the intrinsic value of natural and agricultural ecosystems. The Future Midwestern Landscapes (FML) Study is being undertaken as part of EPA's ESRP. The FML goal is to quantify the current magnitude of ecosystem contribution to human health and to examine how ecosystem services in the Midwest

could change over the next 10 to 15 years, given the growing demand for biofuels, as well as the growing recognition that many different ecosystem services are valuable to society and need to be encouraged. The FML study will examine how the overall complement of ecosystem services provided by the Midwest may be affected. The study will characterize a variety of ecosystem services for the 12-state area of the Midwest.

The significance of reactive nitrogen (Nr), which includes oxidized, reduced, and organic forms, to the environment stems from the duality of its environmental impacts. On the one hand, Nr is one of life's essential nutrient elements. It is required for the growth and maintenance of all of earth's biological systems. For humans, there are several sets of services provided by natural and anthropogenic sources of reactive nitrogen, including the production of plant and animal products (food and fiber) for human consumption and the combustion of fuels that support our energy and transportation needs. Increasing demands for energy, transportation and food lead to greater demand for Nr. Although releases of nitrogen are associated with societal benefits, Nr is a powerful environmental pollutant. Over the past century, human intervention in the nitrogen cycle and use of fossil fuels has led to substantial increases in production of Nr and in human and ecosystem exposure to Nr. The amount of Nr applied to the nation's landscape and released to the nation's air and water has reached unprecedented levels, and projections show that Nr pollution will continue to increase for the foreseeable future. These increases in Nr pollution are accompanied by increased environmental and human health problems. The ESRP Nitrogen Team will address its broad goal of connecting Nr to ecosystem services through a two-pronged effort, with national work where possible and smaller scale, regional studies tackling specific problems and ecosystem types.

Focus areas of the linking to ecosystem services program element include

- characterizing the role of atmospheric nitrogen deposition in the achievement and maintenance of ecosystem resources and services in the Midwestern United States;
- developing the capacity to model air quality response to future emission and land cover scenarios for increased biofuel production to assess the impact of hypothetical policy-driven changes in biofuels and the impact of this response on ecosystem services;
- characterizing 12-km continental U.S. atmospheric deposition of sulfur, oxidized nitrogen, reduced nitrogen, and O₃ for 2002, 2020, and 2030 using CMAQ; and
- assessing regional ecosystem vulnerability to nitrogen and sulfur deposition using CMAQ deposition output

and NADP and Parameter-Elevation Regressions on Independent Slopes Model (PRISM) data

Through the *improvements to CMAQ dry deposition algorithms* program element, the Division develops modeling algorithms, tools, and experiments to evaluate and improve the modeling of the air-surface exchange of pollutants. The interaction between the atmosphere and the underlying surface increasingly is recognized as important in ecosystem health and in air pollution transport processes. Evasion of ammonia (NH₃) and Hg from vegetation, soil and water surfaces is important in the long range transport of these pollutants and can act as a vector of exposure to ecosystems remotely located from anthropogenic sources. A key output of atmospheric models for ecosystem health studies is the dry deposition component of net ecosystem loading (wet + dry + evasion). There is an extreme paucity of measured and monitored dry deposition estimates for use with ecosystem management modeling. The estimates from the atmospheric models fill a critical gap. A targeted focus on creating state-of-the-science dry deposition algorithms for the air quality models has significant importance to ecosystem exposure to air pollution. This is an area of strong collaboration between CMAQ model development and ecosystem exposure programs.

One of the ways EPA assesses the results of air pollution control is through the Clean Air Status and Trends Network (CASTNET). Dry deposition estimates from CASTNET are inferred from measured atmospheric concentrations and a dry deposition velocity estimated from the physical characteristics of the ecosystem and wind velocity measurements. The Multilayer Model (MLM) (Meyers et al., 1998) is used to predict deposition velocity, which then is paired with the measured concentration to calculate the pollutant flux. Air-surface exchange research will continue to develop better models for predicting deposition velocity for network operations. Providing better estimates of deposition flux will improve our ability to forecast ecosystem sustainability.

Excessive loading of nitrogen from atmospheric nitrate and NH₃ deposition to ecosystems can lead to soil acidification, nutrient imbalances, and eutrophication. Accurate net nitrogen flux estimates are important for biogeochemical cycling calculations performed by ecosystem models to simulate ecosystem degradation and recovery. Because of the lack of available monitoring data, these estimates are a high priority for water and soil chemistry modeling of nutrient loading, soil acidification, and eutrophication. A process-level understanding of the biological, chemical, and mechanical processes influencing the soil-vegetation-atmosphere exchange of nitrogen over a variety of managed and natural ecosystems is needed before tenable mitigation strategies can be realized.

Atmospheric loadings of Hg to sensitive ecosystems can lead to methylation and bioaccumulation, adversely affecting wildlife and becoming a vector for human exposure to methylmercury. The transport of Hg in the environment exhibits bidirectional surface exchange, similar to NH₃, and a bidirectional surface exchange model of Hg is needed to estimate the net ecosystem loading of Hg needed by ecosystem managers to assess the vulnerability of ecosystems to Hg exposure.

Focus areas of the improvements to CMAQ dry deposition algorithms program element include those noted below.

- Develop better models for predicting deposition velocities for monitoring network operations
- Collaborate with Federal and academic field scientists to design and conduct experiments to measure air-biosphere exchange parameters based on model sensitivities and hypotheses proposed in the literature
- Develop and refine air-soil and air-vegetation NH₃ exchange algorithms for agricultural and natural ecosystems using the results from intensive measurement campaigns
- Develop an air-biosphere exchange model for Hg emissions from natural processes in CMAQ

Through the *CMAQ ecosystem exposure studies* program element, the Division provides guidance and advice to the ecosystem management community using CMAQ as a laboratory. Atmospheric deposition of sulfur and nitrogen is a key contributor to ecosystem exposure and degradation, adding to the acidification of lakes and streams and eutrophication of coastal systems. Reductions in atmospheric deposition of sulfur and oxidized nitrogen stemming from human-health-driven regulations in the 1990 CAA amendments are expected to significantly benefit efforts to improve water quality. However, water quality managers are not taking advantage of information on anticipated deposition reductions in developing their management plans. Managers need to understand what to expect from atmospheric emissions and deposition. This understanding must come from an air quality model utilized as a laboratory; it cannot come from measurements. The goal is to bring air quality into ecosystem management through regional air quality modeling and to facilitate the air-ecosystem linkage.

The Division's approach is to collaborate with select, motivated air-water partners who are willing to work together to provide a test laboratory with the atmospheric model to explore, assess, and apply improved techniques to advance water quality management goals and test linkage approaches. The Division is developing an understanding of the needs of water quality managers through real-world experience and participation with model applications. We then design model analyses and sensitivity studies to identify

and direct what atmospheric science needs to deliver. Results help provide answers to nearly universal questions uncovered in the course of the application studies: How much is depositing? Who and where is the deposition from? How much will deposition change because of air quality regulations in the face of population and economic growth?

Focus areas of the CMAQ ecosystem exposure studies program element include those that follow.

- Evaluate CMAQ-UCD against the Bay Regional Atmospheric Chemistry Experiment (BRACE) May 2002 data and make any model refinements that may be required
- Assess the relative contributions from the different emissions sectors, particularly mobile sources and utilities, to the annual oxidized nitrogen deposition to Tampa Bay
- Assess the change in annual deposition to Tampa Bay that could be attributed solely to the NO_x emissions reductions by 2010 of the two power plants on its shores
- Assess the change in annual deposition to Tampa Bay that could be attributed to future mobile source and utility reductions of SO₂ and NO_x in 2010
- Develop scenarios estimating the deposition reductions to Chesapeake Bay expected by 2010 and 2020 stemming from Clean Air Act regulations
- Update the Chesapeake Bay scenarios with the configuration of CMAQ that includes bidirectional flux of NH₃ still under development
- Estimate the relative contribution made by NO_x emissions from the six Bay States to the atmospheric deposition of oxidized nitrogen to the Chesapeake Bay watershed and Bay surface after implementation of future reduction scenarios of mobile source and utility emissions

Through the *software tool development* program element the Division develops tools 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.

Focus areas of the software tool development program element include support and development of

- the Visualization Environment for Rich Data Interpretation (VERDI);
- the Watershed Deposition Tool (WDT); and
- the Spatial Allocator vector, raster, and surrogate tools.

