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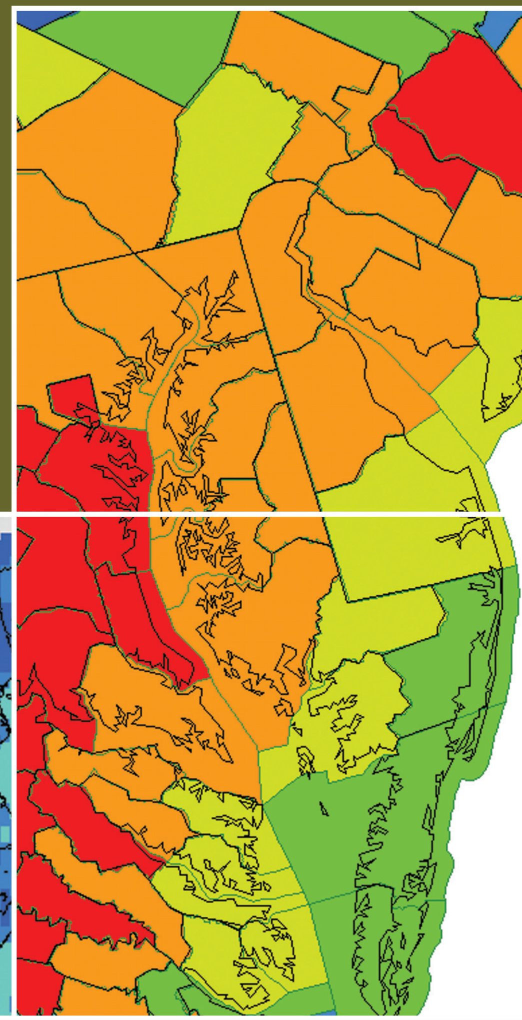
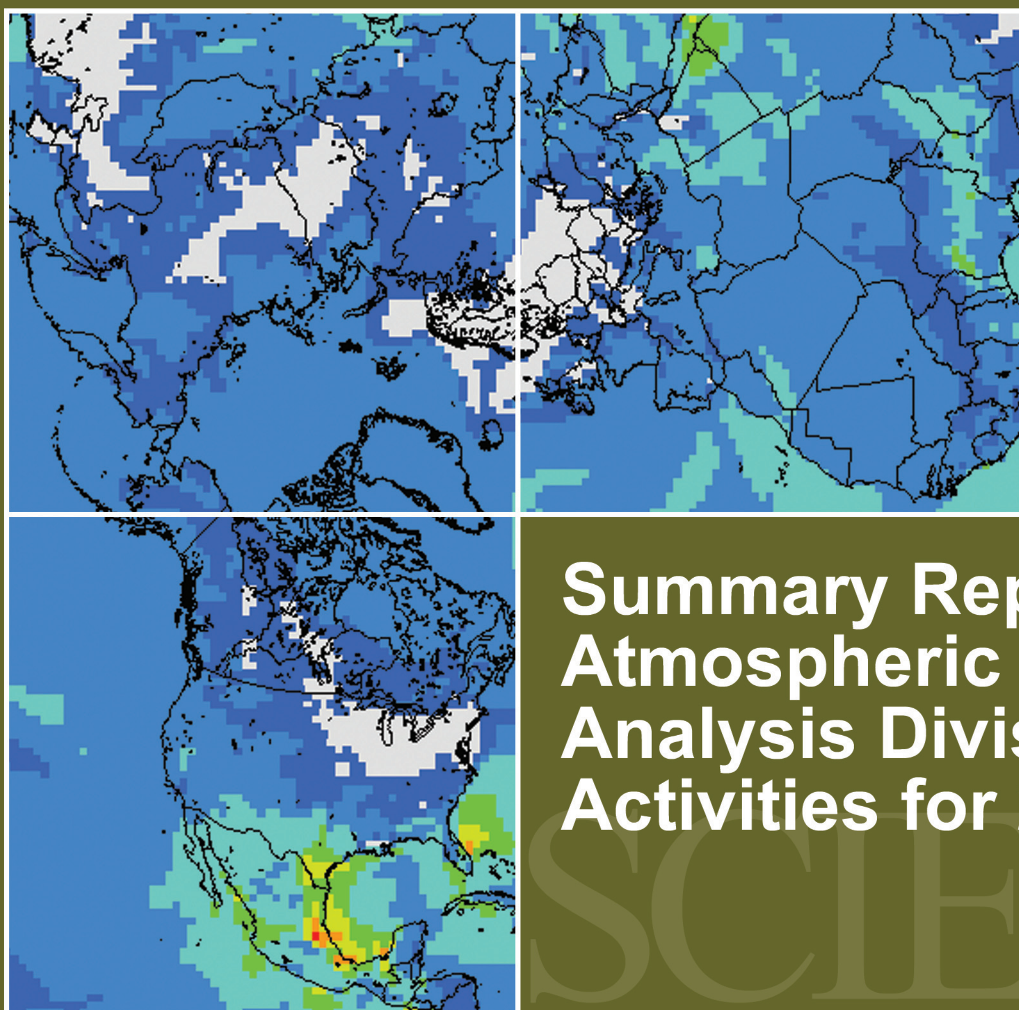
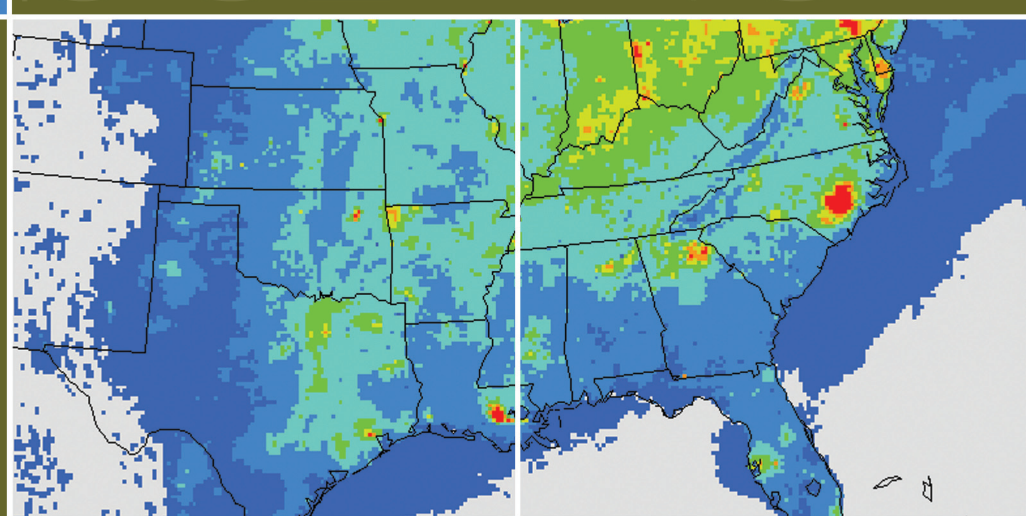




Summary Report of the Atmospheric Modeling and Analysis Division's Research Activities for 2009



ATMOSPHERIC MODELING AND ANALYSIS DIVISION
MOVING SCIENCE INTO APPLICATIONS

Office of
Research and Development
National Exposure
Research Laboratory

EPA/600/R-10/058 June 2010 www.epa.gov/ord

Summary Report of the Atmospheric Modeling and Analysis Division's Research Activities for 2009

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Abstract

The research presented here was performed by the Atmospheric Modeling and Analysis Division (AMAD) of the National Exposure Research Laboratory in the U.S. Environmental Protection Agency's (EPA's) Office of Research and Development in Research Triangle Park, NC. The Division leads the development and evaluation of predictive 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 and reduce exposures to sensitive populations and ecosystems. 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 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, interdisciplinary 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 Community Multiscale Air Quality Model is the flagship model of the Division. This report summarizes the research and operational activities of the AMAD for calendar year 2009.

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CHAPTER 1

Introduction

The research presented here was performed by the Atmospheric Modeling and Analysis Division (AMAD) of the National Exposure Research Laboratory in the U.S. Environmental Protection Agency's (EPA's) Office of Research and Development in Research Triangle Park, NC. This report summarizes the research and operational activities of the Division for calendar year 2009.

The Division structure includes four research branches:

(1) the Atmospheric Model Development Branch (AMDB),
(2) the Emissions and Model Evaluation Branch (EMEB),
(3) the Atmospheric Exposure Integration Branch (AEIB), and
(4) the Applied Modeling Branch (AMB).

Included in this report are a list of Division employees (Appendix A), missions of the Division and its branches (Appendix B), awards earned by Division personnel (Appendix C), citations for Division publications (Appendix D), and a list of acronyms and abbreviations used in this report (Appendix E).

The Division's role within EPA's National Exposure Research Laboratory's (NERL's) "Exposure Framework" and the EPA Office of Research and Development's (ORD'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). 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 emphasizes integration and partnership with EPA and public and private research communities. Specific research and development activities are conducted in-house and externally via external funding.

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 for the peer review, the Division's activities were summarized with 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?

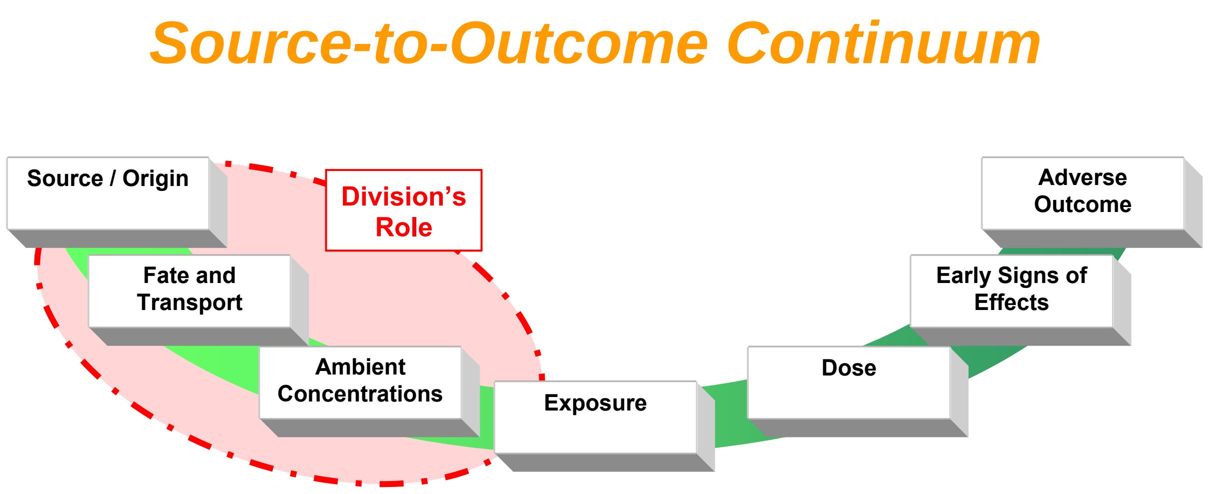


Figure 1-1. The Division's role in the source-exposure-dose-effects continuum from the atmospheric science perspective. (Adapted from "A Conceptional Framework for U.S. EPA's National Exposure Research Laboratory," EPA/600/R-09/003, January 2009)

- 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 above-mentioned 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 2009. 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 (and shown in Figure 1-2).

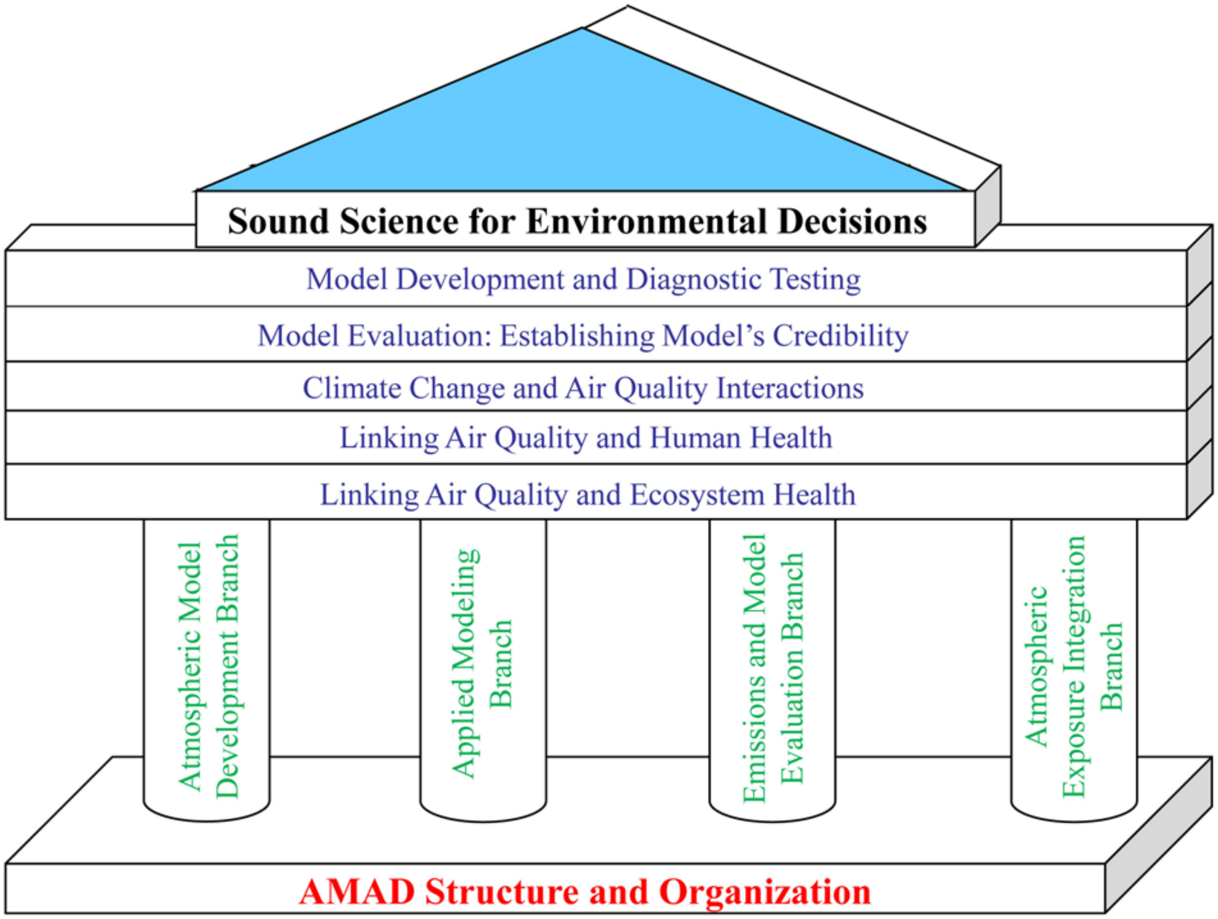


Figure 1-2. The Division's structure and organization.

CHAPTER 2

Summary of Accomplishments for the Division

As a summary of and introduction to the annual report for 2009, the following Division accomplishments are highlighted.

2.1 Division-Wide Accomplishments

1. **Issue:** Strategic thinking regarding air quality monitoring and modeling in the next decades
   Accomplishment: Coordination of papers for the October 2009 issue of the Air and Waste Management Association's *Environmental Manager* (*EM*) on Monitoring and Modeling Needs in the 21st Century
   Findings: Four-dimensional air quality, emissions, and meteorological data are needed with increased spatial and temporal resolution for improving air quality models and future policy decisions.
   Impact: This *EM* special issue provides a thought-provoking set of articles for managers to consider in improving monitoring, modeling, meteorological, emission characterization, and data analysis programs to meet future challenges of the air quality management program. This work led to the preparation of an inter-Divisional collaborative research proposal to AMI, involving program and regional offices, for obtaining 3-D air quality data over the United States using commercial aircrafts.
2. **Issue:** Milestone anniversary meeting of three decades of international cooperation on air pollution modeling (It is the United States' turn to host this North Atlantic Treaty Organization (NATO) meeting.)
   Accomplishment: Development and host of the program for the May 18-22, 2009 Meeting of the 30th NATO/Science for Peace and Security (SPS) International Technical Meeting (ITM) on Air Pollution Modeling and its Applications, in San Francisco, CA
   Findings: The ITM has been broadened (Topic 7) from air quality and human health to cover ecosystems and economy (including air quality trends, cost-benefit analysis of regulatory programs and their effectiveness, and integrated modeling approaches).
   Impact: Over 130 participants from 35 countries attended the NATO/SPS meeting, presenting papers on a wide variety of air pollution modeling topics ranging from local- to global-scale applications. The meeting provided an important forum for synthesizing progress on air quality modeling programs around the world. A book under the NATO banner was published by the conference organizers.
3. **Issue:** January 2009 peer review of NERL's AMAD
   Accomplishment: Preparation of extensive handbook and poster book documentation and posters for the 2009 AMAD Peer Review
   Findings: The draft report of the Peer Review Committee was complimentary of the Division's research and included constructive suggestions.
   Impact: The 2009 AMAD Peer Review confirmed the wisdom of AMAD's strategic research directions and excellence of past accomplishments. Based on the peer review, we prepared three white papers on the Division's new research initiatives.
4. **Issue:** June 2009 Board of Scientific Counselors (BOSC) Review of ORD's Clean Air Research Program
   Accomplishment: Preparation of posters and abstracts for the Air Quality and Multipollutant Sessions; AMAD co-chair of Air Quality Session
   Findings: Multipollutant air quality management is needed.
   Impact: The 2009 BOSC Peer Review of the ORD Air Research Program highlighted AMAD's modeling and analysis contributions to the air quality and multipollutant themes of the program. The Division's contributions to air quality modeling were viewed very favorably by BOSC.
5. **Issue:** Systematic intercomparisons and evaluations are needed for regional air quality models over different continental regions.
   Accomplishment: Initiation of collaborations for the Air Quality Model Evaluation International Initiative (AQMEII) with Canadian and European partners; development of program for first AQMEII Workshop, April 27-29, 2009, Stresa, Italy
   Finding: The AQMEII modeling initiative was begun with a workshop in April 2009, during which North American and European perspectives on model evaluation were discussed.
   Impact: A model intercomparison exercise has been initiated for U.S., Canadian, and European air quality modeling systems to be applied on each continent for full-year simulations for operational and diagnostic evaluations. This is the first of its kind international collaborative effort in air quality modeling using the model evaluation framework developed by AMAD.

2.2 Model Development and Diagnostic Testing

1. **Issue:** As U.S. air quality improves, global background pollutant concentrations play an increasingly more important role in determining compliance with U.S. ambient air standards.
   Accomplishment: Extension of the Community Multiscale Air Quality (CMAQ) model to hemispheric

scales: initial demonstration of the concept for Hg and aerosol radiative effects
Findings: Air quality modeling results for ozone, particulate matter (PM), Hg, and other pollutants over the United States are sensitive to the specification of boundary concentrations.
Impact: CMAQ modeling capability now has been extended to the full Northern Hemisphere, enabling consistent specification of North American boundary concentrations and helping understand how the intercontinental transport of pollution affects air quality over the United States.

2. **Issue:** Chemical kinetic mechanisms are at the heart of air quality models used for National Ambient Air Quality Standard (NAAQS) implementation.
Accomplishment: Testing and initial incorporation of new chemical kinetic mechanisms in CMAQ: SAPRC07 and RACM2
Findings: The latest generation lumped species chemical mechanisms have been tested against smog chamber data and evaluated for incorporation into the CMAQ model.
Impact: The CMAQ model will contain versions of three state-of-the-science chemical mechanisms for use in air quality modeling (CB05, SAPRC07, and RACM2) for testing the robustness of emission control strategies by the program office and States.

3. **Issue:** Engineered nanomaterials can lead to ambient exposures of nanoparticles and health effects.
Accomplishment: Development of a joint AMAD-Human Exposure and Atmospheric Sciences Division (HEASD) research plan for predictive models for the transport, transformation, and fate of engineered nanomaterials
Findings: The initial focus of study will be on cerium oxide, a possible diesel fuel stabilization additive, and titanium dioxide, which is used in paint and other surface coatings.
Impact: The joint research plan will lead to studies on the chemical and physical attributes of these nanomaterials, as well as initial ambient modeling studies.

2.3 Air Quality Model Evaluation

1. **Issue:** EPA-National Oceanic and Atmospheric Administration (NOAA) collaboration in air quality model forecasting has developed an initial capability for $PM_{2.5}$ forecast guidance across the United States. This capability needs comprehensive evaluation before operational deployment.
Accomplishment: Completed Annual Performance Measure (APM) 154: Analysis and evaluation of developmental PM forecast simulations over the continental United States. (This APM reflects the development, deployment, and detailed evaluation of a “developmental” PM forecast modeling system for the continental United States and approaches to produce reliable forecast of air quality index [AQI].)
Findings: Developmental forecast simulations during 2004-2008 continuously were analyzed and evaluated against near real-time measurements from the AIRNOW network. In addition, forecasts of fine-PM speciation were compared against measurements from a variety of other surface PM networks. The systematic errors found in model predictions of both total $PM_{2.5}$ and its constituents have provided guidance for future research and further model development.
Impact: To improve the accuracy and utility of $PM_{2.5}$ forecast guidance obtained from comprehensive atmospheric models in the short-term, postprocessing bias-adjustment techniques that combine the model forecast with near real-time observations from the AIRNOW network were developed to provide reliable operational AQI forecasts. If the proposed method is operationalized by NOAA and EPA, it would enable the development of credible air quality, AQI, and exposure surfaces for the continental United States on a daily basis.

2. **Issue:** CMAQ v4.7 was released to the public in October 2008. Extensive incremental testing was conducted on the model prior to release. Results of the testing and evaluation need to be documented.
Accomplishment: Documentation of extensive process testing and evaluation of CMAQ v4.7 to support its release in October 2008 and multiyear (2002-2006) model evaluations of CMAQ v4.7 in support of the Centers for Disease Control and Prevention (CDC) collaboration on the PHASE project
Findings: The continued evaluation of CMAQ v4.7 has led to the correction of several performance issues with the new model. In addition, as part of the CDC PHASE project, annual CMAQ v4.7 simulations were performed for 2002-2006. This multiyear simulation provided an opportunity to evaluate the CMAQ model under numerous meteorological conditions. The model evaluation revealed several systematic model performance issues that occur each year, while other performance issues appear to occur under specific meteorological conditions.
Impact: Model deficiencies identified from process testing and annual 2002-2006 simulations were corrected and implemented in an interim release of CMAQ v4.7.1 in late 2009, enhancing the scientific credibility for CMAQ.