6.3 Accomplishments

Watershed modeled sensitivities to 2001 to 2003 precipitation data was explored through (1) the use of daily cooperative station data to perform a monthly calibration of the Grid-Based Mercury Model (Tetra Tech, 2006), (2) calibrated model runoff volume response to 36-km simulated daily precipitation and mean daily temperature fields, (3) response to 12-km simulated daily precipitation and mean daily temperature fields, and (4) response to 4-km PRISM-generated precipitation data.

Errors in the simulated meteorology related to timing, spatial coverage, magnitude, and suppressed interannual variability can be observed. The benefit of higher scale meteorological simulations can be noted in cases where model runoff volume driven by the 12-km precipitation is much closer to the U.S. Geological Survey observed runoff than that driven by the 36-km simulation. Exceptions occur where there is little or no runoff response difference between the two meteorological datasets. This happens most often during the fall months and has been traced to a failure of the analysis model used to nudge the meteorological simulation to capture the development of tropical storms off the coast of North Carolina. The PRISM database (Daly et al., 2002) contains 4-km gridded monthly precipitation generated via a set of regression expressions and cooperative station data and represents a more spatially complete dataset that could, perhaps, be used to calibrate the watershed model.

Scenario simulations for the Chesapeake Bay for 2002 and 2010 with CMAQ 4.7 using the new coarse-mode sea salt dynamic mass transfer module were completed. An analysis of the relative contributions of NO_x emissions from six sectors to the atmospheric deposition of oxidized nitrogen to the Chesapeake Bay watershed and Bay surface after the implementation of CAIR was completed. The relative contribution the NO_x emissions from the six Bay states make to the atmospheric deposition of oxidized nitrogen to the Chesapeake Bay watershed and Bay surface after implementation of CAIR was estimated.

The development of the preliminary bidirectional NH₃ exchange and coarse-nitrate model algorithms improved the modeled oxidized and reduced nitrogen budgets and the partitioning between gas and size-segregated aerosol phases. Mechanistic model algorithms developed in collaboration with measurement groups enhances the credibility of the CMAQ nitrogen budget for ecosystem assessments.

Results from the bidirectional NH₃ exchange model helped prioritize current and future measurement needs in field experiments. Scientists from AMAD have collaborated with scientists from EPA's National Risk Management Research Laboratory (NRMRL), Duke University, North Carolina State University, and the

United Kingdom's Center for Hydrology and Ecology to estimate in-canopy and soil NH_3 exchange processes based on field measurements and modeling theory. An analytical in-canopy scalar transport closure model that estimates in-canopy sources and sinks by using measured concentration and wind speed profiles was developed. The above-canopy ammonia flux, in-canopy ammonia sources and sinks, soil chemistry, and leaf chemistry measurements were collected in a fertilized corn (*Zea Mays*) field in Lillington, NC, during the 2007 growing season. Estimates of in-canopy sources and sinks were inferred using measured in-canopy concentration profiles and a simple closure model.

VERDI was developed in 2007 for the EPA by Argonne National Laboratory to improve the capability to visualize data from the CMAQ model and associated programs. In FY08, support for VERDI by the CMAS Center was initiated. Improvements were made to the VERDI software and a Web site was developed to provide information and distribution. VERDI is an open source program, which is licensed under the GPL version 3. A SourceForge repository (<http://sourceforge.net>) for VERDI was created to facilitate distribution and source code version control.

WDT was developed for the EPA by Argonne National Laboratory to provide an easy-to-use tool for mapping the deposition estimates from CMAQ to watersheds to provide the linkage between air and water needed for total maximum daily load (TMDL) and related nonpoint-source watershed analyses. Slight modifications to the program were released in FY08. This tool has been useful in performing analyses and also in providing a means to communicate the strengths of using CMAQ data rather than monitoring data in watershed analyses.

6.4 Next Steps

Over the next several years, advancements are planned for the multimedia theme area to investigate more sophisticated futures scenarios for air-water linkages, to adapt CMAQ to calculate bidirectional exchange of NH_3 and Hg, and to more closely couple to ecosystems models. Some of the planned research goals are as follows.

FY-2009

- Refinement of CMAQ air-canopy bidirectional NH_3 exchange algorithms using the estimated sources and sinks from the 2007 Lillington, NC, study
- Development of an air-soil biogeochemical nitrogen model for fertilizer applications to agricultural ecosystems using data from the 2007 Lillington, NC, study
- Convert mosaic land-use interface to NLCD for consistency with ecosystem models and test CMAQ for land-use-change scenario analysis

- Complete preliminary air-water model linkage for N.C. Albemarle-Pamlico estuarine system
- Collaboration with Federal laboratories and academic institutions to design experiments to measure sources and sinks of NH_3 in forested ecosystems at Duke Forest

FY-2010

- For ESRP place-based scenario analyses (Carolinas, Midwest, Tampa), simulate nitrogen, sulfur, and O_3 deposition futures incorporating land-use changes
- Incorporate into a science version of CMAQ a generalized land-surface layer to support multipollutant bidirectional flux calculations (already in the Hg bidirectional exchange model)
- Adapt and implement an nitrogen fertilizer application scenario tool to produce nationally consistent input required by the improved bidirectional NH_3 exchange algorithms for agricultural ecosystems (see FY-2011)
- Collaboration with Federal laboratories and academic institutions to estimate the sources and sinks of NH_3 in a hardwood and coniferous forested ecosystem
- Annual simulation of CMAQ with bidirectional Hg exchange for 2002 emissions to evaluate the seasonality of the bidirectional and base model with NADP monitoring Hg deposition data
- Simulate Chesapeake Bay futures scenarios with CMAQ at 12-km grid cell size and incorporate NH_3 bidirectional exchange influence for Chesapeake sensitivity
- Improve meteorological precipitation simulations to facilitate better hydrologic linkage with watershed models using higher resolution simulations (4 km) nudged using analyses that include more extensive data assimilation or that employ more advanced data assimilation techniques such as 3-D variational analysis
- Couple VERDI with the watershed deposition tool
- Evaluate the NH_3 bidirectional exchange algorithms over grasslands with data collected at the 2008 Duke Forest measurement campaign
- Annual simulation of CMAQ with bidirectional NH_3 exchange in support of the ESRP FML

FY-2011

- Update CMAQ bidirectional NH_3 exchange algorithms for natural and managed ecosystems
- Development of an updated NH_3 emission inventory for use with CMAQ with bidirectional NH_3 exchange
- Assess the impact of meteorological precipitation errors on the deposition of nitrogen compounds from the atmosphere to underlying soils, vegetation, and water surfaces and their subsequent transport to downstream estuarine end points
- Evaluate the transport and fate of NH_3 in CMAQ using specially collected NASA Tropospheric Emission

Spectrometer (TES) satellite observations and collocated passive monitors

- Evaluate the bidirectional NH_3 exchange algorithms over forested ecosystem with data collected during the 2009 Duke Forest measurement campaign

6.5 Impact and Transition of Research to Applications

Air deposition reductions are now a vital component of the Chesapeake Bay Program's restoration efforts. Critical air deposition information also has been provided to the Tampa Bay Estuary Program to address its TMDL needs and assessment goals. Our efforts have opened the door for water quality managers to include air deposition and make their management plans more efficient and effective. The work has paved the way for

using CMAQ in national NO_x -sulfur oxides regulatory assessments to protect ecosystems and for using CMAQ in U.S. critical loads analyses.

An area where the "one atmosphere" approach of CMAQ helped elucidate the connection between modeled chemical mechanisms and ecosystem exposure through dry deposition was heterogeneous N_2O_5 conversion. The uncertainty in the heterogeneous conversion of N_2O_5 to HNO_3 was examined because it impacts HNO_3 concentrations and deposition. However, this uncertainty has a minor impact on oxidized nitrogen deposition because the deposition pathways among the oxidized nitrogen species rebalance. Zeroing out this conversion reduces HNO_3 and aNO_3^- deposition by 18% and 26%, respectively, whereas total oxidized nitrogen is reduced by only 6%.

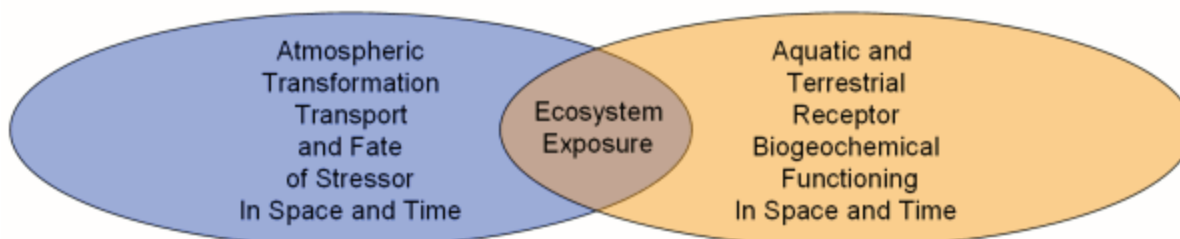


Figure 6-1. A Venn diagram representing ecosystem exposure as the intersection of the atmosphere and biosphere (<http://www.epa.gov/amad/EcoExposure/index.html>).

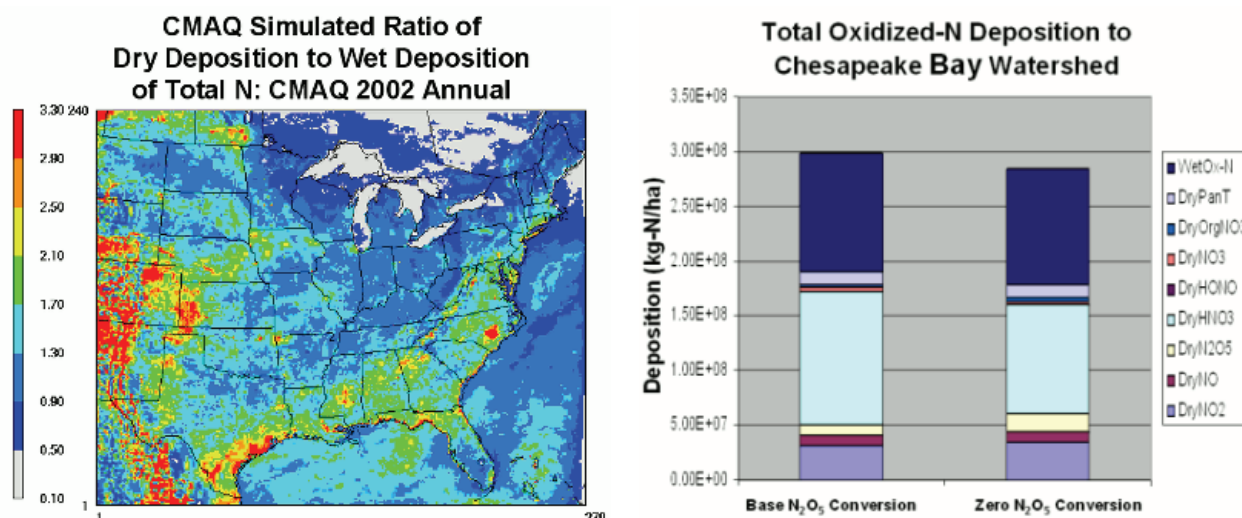


Figure 6-2. CMAQ is a source of data for ecosystem managers that is not available in routine monitoring data, such as (left panel) complete dry and wet deposition estimates, and (right panel) the "one atmosphere" concept of CMAQ is needed to understand the balance between uncertainties in atmospheric reaction rates and deposition pathways (<http://www.epa.gov/amad/EcoExposure/ecoStudies.html>).

References

- Bhave, P.V., G.A. Pouliot, and M. Zheng. Diagnostic Model Evaluation for Carbonaceous PM_{2.5} Using Organic Markers Measured in the Southeastern U.S. *Environmental Science and Technology*, 41:1577-1583 (2007).
- Bullock, O.R., and K.A. Brehme. Atmospheric Mercury Simulation Using the CMAQ Model: Formulated Description and Analysis of Wet Desposition Results. *Atmos. Environ.*, 36:2135-2146 (2002).
- Bullock, R., D. Atkinson, T. Braverman, K. Civerolo, A. Dastoor, D. Davignon, J. Ku, K. Lohman, T.C. Meyer, R.J. Park, C. Seigneur, N.E. Selin, G. Sistla, and K. Vijayaraghavan. The North American Mercury Model Intercomparison Study (NAMMIS). Study Description and Model-to-Model Comparison. Mercury Fate and Transport in the Global Atmosphere, Chapter 13. *Journal of Geophysical Research*, American Geophysical Union, Washington, DC, 113(D17310):1-17 (2008).
- Bullock, O.R., Jr., D. Atkinson, T. Braverman, K. Civerolo, A. Dastoor, D. Davignon, J.-Y. Ku, K. Lohman, T.C. Myers, R.J. Park, C. Seigneur, N.E. Selin, G. Sistla, and K. Vijayaraghavan. An Analysis of Simulated Wet Deposition of Mercury from the North American Mercury Model Intercomparison Study (NAMMIS). *Journal of Geophysical Research*, 114, D08301, doi:10.1029/2008JD011224 (2009).
- Carlton, A.G., H.-J. Lim, K. Altieri, S. Seitzinger, and B.J. Turpin. Link Between Isoprene and Secondary Organic Aerosol (SOA): Pyruvic Acid Oxidation Yields Low Volatility Organic Acids in Clouds. *Geophysical Research Letters*, 33: L06822, doi:10.1029/2005GL025374 (2006).
- Carlton, A.G., B.J. Turpin, K. Altieri, S. Seitzinger, A. Reff, H.-J. Lim, and B.E. Ervens. Atmospheric Oxalic Acid and SOA Production from Glyoxal: Results of Aqueous Photooxidation Experiments. *Atmos. Environ.*, 41:7588-7602 (2007).
- Carlton, A.G., B.J. Turpin, K. Altieri, S. Seitzinger, R. Mathur, S. Roselle, and R.J. Weber. "CMAQ Model Performance Enhanced when In-Cloud SOA Is Included: Comparisons of OC Predictions with Measurements." *Environ. Sci. Technol.* 42(23):8798-8802 (2008).
- Ching, J., M. Brown, S. Burian, F. Chen, R. Cionco, A. Hanna, T. Hultgren, T. McPherson, D. Sailor, H. Taha, and D. Williams. National Urban Database and Access Portal Tool, NUDAPT. *Bulletin of the American Meteorological Society*, 90(8):1157-1168 (2009).
- Daly, C., W.P. Gibson, G.H. Taylor, G.L. Johnson, and P. Pasteris. A Knowledge-Based Approach to the Statistical Mapping of Climate. *Clim. Res.*, 22: 99-113 (2002).
- Dentener, F.J., and P.J. Crutzen. Reaction of N₂O₅ on Tropospheric Aerosols: Impact on the Global Distributions of NO_x, O₃ and OH. *J. Geophys. Res.*, 98:7149-7163 (1993).
- Evans, M.J. and D.J. Jacob. Impact of New Laboratory Studies of N₂O₅ Hydrolysis on Global Model Budgets of Tropospheric Nitrogen Oxides, Ozone and OH. *Geophys. Res. Lett.*, 32, L09813 (2005).
- Gégo, E., P.S. Porter, A. Gilliland, and S.T. Rao. Observation-Based Assessment of the Impact of Nitrogen Oxides Emissions Reductions on O₃ Air Quality over the Eastern United States. *Journal of Applied Meteorology and Climatology*, 46:994-1008 (2007).
- Gilliam, R.C., and J.E. Pleim. Performance Assessment of New Land-Surface and Planetary Boundary Layer Physics in the WRF-ARW. *J. Appl. Meteor. and Clim.*, (in press).
- Gilliland, A.B., C. Hogrefe, R.W. Pinder, J.M. Godowitch, K.L. Foley, and S.T. Rao. Dynamic Evaluation of Regional Air Quality Models: Assessing Changes in O₃ Stemming from Changes in Emissions and Meteorology. *Atmospheric Environment*, 42:5110-5123 (2008).
- Godowitch, J.M., C. Hogrefe, and S.T. Rao. Diagnostic Analyses of Regional Air Quality Model: Changes in Modeled Processes Affecting Ozone and Chemical-Transport Indicators from NO_x Point Source Emission Reductions. *Journal of Geophysical Research*, 113: D19303, doi:10.1029/2007JD009537 (2008).
- Isakov, V., J. Touma, J. Burke, D. Lobdell, T. Palma, A. Rosenbaum, and H. Özkaynak. Combining Regional and Local Scale Air Quality Models with Exposure Models for Use in Environmental Health Studies. *J. AandWMA*, 59:461-472 (2009).
- Kleindienst, T.E., M. Jaoui, M. Lewandowski, J.H. Offenberg, C.W. Lewis, P.V. Bhave, and E.O. Edney. Estimates of the Contributions of Biogenic and Anthropogenic Hydrocarbons to Secondary Organic Aerosol at a Southeastern US Location, *Atmospheric Environment*, 41:8288-8300 (2007).
- Lewis, C.W., G.A. Klouda, and W.D. Ellenson. Radiocarbon Measurement of the Biogenic Contribution to Summertime PM_{2.5} Ambient Aerosol in Nashville, TN. *Atmospheric Environment*, 38:6053-6061 (2004).
- Meyers, T.P., P. Finkelstein, J. Clarke, T.G. Ellestad, and P.F. Sims. A Multilayer Model for Inferring Dry Deposition Using Standard Meteorological Measurements. *J. Geophys. Res.*, 103(D17):22645-22661 (1998).
- Nakicenovic, N., J. Alcamo, G. Davis, B. de Vries, J. Fenhann, S. Gaffin, K. Gregory, A. Grübler, T. Jung, T. Kram, E. La Rovere, L. Michaelis, S. Mori, T. Morita, W. Pepper, H. Pitcher, L. Price, K. Riahi, A. Roehrl, H. Rogner, A. Sankovski, M. Schlesinger, P. Shukla, S. Smith, R. Swart, S. van Rooijen, N. Victor, and Z. Dadi. Special Report on Emissions Scenarios, Intergovernmental Panel on Climate Change. Available at http://www.grida.no/publications/other/ipcc_sr/ (2000).
- Ng, N.L., P.S. Chhabra, A.W.H. Chan, J.D. Surratt, J.H. Kroll, A.J. Kwan, D.C. McCabe, P.O. Wennberg, A. Sorooshian, S.M. Murphy, N.F. Dalleska, R.C. Flagan, and J.H. Seinfeld. Effect of NO_x Level on Secondary Organic Aerosol (SOA) Formation from the Photooxidation of Terpenes. *Atmos. Chem. Phys.*, 7:5159-5174 (2007).
- Nolte, C.G., A.B. Gilliland, C. Hogrefe, and L.J. Mickley. Linking Global to Regional Models To Assess Future Climate Impacts on Surface Ozone Levels in the United States. *Journal of Geophysical Research*, 113:D14307 (2008).