3. **Issue:** The quantification of uncertainty in air quality modeling results has been an important goal, but there has been little progress in this area.
Accomplishment: Demonstration of probabilistic model evaluation of the CMAQ model using an ensemble of model configurations and direct sensitivity analysis
Findings: Advances in probabilistic modeling approaches include improved methods for characterizing and understanding the sources of

uncertainty. Using Bayesian Parameter Estimation, advanced methods have been developed for translating an ensemble of CMAQ model simulations into a probability distribution.
Impact: The Direct Decoupled Method (DDM) has been incorporated in CMAQ v4.7, which is used to calculate the sensitivity of ozone to specific emission sources and model parameters. Further, these techniques have been applied to identify emission source sectors that have significant contributions to ozone sensitivity. This work is helping us in testing the robustness of the response of CMAQ to emission reductions.

2.4 Climate and Air Quality Interactions

1. **Issue:** Future air quality is expected to be affected both by climate change and by emissions changes. Phase 1 of the Climate Impacts on Regional Air Quality (CIRAQ) project focused on the potential impacts of climate change on air quality. Phase 2 has added regional emissions projections for the future on top of climate change.
Accomplishment: Completed APM 258: The impact of climate change on U.S. PM concentrations: Model sensitivity tests and PM concentration changes in the United States under a future climate scenario with and without future emission scenarios
Findings: In Phase 1 (climate change only), CMAQ modeling under the future (2050) scenario resulted in average ozone increases of approximately 2 to 5 ppb and 95th percentile (i.e., fourth highest) ozone increases greater than 10 ppb in some regions. In Phase 2, with emissions projections added, it was found that the magnitude of the decrease in ozone resulting from changing emissions is much larger than the increase resulting from climate change. The effect of climate change on PM concentrations appears to be driven primarily by changes in precipitation patterns, which are highly uncertain. For these simulations, increased future precipitation leads to decreased PM concentrations, so that the effect of changing emissions and climate are in the same direction.
Impact: This initial CIRAQ study has laid the foundation for future air quality-climate change assessments. Large uncertainties exist in future projections from any single global climate model (GCM), so research planning has taken into account the use of up to three GCMs from which to simulate regional climate. Various downscaling techniques will be tested, including dynamical and statistical. Screening tools and comprehensive modeling tools will be developed to assess the potential impacts of air quality on global and regional climate.
2. **Issue:** Regional downscaling of GCM results must begin with global model data. AMAD must establish strong working relationships with global modeling groups to acquire the appropriate data for downscaling.
Accomplishment: Establishment of collaboration with the National Aeronautics and Space Administration (NASA) Goddard Institute for Space Studies (GISS) on global to regional downscaling of upcoming GCM simulations covering the 21st century
Findings: NASA/GISS, under the leadership of Dr. James Hansen, is one of the premier global climate modeling centers in the world. Their latest global model, Model E, will be used for simulations to inform the next International Panel on Climate Change (IPCC; the fifth) Assessment Report.
Impact: An interagency agreement with NASA is being established, with a postdoctoral fellow to work between both NERL/AMAD and NASA/GISS, to obtain high temporal resolution Model E results for AMAD’s regional model downscaling with weather research and forecasting (WRF). This demonstrates the value of cross-agency collaboration.
3. **Issue:** Traditional techniques for dynamical downscaling of global model results to the regional scale have relied only on specification of boundary conditions for the regional model. However, this specification in itself is insufficient to constrain the regional model. New techniques are needed to assure better consistency between global and regional model results.
Accomplishment: Regional Climate Downscaling with WRF has been tested using both global reanalysis data and output from the GISS Model-E GCM. Most of the testing thus far has focused on spectral and analysis nudging.
Findings: Initial testing of dynamical downscaling from GISS Model E to WRF using various nudging techniques has shown much better correspondence between global and regional meteorological patterns. Results are sensitive to the nudging parameters; thus, more testing is needed to determine best configuration.
Impact: AMAD’s experiments with data assimilation in the process of downscaling from global to regional climate models (RCMs) have shown much promise in moving this discipline forward. Initial results presented at recent conferences have generated much discussion and interest in the scientific community.
4. **Issue:** Thus far, AMAD’s air quality-climate research has focused on the potential impacts of future global climate change on air quality. The reverse process (i.e., the impacts of local and regional air pollution on climate) is also of intense scientific interest.
Accomplishment: The WRF-CMAQ coupled meteorology-chemistry model has been tested, including direct aerosol feedback on shortwave (SW) radiation and ozone feedback on longwave (LW) radiation. Indirect feedback is under development.
Findings: The WRF-CMAQ coupled meteorology-chemistry model has been tested, including direct

aerosol feedback on SW radiation and ozone feedback on LW radiation. Indirect feedback is under development.

Impact: The 2-way coupled WRF-CMAQ system provides a framework to properly characterize the spatial heterogeneity in radiative forcing associated with short-lived aerosol and gases and, consequently, to better understand their aggregate influence on the earth's radiation budgets. This evolving system is expected to play a critical role in the Agency's evolving research and regulatory applications exploring air quality-climate interactions. The flexible design of the system facilitates coupling meteorological and chemical calculations at finer temporal resolutions, which enables more consistent applications at fine spatial scales to better characterize variability in air quality and its linkage with health studies. This work led to the preparation of a research proposal to build EPA-U.S. Department of Energy collaboration in the climate change arena.

2.5 Linking Air Quality to Human Exposure

1. **Issue:** Methods are needed for verifying the impact of emissions control programs on air quality ambient concentrations, human exposures, and health outcomes

   Accomplishment: Completed APM 155: Develop a Mesoscale Pilot of Approaches for Identifying and Tracking Regulatory Impacts (This APM reflects the culmination of several research projects that have resulted in approaches for identifying and tracking air quality impacts of regional-scale regulatory emissions control programs. These approaches were applied to examine the impact of the NO_x Budget Trading Program [NBP].)

   Findings: The CMAQ model was used to characterize air quality before and after the implementation of the NBP 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 seasonal variations. Trajectory models were used to investigate the transport of primary and secondary pollutants from their emission sources to downwind regions. In addition, research has focused on relating NO_x emissions and ambient ozone concentrations to human exposure and health end points.

   Impact: Combined modeled/measured high-resolution air quality surfaces were used in human exposure models, epidemiological health studies, and health risk assessments. The preliminary results indicate that the NBP might have contributed to reduced respiratory-related hospital admissions in some regions of New York State. This effort led to the development of an innovative method to understand air quality and human health linkages.

2. **Issue:** Ambient air pollutant concentrations are needed to assess exposures but are not equivalent to them. Methods are needed to develop exposure estimates informed by modeled ambient concentrations.

   Accomplishment: Development and demonstration of a methodology to link regional- and local-scale air quality models with human exposure models for improving community level environmental health studies, involving near-source exposures to multiple pollutants

   Findings: A 2009 *Journal of the Air & Waste Management Association* paper by Isakov and co-investigators presents an innovative methodology to link regional- and local-scale air quality models with human exposure models. It shows the existence of strong spatial gradients in exposures near roadways and industrial facilities that can vary by almost a factor of two across the urban area and much higher at the high end of the exposure distribution.

   Impact: The complexity in the spatial variation of exposures among different population cohorts, especially in the context of cross-sectional or intra-urban analysis of air pollution health effects, could be quite challenging. The information derived from this study will be used by EPA as a resource for future air accountability research planning. Through this effort, the Division has helped to advance exposure science.

3. **Issue:** A principal route of human exposure to pollutants occurs for those living and working within several hundred meters of roadways. A better understanding of the mechanisms of such exposure is needed.

   Accomplishment: For the near-road research program, developed wind tunnel and field study databases and improved algorithms for urban roadways in the American Meteorological Society (AMS)/EPA Regulatory Model (AERMOD) in support of human exposure and health assessments.

   Findings: The new line source algorithm significantly advances the assessment tools for near-road application. To be approved for inclusion in AERMOD, this algorithm and the work described underwent extensive internal and external peer review. This review and approval process included input from the AMS/EPA Regulatory Model Improvement Committee that provided scientific advice and support to EPA in the area of near-source/short-range dispersion modeling. This work supports EPA offices and programs needing to simulate short-range dispersion in relation to permit applications, exposure research, and human health risk assessments by ensuring that short-range

dispersion programs incorporate peer-reviewed science. This research assists with the transfer of state-of-the-art science and modeling techniques into practical, workable tools applicable to key programs, such as regulatory modeling. The improved model provides EPA and other stakeholders with the information needed to identify potential health risks for near-road populations and to develop air pollution control programs to address these risks. In addition, it enables the modeling of air quality impacts for regulatory programs under the Federal Highway Administration's (FHA's) Transportation Conformity Rule and the National Environmental Policy Act.
Impact: The importance of this work was recognized by EPA and external stakeholders by its inclusion in the proposed nitrogen dioxide (NO_2) NAAQS for near-road monitoring requirements. Results from this work also were used by the FHA in addressing near-road monitoring needs associated with their settlement agreement litigation. The FHA requested EPA's guidance and expertise in implementing their near-road research requirements as part of this litigation, and an inter-agency agreement has been established to that end. In addition to regulatory applications, the nominated papers have been cited in numerous other peer-reviewed journal articles related to near-road and local-scale dispersion topics.

2.6 Linking Air Quality and Ecosystems

1. **Issue:** Existing treatment of ammonia (NH_3) flux in the CMAQ model consists of a specified emissions term and a computed deposition. More realistic treatment is needed considering the compensation points for NH_3 in soil and the plant canopy allowing for two-way flux.
Accomplishment: Development of new CMAQ NH_3 bidirectional exchange algorithms through joint AMAD-National Risk Management Research Laboratory (NRMRL) collaboration on field data analyses and model development
Findings: Critical data needed to parameterize a two-layer deposition model was collected, and it was shown that it was feasible to parameterize a model that accounts for bidirectional exchange and include it in CMAQ. The need for a fertilization model to provide an estimate of the soil compensation point was identified.
Impact: The foundation is laid for a more sophisticated approach to air-surface exchange within CMAQ, and a strong rationale is provided to bring air-surface exchange calculations fully into CMAQ. Incorporating bidirectional exchange of NH_3 is expected to significantly impact the range of influence of NH_3 emissions.
2. **Issue:** Biases and/or errors in the Fifth-Generation Pennsylvania State University/National Center for Atmospheric Research (NCAR) Mesoscale Model (MM5) or WRF modeled precipitation can cause problems for calibrated watershed models that typically use observed precipitation data for calibration.
Accomplishment: Identification of the need for WRF-consistent hydrology to address linkage disparities through collaboration between AMAD and the Ecological Research Division (ERD) on analysis of the effect of MM5 precipitation errors on watershed hydrology
Findings: Errors in MM5 or WRF modeled precipitation timing, location, and amount are too large to be handled by calibrated watershed models, making the direct use of CMAQ wet deposition for air-water linkage very problematic.
Impact: A key new AMAD research area is identified, linking a hydrology model to WRF/CMAQ, which is needed for CMAQ to successfully support atmosphere-ecosystem linkage. This effort would help advance ecological exposure assessments.
3. **Issue:** Future deposition is expected to be significantly reduced by Clean Air Act (CAA) regulations that address ozone and $PM_{2.5}$ attainment. Finer resolution grids (12-km) match better to watershed segments and better resolve coastal estuaries for linking atmospheric deposition to coastal systems.
Accomplishment: Delivery of nitrogen deposition futures scenarios for 2009, 2020, and 2030 to Chesapeake Bay Program
Findings: The CAA Amendments are anticipated to make major reductions (>50%) in oxidized nitrogen deposition to coastal estuaries across the eastern United States. Such reductions are very important to restoration efforts. However, these gains are offset to a significant degree by the expected future increases in ammonia emissions.
Impact: Linked the latest CMAQ with the latest Chesapeake watershed model—both at higher spatial resolution. The Division provided Chesapeake Bay Program a complete set of deposition scenarios that provides a best estimate of the benefits of CAA regulations on deposition for Chesapeake Bay Program Office total maximum daily load (TMDL) analyses and other management analyses.
4. **Issue:** MM5 or WRF modeled precipitation errors cause a problem for providing deposition inputs to critical loads models that require the most accurate deposition inputs possible for their biogeochemical mass balance calculations.
Accomplishment: Development of approach to postprocess CMAQ wet deposition to reduce errors and delivery of postprocessed CMAQ deposition fields to EPA and the National Park Service (NPS) for national critical loads analysis
Findings: Use of Parameter-Elevation Regressions on Independent Slopes Model (PRISM) data to correct for modeled precipitation error, plus simple

bias corrections, enables reduction and smoothing out wet deposition error and inclusion of orographic effects on wet deposition. This approach appears to be preferable to data fusion for providing modeled fields to better fill in for sparse monitoring of wet deposition.

Impact: The postprocessing approach was applied successfully to 2002 annual deposition data to create acceptable national deposition fields for EPA and NPS critical loads analyses. The critical loads models for the first time used CMAQ wet and dry deposition fields for input, successfully demonstrating the capability to use CMAQ for these critical loads analyses.

CHAPTER 3

Model Development and Diagnostic Testing

3.1 Introduction

EPA and the States are responsible for implementing the NAAQS for ozone and PM. New standards for 8-h average ozone and daily average $PM_{2.5}$ concentrations recently have been promulgated. Air quality simulation models, such as the CMAQ modeling system, are central components of the air quality management process at the national, State, and local levels. CMAQ, which is used for research and regulatory applications by the EPA, States, and others, 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.

- Develop, evaluate, and refine scientifically credible and computationally efficient process simulation and numerical methods for the CMAQ air quality modeling system
- 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)
- 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 processes or data sensitivities and uncertainties related to the problem
- Evaluate the CMAQ modeling system using operational and diagnostic methods and to identify needed model improvements
- Use CMAQ to study the interrelationships between different chemical species, as well as the influence of uncertainties in meteorological predictions and emission estimates on air quality predictions
- Collaborate with research partners to include up-to-date science process modules within the CMAQ model system
- Pursue computational science advancements (e.g., parallel processing techniques) to maintain the efficiency of the CMAQ modeling system

The CMAQ modeling system outlined in Figure 3-1 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, which provides user support for the CMAQ system and holds an annual CMAQ users conference, have helped to create a dynamic and diverse CMAQ community of over 2000 users in 90 countries. CMAQ has been and continues to be used extensively by EPA and the States for air quality management analyses, 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 WRF (meteorological

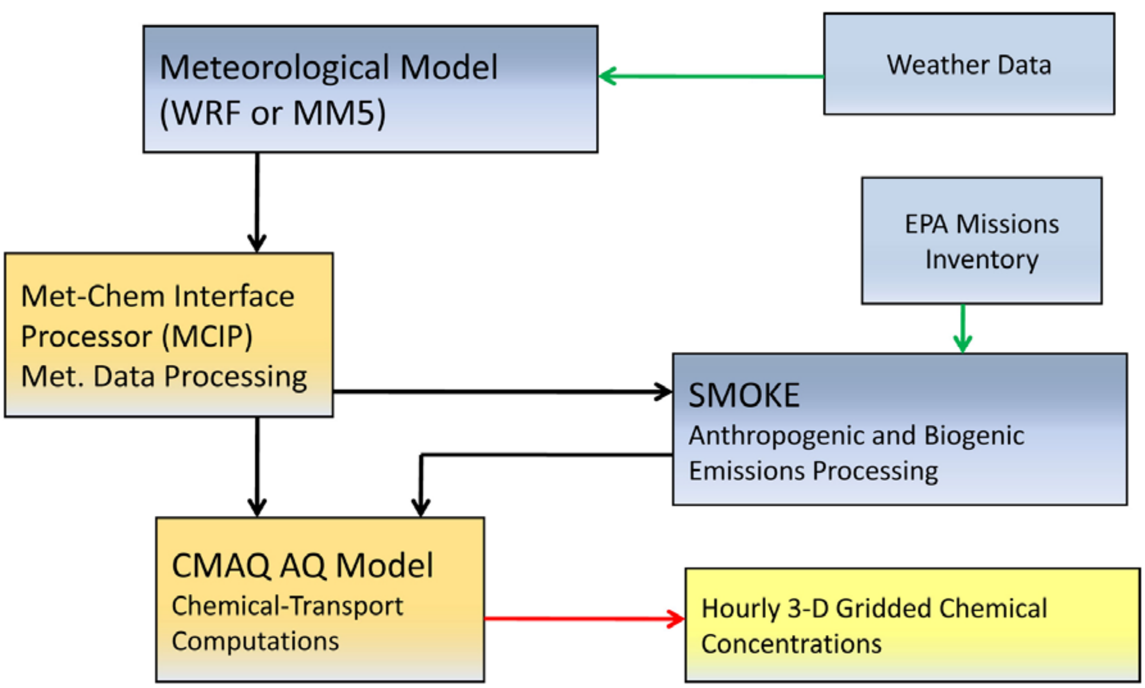


Figure 3-1. A flowchart that outlines the various components of the CMAQ modeling system.

model)-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.

3.2 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 (Figure 3-2) by advancing the scientific algorithms, computational efficiency, and numerical stability of the CMAQ aerosol module.

To achieve this objective, we have focused efforts in five areas to improve 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 dinitrogen 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.

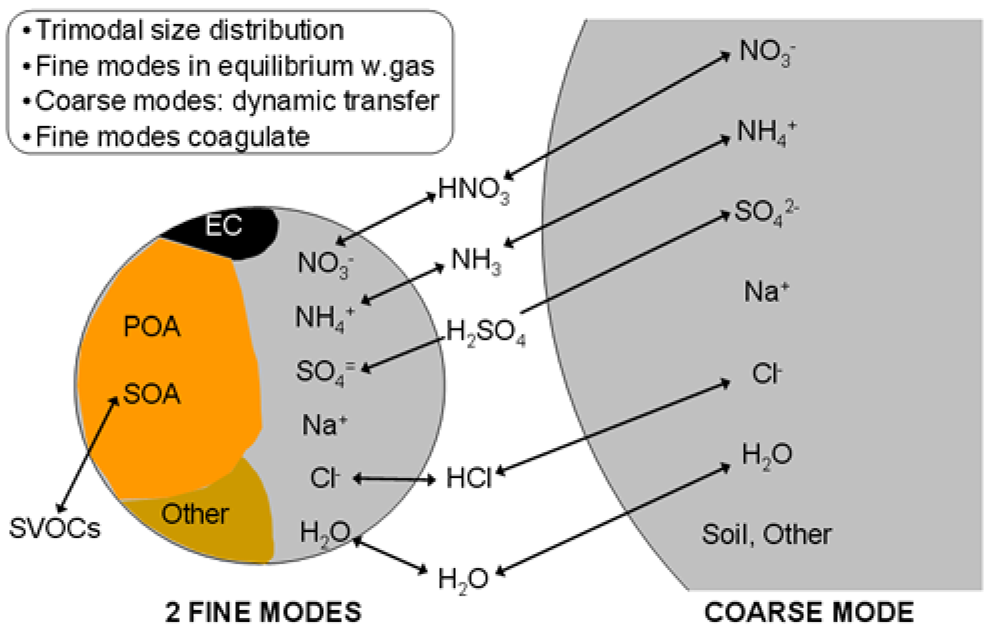


Figure 3-2. Representation of PM size and composition in CMAQ v4.7.

As a result of this research, the CMAQ aerosol module has been enhanced and greatly improved over the past 5 years. During that time, the aerosol module has been used for regulatory and forecasting applications (e.g., EPA's Clean Air Interstate Rule [CAIR], NOAA's National Centers for Environmental Prediction) 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 Standard rulemaking). Meanwhile, the community of CMAQ users outside EPA continues to grow rapidly.

3.3 CMAQ Gas and Aqueous Chemical 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 since has become clear that it is more appropriate to treat chemistry in an integrated, multiphase, multipollutant manner (National Research Council, 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 ozone, SOA, and secondary toxics formation (Ng et al., 2007; Luecken et al., 2008). Our research and implementation program for chemical mechanisms accounts for production of pollutants in the gas and aqueous phase, as well as for precursors to aerosol production, as shown in Figure 3-3.

In addition, the requirements for air quality modeling also have changed: The new NAAQS for ozone and $PM_{2.5}$ have shifted our focus from urban-scale ozone episodes (~7 days) to regional/continental-scale simulations over longer time 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 impacts of biofuels.

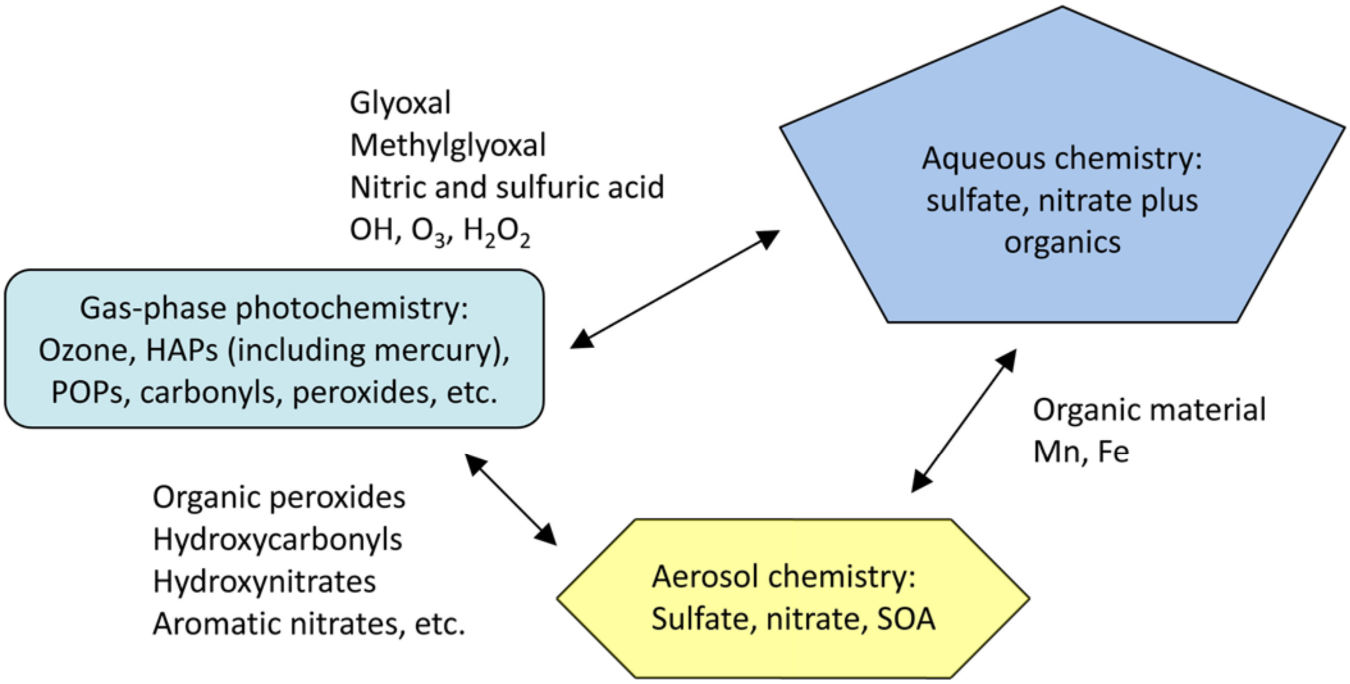


Figure 3-3. Current interactions between gas, aqueous, and aerosol chemistry in CMAQ base (criteria pollutants) and multipollutant (including HAPs) models.