- NRC. National Research Council of the National Academies. *Air Quality Management in the United States*. The National Academies Press: Washington, DC (2004).
- Pleim, J.E. A Combined Local and Nonlocal Closure Model for the Atmospheric Boundary Layer. Part I: Model Description and Testing. *J. Appl. Meteor. Clim.*, 46:1383-1395 (2007a).
- Pleim, J.E. A Combined Local and Nonlocal Closure Model for the Atmospheric Boundary Layer. Part II: Application and Evaluation in a Mesoscale Meteorological Model. *J. Appl. Meteor. Clim.*, 4:1396-1409 (2007b).
- Pleim, J.E., and R. Gilliam. An Indirect Data Assimilation Scheme for Deep Soil Temperature in the Pleim-Xiu Land Surface Model. *J. Appl. Meteor. Clim.*, 48:1362-1376 (2010).
- Rierner, N., H. Vogel, B. Vogel, B. Schell, I. Ackermann, C. Kessler, and H. Hass, Impact of the Heterogeneous Hydrolysis of N_2O_5 on Chemistry and Nitrate Aerosol Formation in the Lower Troposphere under Photosmog Conditions, *J. Geophys. Res.*, 108(D4), 4144, doi:10.1029/2002JD002436 (2003).
- Ryaboshapko, A., O.R. Bullock, R. Ebinghaus, I. Ilyin, K. Lohman, J. Munthe, G. Petersen, C. Seigneur, and I. Wängberg. Comparison of Mercury Chemistry Models. *Atmos. Environ.*, 36:3881-98 (2002).
- Ryaboshapko, A., R. Bullock, J. Christensen, M. Cohen, A. Dastoor, I. Ilyin, G. Petersen, D. Syrakov, R.S. Artz, D. Davignon, R.R. Draxler, and J. Munthe. Intercomparison Study of Atmospheric Mercury Models: 1. Comparison of Models with Short-Term Measurements. *Science of the Total Environment*, 376(1-3):228-240 (2007a).
- Ryaboshapko, A., R. Bullock, J. Christensen, M. Cohen, A. Dastoor, I. Ilyin, G. Petersen, D. Styakov, R.S. Artz, D. Davignon, R.R. Draxler, and J. Munthe. Intercomparison Study of Atmospheric Mercury Models: 2. Modeling Results Versus Long-Term Observations and Comparison of Country Atmospheric Balances. *Science of the Total Environment*, 377(2-3):319-333 (2007b).
- Stein, A.F., V. Isakov, J. Godowitch, and R.R. Draxler. A Hybrid Approach To Resolve Pollutant Concentrations in an Urban Area. *Atmospheric Environment*, 41: 9410-9426 (2007).
- Sullivan, T.J., B.J. Cosby, J.R. Webb, R.L. Dennis, A.J. Bulger, and F.A. Deviney, Jr. Streamwater Acid-Base Chemistry and Critical Loads of Atmospheric Sulfur Deposition in Shenandoah National Park, Virginia. *Environ. Monit. Assess.*, 137:85-99 (2008).
- Tetra Tech. *Development of a Second-Generation of Mercury Watershed Simulation Technology: Grid Based Mercury Model, Users Manual, Version 2.0*. Fairfax, VA (2006).
- USEPA. U.S. Environmental Protection Agency. *NO_x Budget Trading Program*, EPA-430-R-07-009. <http://www.epa.gov/airmarkets> (2007).
- Yu, S., P.U. Behave, R.L. Dennis, and R. Mathur. Seasonal and Regional Variations of Primary and Secondary Organic Aerosols over Continental U.S.: Semi-empirical Estimates and Model Evaluation. *Environmental Science and Technology*, 41:4690-4697 (2007).

APPENDIX A

Atmospheric Modeling and Analysis Division Staff Roster

(as of December 31, 2008)

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S. T. Rao, Director
David Mobley Deputy Director
Patricia McGhee, Assistant to the Director
Sherry Brown
Veronica Freeman-Green
Linda Green
Ken Schere, Science Advisor
Gary Walter, IT Manager
Jeff West, QA Manager

Emissions and Model Evaluation Branch

Tom Pierce, Chief
Jane Coleman (SEEP¹), Secretary
Wyat Appel
Brian Eder
Kristen Foley
Jim Godowitch
Steve Howard
Sergey Napelenok
George Pouliot
Alfreida Torian

Atmospheric Exposure Integration Branch

Val Garcia, Chief
Jesse Bash
Jason Ching
Ellen Cooter
Jim Crooks (postdoctoral fellow)
Robin Dennis
Vlad Isakov
Wilma Jackson (contractor)
Donna Schwede
Joe Touma
Adrienne Wootten (contractor)
David Heist, Fluid Modeling Facility
Ashok Patel (SEEP), Fluid Modeling Facility
Steve Perry, Fluid Modeling Facility

Bill Peterson (contractor), Fluid Modeling Facility
John Rose (SEEP), Fluid Modeling Facility

Atmospheric Model Development Branch

Rohit Mathur, Chief
Shirley Long (SEEP), Secretary
Prakash Bhawe
Ann Marie Carlton
Tianfeng Chai (contractor)
Garnet Erdakos (NRC² postdoctoral fellow)
Rob Gilliam
Bill Hutzell
Daiwen Kang (contractor)
Hsin-mu Lin (contractor)
Deborah Luecken
Harshal Parikk (contractor)
Jon Pleim
Shawn Roselle
Golam Sarwar
Heather Simon (postdoctoral fellow)
John Streicher
Daniel Tong (contractor)
David Wong
Jeff Young
Shaocai Yu (contractor)

Applied Modeling Branch

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Melanie Ratteray (SEEP), Secretary
Bill Benjey
Jared Bowden (NRC postdoctoral fellow)
Russ Bullock
Barron Henderson (ORISE³)
Jerry Herwehe
Chris Nolte
Tanya Otte
Rob Pinder
Jenise Swall

¹SEEP—Senior Environmental Employee Program

²NRC—National Research Council

³ORISE—Oak Ridge Science and Education Program

APPENDIX B

Division and Branch Descriptions

The **Atmospheric Modeling Analysis Division** leads the development and evaluation of atmospheric models on all spatial and temporal scales for assessing changes in air quality and air pollutant exposures, as affected by changes in ecosystem management and regulatory decisions, and for forecasting the Nation's air quality. AMAD is responsible for providing a sound scientific and technical basis for regulatory policies to improve ambient air quality. The models developed by AMAD are being used by EPA, NOAA, and the air pollution community in understanding and forecasting not only the magnitude of the air pollution problem but also in developing emission control policies and regulations for air quality improvements. AMAD applies air quality models to support key integrated, multidisciplinary science research. This includes linking air quality models to other models in the source to outcome continuum to effectively address issues involving human health and ecosystem exposure science.

The **Atmospheric Model Development Branch** (AMDB) develops, tests, and refines analytical, statistical, and numerical models used to describe and assess relationships between air pollutant source emissions and resultant air quality, deposition, and pollutant exposures to humans and ecosystems. The models are applicable to spatial scales ranging from local/urban and mesoscale through continental, including linkage with global models. AMDB adapts and extends meteorological models to couple effectively with chemical-transport models to create comprehensive air quality modeling systems, including the capability for two-way communication and feedback between the models. The Branch conducts studies to describe the atmospheric processes affecting the transport, diffusion, transformation, and removal of pollutants in and from the atmosphere using theoretical approaches, as well as from analyses of monitoring and field study data. AMDB converts these and other study results into models for simulating the relevant physical and chemical processes and for characterizing pollutant transport and fate in the atmosphere. The Branch conducts model exercises to assess the sensitivity and uncertainty associated with model input databases and applications results. AMDB's modeling research is designed to produce tools to serve the nation's need for science-based air quality decision-support systems.

The **Emissions and Model Evaluation Branch** (EMEB) develops and applies advanced methods for

evaluating the performance of air quality simulation models to establish their scientific credibility. Model evaluation includes diagnostic assessments of modeled atmospheric processes to guide the Division's research in areas such as land use and land cover characterization, emissions, meteorology, atmospheric chemistry, and atmospheric deposition. The Branch also advances the use of dynamic and probabilistic model evaluation techniques to examine whether the predicted changes in air quality are consistent with the observations. By collaborating with other EPA offices that provide data and algorithms on emissions characterization and source apportionment and with the scientific community, the Branch evaluates the quality of emissions used for air quality modeling and, if warranted, develops emission algorithms that properly reflect the effects of changing meteorological conditions.

The **Atmospheric Exposure Integration Branch** (AEIB) develops methods and tools to integrate air quality process-based models with human health and ecosystems exposure models and studies. The three major focus areas of this Branch are (1) linkage of air quality with human exposure, (2) deposition of ambient pollutants onto sensitive ecosystems, and (3) assessment of the impact of air quality regulations (accountability). AEIB's research to link air quality to human exposure includes urban-scale modeling, atmospheric dispersion studies, and support of exposure field studies and epidemiological studies. The urban-scale modeling program (which includes collection and integration of experimental data from its Fluid Modeling Facility) is focused on building "hot-spot" air toxic analysis algorithms and linkages to human exposure models. The deposition research program develops tools for assessing nutrient loadings and ecosystem vulnerability, and the accountability program develops techniques to evaluate the impact of regulatory strategies that have been implemented on air quality and conducts research to link emissions and ambient pollutant concentrations with exposure and human and ecological health end points.

The **Applied Modeling Branch** (AMB) uses atmospheric modeling tools to address emerging issues related to air quality and atmospheric influences on ecosystems. Climate change, growing demand for biofuels, and emission control programs and growth all affect air quality and ecosystems in various ways that require integrated assessment. Fundamental to these

studies is the development of credible scenarios of current and future conditions on a regional scale and careful consideration of global scale influences on air pollution and climate. Scenarios of climate, growth and

development, and regulations will be used with regional atmospheric models to investigate potential changes in exposure risks related to air quality and meteorological conditions.

APPENDIX C

Awards and Recognition for 2008

EPA Gold Medal

Annmarie Carlton, Brian Eder, Jerold Herwehe, Rohit Mathur, Tanya Otte, Thomas Pierce, Jonathan Pleim, George Pouliot, S.T. Rao, Kenneth Schere, David Wong, and Jeffrey Young — Air Quality Forecasting Team

EPA Silver Medal

Valerie Garcia and Alice Gilliland—Public Health Air Surveillance Valuation (PHASE) Team

EPA Bronze Medal

Russ Bullock, Bill Hutzell, Deb Luecken, Rohit Mathur, Shawn Roselle, Golam Sarwar, and Ken Schere—CMAQ Multipollutant Model Team

Kristen Foley, Val Garcia, Alice Gilliland, Jim Godowitch, S.T. Rao, and Jenise Swall—Accountability: Evaluating the Effectiveness of the NO_x SIP Call Program in Improving Ozone Air Quality Over the Eastern United States

Russ Bullock, Robin Dennis, and Donna Schwede—Nitrogen and Mercury Watershed TMDL Assessment Team

Vlad Isakov—Near Roadway Research Team

Jonathon Pleim—Exhaled Breath Condensate Research

ORD Technical Assistance to the Regions or Program Offices Award

David Mobley, Tom Pierce, and George Pouliot—National Fire Emissions Inventory Team

Wyatt Appel, Jesse Bash, William Benjey, Prakash Bhawe, Russell Bullock, Annmarie Carlton, Robin Dennis, Kristen Foley, Alice Gilliland, Bill Hutzell, Deborah Luecken, Rohit Mathur, Sergey Napelenok, Chris Nolte, Tanya Otte, Tom Pierce, Rob Pinder, Jonathon Pleim, George Pouliot, Shawn Roselle, Golam Sarwar, Kenneth Schere, Donna Schwede, David Wong, and Jeff Young—CMAQ Model Team

ORD Scientific Communication Award

Robin Dennis, Valerie Garcia, Rohit Mathur, Patriacia McGhee, David Mobley, and S.T. Rao—*EM Magazine* Team

Scientific and Technological Achievement Awards (STAA) Winners

David Mobley—A Critical Overview of Air Emission Inventories with Recommendations To Improve Their Value to Air Quality Management

Recognition

Support to 2007 Nobel Peace Prize to Intergovernmental Panel on Climate Change—David Mobley

Embassy Science Fellow-New Zealand—David Mobley (January-May 2008)

Embassy Science Fellow-Hong Kong—Golam Sarwar (September-November 2008)

APPENDIX D

Publications for FY and CY 2008

(Division authors are in bold.)