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

- ensure that CMAQ and other regional 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 accounted for adequately, so that we can better predict multimedia chemical effects of emissions changes;
- develop techniques, tools, and strategies, so that we are able to efficiently expand current mechanisms to predict the chemistry of additional atmospheric pollutants that we anticipate 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 ozone and PM. These efforts are linked closely to the research that we perform in developing the secondary organic aerosol module. We continue to improve the base photochemical mechanisms that drive the oxidant and radical chemistry. Because our models are used for both research and regulations, we constantly strive for a balance between stability and response to new scientific information. We partner with other EPA researchers and outside experts to develop state-of-the-science chemistry descriptions that we implement in CMAQ to provide more accurate descriptions of important chemical pathways. Table 3-1 shows the base photochemical mechanisms currently maintained and released in CMAQ and some of the most important species predicted by these CMAQ mechanisms. In addition, variants of other mechanisms, including portions of the Master Chemical Mechanism, are being used in CMAQ by outside groups. The different mechanisms predict slightly different values of ozone and other gas phase species and also can affect PM formation, as shown in Figure 3-4, where the sulfate production pathways differ widely depending on the particular chemical mechanism used.

Clouds cover roughly 60% of the Earth's surface, yet aqueous phase cloud chemistry is poorly understood and not well characterized in atmospheric models. Recently, CMAQ's aqueous chemistry was expanded to

Table 3-1. Base Photochemical Mechanisms in CMAQ and the Species Commonly Predicted by Each Mechanism

Mechanism	Notes
CB05	Standard with chlorine chemistry, used for regulatory application
SAPRC-99	Used for research applications
SAPRC07	Customized version with chlorine chemistry, in testing phase
RACM2	Customized version, currently in testing phase
CB4	To be phased out in 2011 release of CMAQ

Major Species Predicted in CMAQ
Ozone (O_3)
Nitrogen oxide and nitrogen dioxide (NO and NO_2)
Other oxidized nitrogen (PAN, HONO, N_2O_5, and organic nitrates)
Fine and coarse particulate matter ($PM_{2.5}$ and PM_{10})
Sulfur dioxide and sulfate (SO_2 and SO_4)
Nitric acid and nitrate (HNO_3 and NO_{3-})
Hydrogen peroxide (H_2O_2)
Carbon monoxide (CO)
Biogenic VOCs (isoprene, pinene, and sesquiterpenes)
Aromatic compounds (benzene, xlenes, and toluence)
Radicals (such as OH, HO_2, and NO_3)
Number of gas phase species: 86 (CB05), 94 (SAPRC-99)
Number of aerosol species: 75

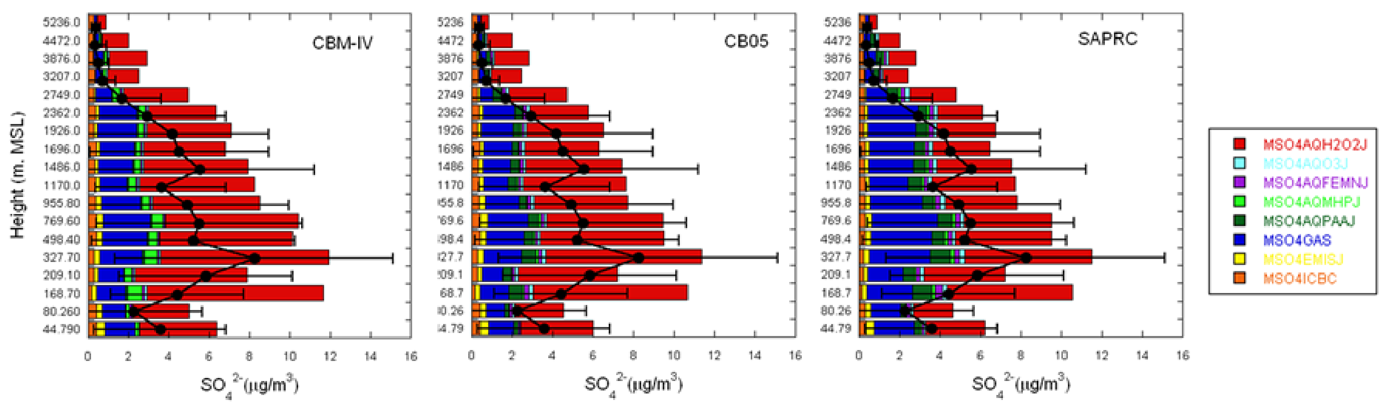


Figure 3-4. Comparison of average modeled (bars) vertical profiles of sulfate with NOAA WP-3D aircraft measurements (black line; July-August 2004).

include cloud production of SOA via two in-cloud organic reactions: (1) glyoxal with hydroxyl radical (OH) and (2) methylglyoxal with OH.

The cloud processing hypothesis for SOA formation is that water-soluble oxidation products of reactive organic compounds partition into cloud droplets, oxidize further, and create low-volatility compounds that remain, in part, in the particle phase on droplet evaporation (>90% of cloud droplets evaporate).

When SOA formation from these organic aqueous phase reactions was added, CMAQ model performance for particulate organic carbon (OC) improved. This is most noticeable when comparing the vertical profile of CMAQ-predicted OC with WSOC measurements from a NOAA P3 “cloud experiment” flight during the International Consortium for Atmospheric Research on Transport and Transformation (ICARTT) in 2004, as shown in Figure 3-5.

The inclusion of chlorine reactions and the explicit chemistry for 43 Hazardous Air Pollutants (HAPs) has helped to expand the applications for which CMAQ can be used. More detail on the HAPs portion of the CMAQ mechanism can be found in section 2.8 of this chapter.

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.

Future Directions

Because atmospheric chemistry is central to air quality models, our future efforts in atmospheric chemistry mechanisms will continue to evolve and fully employ our expertise in gas, aqueous, and aerosol chemistry. Future efforts will involve reducing known uncertainties in current chemical mechanisms and improving gas-aerosol-aqueous chemistry linkages.

We will continue to monitor in-house and external research in atmospheric chemistry, toxic air pollutants, aerosol formation, and aqueous chemistry. We will assess the robustness and importance of new discoveries, and partner with leading researchers to direct research in areas that will provide the greatest improvements in air quality model predictions. We will modify the mechanisms to include new information (such as new reactions) to keep our mechanisms at state of the science.

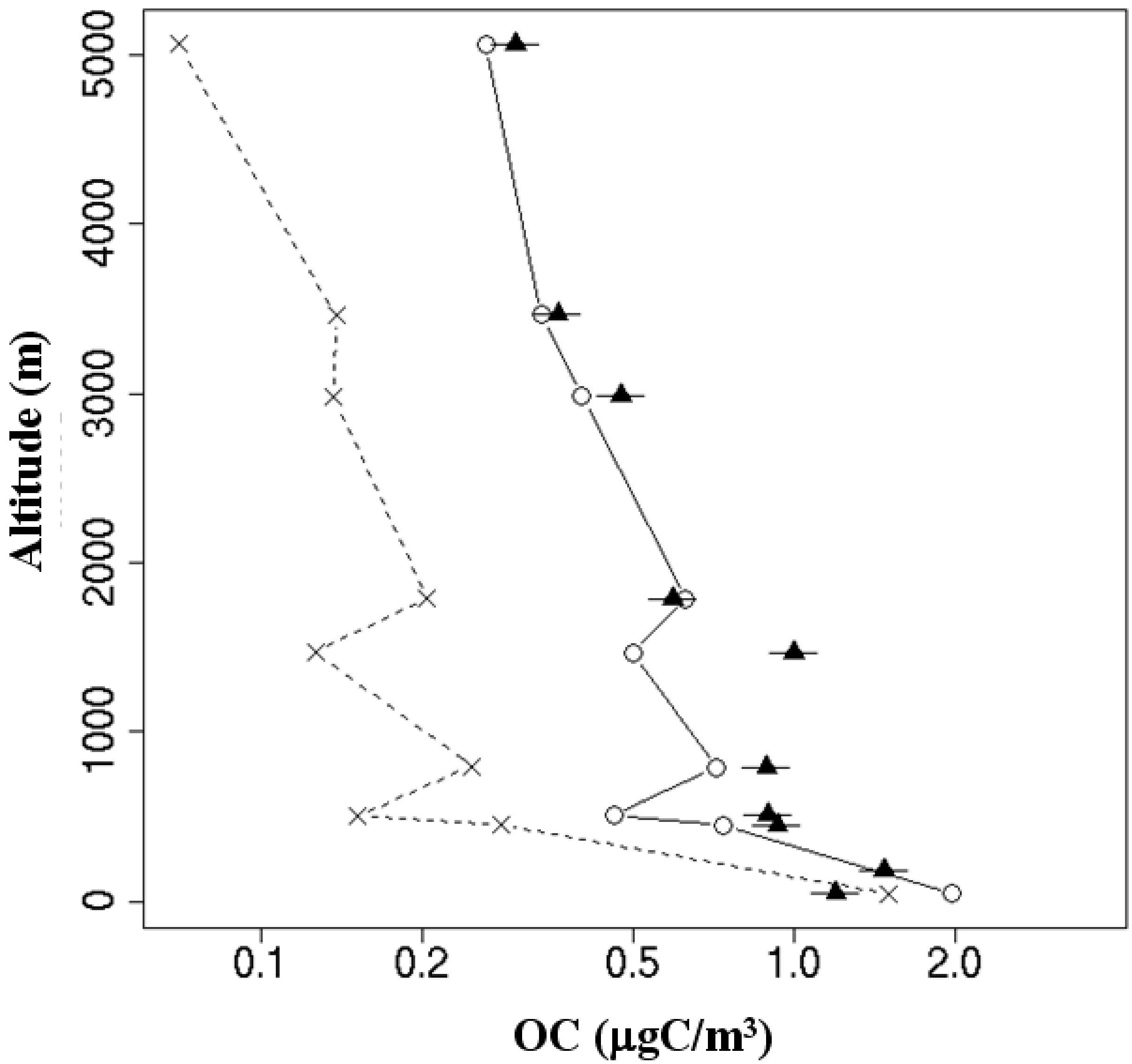


Figure 3-5. Layer-averaged vertical profiles of OC and WSOC on August 14, 2004. Normalized mean bias for layer-average values for this flight was reduced from –65% to –15% when SOA_{cld} was included. Note: Dashed line and "x" indicate layer-averaged base CMAQ OC prediction. Solid line and "o" indicate CMAQ OC prediction with cloud-produced SOA included. WSOC observations from the NOAA P3 flight are indicated with "▲". The x-axis is log scale. (Adapted from Carlton et al. [2008])

We also anticipate that our future efforts will involve extending the chemistry beyond "traditional" pollutants to address newly emerging issues such as biofuels, pesticides, and chemicals that contribute to global warming.

3.4 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 planetary boundary layer (PBL), which extends from the ground up to ~1 to 3 km during the daytime but is only tens or hundreds of meters deep at night.

The modeling of the atmospheric boundary layer, particularly during convective conditions, long has 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, cannot simulate convective conditions realistically. Simple nonlocal-closure PBL models, such as the Blackadar convective model, which has been a mainstay PBL option in NCAR's mesoscale model (MM5) for many years, and the original Asymmetric Convective Model (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, ACM2 can represent both the super-grid-scale and subgrid-scale components of turbulent transport in the CBL. Testing ACM2 in one-dimensional form and comparing to large-eddy simulations (LES) and field data from the second and third Global Energy and Water Cycle Experiment Atmospheric Boundary Layer Study, known as the GABLS2 (CASES-99) and GABLS3 (Cabauw, The Netherlands) experiments demonstrate that the new scheme accurately simulates PBL heights, profiles of fluxes and mean quantities, and surface-level values. 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.

ACM2 is in the latest releases of the WRF model and the CMAQ model and is being used extensively by the air quality and research communities. 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.

3.5 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 systems 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 air quality 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 MM5 mesoscale model system to the WRF model that represents the current state of science. Part of this effort was to implement in WRF the land-surface (Pleim-Xiu [PX]), surface-layer (Pleim), and PBL (ACM2) schemes that have been used in MM5 and are designed for retrospective air quality simulations. Part of this effort included improving the PX land-surface physics that included a deep-soil-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 4D data assimilation (FDDA) capability that had been available in MM5. Another effort has been a reexamination of FDDA techniques, including the use of an objective reanalysis package for WRF (OBS-GRID) to lower the error of analyses that are used to nudge the model toward the observed state. RAWINS was the equivalent package used by MM5.

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 the uncertainty or error in near-surface variables like 2-m temperature, 2-m moisture, and 10-m wind as indicated in Table 3-2. 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. Figure 3-7 shows error differences between WRF and MM5, where both models were configured as similar as possible (i.e., PX land surface model [LSM], ACM2 PBL, etc.). The large number of dark blue and purple areas indicate WRF has a much lower temperature error than MM5. In Table 3-2 and Figure 3-9, PXACM is the simulation that used the PX LSM and ACM2 PBL scheme, whereas the terminology NOAHYSU indicates the simulation that used NOAA's land surface model (NOAH) LSM and Yonsei University (YSU) PBL scheme.

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 PBL 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 or less), wind speed (<2.0 m/s), and wind direction (<30 deg) in the PBL, which is generally less than the error near the surface (Figure 3-8). The model also simulates the evolution of the wind structure, including features like nocturnal jets and the convective mixed layer (see Figure 3-9), with low error (<2.0 m s^{-1}). Our current configuration of WRF has met the requirements for the transition from MM5.

Table 3-2. Summary of Surface-Based Model Performance Statistics for Each Simulation (Also provided is the RMSE [2-m temperature only] of analysis dataset that was used for the indirect soil moisture and temperature nudging of the PX LSM.)

RMSE	WRF PXACM	MM5 PXACM	WRF NOAHYSU	Obsgrid Analysis	RAWINS Analysis
2-m Temperature (K)					
January	2.48	2.52	2.33	1.29	1.47
August	1.94	2.00	2.31	1.22	1.31
2-m Mixing ration (g kg^{-1})					
January	0.92	0.84	0.78		
August	1.86	1.92	2.11		
10-m Wind speed (m s^{-1})					
January	1.64	1.79	1.78		
August	1.47	1.49	1.60		
10-m Wind direction (deg)					
January (MAE)	21	25	23		
August (MAE)	30	33	32		

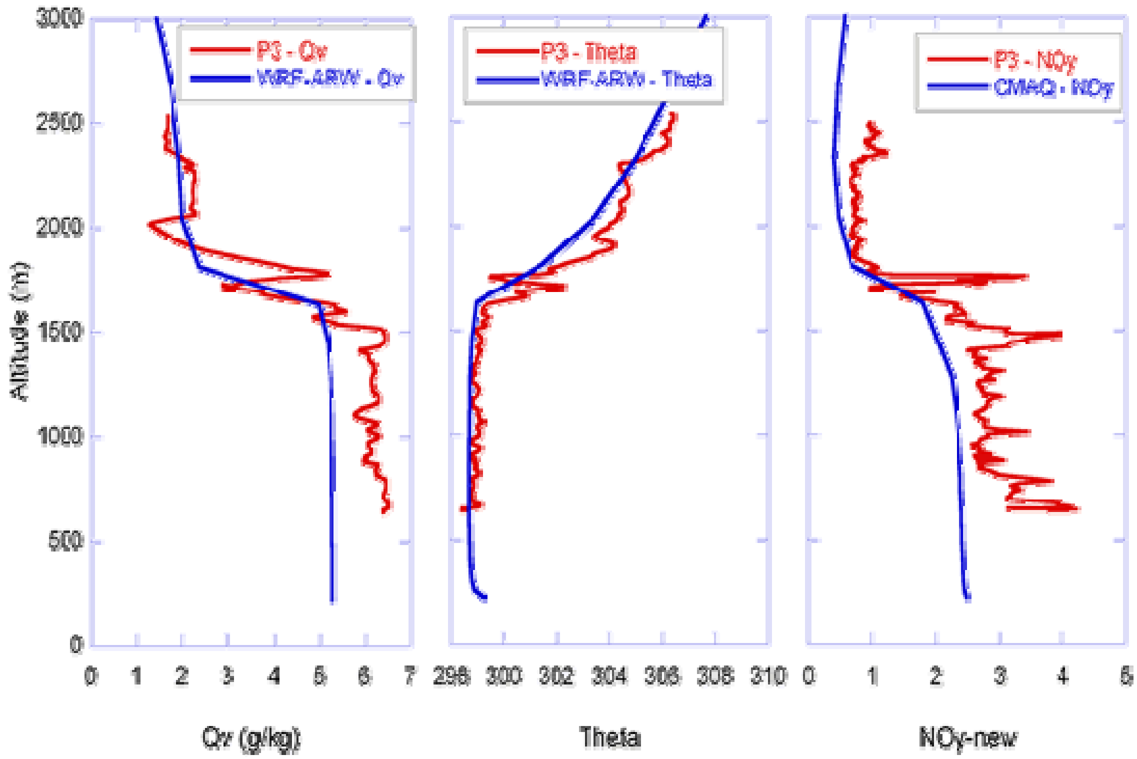


Figure 3-6. The most direct measure of success for a PBL model for both meteorology and air quality is its ability to accurately simulate the vertical structure of both meteorological and chemical species. The figure above shows an example of WRF and CMAQ profiles (both use the ACM2 scheme) compared with aircraft measurements. The top of the PBL mixed layer is well defined and modeled for both meteorology variables (Qv and Theta) and chemical variables (NO_y). Although such simultaneous measurements of vertical profiles of meteorology and chemistry are very rare, these limited results are encouraging.

3.6 Coupled WRF-CMAQ Modeling System

Although the role of long-lived greenhouse gases in modulating the Earth's radiative budget long has 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

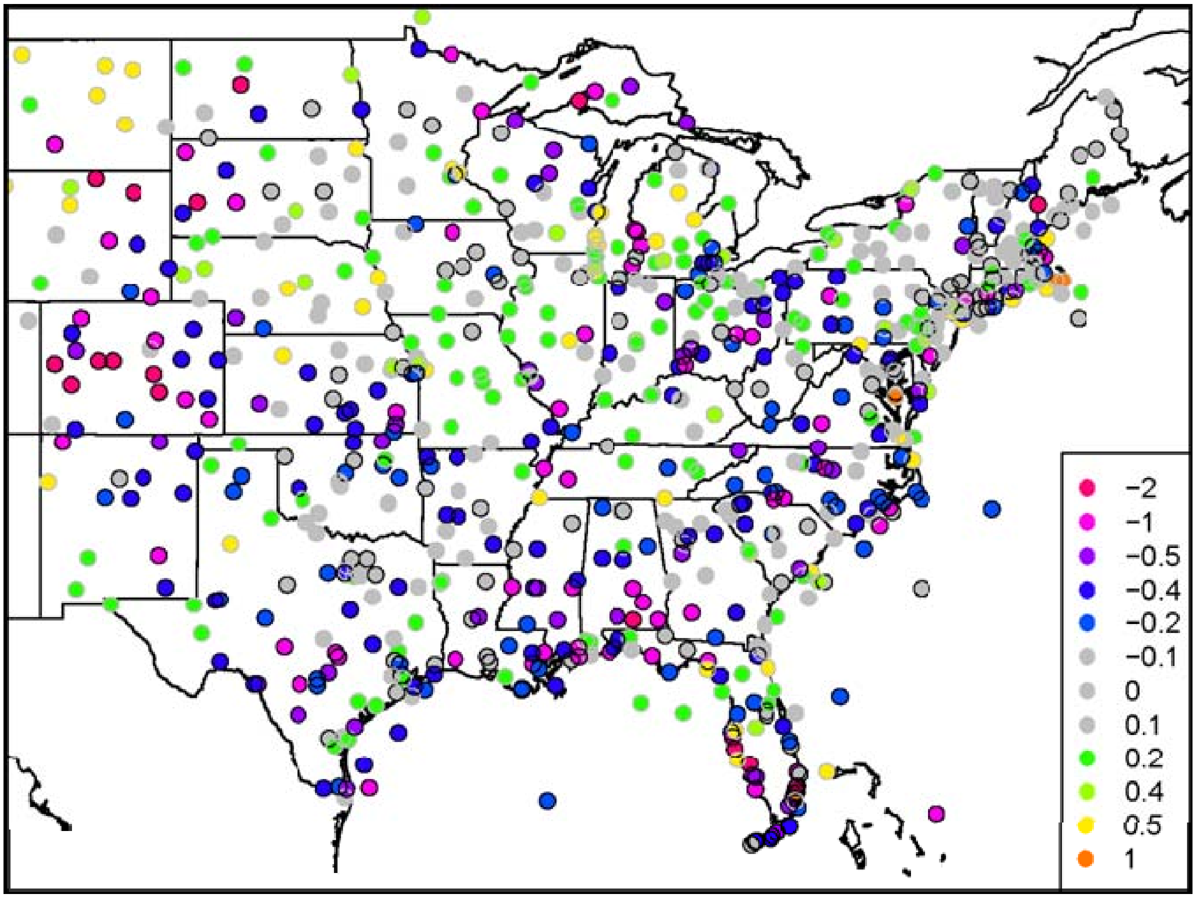


Figure 3-7. Spatially distributed root mean square error (RMSE) difference (2-m temperature) between the WRF and MM5 for August 2006. Negative values indicate WRF has a lower error, and positive values indicate MM5 has a lower error.