Journal Articles

- Altieri, K. E., S. P. Seitzinger, **A. G. Carlton**, B. J. Turpin, G. C. Klein, A. G. Marshall. Oligomers formed through in-cloud methylglyoxal reactions: Chemical composition, properties, and mechanisms investigated by ultra-high resolution FTICR mass spectrometry. *Atmospheric Environment*, 42 (7): 1476-1490, (2008).
- Appel, W., A. Gilliland, G. Sarwar, and R.C. Gilliam.** Evaluation of the community multiscale air quality (CMAQ) model version 4.5: Uncertainties and sensitivities impacting model performance: Part I – ozone. *Atmospheric Environment*, 41(40):9603-9613, (2007).
- Appel, K.W., P.V. Bhave, A. B. Gilliland, G. Sarwar, and S.J. Roselle.** Evaluation of the community multi-scale air quality (CMAQ) model version 4.5: Sensitivities impacting model performance; Part II - particulate matter. *Atmospheric Environment*, 42(24): 6057-6066, (2008).
- Boersma, K.F., D.J. Jacob, H. J. Eskes, **R. W. Pinder**, J. Wang, and R. J. Van Der A. Intercomparison for SCIAMACHY and OMI tropospheric NO₂ columns: Observing the diurnal evolution of chemistry and emissions from space. *Journal of Geophysical Research*, 113 (D16S26): 1-14, (2008).
- Bowker, G., D. A. Gillette, G. Bergametti, B. Marticorena, and D. K. Heist.** Fine-scale Simulations of Aeolian sediment dispersion in a small area of the northern Chihuahuan Desert. *Journal of Geophysical Research*. 113(F02S11):1-28, (2008).
- Bullock, R., D. Atkinson, T. Braverman, K. Civerolo, A. Dastoor, D. Davignon, J. Y. Ku, K.Lohman, T. Myers, R. Park, C. Seigneur, N. E. Selin, G. Sistla, and K. Vijayaraghavan.** The North American mercury model intercomparison (NAMMIS). Study description and model-to-model comparisons. *Journal of Geophysical Research*, 113(D17310): 1-17, (2008).
- Carlton, A.G.,** B. Turpin, K.E. Altieri, S. Seitzinger, A.H. Reff, H. Lim, and B. Ervens. Atmospheric oxalic acid and SOA production from glyoxal: Results of aqueous Photooxidation experiments. *Atmospheric Environment*, 1(35):7588-7602, (2007).
- Carlton, A. G.,** B. J. Turpin, K. E. Altieri, Sybil P. Seitzinger, **R. Mathur, S. Roselle,** and R. J. Webber. CMAQ Model performance enhanced when in-cloud secondary organic aerosol is included: Comparisons of organic carbon predictions with measurements. *Environmental Science and Technology*, 42(23): 8798-8802, (2008).
- Chow, J.C., J.L. Watson, H.J. Feldman, J.E. Nolen, B. Wallerstein, G. Hidy, P.J. Lioy, **D. Mobley,** K. Baugues, and J.D. Bachmann. Will the circle be unbroken: A history of the U.S. National Ambient Air Quality Standards. *Journal of Air and Waste Management*, 57(10):1151-1163, (2007).
- Cook, R., **V. Isakov, J. S. Touma, W. Benjey, J. Thurman, E. Kinnee, and D. Ensley.** Resolving local scale emissions for near roads modeling assessments. *Journal of the Air and Waste Management Association*, 58(3):451-461, (2008).
- Cooter, E., J. Swall, and R.C. Gilliam.** Comparison of 700-hPa NCEP-R1 and AMIP-R2 wind Patterns over the continental U.S. using the cluster analysis. *Journal of Applied Meteorology and Climatology*, 46(11):1744-1758, (2007).
- Davis, J. M., **P. V. Bhave, and K. M. Foley.** Parameterization of N₂O₅ reaction probabilities on the surface of particles containing ammonium, sulfate, and nitrate. *Atmospheric Chemistry and Physics*, 8(17): 5295-5311, (2008).
- Dennis, R.L.,** R. Haeuber, T. Blett, J. Cosby, C. Driscoll, J. Sickles, and J.M. Johnston. Sulfur and nitrogen deposition on ecosystems in the United States. *EM: Air and Waste Management Associations Magazine for Environmental Managers*, 12-17, (2007).

Dennis, R., P. V. Bhawe, and R. W. Pinder.

Observable indicators of the sensitivity of PM_{2.5} nitrate to emission reductions, Part II: Sensitivity to error in total ammonia and total nitrate of the CMAQ-predicted nonlinear effect of SO₂ emission reductions on PM_{2.5} nitrate. *Atmospheric Environment*, 42(6): 1287-1300, (2008).

Ervens, B., **A. G. Carlton**, B.J. Turpin, K.E. Altieri, S. M. Kreidenwies, and G. Feingold. Secondary organic aerosol yields from cloud-processing of isoprene oxidation products. *Journal of Geophysical Research Letters*. 35 L02816: 1-20, (2008).

Garcia, V., N. Fann, R. Haeuber, and P. Lorang. Assessing the public health impact of regional-scale air quality regulations. *EM, Air and Waste Management Association Magazine for Environmental Managers*, 25-30, (2008).

Gego, E., S. Porter, **A. Gilliland**, C. Hogrefe, **J. Godowitch**, and **S. T. Rao**. Modeling analysis of the effects of changes in nitrogen oxides emission from the electric power sector on ozone levels in the eastern United States. *Journal of Air and Waste Management Association*, 58(4): 580-588, (2008).

Gilliland, A.B., C. Hogrefe, **R. W. Pinder, J. M. Godowitch, K.M. Foley**, and **S.T. Rao**. Dynamic evaluation of regional air quality models: Assessing changes in O₃ stemming from changes in emissions and meteorology. *Atmospheric Environment*, 42(20): 5110-5123 (2008).

Godowitch, J., A. Gilliland, R. Draxler, and **S.T. Rao**. Modeling assessment of point source NO_x emission reductions on ozone air quality in the eastern United States. *Atmospheric Environment*, 42(1): 87-100, (2008).

Godowitch J. M., C. Hogrefe, and **S. T. Rao**. Diagnostic analyses of regional air quality model: Changes in modeled processes affecting ozone and chemical-transport indicators from NO_x point source emission reductions. *Journal of Geophysical Research*, 113(D19303): 1-15, (2008).

Hutzell, W. T., and D. Luecken. Fate and transport of emissions from several trace metals over the United States. *Science of the Total Environment*. 396(2-3):164-179, (2008).

Irwin, J. S., K. Civerolo, C. Hogrefe, **W. Appel, K. Foley**, and **J. Swall**. A procedure for inter-comparing the skill of regional-scale air quality model simulations of daily maximum 8-hour ozone values. *Atmospheric Environment*, 42(21): 5403-5412, (2008).

Isakov, V., J. Touma, and A. Khlystov. A method of assessing air toxics concentrations in urban areas using mobile platform measurements. *Journal of Air and Waste Management*, 57(11):1287 – 1295, (2007).

Kang, D., **R. Mathur, S.T. Rao**, and S. Yu. Bias-adjustment techniques for improving ozone air quality forecasts. *Journal of geophysical Research*, 113(D23308): 1-17, (2008).

Liao, K., E. Tagaris, K. Manomaiphiboon, **S. Napelenok**, J. Woo, S. He, P. Amar, and A. Russell. Sensitivities of ozone and fine particulate matter formation to emission under the impact of potential future climate change. *Environmental Science and Technology*, 41(24):8355-8361, (2007).

Liao, K.J., E. Tagaris, **S. L. Napelenok**, K. Manomaiphiboon, J. H. Woo, P. Amar, S. He, and A. G. Russell. Current and future linked responses of ozone and PM_{2.5} to emissions controls. *Environmental Science and Technology*, 42(13): 4670-4675, (2008).

Lin, C., P. Pongprueksa, **R. Bullock**, S. Lindberg, S.O. Pehkonen, C. Jang, T. Braverman, and T.C. Ho. Scientific Uncertainties in atmospheric mercury models II: Sensitivity analysis in the conus domain. *Atmospheric Environment*. 41(31):6544-6560, (2007).

Luecken, D. J. and A. Cimorelli. CO-Dependencies of Reactive Air Toxic and Criteria Pollutants on Emission Reductions. *The Journal of Air and Waste Management Association*, 58(5):693-701, (2008).

Luecken, D. L., and M. R. Mebust. Technical challenges involved in implementation of VOC reactivity-based control of ozone. *Environmental Science and Technology*. 42(5): 1615-1622, (2008).

Luecken, D. J., S. Phillips, **G. Sarwar**, and C. Jang. Effects of using the CB05 versus SAPRC99 versus CB4 chemical mechanism on model predictions: ozone and gas-phase photochemical precursor concentrations. *Atmospheric Environment*, 42(23): 5805-5820, (2008).

Mathur, R., W.E. Frick, G. Lear, and **R.L. Dennis**. Ecological Forecasting: Microbial Contamination and Atmospheric Loadings of Nutrients to Land and Water. *EM: Air and Waste Management Associations Magazine for Environmental Managers*, 36-40, (2007).

Mathur, R. Estimating the impact of the 2004 Alaskan forest fires on episodic particulate matter pollution over the eastern United States through assimilation of satellite-derived aerosol optical depths in a regional air quality model. *Journal of Geophysical Research*, 113(D17302): 1-14, (2008).

Mathur, R., S. Yu, D. Kang, and K.L. Schere. Assessment of the winter-time performance of developmental particulate matter forecasts with the Eta-CMAQ modeling system. *Journal of Geophysical Research-Atmospheres (JGR-Atmospheres)*, 113(D02303): 1 -15, (2008).

Mobley, D. and P. Gurnsey. New Zealand's innovative approach to emissions trading for addressing global climate change. *EM, Air and Waste Management Association Magazine for Environmental Managers*, 14-19, (2008).

Napelenok, S.L., D. S. Cohan, M.T. Odman, and S. Tonse. Extension and evaluation of sensitivity analysis capabilities in a photochemical model. *Environmental Modeling and Software*. 23(8):994-999, (2008).

Napelenok, S. L., R. Pinder, A. B. Gilliland, and R. V. Martin. A method of evaluating spatially-resolved NO₂ emissions using Kalman filter inversion, direct sensitivities, and space-based NO₂ observations. *Atmospheric Chemistry and Physics*, 8: 5603-5614, (2008).

Nolte, C.G., A. B. Gilliland, C. Hogrefe and L.J. Mickley. Linking global to regional models to assess future climate impacts on surface ozone levels in the United States. *Journal of Geophysical Research*, 113(D14307): 1-14, (2008).

Nolte, C.G., P.V. Bhave, J. R. Arnold, R. L. Dennis, K. Max Zhang, and A. S. Wexler. Modeling urban and regional aerosols –Application of the CMAQ-UCD aerosol model to Tampa, a coastal urban site. *Atmospheric Environment*, 42(13):3179-3191, (2008).

Otte, T.L. The Impact of nudging in the meteorological model for retrospective air quality simulations. Part I: Evaluation against national observation networks. *Journal of Applied Meteorology and Climatology*, 47(7): 1853-1867, (2008).

Otte, T.L. The Impact of nudging in the meteorological model for retrospective air quality simulations. Part II: Evaluating collocated meteorological and air quality observations. *Journal of Applied Meteorology and Climatology*, 47(7): 1868-1887, (2008).

Pinder, R., A. B. Gilliland, and R. Dennis. Environmental impact of atmospheric NH₃ emissions under present and future conditions in the Eastern United States. *Geophysical Research Letter*, 35(L 12808): 1-6, (2008).

Pinder, R.W., R. L. Dennis, and P. V. Bhave. Observable indicators of the sensitivity of PM_{2.5} nitrate to emission reductions: Part I: Derivation of the adjusted gas ratio and applicability at regulatory-relevant time scales. *Atmospheric Environment*, 42(6): 1275-1286, (2008).

Pongprueksa, P. C-J, Lin, S. E. Lindberg, C. Jang, T. Braverman, **O.R. Bullock, Jr.**, T. C. Ho, and H-W.Chu. Scientific uncertainties in atmospheric mercury models III: Boundary and initial conditions, model grid resolutions, and Hg (II) reduction mechanisms. *Atmospheric Environment*. 42(8): 1828-1845, (2008).

Pouliot, G., T. Pace, B. Roy, T. Pierce, and D. Mobley. Development of a biomass burning emissions inventory by combining satellite and ground-based information. *Journal of Applied Remote Sensing*, 2(1): 021501, (2008).

Pullen, Julie, **J. Ching**, W. Sailor, W. Thompson, B. Bornstein, and D. Koracin. Progress toward meeting the challenges of our coastal urban future. *Bullentin of the American Meteorological Society*, 89(11): 1727-1731, (2008).

Queen, A., Y. Zhang, **R. Gilliam, and J. Pleim.** Examining the sensitivity of MM5-CMAQ predictions to explicit, microphysics schemes, Part I - Database description, evaluation protocol and precipitation predictions. *Atmospheric Environment*, 42(16): 3842-3855, (2008).

Rao, S. Linking air, land, and water pollution for effective environmental management. *EM: Air and Waste Management Associations Magazine for Environmental Managers*, 5 (2007).

Rao, S. T. Exposure science and its applications for effective environmental management. *EM, Air and Waste Management Association Magazine for Environmental Managers*, July 2008, 7, (2008).

Sarwar, G., D. Luecken, G. Yarwood, G. Z. Whitten, S. Reyes, and W. P. L. Carter. Impact of an updated carbon bond mechanism on predictions from the Community Multi-scale Air Quality (CMAQ) modeling system: Preliminary assessment. *Journal of Applied Meteorology and Climatology*. 47(1): 3-14, (2008).

Sarwar, G., S.J. Roselle, R. Mathur, W. Appel, R.L. Dennis, and B. Vogel. A Comparison of CMAQ HONO Predictions with Observations from the Northeast Oxidant and Particle Study. *Atmospheric Environment*, 42(23):5760-5770, (2008).

Smolarkiewicz, P.K., R. Sharman, J. Weil, **S.G. Perry, D. Heist,** and **G.E. Bowker.** Building resolving large-eddy simulation and comparison with wind tunnel experiments. *Journal of Computational Physics*, 227(1):633-653, (2007).

Stein, A.F., **V. Isakov, J.M. Godowitch,** and R.R. Draxler.

A hybrid modeling approach to resolve pollutant concentrations in an urban area. *Atmospheric Environment*. 41(40):9410-9426, (2007).

Sullivan, T. J., B. J. Cosby, J. R. Webb, **R. L. Dennis,** A. J. Bulger, and F. A. Deviney. Streamwater acid-base chemistry and critical loads of atmospheric sulfur deposition in Shenandoah National Park, Virginia. *Journal of Environmental Monitoring and Assessment*. 137(1-3): 85-99, (2008).

Tiwar, A., **A. Reff,** and J. J. Colls. Collection of ambient particulate matter by porous vegetation barrier: Sampling and characterization methods. *Journal of Aerosol Science*, 39(1): 40-47, (2008).

Tong, D., **R. Mathur, K.L. Schere,** D. Kang, and S. Yu. The use of air quality forecasts to assess impacts of air Pollution on crops: Methodology and case study. *Atmospheric Environment*, 41(38):8772-8784, (2007).

Venkatram, A., **V. Isakov,** E.D. Thoma, and R.W. Baldauf. (AMD) Analysis of air quality data near roadways using a dispersion model. *Atmospheric Environment*. 41(40):9481-9497, (2007).

Book Chapters

Baklanov, A., **J. Ching,** C.S. B. Grimmmond, and A. Martilli. Cost 728 Action Report: Urbanization of meteorological and air quality models - Chapter 5 - Model Urbanization strategy: Summaries, recommendation, and requirements. *Urbanization of meteorological and air quality models, The Danish Meteorological Institute*, Copenhagen, Denmark, 118-127, (2008).

Bullock, R. The Effect of Lateral Boundary Values on Atmospheric Mercury Simulations with the CMAQ Model. Chapter 2, Carlos Borrego; Ana Isabel Miranda (ed.), *Air Pollution Modeling and its Application XIX*. Springer, New York, NY, (Series C):173-181, (2008).

Davidson, P., **K. L. Schere,** R. Draxter, S. Kondragunta, R. Wayland, J. F. Meagher, and **R. Mathur.** Toward a US National Air Quality Forecast Capability: Current and Planned Capabilities. Chapter 2, Carlos Borrego; Ana Isabel Miranda (ed.), *Air Pollution Modeling and its Application XIX*. Springer, New York, NY. 226-234, (2008).

Gego, E., P.S. Porter, **V. Garcia,** C. Hogrefe, and **S.T. Rao.** Fusing Observations and Model Results for Creation of Enhanced Ozone Spatial Fields: Comparison of Three Techniques. Chapter 3, Carlos Borrego; Ana Isabel Miranda (ed.), *Air Pollution Modeling and Its Application XIX*. Springer, New York, NY, 339-346, (2008).

Gilliland, A., J. M. Godowitch, C. Hogrefe, and **S.T. Rao.** Evaluating Regional-Scale Air Quality Models. Chapter 4, Carlos Borrego; Ana Isabel Miranda (ed.), *Air Pollution Modeling and Its Application XIX*. Springer, New York, NY. 412-419, (2008).

Hogrefe, C., J. Ku, G. Sistla, **A. Gilliland,** J. Irwin, P. S. Porter, E. Gego, P. Kasibhatla, and **S.T. Rao.** Has the Performance of Regional-Scale Photochemical Modeling Systems Changed over the Past Decade? Chapter 4, Carlos Borrego; Ana Isabel Miranda (ed.), *Air Pollution Modeling and Its Application XIX*. Springer, New York, NY. 394-403, (2008).

Isakov, V. and H. A. Ozkaynak. A Modeling Methodology to Support Evaluation PublicHealth Impacts on Air Pollution Reduction Programs. Chapter 7, Carlos Borrego; Ana Isabel Miranda (ed.), *Air Pollution Modeling and Its Application XIX*. Springer, New York, NY. 614-622, (2008).

Luecken, D. J., A. Cimorelli, C. Stahl, and D. Tong. Evaluating the Effects of Emission Reductions on Multiple Pollutants Simultaneously. Chapter 7, Carlos Borrego; Ana Isabel Miranda (ed.), *Air Pollution Modeling and its Application XIX*. Springer, New York, NY. 623-631, (2008).