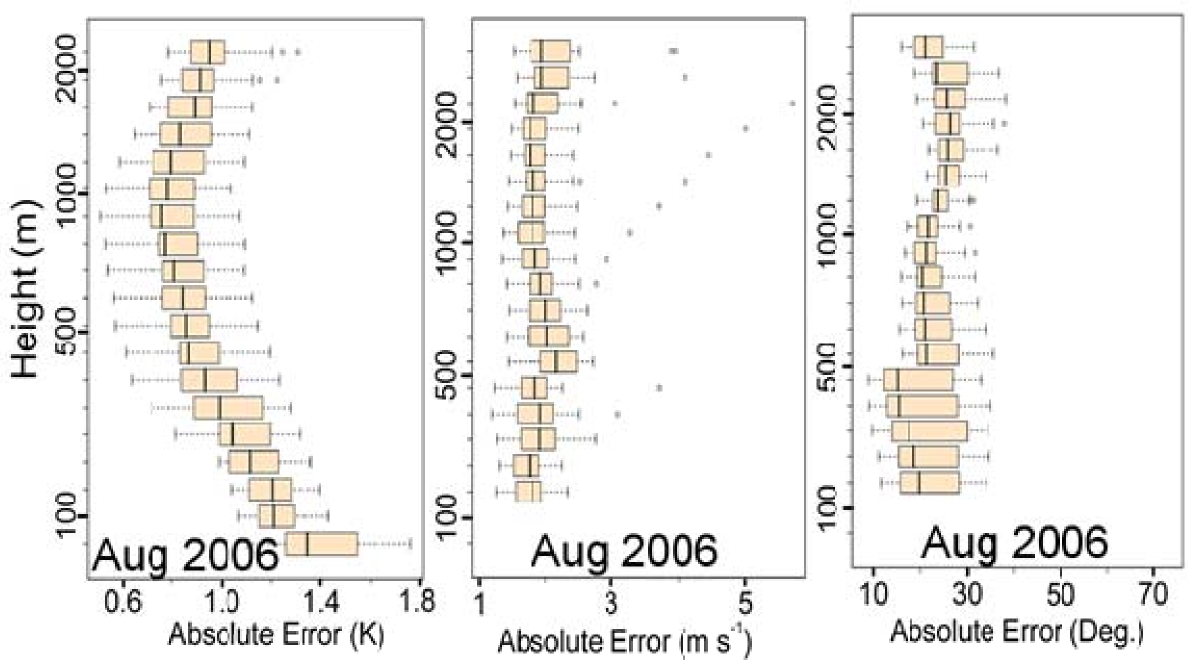


Figure 3-8. Mean absolute error (MAE) profiles of model-simulated temperature, wind speed, and wind direction for August 2006. The observations used to compute MAE include 19 NOAA wind profilers located in the central United States.

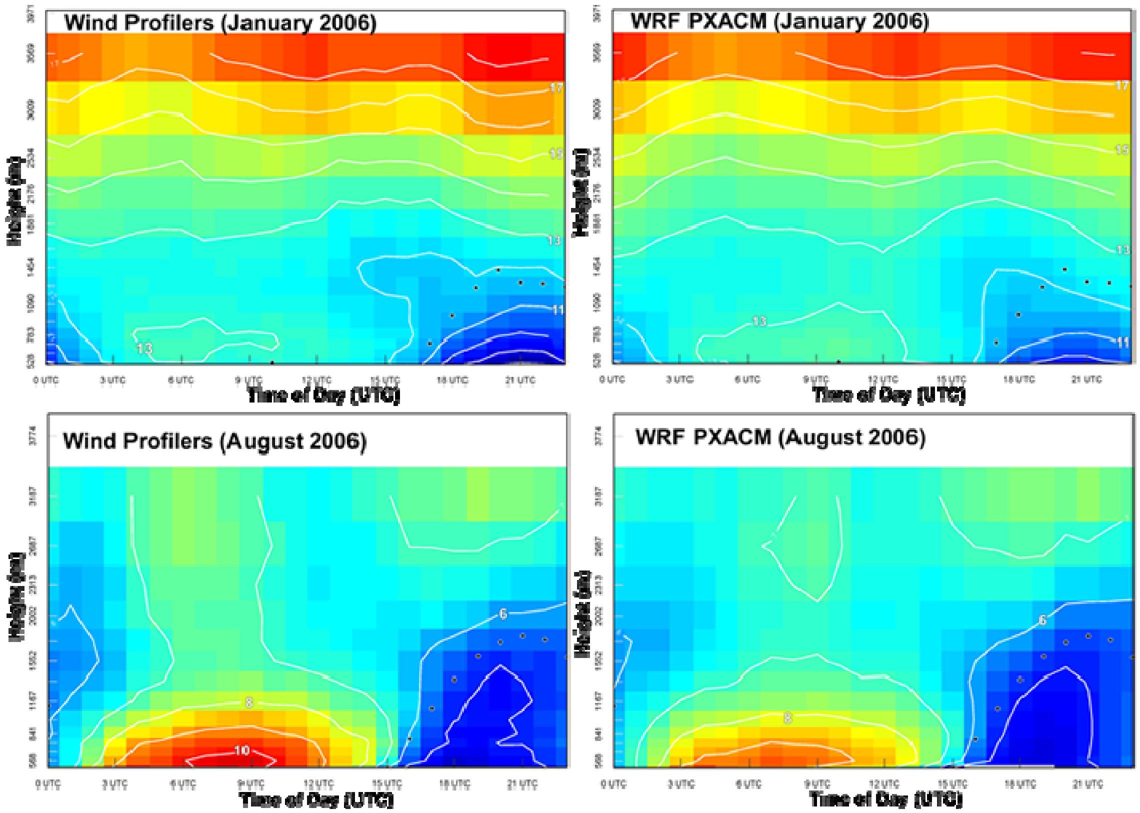


Figure 3-9. **Diurnal mean wind speed profiles (height above ground level) for January and August 2006. The left column represents the mean observed wind speed computed using 19 NOAA wind profilers located in the central United States. The right column is the corresponding model-simulated mean wind speed using the grid points closest to the wind profiler sites. Small dots indicate the mean PBL height of the WRF.**

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 off-line 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 and, thus, facilitates consistent use of data; (3) reduces the disk-storage requirements typically associated with off-line 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 off-line modeling.

In the prototype coupled WRF-CMAQ system, the simulated aerosol composition and size distribution are used to estimate the optical properties of aerosols, which then are 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 as demonstrated in Figure 3-10. 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.

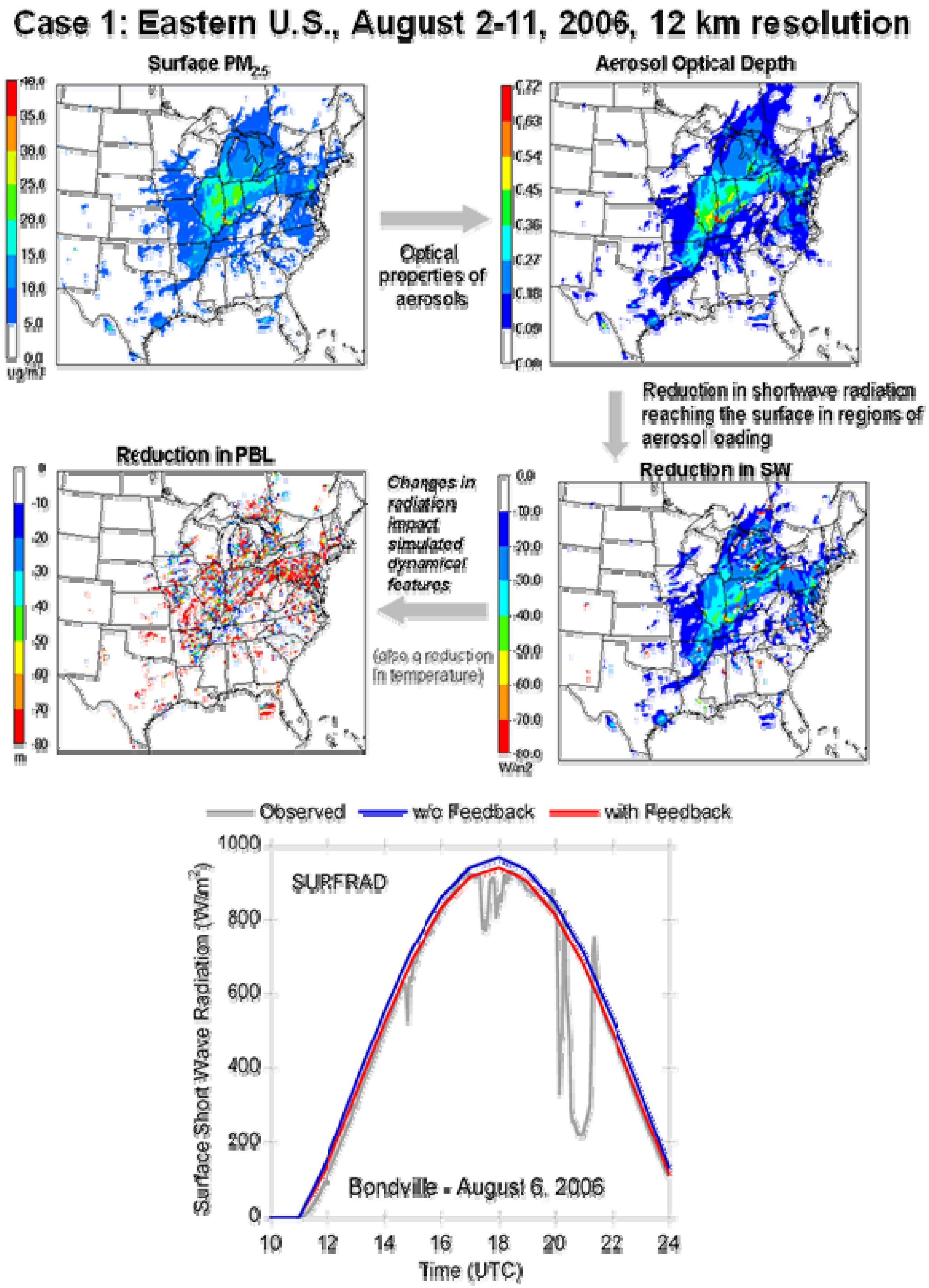


Figure 3-10. Two sets of initial simulations have been conducted to test the evolving coupled WRF-CMAQ modeling system and to systematically assess the impacts of coupling and feedbacks. The upper panels in the figure above demostrate the impact that aerosols estimated by CMAQ have on the meteorological models' estimates of planetary boundary layer (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.

3.7 Mercury Modeling

AMAD has been working on the development of atmospheric mercury models since the early 1990s, when the Regional Lagrangian Model of Air Pollution (RELMAP) was adapted to simulate mercury in support of EPA's Mercury Study Report to Congress. As the scientific understanding of atmospheric mercury 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 mercury with other pollutants that were being discovered. Thus, AMAD's focus for atmospheric mercury model development was moved to the CMAQ model. That model simulates atmospheric processes within a 3-D array of predefined finite volume elements and can model complex interactions between all of the pollutants that might exist within each volume element. The CMAQ model was developed to simulate photochemical oxidants, acidic and nutrient pollutants, and aerosol PM, all of which have been shown to interact with mercury in air and in cloud water and influence its 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 mercury modeling at AMAD.

A number of modifications were made to the standard CMAQ model to enable it to simulate atmospheric mercury; these are described in detail in Bullock and Brehme (2002). Because new information about chemical and physical processes affecting atmospheric mercury continually is being published, refinement of the model code is an ongoing process. Further modification of the CMAQ-Hg 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 mercury in the multipollutant version of the model. We found this to be the most efficient way to maintain and disseminate mercury simulation capabilities in CMAQ because of the increasing number of pollutants with which mercury is known to react.

AMAD has participated in two major model intercomparison studies for atmospheric mercury. 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 mercury chemistry in a closed cloud volume given a variety of initial conditions, and results were published in Ryaboshapko et al. (2002). The second phase of the study involved full-scale model simulations of the emission, transport, transformation, and deposition of mercury over Europe for two short periods of 10 to 14 days each. Model simulations were compared to field measurements of elemental mercury gas, reactive gaseous mercury, and particulate mercury in air. Results from this phase of the study 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 to observations of the wet deposition of mercury. Results from this phase of the study were reported in Ryaboshapko et al. (2007b).

As the EMEP study was nearing completion, AMAD organized a second mercury 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 the NAMMIS; the Regional Modeling System for Aerosols and Deposition (REMSAD), and the Trace Element Analysis Model (TEAM). All three models were each applied to simulate the entire year of 2001 three times, each time using initial condition and boundary conditions developed from a different global model. The NAMMIS provided not only a comparison between regional atmospheric mercury models but also a measure of the sensitivity of each regional model to uncertainties regarding intercontinental transport. The NAMMIS evaluated each regional model for its agreement to observations of wet deposition of mercury from the MDN and Underhill observations. Results from the NAMMIS statistical model evaluation are shown in the Table 3-3. For most of the evaluation metrics, CMAQ was found to have superior agreement to the observations.

Results from all three of the regional models tested (CMAQ, REMSAD, and TEAM) varied depending on the global model used to define lateral boundary concentrations for mercury. These global models included Chemical Tansport Model for Mercury (CTM-Hg), Goddard Earth Observing System's Chemistry (GEOS-Chem) model, and the Global/Regional Atmospheric Heavy Metals (GRAHM) model. All of the regional models used meteorological data provided by the MM5 model. Statistics for the precipitation data obtained from MM5 also are shown in the table. Obviously, the level of accuracy one can expect from the regional air quality models is limited by the accuracy of the input precipitation data. It does appear that the best performing air quality simulations have about the same level of accuracy as the precipitation data provided to those simulations. Thus, it can be reasoned that significant improvements in the simulation of mercury wet deposition are contingent on improvements in the modeling of physical meteorology. Complete descriptions of the NAMMIS study design, participating models, and modeling results are available in two articles published in the *Journal of Geophysical Research* (Bullock et al., 2008; Bullock et al., 2009).

CMAQ mercury modeling capabilities have been applied to support various EPA regulatory actions for mercury. They also have been used to provide information regarding mercury deposition from global background concentrations to tribal, State, and regional environmental authorities in the development of their water quality protection strategies. EPA currently is working with the United Nations Environment Program toward the development of international treaties to reduce mercury emissions to the environment. AMAD is working to expand the CMAQ modeling domain to cover the Northern Hemisphere. This will allow CMAQ to provide modeling assessments of the intercontinental transport of mercury and its importance as a global pollutant.

Table 3-3. Evaluation Statistics from the North American Mercury Model Intercomparison Study

Model	CMAQ			REMSAD			TEAM			MM%
Test Case	**CTM**	**GEOS-Chem**	**GRAHM**	**CTM**	**GEOS-Chem**	**GRAHM**	**CTM**	**GEOS-Chem**	**GRAHM**	**Precip.**
r^2	0.15	0.12	0.14	0.16	0.15	0.16	0.14	0.12	0.18	0.35
Mean Bias ($ng\ m^{-2}$)	-12.2	46.9	40.2	67.8	10.2	41.3	164.2	220.3	155.2	1.9 (mm)
Mean Normalized Bias	178.1	213.0	207.0	226.0	248.7	213.8	278.8	326.3	264.8	15.3 (mm)
Mean Normalized Error	1.580	2.031	2.020	2.292	2.593	2.133	3.298	3.804	3.091	1.681
Normalized Mean Bias	-0.049	0.187	0.160	0.270	0.399	0.164	0.653	0.876	0.617	0.078
Normalized Mean Error	0.708	0.847	0.823	.899	0.989	0.850	1.109	1.298	1.053	0.620
Mean Fractional Bias	0.142	0.279	0.247	0.167	0.242	0.103	0.602	0.670	0.593	0.098
Mean Fractional Error	0.725	0.771	0.771	0.839	0.861	0.835	0.885	0.928	0.867	0.641

3.8 CMAQ for Air Toxics and Multipollutant Modeling

In the past, chemical mechanism and air quality development have focused on ozone and primary inorganic PM, we are expanding the scope of the atmospheric photochemistry in CMAQ to include predictions for a large number of HAPs. More information on air toxics and EPA's important role in identifying and mitigating high concentrations of air toxics can be found at EPA's air toxics Web site (http://www.epa.gov/ttn/atw/index.html).

We build on the base photochemical mechanisms in CMAQ by adding explicit chemical characterizations for HAPs. The multipollutant version of CMAQ (CMAQ-MP) currently predicts the 44 individual HAPs shown in Table 3-4.

In addition to HAPs explicitly listed in the CAA Section 112(b), research versions of CMAQ have been modified to model additional, potentially toxic compounds that are emerging pollutants, such as pesticides (dioxin), herbicides (atrazine), and hydrofluorocarbons (tetrafluoropropene).

In CMAQ-MP, the chemistry was harmonized with the regulatory model for ozone and $PM_{2.5}$, allowing the Agency to analyze simultaneous effects of emission control strategies on all high-priority pollutants. This chemistry accounts for interactions and feedbacks between multiple pollutants, which would not be possible in separate simulations. CMAQ-MP provides a tool that can be used to help answer the following questions.

- What tools can we provide to help the Agency to evaluate the true overall effects of an emission control strategy, and, therefore, develop strategies that optimize human and ecological health?
- How do we ensure that the chemistry that is used in regulatory and research models is rigorous and state of the science?
- How do changes in one air pollutant affect other pollutants?
- What is the best way to incorporate flexibility into the chemistry, so that the Agency can quickly respond to emerging issues and new atmospheric pollutants?

Two examples of output from one multipollutant modeling simulation are shown in Figure 3-11.

Future Directions

Because chemistry impacts every component of air quality models, our future efforts in atmospheric chemistry mechanisms will continue to evolve and fully employ our expertise in gas, aqueous, and aerosol chemistry. Future efforts will involve reducing known uncertainties in current chemical mechanisms and improving gas-aerosol-aqueous chemistry linkages.

We will continue to monitor internal and external research in atmospheric chemistry, toxic air pollutants, aerosol formation, and aqueous chemistry. We will assess the robustness and importance of new discoveries and partner with leading researchers to direct research in areas that will provide the greatest improvements in air quality model predictions. We will modify the mechanisms to include new information (such as new reactions) to keep our mechanisms at state of the science.

We also anticipate that our future efforts will involve extending the chemistry beyond "traditional" pollutants to

Table 3-4. Hazardous Air Pollutants Represented in the Current CMAQ Multipollutant Model

Gas-Phase HAPS		Multiphase and Aerosol HAPS
Formaldehyde	Carbon tetrachloride	Diesel PM
1,3-butadiene	Dichloromethane	Beryllium compounds
Naphthalene	1,1,2,2-Tetrachloroethane	Cadmium compounds
Acrolein	Chloroform	Lead
Acetaldehyde	2,4-Toluene diisocyanaate	Manganese compounds
1,3-Dichloropropene	Hexamethylene 1-6-diisocyanate	Nickel compounds
Quinoline	Maleic anhydride	Chromium 3
Vinyl chloride	Triethylamine	Chromium 6
Acrylonitrile	Chlorine	Elemental mercury
Trichlorethylene	Hydrazine	Reactive gaseous mercury
Benzene	Hydrochloric acid	Particulate mercury
1,2-Dichloropropane	p-Dichlorobenzene	
Ethylene oxide	Xylene (o,m, and p explicitly)	
1,2-Dibromoethane	Toluene	
1,2-Dichloroethane	Methanol	
Tetrachlo[1]-oethylene		

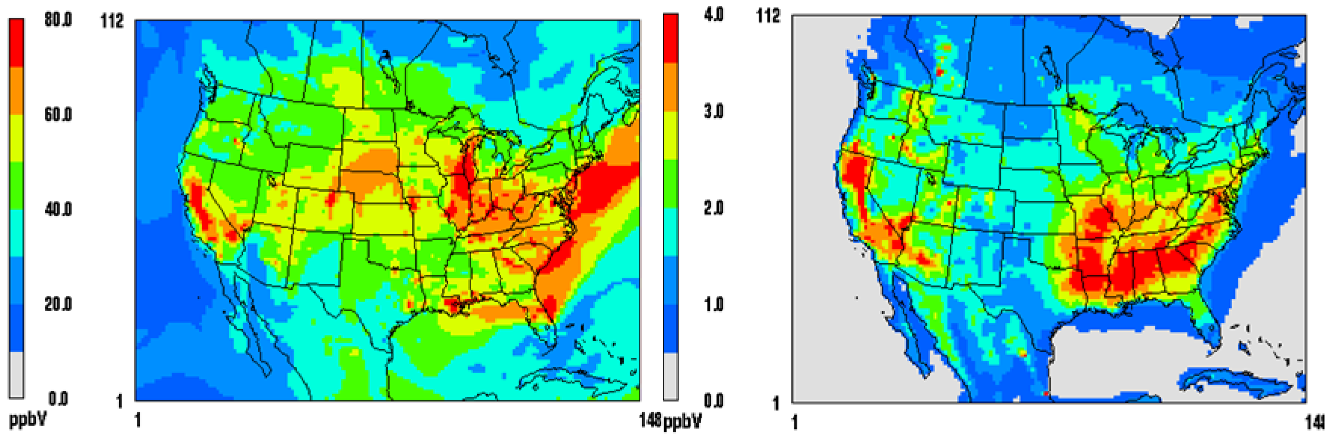


Figure 3-11. CMAQ multipollutant model predictions for ozone (left), as maximum 8-h value, and formaldehyde (right), as monthly average for July 2002.

address new, emerging issues, such as biofuels, pesticides, and chemicals that contribute to global warming.

3.9 Emissions Modeling Research

Emission data input is one of the principal drivers of the CMAQ modeling system. However, estimates of emissions data are subject to a large degree of uncertainty, as noted in the NARSTO (formerly the North American Research Strategy for Tropospheric Ozone) Emission Inventory Assessment (http://www.narsto.org/section.src?SID=8), particularly for precursors of airborne fine PM and for sources of organic and elemental carbon (EC) and ammonia. Most anthropogenic emissions used in the CMAQ system are available from EPA's National Emissions Inventory (NEI) (http://www.epa.gov/ttn/chief/eiinformation.html). AMAD focuses on the evaluation and improvement of emission categories that respond to meteorology and/or that are natural or quasi-natural in character, and that are not readily available in the NEI. Our work includes the development, evaluation, and implementation of emission models for biomass burning, fugitive dust, lightning, and biogenic sources. These sources emit ozone precursors (volatile organic compounds [VOCs] and nitrogen oxides), PM, and some air toxins.

After working with EPA's OAQPS to release an operational satellite-based biomass burning emission estimation system for the NEI, the Division focused on evaluating the emissions from this system in the context of air quality modeling and in working with other researchers in improving areas of greatest uncertainty. We continued to compare emissions from alternative methodologies and to evaluate CMAQ model performance with these alternative emissions, and we began to collaborate with the NPS to compare carbon aerosol concentrations from two different air quality modeling systems with IMPROVE measurement data. Collaborations with NASA (as well as with researchers at Michigan Tech and the University of Kentucky) also began under a NASA-funded grant. Objectives of the NASA research include evaluation of plume rise and refinement of rangeland/cropland biomass burning emission estimates.