Luecken, D. J. Comparison of Atmospheric Chemical Mechanisms for Regulatory and Research Applications. NATO Advanced Research Workshop on Simulation and Assessment of Chemical Processes in Multiphase Environment, Alushta, Ukraine, October 01 - 04, 2007. Springer Science + Business Media, LLC, New York, NY, 95-106, (2008).

Mathur, R., S. J. Roselle, G. Pouliot, and G. Sarwar. Diagnostic Analysis of the Three-Dimensional Sulfur Distributions over the Eastern United States Using the CMAQ Model and Measurements from the ICARTT Field Experiment. Chapter 5, Carlos Borrego; Ana Isabel Miranda (ed.). *Air Pollution Modeling and its Application XIX*. Springer, New York, NY. 496-504, (2008).

Mobley, J. D., L.L. Beck, G. Sarwar, A. Reff, and M. Houyoux. SPECIATE – EPA's Database of speciated emission profiles. P2.4, Carlos Borrego; Ana Isabel Miranda (ed.). *Air Pollution Modeling and its Application XIX*. Springer, New York, NY, 665-666 (2008).

Napelenok, S., R. W. Pinder, A. Gilliland, and R. V. Marin. Developing a Method for Resolving NO_x Emission Inventory Biases Using Discrete Kalman Filter Inversion, Direct Sensitivities, and Satellite-Based Columns. Chapter 3, Carlos Borrego; Ana Isabel Miranda (ed.). *Air Pollution Modeling and its Application XIX*. Springer, New York, NY. 322-330, (2008).

Nolte, C., A. Gilliland, and C. Hogrefe. Linking Global and Regional Models to Simulate U.S. Air Quality in the Year 2050. Chapter 6, Carlos Borrego; Ana Isabel Miranda (ed.). *Air Pollution Modeling and Its Application XIX*. Springer, New York, NY. 559-567, (2008).

Pleim, J. A., J. O. Young, D. Wong, R. C. Gilliam, T. L. Otte, and R. Mathur. Two-Way Coupled Meteorology and Air Quality Modeling. Chapter 2, Carlos Borrego; Ana Isabel Miranda (ed.). *Air Pollution Modeling and its Application XIX*. Springer, New York, NY. 235-242, (2008).

Pouliot, G., T. Pierce, X. Zhang, S. Kondragunta, C. Wiedinmer, T. Pace and D. Mobley. The Impact of satellite-derived biomass burning emission estimates on air quality. *SPIE/International Society for Optical Engineering*, Vol. 7089(1): 7089F 1-12 (2008).

Rao, S.T., C. Hogrefe,, and G. Kallos. Long –range transport of atmospheric pollutant's and transboundary pollution. *Anthem Press, World Atlas of Atmospheric Pollution*, Chapter 3, 35-45 (2008).

Roy, D., G. Pouliot, D. Mobley, G. Thompson, T. E. Pierce, A. J. Soja,, J. J. Szykman, and J. Al-Saadi. Development of Fire Emissions Inventory Using Satellite Data. Chapter 2, Carlos Borrego; Ana Isabel Miranda (ed.). *Air Pollution Modeling and its Application XIX*. Springer, New York, NY, 217-225, (2008).

Sarwar, G., R. L. Dennis, and B. Vogel. The Effect of Hetrogeneous Reactions on Model Performance for Nitrous Acid. Chapter 4, Carlos Borrego; Ana Isabel Miranda (ed.). *Air Pollution Modeling and its Application XIX*. Springer, New York, NY. 349-357, (2008).

Published Reports

Pierce, T.E., V. Isakov, B. Haneke, and J. Paumier. Emission and Air Quality Modeling Tools for Near-Roadway Applications. U.S. Environmental Protection Agency, Washington, D.C., EPA/600/R-09/001 (NTIS PB2009-103941), 2008.

Rao, S., R.L. Dennis, V. Garcia, A. Gilliland, R. Mathur, D. Mobley, T.E. Pierce, and K.L. Schere. Summary Report of Air Quality Modeling Research Activities for 2006. U.S. Envirnmntal Protection Agency, Washington, D.C., EPA/600/R-07/103 (NTIS PB2008-110094), 2008.

APPENDIX E

Acronyms and Abbreviations

ACM	Asymmetric Convective Model	IC/BC	initial condition/boundary condition
AERMOD	AMS/EPA Regulatory Model	IMPROVE	Interagency Monitoring of Protected Visual Environment Network
AMAD	Atmospheric Modeling and Analysis Division	INTEX	Intercontinental Chemical Transport Experiment
AMB	Applied Modeling Branch	INTEX-NA	Intercontinental Chemical Transport Experiment—North America
AMD	Atmospheric Modeling Division	ISORROPIA	thermodynamics module
AMDB	Atmospheric Model Development Branch	LES	large-eddy simulation
AMET	Atmospheric Model Evaluation Tool	LIDAR	light detecting and ranging
ASMD	Atmospheric Sciences and Modeling Division	MLM	multilayer model
BELD3	Biogenic Emissions Land Cover Database, v3	MM5	fifth generation of the Penn State/UCAR Mesoscale Model
BRACE	Bay Regional Atmospheric Chemistry Experiment	MPI	message-passing interface
CAA	Clean Air Act	MYSQL	open-source database software
CAIR	Clean Air Interstate Rule	NAAQS	National Ambient Air Quality Standard
CASTNET	EPA's Clean Air Status and Trends Network	NADP	National Acid Deposition Program
CBL	convective boundary layer	NAMMIS	North American Mercury Model Intercomparison Study
C-CAP	Coastal Change Analysis Program	NASS	National Agricultural Statistics Service
CCTM	CMAQ Chemistry-Transport Model	NCAR	National Center for Atmospheric Research
CIRAQ	Climate Impacts on Regional Air Quality	NCEP	National Centers for Environmental Prediction
CMAQ	Community Multiscale Air Quality Model	NERL	National Exposure Research Laboratory
CMAQ-UCD	University of California Davis Aerosol Module coupled to the Community Multiscale Air Quality Model	NGA	National Geospatial Agency
CMAS	Community Modeling and Analysis System	NH ₃	ammonia
DDM-3D	Decoupled Direct Method—three-dimensional	NLCD	National Land Cover Dataset
DEM	digital elevation model	NO ₂	nitrogen dioxide
DTM	digital terrain model	NO ₃ ⁻	nitrate ion
EC	elemental carbon	N ₂ O ₅	nitrogen pentoxide
EMEP	European Monitoring and Evaluation Programme	NOAA	National Oceanic and Atmospheric Administration
EPA	U.S. Environmental Protection Agency	NO _x	oxides of nitrogen
ESRP	Ecological Services Research Program	NO _y	total reactive oxides of nitrogen
FDDA	four-dimensional data assimilation	Nr	reactive nitrogen
FMF	fluid modeling facility	NRC	National Research Council
FML	Future Midwestern Landscapes	NRMRL	National Risk Management Research Laboratory
FY	fiscal year	NUDAPT	National Urban Database and Access Portal Tool
GCM	global climate model	O ₃	ozone
GPL	Gnu public license	OAQPS	Office of Air Quality Planning and Standards
HAP	hazardous air pollutant	OC	organic carbon
HAPEM	Hazardous Air Pollutant Exposure Model	ORD	Office of Research and Development
HNO ₃	nitric acid	ORISE	Oak Ridge Science and Education Program
ICARTT	International Consortium for Atmospheric Research on Transport and Transformation	O _v	water vapor mixing ratio
		PAN	peroxyacetyl nitrate

PBL	planetary boundary layer	SIP	state implementation plan
PM	particulate matter	SO ₂	sulfur dioxide
PRISM	Parameter-Elevation Regressions on Independent Slopes Model	SOA	secondary organic aerosol
PX LSM	Pleim-Xiu Land Surface Model	STENEX	Stencil Exchange
RELMAP	Regional Lagranian Model of Air Pollution	STN	Speciated Trends Network
REMSAD	Regional Modeling System for Aerosols and Deposition	TEAM	Trace Element Analysis Model
SCIAMACHY	scanning imaging absorption spectrometer for atmospheric cartography	TES	Tropospheric Emission Spectrometer
SEEP	Senior Environmental Employee Program	TexAQS	Texas Air Quality Study
SGV	subgrid variability	TMDL	total maximum daily load
SHEDS	Stochastic Human Exposure and Dose Simulation	UCP	urban canopy parameter
		USDA	U.S. Department of Agriculture
		VERDI	Visualization Environment for Rich Data Interpretation
		WDT	Watershed Deposition Tool
		WRF	weather research and forecasting



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