The 2011 release of CMAQ is scheduled to offer two alternatives for biogenic emissions: NCAR's Model for Emissions of Gases and Aerosols from Nature (MEGAN) and Biogenic Emissions Inventory System (BEIS) v3.14. Both models are now being tested in CMAQ. In concert with the Division's ecosystems-related research, we worked with UNC's Institute for the Environment (IE) to incorporate updated agricultural data and information from EPA and the U.S. Geological Survey's (USGS's) 30-m National Land Cover Database (NLCD). We then worked further with UNC-IE to design a plan for incorporating updated forest inventory data and for possibly harmonizing the vegetation cover data in MEGAN with that in BEIS v3.14. Under a NASA-funded grant with the University of Maryland, we collaborated on the use of satellite imagery to evaluate soil NO_x emissions.

Via a collaboration with NASA and the University of Maryland, we continued to explore the development and evaluation of an algorithm to estimate nitric oxide production from lightning using meteorological parameters available from the MM5 and WRF meteorological models. Early results indicate that the NO_x profile simulated by CMAQ in the middle troposphere—which had been underestimated by CMAQ—compares much better with observations when lightning-generated NO_x is included in the model.

The Division continued to interact with NOAA's air quality forecast model research program to develop and evaluate a wind-blown dust algorithm based on land cover data and meteorological variables (notably wind speed and precipitation). In addition, we began to assess the use of alternative temporal profiles for computing fugitive dust emissions to possibly correct for temporal biases that have been observed with urban $PM_{2.5}$ measurement data.

The Division is continuing to work with other partners in EPA to improve the SPECIATE database, which is central to speciating VOC and PM gas and aerosols for emissions used in the CMAQ modeling system.

In future years, the Division's priorities in emissions research will be on improving and evaluating components of the emission modeling system used in CMAQ and where other organizations, such as OAQPS, are unable to provide support. Where resources permit, we will improve the scientific content, accuracy, and efficiency of emission models that are required for the development, testing, and evaluation of the CMAQ modeling system.

Future Directions

The Division's research is organized around several model evaluation studies addressing ozone and PM predictions of CMAQ and characterization of CMAQ performance for client groups, particularly OAQPS. Work is planned to improve process-based emission algorithms and the use of geographical data. Many of these improvements likely will depend on outside funding and continued collaboration with OAQPS and NRMRL. The NARSTO Emission Inventory Assessment recommends that inventory builders "Develop and/or improve source profiles and emission factors plus the related activity data to estimate emissions for particulate matter, volatile organic compounds, ammonia, and air toxics." Outputs from this research will create tools for directly modeling hourly values of PM (from dust and wild fires), VOCs from biogenic sources, and from lightning NO_x. The Division plans to further develop and test emission modeling tools for episodic modeling (hourly) of the emissions of biogenic emissions, wildland fires, lightning NO_x, and fugitive dust. In collaboration with OAQPS, these advances will be incorporated into the Sparse Matrix Operator Kernel Emission (SMOKE) modeling system, which processes emissions data for CMAQ. All of the planned emissions research directly supports the major release of CMAQ in 2011.

Biomass burning emissions. We plan to continue our work with OAQPS and the U.S. Forest Service to evaluate information on fire activity, fuel loadings, and climatological patterns associated with biomass burning emission estimates. Sensitivity tests and model evaluation of CMAQ are planned to examine whether improvements in the fire emission estimation methods will improve air quality model simulations. Figure 3-12 is an example of biomass burning emissions. We plan to prepare one or more publications for submittal to a peer-reviewed journal related to this effort.

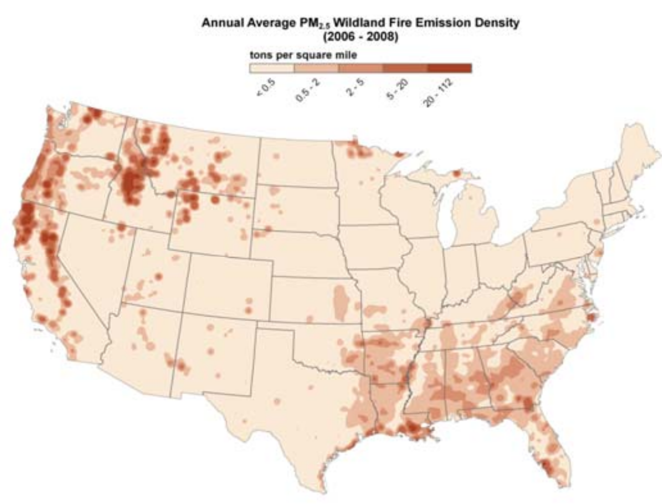


Figure 3-12. AMAD's research contributed to the NEI's Wildfire Emissions Inventory. (Plot courtesy of S. Raffuse, STI, Inc.)

We also plan to continue our collaboration with scientists at NASA in Langley, VA, as well as with NERL's Environmental Sciences Division, to evaluate and possibly improve plume rise estimates for biomass burning events and to improve temporal/spatial estimates of rangeland/cropland burn emissions.

Biogenic emission modeling. Biogenic emission estimates can strongly affect the assessment of the anthropogenic activities on tropospheric chemistry. Yet, large uncertainties persist in biogenic emission estimates. Figure 3-13 shows the differences of isoprene between MEGAN and BEIS, for example. We plan to continue work with EPA's NRMRL and scientists at NCAR to integrate and evaluate MEGAN in the CMAQ modeling system. Building off previous progress, we plan to evaluate model performance with MEGAN and submit a publication for consideration to a peer-reviewed journal to report our findings and recommendations. We intend to include MEGAN and BEIS v3.14 in the 2011 release of CMAQ.

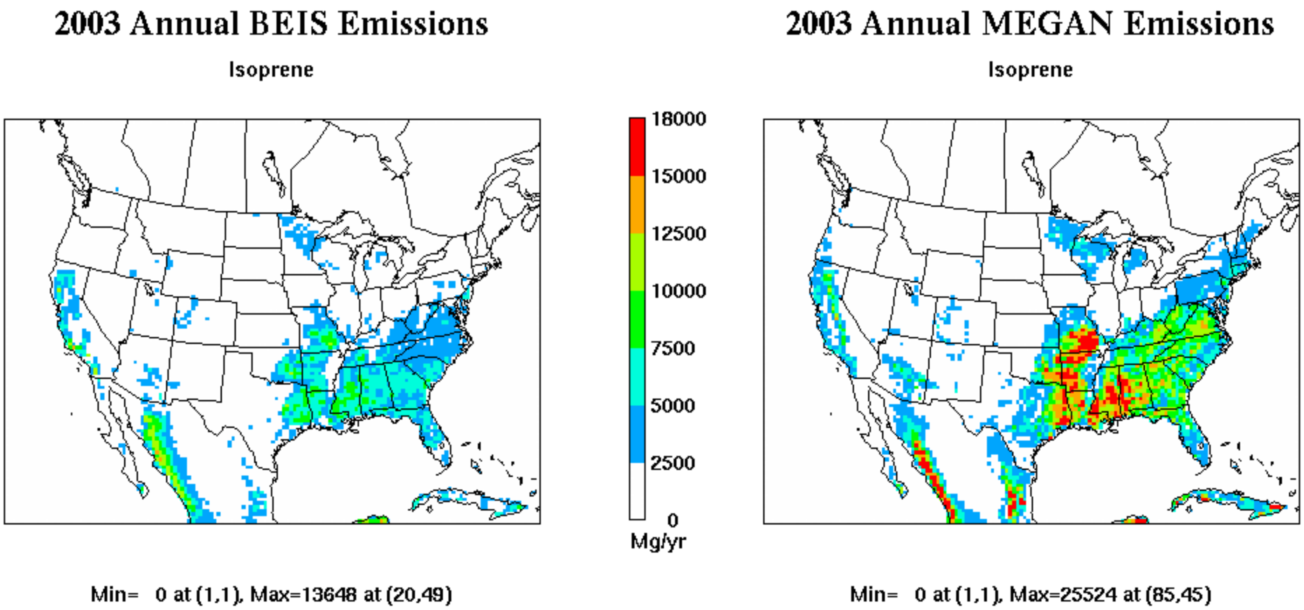


Figure 3-13. Comparison of isoprene emissions estimated by BEIS and MEGAN.

Working with scientists at the University of North Carolina, we will continue to explore updates of the vegetation landcover with the 30-m resolved land cover classes in the EPA/USGS NLCD. During 2011, we plan to focus on collaborating with NCAR via the UNC contract to harmonize the vegetation cover datasets in MEGAN and BEIS. Time and resources permitting, we will include an updated vegetation cover dataset in BEIS for the 2011 release of CMAQ—but, at the time of this writing, achieving this goal appears to be a challenge.

Lightning NO_x. In collaboration with NASA, an algorithm for estimating NO production from lightning in the CMAQ modeling system will continue to be refined and tested. As of the winter 2009/2010, NASA has provided the Division with initial estimates, so that we can perform testing with CMAQ. NASA has indicated that a draft journal article on this work is in preparation. We plan to incorporate an online version of the lightning NO_x algorithm in the 2011 release of CMAQ.

Geogenic dust. Depending on our ability and the time available to interact with NOAA's air quality modeling forecast research team, a publication will be prepared and an algorithm for improved estimates of fugitive dust will be integrated into the CMAQ modeling system. The Division will continue to assess alternative temporal profiles and to provide appropriate recommendations to OAQPS to improve the NEI. We are also testing an in-line windblown fugitive dust emission algorithm in the CMAQ code. Accelerated progress in this area, particularly to support hemispheric and/or global climate research, may require allocation of additional resources.

Speciation of emissions. The Division plans to continue to champion improvements in the speciation of VOCs and PM. This work will be accomplished largely through collaborative work with NRMRL and OAQPS. Meanwhile, scientists in the Division will attempt to use the CMAQ modeling system to assess the contributions from and the uncertainties of various aspects of the NEI. An emissions inventory of fine-particulate trace elements (e.g., calcium, iron, silver, tin, antimony, etc.) has been developed using the 2001 NEI in combination with emission profiles in the SPECIATE v4.0 database. This inventory is now being evaluated against trace-elemental measurements collected at urban sites in the Speciated Trends Network (STN). The inventory will be refined as necessary and then used as input to the CMAQ source-apportionment model to compute atmospheric concentrations of various trace elements in $PM_{2.5}$. These modeled concentrations will be compared against corresponding measurements taken across the major monitoring networks (e.g., IMPROVE, STN, SEARCH, and NADP).

Fairbanks, Alaska. Based on raw emissions information supported under a contract by EPA Region 10, we plan to assess and integrate emissions for fine-scale CMAQ modeling of fine particulates during stable, wintertime conditions in Alaska. This effort will require innovative approaches with different source categories and at fine vertical resolution

Air Quality Model Evaluation

4.1 Introduction

To ensure that we provide quality products to regulatory, academic, and other end users, we conduct extensive evaluation studies to rigorously assess air quality model performance in simulating the spatio-temporal features embedded in the air quality observations. We comprehensively analyze the performance of meteorology, emissions, and chemical transport models to not only characterize model performance but also identify what model improvements (inputs or processes) are needed. Thus, model evaluation efforts are tied directly with model development.

The Division has developed a framework (Dennis et al., 2010) to classify the different aspects of model evaluation under four general categories: (1) operational, (2) diagnostic, (3) dynamic, and (4) probabilistic. Operational evaluation is a comparison of model predicted and observed concentrations of the end-point pollutant(s) of interest and is a fundamental first phase of any model evaluation study. Diagnostic evaluation investigates the processes and input drivers that affect model performance. Dynamic evaluation focuses on assessing the model's air quality response to changes in emissions and meteorology, which is central to applications in air quality management. Probabilistic evaluation characterizes the uncertainty of air quality model predictions and is used to provide a credible range of predicted values rather than a single "best-estimate." Because these four types of model evaluations are not necessarily mutually exclusive, research studies often incorporate aspects from more than one category of evaluation.

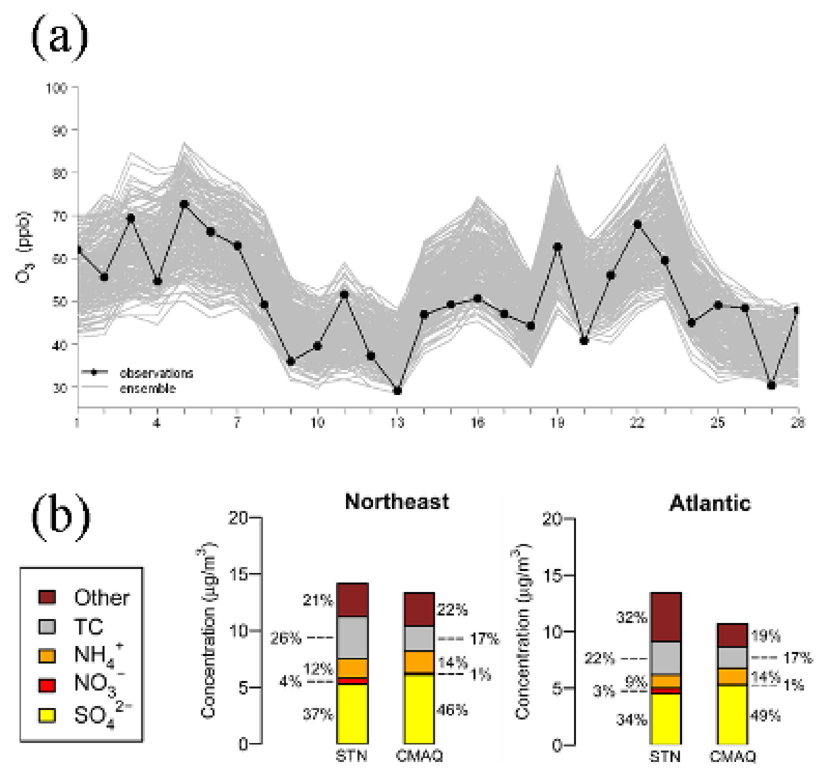


Figure 4-1. Model outputs are compared to observations using various techniques, including (a) time series of daily maximum 8-h ozone concentrations from a 200-member CMAQ model ensemble at a monitoring site in an urban location and (b) percent contribution of individual aerosol species comprising the total average regional $PM_{2.5}$ mass concentrations predicted by CMAQ and measured by the Speciated Trends Network (STN) sites.

4.2 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 against observed data. This type of evaluation is referred to as operational evaluation. A similar evaluation of the air quality model simulation is also performed using available observed air quality measurements.

As the developer of the CMAQ model, AMAD is frequently 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) over time, the frequency of model simulations has increased, whereas 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.

AMET is a combination of an open-source database software (MYSQL), the R statistics software, and

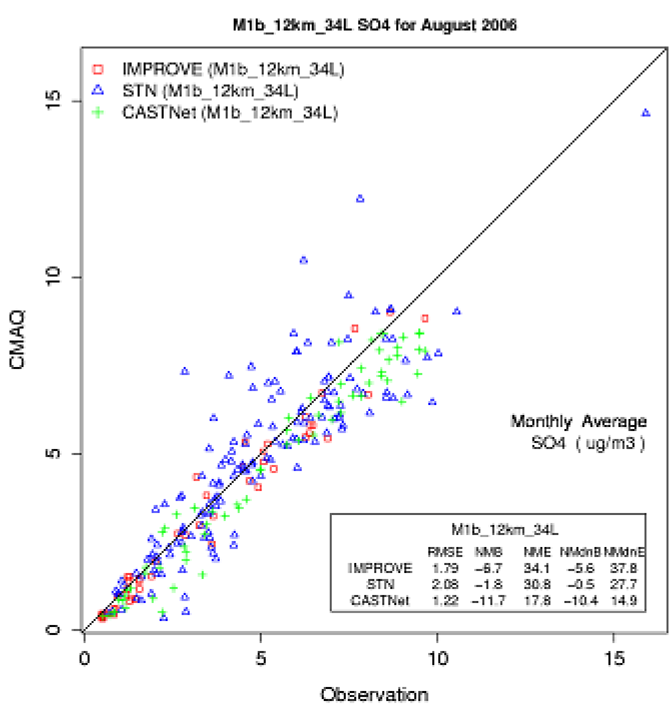


Figure 4-2. Scatter plot of observed versus CMAQ-predicted sulfate for August 2006 created by AMET.

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.

4.3 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 NO_y between NO_2, HNO_3, and PAN. 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 ICARTT, 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.

4.4 Diagnostic Evaluation of the Carbonaceous Fine Particle System

Routine measurements of speciated $PM_{2.5}$ (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 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.

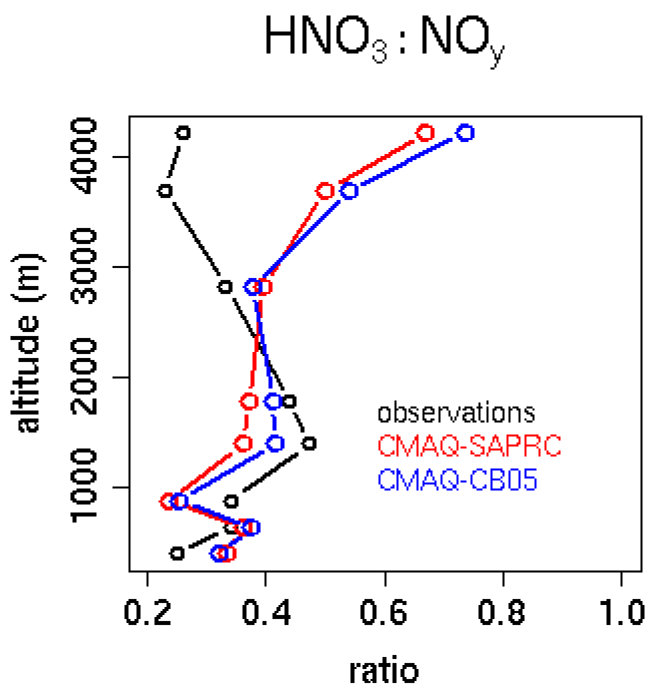


Figure 4-3. Vertical profile of the ratio of nitric acid (HNO_3) to total oxidized nitrogen (NO_y) as sampled during the August 8, 2004, ICARTT flight over the Northeastern United States. When the observations are paired in time and space with the CMAQ simulations, we find that the chemical mechanisms used in CMAQ over-estimate the contribution of nitric acid to total NO_y, especially in the free troposphere.

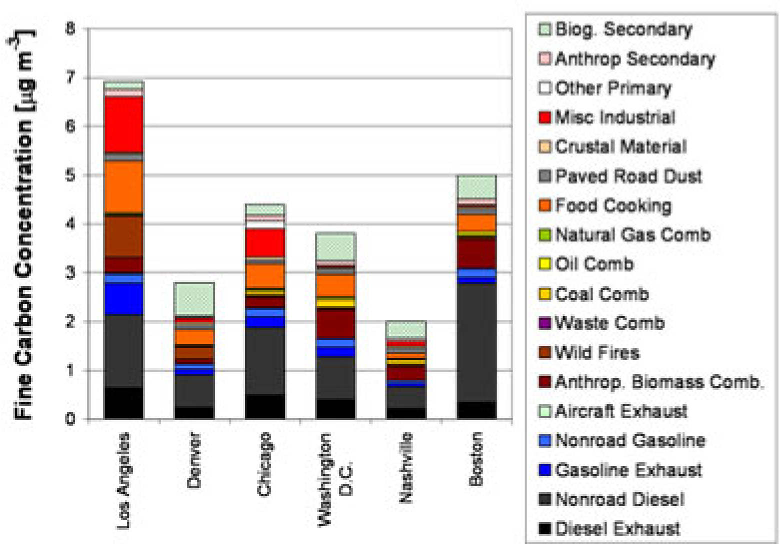


Figure 4-4. Source contributions to the modeled concentrations of fine-particulate carbon in six U.S. cities.

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 to August 1999 period in the southeastern United States. (Bhave et al., 2007).

Fossil fuel versus modern carbon predictions. Measurements of radiocarbon ($_{14}C$ isotope) enable one to distinguish fossil fuel carbon (e.g., motor vehicle exhaust, coal and oil combustion) from modern carbon (e.g., biomass combustion, biogenic SOA). summer of 1999 (Lewis et al., 2004) are being used to evaluate model predictions of these two types of carbon.

Tracers of anthropogenic and biogenic secondary organic aerosol (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 were 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).

Many of these exploratory projects are in collaboration with scientists in NERL HEASD.

4.5 Inverse Modeling To Evaluate and Improve Emission Estimates

Although continuously updated and improved, emission inventories are still considered to be one of the largest sources of uncertainty in air quality modeling. It is often difficult to measure 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 Measurements of this type at Nashville, TN, in the 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-observed NO_2 column density to attempt to identify any possible bias in the NO_x emission inventories over several regions in the southeastern United States. Figure 4-5 shows a model comparison of satellite observations (from SCIAMACHY retrieval) and CMAQ prediction. This application relies on the adaptive-iterative Kalman filter as an inverse method and decoupled direct method in 3D (Decoupled Direct Method [DDM]-3D) as a way to quantify the relationship between emission rates of NO_x and atmospheric concentrations of NO_2. We find that urban emissions in Atlanta, GA, and Birmingham, AL, are likely to be overestimated, whereas more rural concentrations of NO_2 are likely to be low because of missing emissions and chemical processes aloft in the CMAQ model.

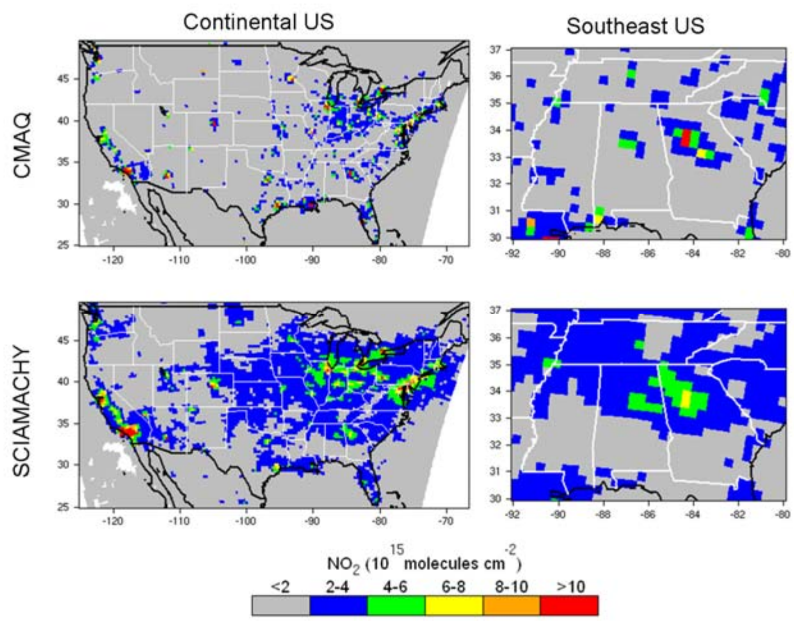


Figure 4-5. Comparison of modeled and observed NO_2 column concentrations.

4.6 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 these 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 have 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 is frequently 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 while 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 4-6 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 NOx emissions (bottom). Compared with 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.

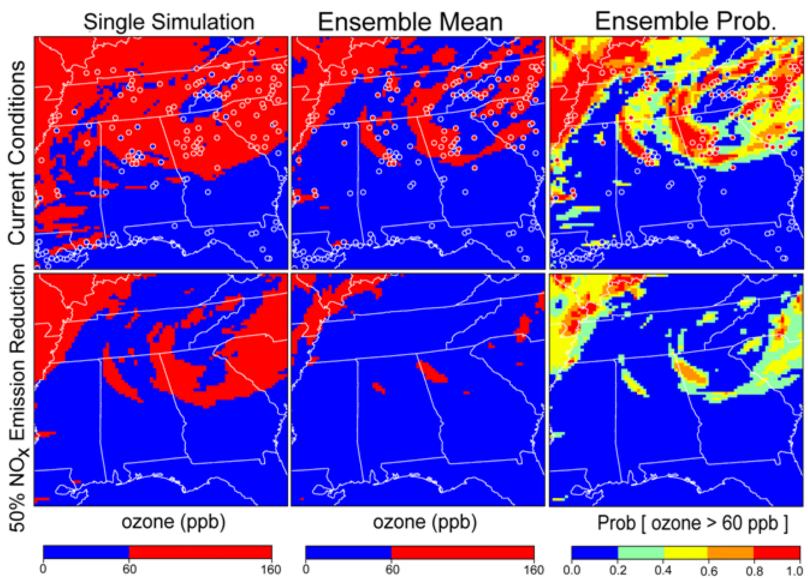


Figure 4-6. Spatial plots of ozone and probability of exceeding the threshold concentration for July 8, 2002, at 5 p.m. EDT. Observations are shown in white circles.

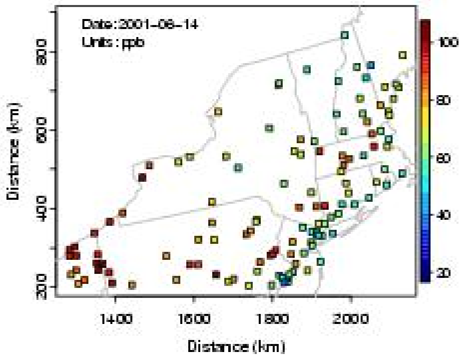
4.7 Statistical Methodology for Model Evaluation

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 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.

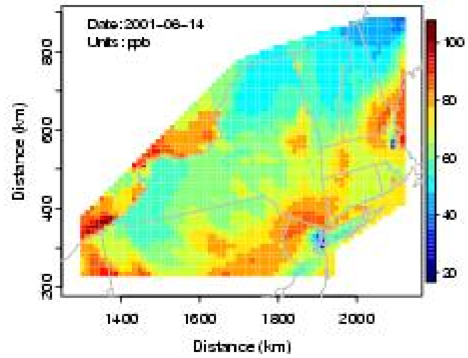
Although a variety of approaches reasonably could be utilized, we have focused on methods that allow us to better understand and utilize the spatial correlation of pollutant fields, such as kriging-based methods. For example, we have used Bayesian kriging to investigate the relationship between ammonium wet deposition and precipitation and kriging with adjustments for anisotropy to better understand ozone and $PM_{2.5}$ concentrations in the northeastern United States. In addition, recent work (Figure 4-7) has explored the impact on model evaluation of incommensurability (i.e., the mismatch between point-based measurements and areal averages (model output).

4.8 Dynamic Evaluation of a Regional Air Quality Model

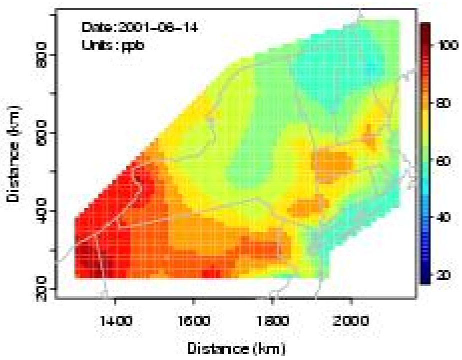
The dynamic evaluation approach explicitly focuses on assessing the model-predicted pollutant responses stemming from changes in emissions or meteorology. However, the emergence of the dynamic evaluation approach introduces new challenges. In particular, retrospective case studies are needed that provide observable changes in air quality that can be related closely to known changes in emissions or meteorology. The NO_x State Implementation Plan (SIP) Call has



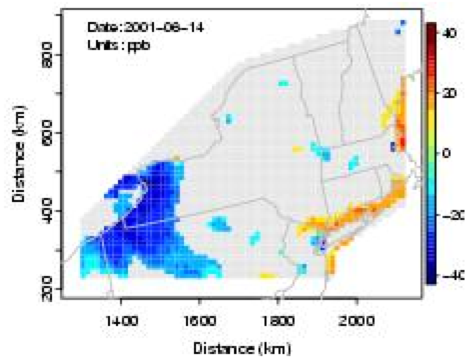
(a) Observed concentrations



(b) Modeled concentrations



(c) Block kriging estimates based on observations



(d) Grid cells of interest for further investigation

Figure 4-7. Assessment of CMAQ's performance in estimating maximum 8-h ozone in the northeastern United States on June 14, 2001, by Swall and Foley.

offered a very strong initial case study to test model responses via dynamic evaluation.

EPA's NO_x SIP call required substantial reductions in NO_x emissions from power plants in the eastern United States during summer ozone seasons, with the emission controls being implemented during 2003 through May 31, 2004. Gégo et al. (2007) and USEPA (2007) show examples of how observed ozone 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 ozone response to known and quantifiable observed ozone changes. An example of a dynamic evaluation study is described in Gilliland et al. (2008), where air quality model simulation results with the CMAQ model were evaluated before and after major reductions in NO_x emissions. Figure 4-8 provides an example from this prototype modeling study, where changes in maximum 8-h ozone are compared from the summer 2005 period (after the NO_x controls) with those from the summer 2002 period (before the NO_x emission reductions occurred). The spatial patterns of percentage decreases in ozone derived from observations and the model exhibit strong similarities. However, these results also revealed model underestimation of ozone decreases as compared to observations, especially in the 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 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 ozone 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

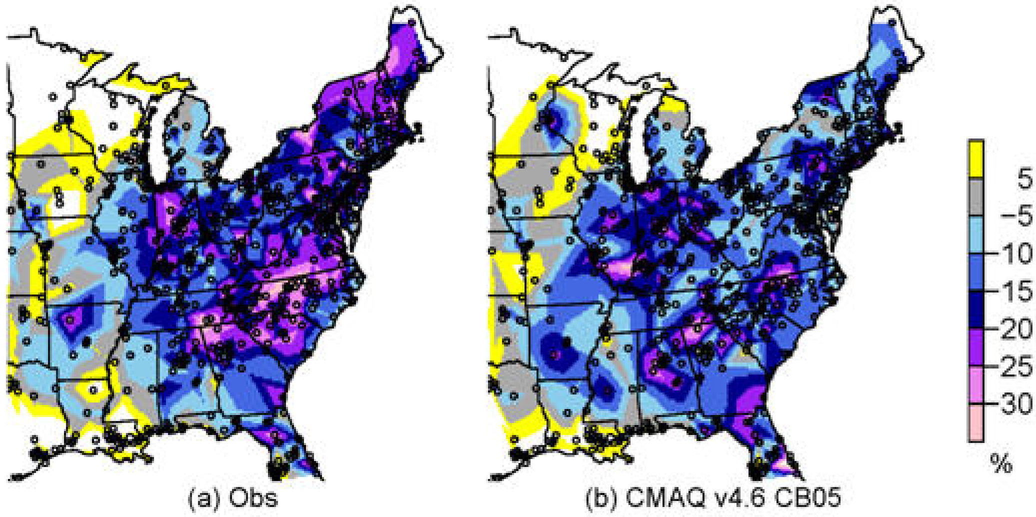


Figure 4-8. Example of dynamic evaluation showing (a) observed and (b) air quality model-predicted changes (%) from differences between summer 2005 and summer 2002 ozone concentrations from Gilliland et al. (2008). The results illustrate the relative change in ozone when comparing the 95th percentile daily 8-h maximum levels between the two summers.

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.

CHAPTER 5

Climate and Air Quality Interactions

5.1 Introduction

AMAD has been working on improving our understanding of the interactions between air pollution and climate change. Below are some of the science questions we are addressing.

- How will future climate change affect air quality?
- How do short-lived air pollutants impact atmospheric dynamics on regional and global scales?
- What will be the regional-scale impact of climate change on precipitation patterns?
- How will emission controls implemented for air quality management impact climate change?
- What are the most cost-effective ways to mitigate climate change by reducing concentrations of pollutants that contribute to radiative forcing while meeting air quality goals?

The first phase of the CIRAQ pilot study has been completed. Other projects that are in progress include the the ones noted below.

- Developing alternative scenarios for future U.S. emissions of ozone precursors and species that form atmospheric PM
- Developing methods to generate a range of future regional-scale climate scenarios via dynamic downscaling and statistical downscaling
- Developing integrated decision support tools for rapid assessment of emission scenarios designed for improving air quality and mitigating climate change
- Using the coupled WRF-CMAQ meteorology and chemistry model to investigate feedbacks of future emission scenarios on radiative budget
- Developing improved atmospheric chemistry models for understanding the impact of biogenic isoprene and anthropogenic NO_x on short-lived, radiatively active species.

5.2 Climate Impact on Regional Air Quality

Air quality is determined both by emissions of air pollutants, including ozone and PM precursors, 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 given emission control strategies will result in compliance with the relevant NAAQS. These modeling applications typically assume present meteorological conditions, which means that potential changes in climate are not included in air quality assessment. With emission controls that are implemented over several decades, however, future climate trends could impact the effectiveness of these controls.

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 (STAR) grant program.

The GISS GCM v2' was used to simulate the period from 1950 to 2055 at 4° latitude × 5° longitude resolution. Historical values for greenhouse gases (as CO_2 equivalents) were used for 1950 to 2000, with future greenhouse gas forcing following the IPCC's A1B 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 climate change alone was considered, without attempting to account for changes in emissions of ozone and PM precursors. Hourly emissions were simulated using the SMOKE model. Anthropogenic emissions were based on the EPA 2001 modeling inventory, projected from the 1999 National Emission Inventory (NEI) version 3. Biogenic emissions were calculated using the BEIS model and the simulated future meteorology. Air quality was simulated for two 5-year periods (1999 to 2003 and 2048 to 2052) using CMAQ v4.5. Figure 5.1 shows changes in simulated average and 95th percentile values of the maximum daily 8-h average (MDA8) ozone concentrations for both summer and fall.

5.3 Emission Scenario Development

For the first phase of the CIRAQ study, AMAD examined air quality under a future climate scenario with anthropogenic emissions of ozone and aerosol precursors fixed at 2001 levels and biogenic emissions from vegetation and soils allowed to vary with the simulated meteorology (Nolte et al., 2008). For the second phase of CIRAQ, future air quality is simulated using the same meteorology from phase 1 and alternative projections of future anthropogenic emissions.

Emission projections for different scenarios of economic growth and technological utilization have been developed by colleagues at NRMRL using the EPA 9-region MARKAL energy system model. MARKAL outputs were converted to source classification code-specific growth factors, which then were used with the SMOKE model to generate emissions inputs for use by the CMAQ chemical transport model.

Air quality simulations using these emissions projections and the climatological meteorology described above have been conducted using CMAQ v4.7. Analysis of these simulations is in progress.

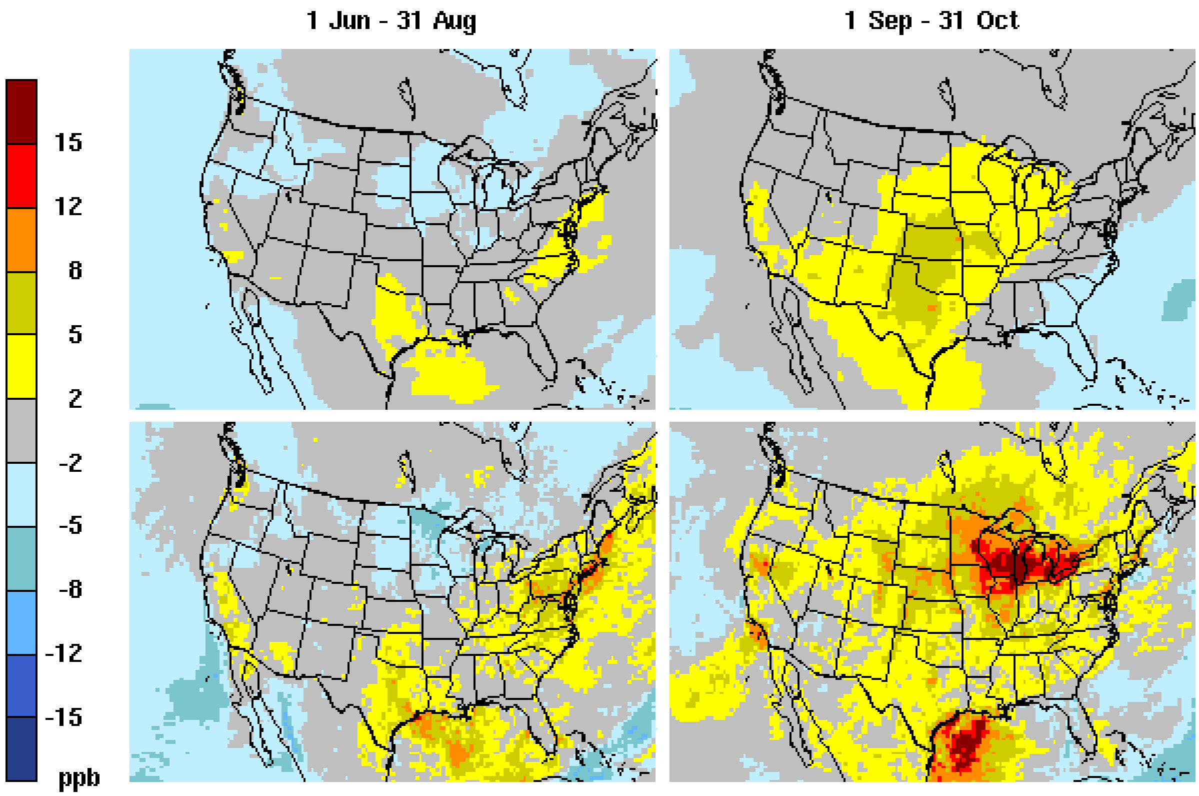


Figure 5-1. Differences (5-year future − 5-year current) in mean (top) and 95th percentile (bottom) maximum daily 8-h average (MDA8) ozone concentrations. Results show summertime increases of 2 to 5 ppb in mean MDA8 concentrations in Texas and parts of the eastern United States and even larger increases 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).

5.4 Regional Climate Downscaling

To meet EPA's growing need for regional climate projections to support impact assessments, AMAD is developing climate downscaling capabilities using both dynamic downscaling and statistical downscaling techniques. AMAD is developing a methodology for using the WRF model to downscale GCM simulations provided by colleagues at NASA's Goddard Institute for Space Studies.

When using coarse-scale data (either from a reanalysis or a GCM) as lateral boundary conditions (LBCs) for a regional model without any further constraint, the interior meteorological fields simulated by the regional model can deviate significantly from those of the driving fields. Four-dimensional data assimilation (FDDA) techniques provide one way to constrain the RCM and keep it from diverging too far from the coarse-scale fields. If the regional model is constrained too strongly to the GCM fields, however, there is the possibility that the benefit of using the higher resolution RCM will not be realized. What is needed is a delicate balance between the amount of constraint given to the RCM and the freedom of the RCM to simulate its own mesoscale features.

Analysis nudging and spectral nudging are two forms of interior nudging available within the WRF model. These methods have been applied in the literature (e.g., Miguez-Macho et al., 2004; Lo et al., 2008), but they rarely have been compared to each other for climate simulations. Our research will apply each nudging method to reanalysis- and GCM-driven WRF model simulations, with physics options chosen for air quality applications.

Preliminary simulations (Figures 5-2, 5-3, and 5-4) indicate that nudging is likely needed for both reanalysis- and GCM-driven simulations to maintain large-scale consistency between the driving fields and those simulated within the WRF model.

5.5 Statistical Climate Downscaling

Statistical downscaling methods use correlations among observed and modeled meteorological variables to predict regional and local patterns and events that are likely to occur based on the broader-scale GCM simulations. Typically, these approaches do not use the same detailed information that is used in dynamical downscaling, such as physical equations, orographic data, or extensive land-use information. The advantages of statistical downscaling methods lie in their efficiency and speed, and these methods could be particularly attractive if numerous climate scenarios need to be investigated. Statistical methods are not limited by the resolution achievable by the nested regional dynamical model. Thus, statistical methods possibly could be used

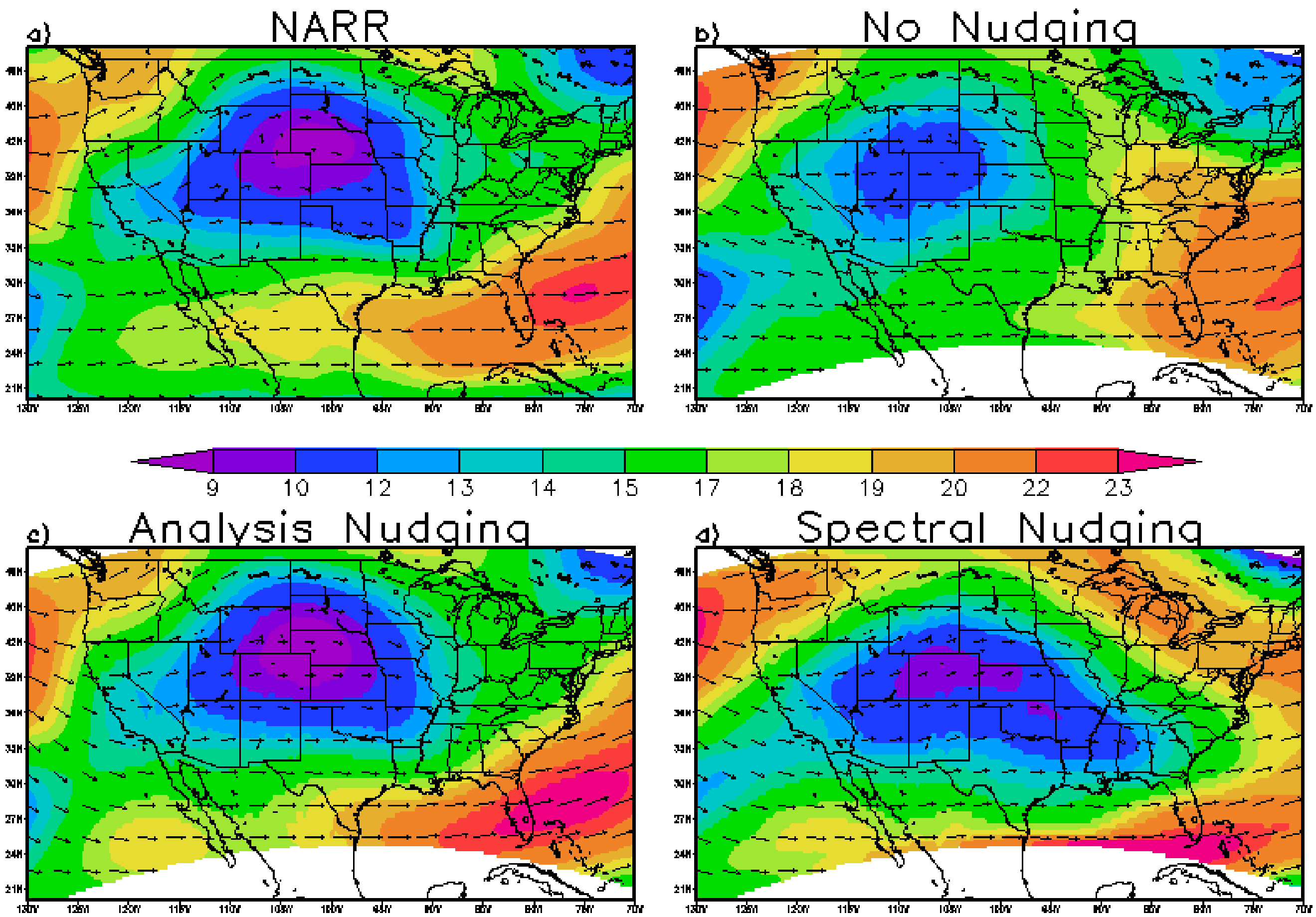


Figure 5-2. Seasonally-averaged (April-June) wind fields at 300 hPa as simulated by (a) North American Regional Reanalysis, (b) WRF without nudging, (c) WRF with analysis nudging, and (d) WRF with spectral nudging. Analysis nudging improves WRF's ability to simulate the location and intensity of the jet stream.

to gain a better understanding of fine-scale variability, even down to point locations.

It has been reported in the literature that the performances of dynamical and statistical downscaling are comparable for current climatic conditions. However, it is questionable whether statistical models can perform as well under future conditions (Wilby et al., 2002) because statistical downscaling methods rely on associations among meteorological variables. These relationships do not explain all of the inherent variability in atmospheric phenomena; in fact, the choice of variables to be used as the "predictors" in such approaches is a difficult part of the statistical downscaling process. Once a statistical model has been developed for a particular time period (e.g., using current climate), it is unclear whether the relationships it incorporates will remain the same under different climatic conditions (e.g., in future decades). However, statistical downscaling makes this assumption as it extrapolates to future conditions.

Current research interests in statistical downscaling include the following.

- Evaluating the performance of statistical downscaling methods in estimating the frequency, duration, and intensity of extreme meteorological events
- Developing at least a rough understanding of how the uncertainty affects estimates, and, particularly, how the uncertainty may change when applied to future-year GCM simulations
- Identifying the relative strengths and weaknesses of the dynamical and statistical approaches to downscaling
- Determining whether hybrid downscaling approaches may be able to capitalize on the strengths of both methods

5.6 Integrated Tools for Scenario Discovery

Because climate change occurs over decades, scenarios are used to understand the impacts of policy decisions on a range of future outcomes. However, fully assessing the air quality and climate change impacts of a given emission scenario requires extensive computational modeling and analysis. Tools that can rapidly inform decisionmakers and stakeholders are a first-order need.

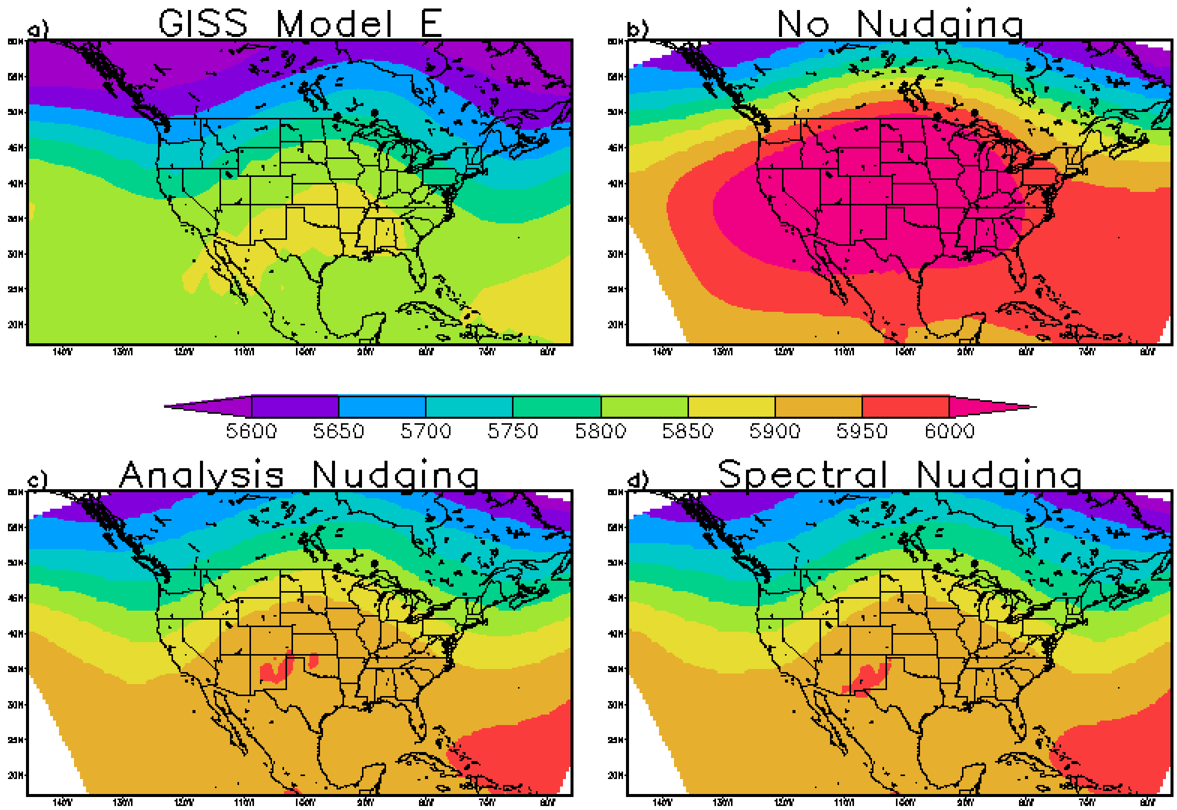


Figure 5-3. Mean July 500-hPa geopotential height (m) for (a) GISS ModelE, (b) base WRF run without any interior nudging, (c) WRF with analysis nudging, and (d) WRF with spectral nudging. Although both nudging techniques are applied only above the planetary boundary layer, both serve to keep the 500-hPa geopotential height simulated by WRF closer to that simulated by ModelE.

To meet this need, we are developing GLIMPSE (GEOS-CHEM LIDORT Integrated with MARKAL for the Purpose of Scenario Exploration), a framework for connecting atmospheric chemistry, radiative forcing, and energy-economy models to *rapidly* understand the integrated air quality and climate change impacts of U.S. emission scenarios. Its four components, as depicted in Figure 5-5, are as follows.

(1) GEOS-Chem, global chemical transport model to simulate the global impacts of U.S. emissions
(2) LIDORT, a radiative transfer model to calculate the radiative forcing impacts from short-lived species, such as black carbon
(3) Adjoint calculations of GEOS-Chem LIDORT to explicitly attribute the contribution from U.S. emission sources to global changes in radiative forcing
(4) EPA 9-Region MARKAL energy system model to discover the technologies, activities, and policy options that jointly achieve our air quality and climate change goals

In the first version of GLIMPSE, we will use the adjoint version of GEOS-Chem LIDORT adjoint model developed by Daven Henze at the University of Colorado. This model will calculate the change in sulfate and black carbon direct radiative forcing resulting from emissions from U.S. sources. These data will be used by MARKAL to find emission scenarios that achieve a given reduction in radiative forcing for minimal cost. The key assumptions driving these emission scenarios will be further analyzed to find emission scenarios that robustly achieve reductions in radiative forcing despite uncertainties in future projections. Once such a subset of robust emission scenarios is determined, it will be used as input to more complete global and regional climate models to fully quantify the impacts.

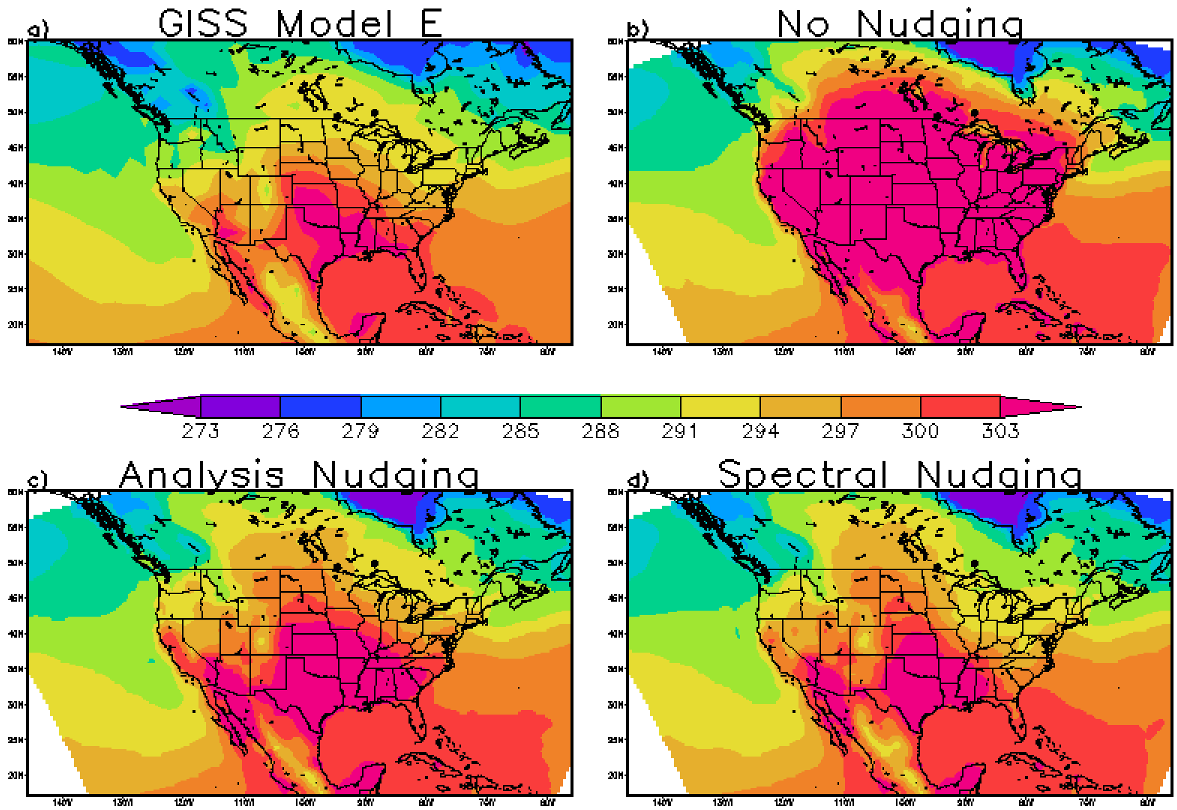


Figure 5-4. Mean July 2-m temperature (K) for (a) GISS ModelE, (b) base WRF run without any interior nudging, (c) WRF with analysis nudging, and (d) WRF with spectral nudging. Without nudging, average near-surface temperatures simulated by WRF for the Pacific Northwest are more than 6 K warmer than in the GCM.

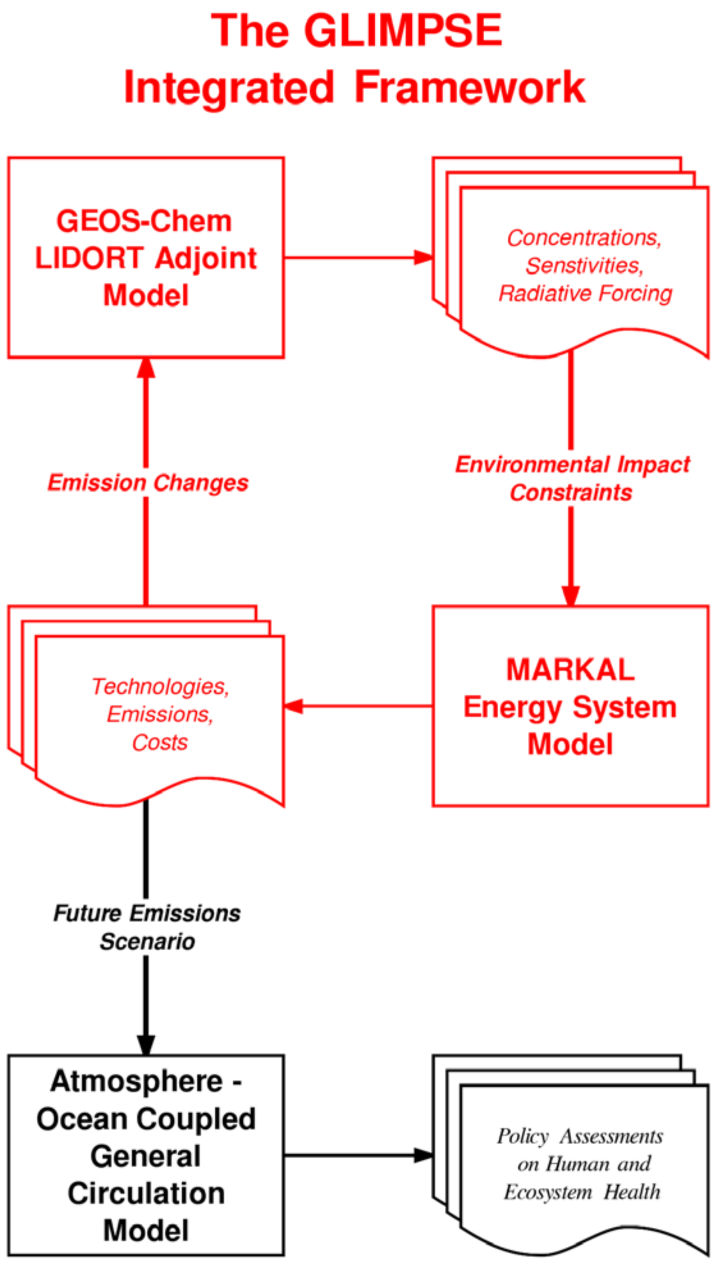


Figure 5-5. GLIMPSE data flow: GEOS-Chem LIDORT Adjoint model is used to attribute radiative forcing changes to U.S. emission sectors. These data are used in conjunction with greenhouse gas emissions as constraints for the MARKAL model, which, in turn, is used to generate scenarios that meet these constraints.

CHAPTER 6

Linking Air Quality to Human Health

6.1 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 can be influenced by the infiltration of ambient concentrations into indoor facilities (such as automobiles, homes, schools, and workplaces) 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 (Figure 6-1). 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.

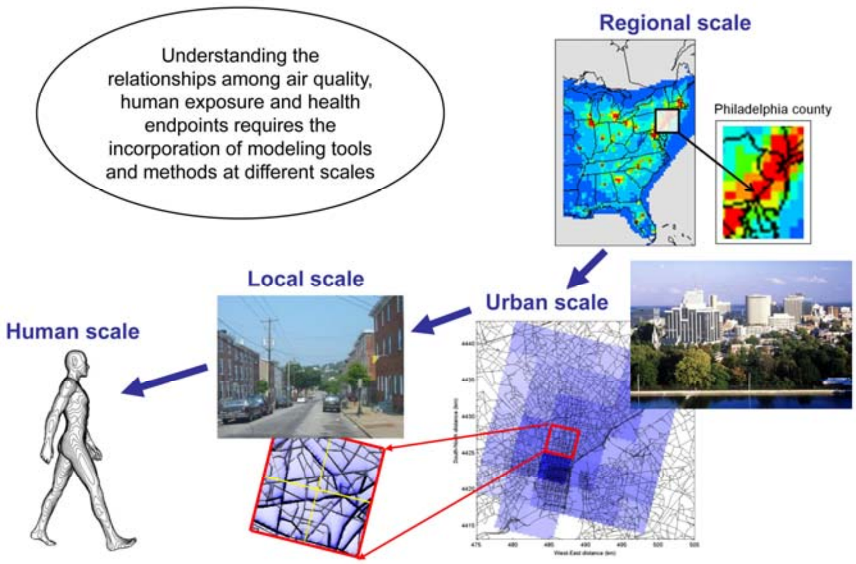


Figure 6-1. Linking local-scale and regional-scale models for exposure assessment characterizing spatial variation of air quality near roadways assessing the effectiveness of regional-scale air quality regulations. (Source: Stein et al., 2007)

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 exposure issues, such as exposure to multiple pollutants and for multiple scales.

6.2 Near-Roadway Environment

Recent studies have identified increased adverse health effects in the population that lives, works, and attends school near 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 purpose of the effort described here is to better 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., noise barriers, depressed roads, 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 near roadways.

The AERMOD dispersion model is one of the modeling approach that is being used to link between urban sources (particularly mobile emissions) and human exposure assessments and human health outcomes. As part of ORD's Near-Road Research Program, laboratory, field, and numerical modeling studies are underway to better characterize the concentration distributions surrounding the wide variety of complex roadway configurations found in urban areas. These studies include an examination of wind direction and roadway configuration effects in the Division's meteorological wind tunnel located at the Fluid Modeling Facility (Figure 6-2).

Figure 6-2. The Fluid Modeling Facility houses the Division's meteorological wind tunnel used to study the effect of roadway configuration and wind direction on near-road dispersion.

A research project has been initiated to characterize the impact of mobile sources on near-road air quality and exposures for children with persistent asthma who live near major roadways in Detroit, MI. Exposure metrics developed in this project will be coupled with health outcomes determined in the Childhood Health Effects from Roadway and Urban Pollutant Burden Study (CHERUBS). Modeled and monitored air quality and exposure data will be used with assessments of respiratory effects to investigate the relationships between traffic-related exposures and observed health effects. Air quality modeling will be conducted with the AERMOD dispersion model. Additionally, wind tunnel simulations of flow and dispersion near roadway configurations characteristic of area in the health study will be conducted at the Division's Fluid Modeling Facility. Wind tunnel studies will support the development and evaluation of the AERMOD model for urban, near-road applications and assist in the interpretation of site-specific monitoring. The air quality modeling and wind tunnel simulations of the Detroit area are critical links between traffic-related emissions and human exposures and health outcomes.

6.3 Evaluating Regional-Scale Air Quality Regulations

A core objective of the CAA 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. This research moves beyond characterizing emission and ambient concentration changes because of regulatory control actions to linking these changes to human exposure and health end points.

The NO_x SIP Call recently was implemented by EPA to reduce the emissions of NO_x and the secondarily formed ozone and to decrease the formation and transport of ozone 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

(Figure 6-3). 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.

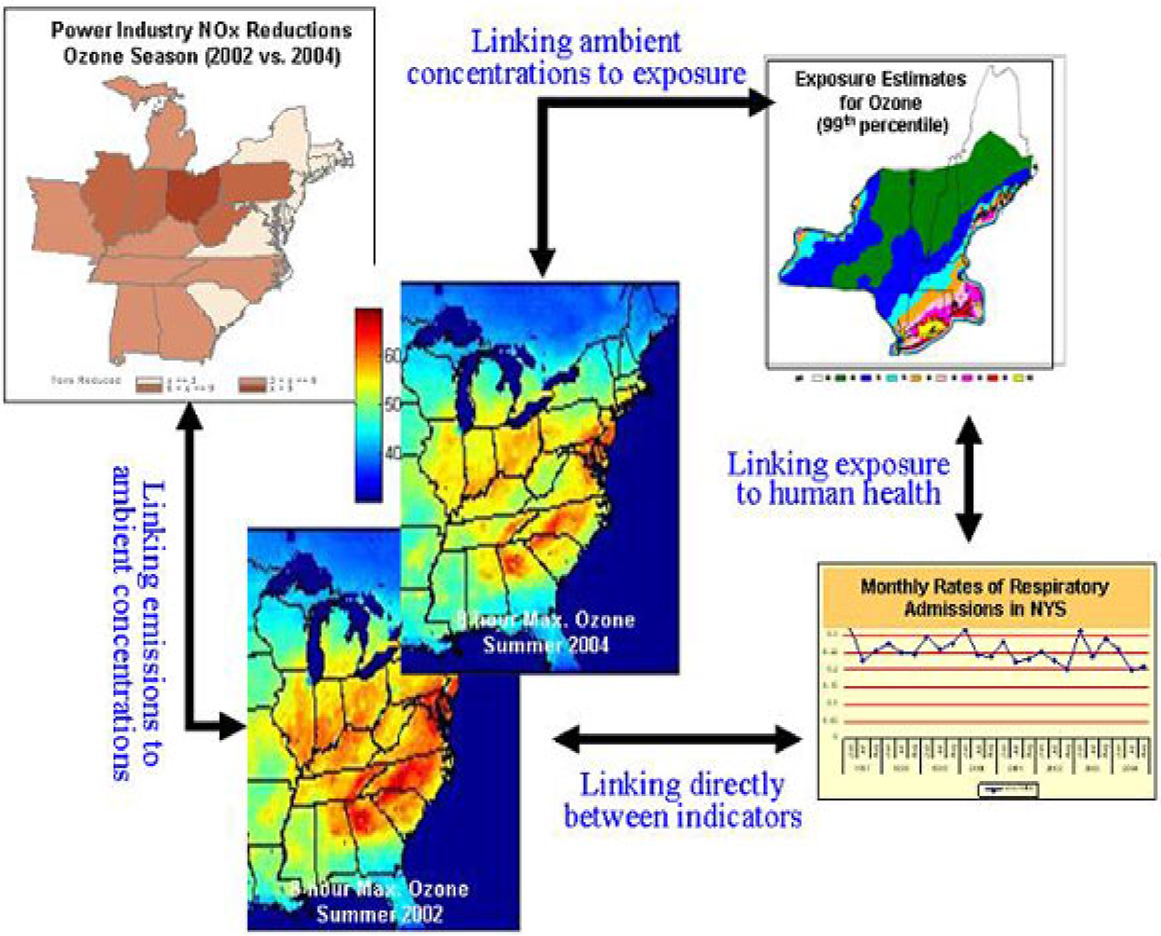


Figure 6-3. Assessing the impact of regulations on ecosystems and human health end points showing the indicators (boxes) and process linkages (arrows) associated with the Nox Budget Trading Program. (Source: Garcia et al., 2008)

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 ozone 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 ozone 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 the 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).

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

EPA and State and local governments increasingly need urban-scale air quality assessments that capture spatial heterogeneity, identify highly exposed subpopulations, and support public health studies. Air quality modeling estimates should account for local-scale features, long-range transport, and photochemical transformations. Therefore, a hybrid air quality modeling approach is under development to integrate results from a grid-based chemical-transport model with a local plume dispersion model to provide these spatially and temporally resolved air quality concentration estimates (Figure 6-4). Such capabilities are also critical to support human exposure and environmental health studies and to help identify air pollutant sources of greatest risk to humans. The coupling and appropriate application of these models will improve estimates, demonstrate utility in environmental health accountability programs, assist in the development of risk mitigation strategies, and improve epidemiology and community health studies.

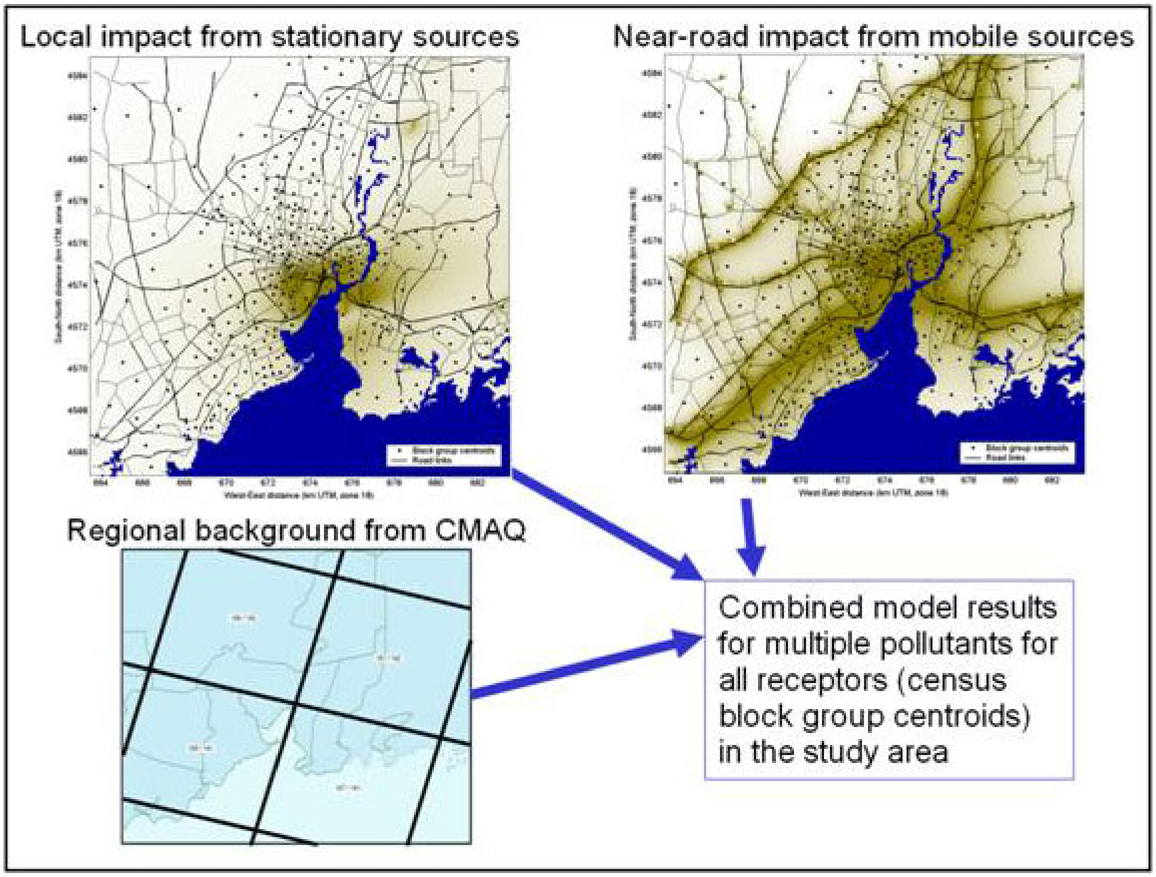


Figure 6-4. **Schematics of the hybrid modeling approach showing (a) local impact from stationary sources, (b) near-road impact from mobile sources, and (c) regional background from CMAQ. (Source: Isakov et al., 2009)**

AMAD scientists currently are involved in several activities to develop and evaluate techniques in support of exposure and health studies. This research is focused on integrating air quality modeling into exposure and health studies. Critical to that is the improvement of fine-scale air quality models. 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 regional- and local-scale air quality models (the CMAQ chemistry-transport model and the AERMOD dispersion model). An important component of this research is an EPA feasibility study conducted in New Haven, CT, that examines 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 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 resulting from 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 or industrial growth on human exposures and health in the community.

AMAD's scientists also are participating in several cooperative research projects to test the newly developed techniques in support of exposure and health studies involving three major academic institutions: (1) Emory University, (2) Rutgers University, and (3) the University of Washington. NERL also has initiated another cooperative research project (CHERUBS) with the University of Michigan. This project is focused on health effects of near-roadway exposures to air pollution. The overall goal of these activities is to enhance the results from epidemiologic studies of ambient PM and gaseous air pollution through the use of more reliable approaches for characterizing personal and population exposures.

6.5 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 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 (Figure 6-5). Urbanization schemes have been introduced into MM5, WRF, and other models and are being tested and evaluated for grid sizes on the 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.

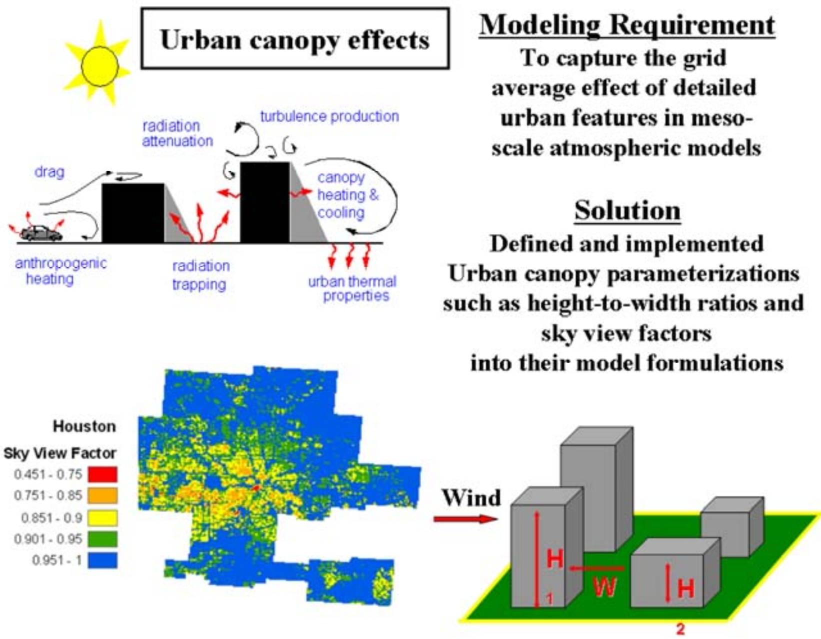


Figure 6-5. Urban canopy effects. (Source: Ching et al., 2009)

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 Detection 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 produces data of 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.

CHAPTER 7

Linking Air Quality and Ecosystems

7.1 Introduction

Ecological resources are exposed to atmospheric pollutants through wet and dry deposition processes. A long-term goal of multimedia environmental management is to achieve sustainable ecological resources. Progress toward this goal rests on a foundation of science-based methods and data integrated into predictive multimedia, integrated multidisciplinary, multistressor, open architecture modeling systems. The strategic pathway aims at progressing from addressing one stressor at a time to a comprehensive multimedia-multistressor assessment capability for current and projected ecosystem health.

Over the next several years, the AMAD's goal for air-ecosystem linkage is the consistent interfacing of weather, climate, and air quality models with aquatic and terrestrial ecosystem models to provide the local atmosphere-biogeochemical drivers of ecosystem exposure and resultant effects. A goal is also to harmonize the connection of the local ecosystem scale (tens of kilometers) with the regional airshed scale (thousands to millions of kilometers). The physically consistent linkage of atmospheric deposition and exposure with aquatic/watershed and terrestrial models is central, has not received adequate attention to date, and needs further development.

7.2 Linking Air Quality to Aquatic and Terrestrial Ecosystems

Ecosystem exposure occurs when stressors and receptors occur at the same time and place (Figure 7-1). To model the exposure, models for different media (e.g., air, water, land) must be linked together. Linkages among 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.

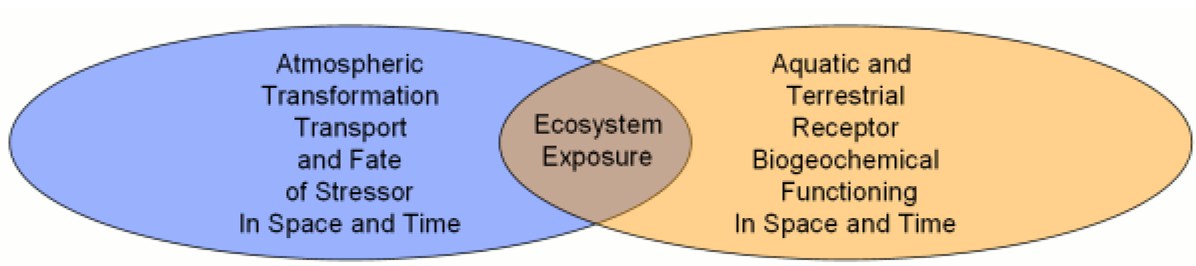


Figure 7-1. A Venn diagram representing ecosystem exposure as the intersection of the atmosphere and biosphere (http://www.epa.gov/amad/EcoExposure/index.html).

Improved Spatial Distribution of Terrestrial Receptors

Dry deposition velocity varies with underlying vegetation type because of differences in leaf area index, canopy height, and plant characteristics, such as minimum stomatal resistance. CMAQ v4.7 relies on the 1992 National Land Cover Dataset to identify the location of land cover types. USGS 2001 National Land Cover Database (NLCD) and 2001 to 2006 NOAA coastal lands (C-CAP) databases provide higher resolution information. The Spatial Allocator Raster Tool can be used to compute CMAQ modeling-domain-gridded land use information based on these input image data. As an example, Figure 7-2 illustrates our improved ability to identify the extent of deciduous forest cover areas in North Carolina over earlier lower resolution estimates. Colors indicate the percentage of each 1-km rectangular grid containing deciduous trees.

The second stage of this spatial improvement is to update the 1-km resolution Biogenic Emissions Landcover Database v3 (BELD3) dataset agricultural species distributions. The current distribution is based on 1995 National Agricultural Statistics Service surveys. These estimates are being updated to reflect 2001 crop distributions in combination with the 2001 NLCD imagery. At present, the BELD3 data are used to determine bioemission input for CMAQ. We anticipate its more extensive use in the estimation of species-specific exposure to atmospheric nitrogen and mercury deposition.

Improved Estimates of Receptor-Specific Atmospheric Deposition

The deposition velocity calculation for CMAQ v4.7 is a combination of processes modeled in the meteorological model and the chemical transport model. Because CMAQ is a grid-based model, the influence of the different land covers that comprise a grid cell are averaged in the meteorological model for use in the deposition velocity calculations. These grid-average values are carried forth from the meteorological model to the chemical transport model where chemical specific

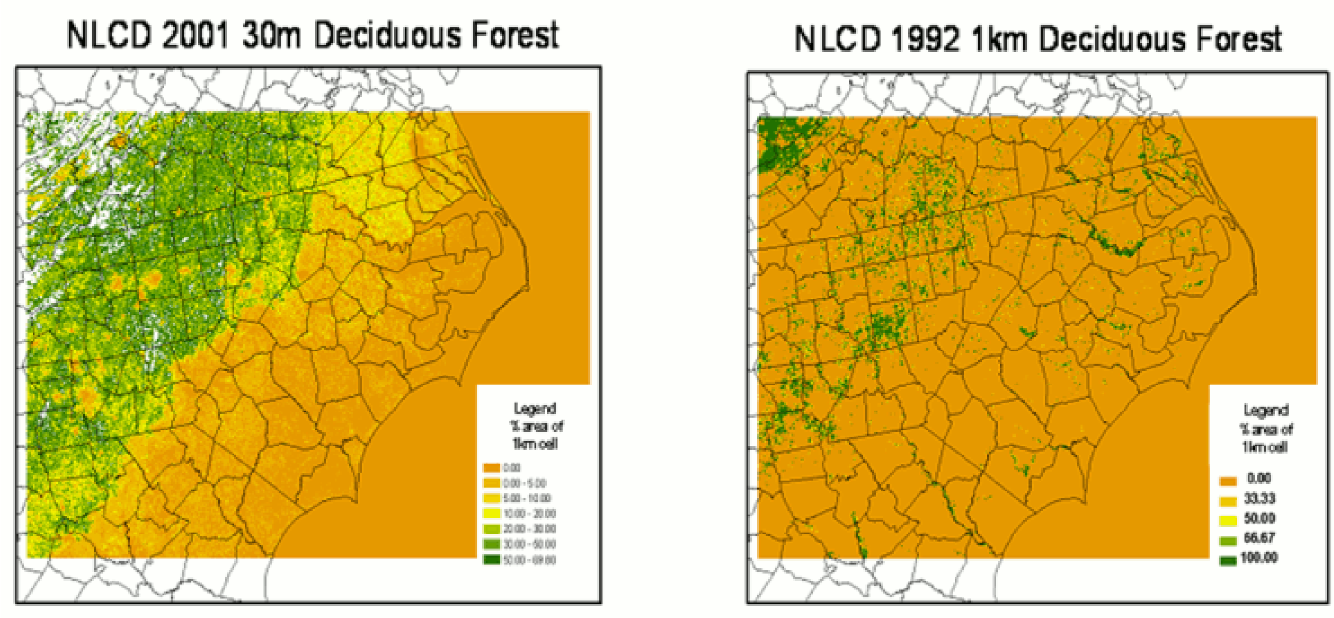


Figure 7-2. Fractional deciduous forest coverage as represented in the 30-m resolution 2001 NLCD based on Landsat 7 satellite imagery (right panel) and in the 1-km resolution 1992 NLCD based on Landsat TM satellite imagery (left panel).

deposition velocity calculations are done. Ecological applications need information regarding the amount of deposition to the individual land cover categories. To be able to provide this information without requiring modification of the meteorological model, an approach has been implemented in CMAQ that disaggregates these grid-average values within CMAQ to allow output of deposition estimates for each land cover type within a grid in a manner consistent with meteorological model flux calculations. Figures 7-3 and 7-4 illustrate deposition velocity dependence on vegetation type for ozone.

7.2.1 Linking Air and Water Quality Models

Linking Air Quality and Watershed Models—Collaborative Research with the ERD

AMAD and ERD have been collaborating to explore air-water model linkage. The present focus is on how best this might be accomplished now that multiple years of CMAQ deposition are feasible, and grid sizes are shrinking because of increasing computational capability. 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 (e.g., 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 future cases are not consistent. This raises several questions: How sensitive are watershed models to this error? Can the watershed models tolerate these errors in scenario mode? Can we create greater consistency by using the CMAQ meteorological inputs for all watershed simulations?

As a first step, we have explored with 2001-2003 data (1) the use of daily cooperative station data to perform a monthly calibration of the Grid Based Mercury Model (GBMM; 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 Parameter-Elevation Regressions on Independent Slopes Model (PRISM)-generated precipitation data. Figure 7-5 shows preliminary results for the hydrologic response to these various sources of 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 USGS 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. MM5 precipitation errors were found to be a serious problem when linking MM5 to calibrated watershed models, indicating the need to develop hydrology that is consistent with MM5/WRF precipitation. 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. PRISM

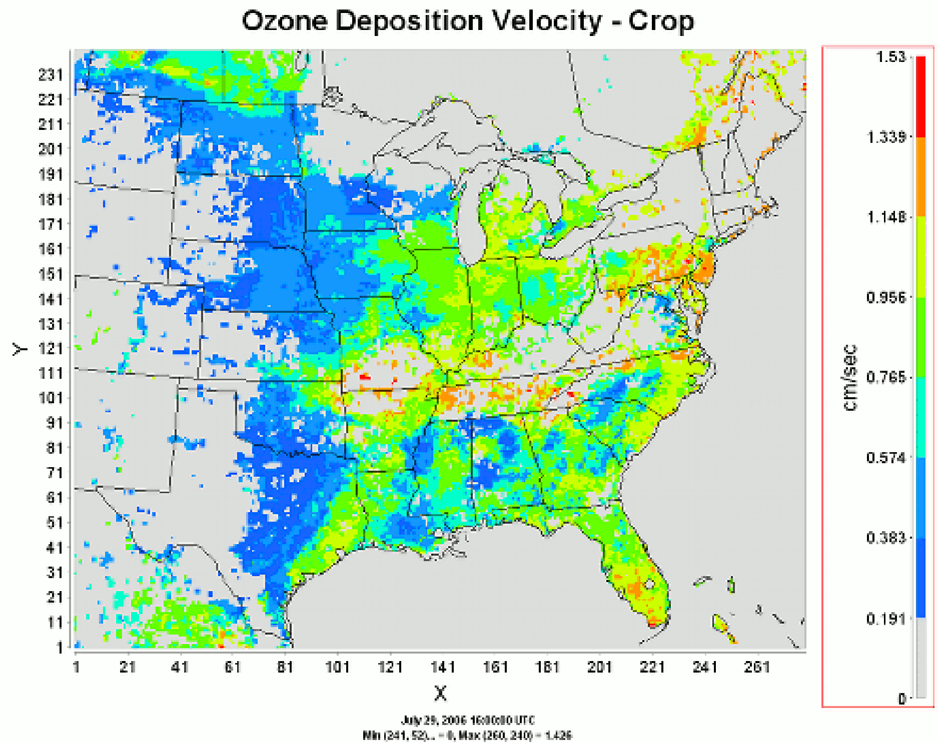


Figure 7-3. Receptor-specific ozone deposition velocities to croplands.

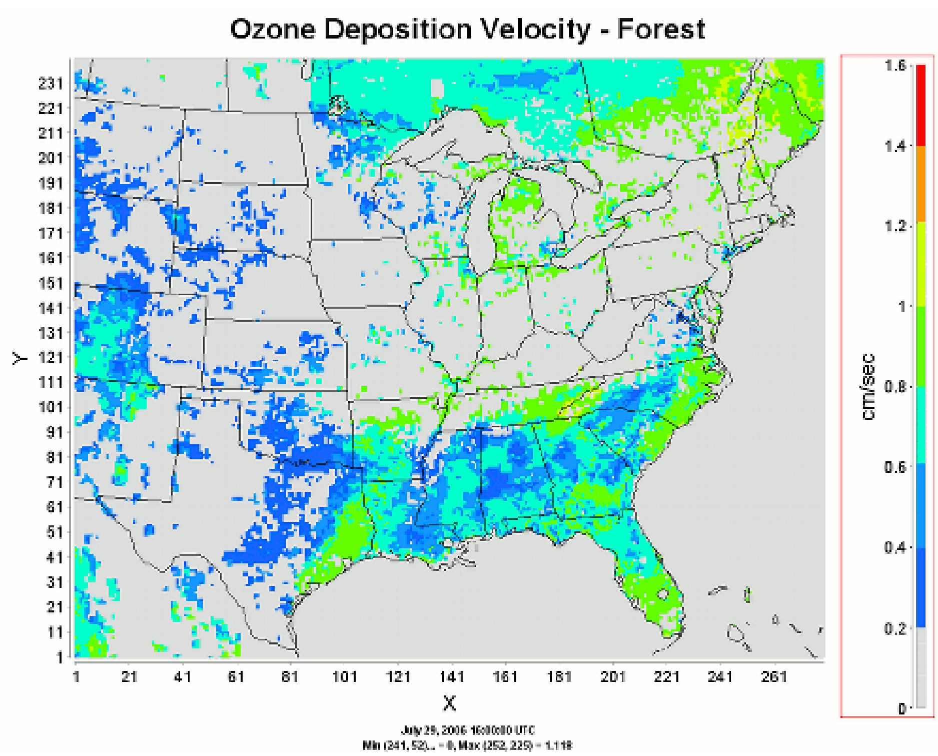


Figure 7-4. Receptor-specific ozone deposition velocities to forested ecosystems.

data were found to be useful in adjusting modeled precipitation errors.

Ongoing research within AMAD is focusing on ways to improve meteorological precipitation simulations to facilitate better hydrologic linkage with watershed models. The use of higher resolution simulations (4-km) nudged using analyses that include more extensive data assimilation (OBS-GRID) or that employ more advanced

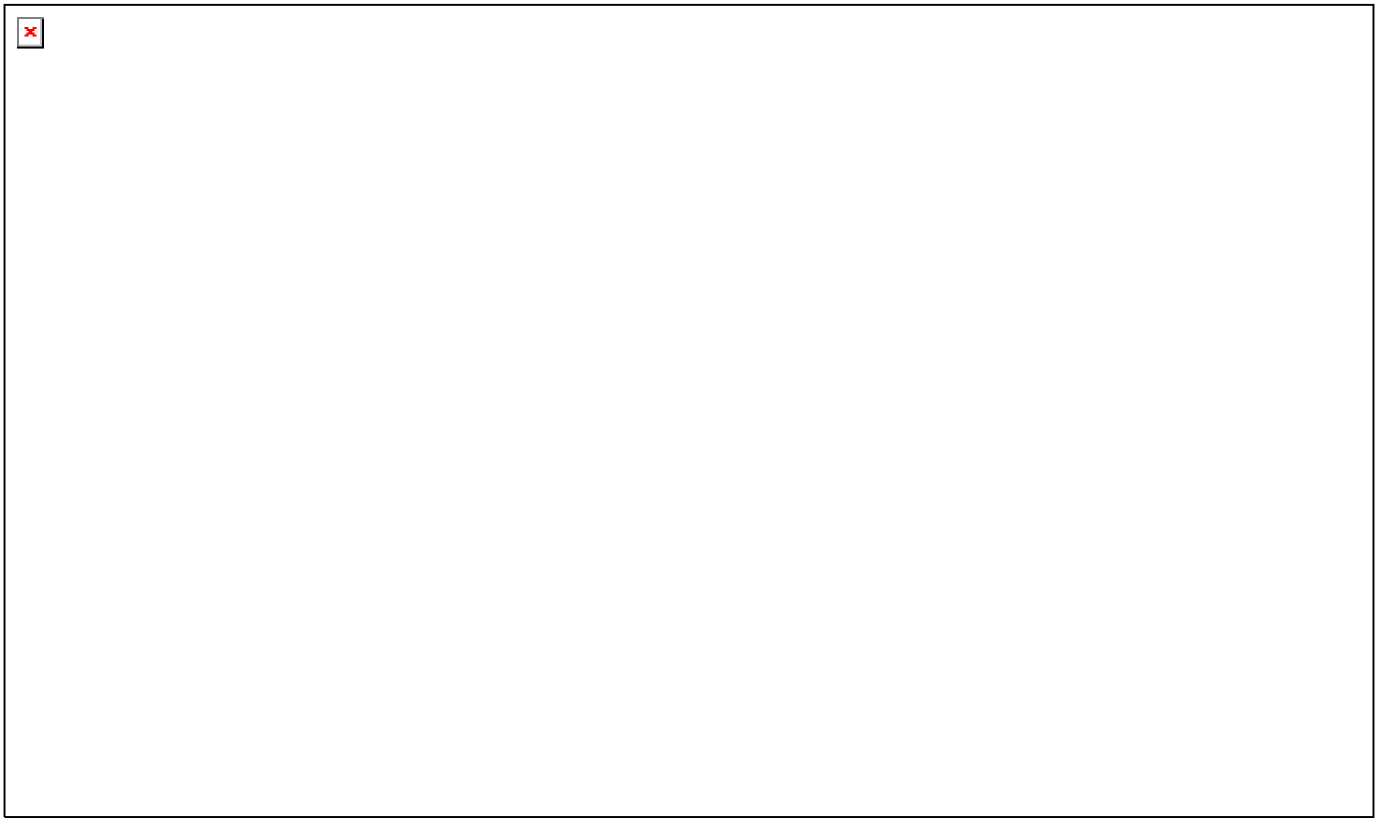


Figure 7-5. Left panel is a map of the Deep River and Haw River watersheds within the Cape Fear River Basin. Right panel shows time series of the simulated monthly runoff for the Deep and Haw watersheds during the 2001-2003 period for the different precipitation datasets. Runoff for each precipitation dataset is compared to the USGS gage value for each watershed.

data assimilation techniques, such as 3D variational analysis, are being explored. Outcomes of these experiments will be evaluated and, if significant improvement is noted, will be tested within the GBMM.

CMAQ deposition datasets are being developed for terrestrial and aquatic critical loads assessments and for linking with USGS's SPARROW model. CMAQ deposition datasets are planned to transition to those with the land use mosaic approach and bidirectional ammonia deposition. The initial emphasis for a core capability would be off-line approaches to atmospheric deposition that address bidirectional exchange and land use. To further support trend analysis, sensitivity testing to illustrate the response of atmospheric deposition to various land use changes is planned.

7.3 Linking to Ecosystem Services

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 functions because there is human demand for and benefit from 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. The overarching ESRP research questions are as follows.

- What are the effects of multiple stressors on ecosystem services, at multiple scales, over time?
- What is the impact of various plausible changes in these services on human well-being and on the value of the services?

7.3.1 Future Midwestern Landscapes

The Future Midwestern Landscapes (FML) Study is being undertaken as part of ESRP. The study examines the variety of ways in which the landscapes of the Midwest, including working lands, conservation areas, wetlands, lakes, and streams, contribute to human well-being. The FML goal is to quantify the current magnitude of those contributions, 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 a 12-State area of the Midwest (see Figure 7-6).

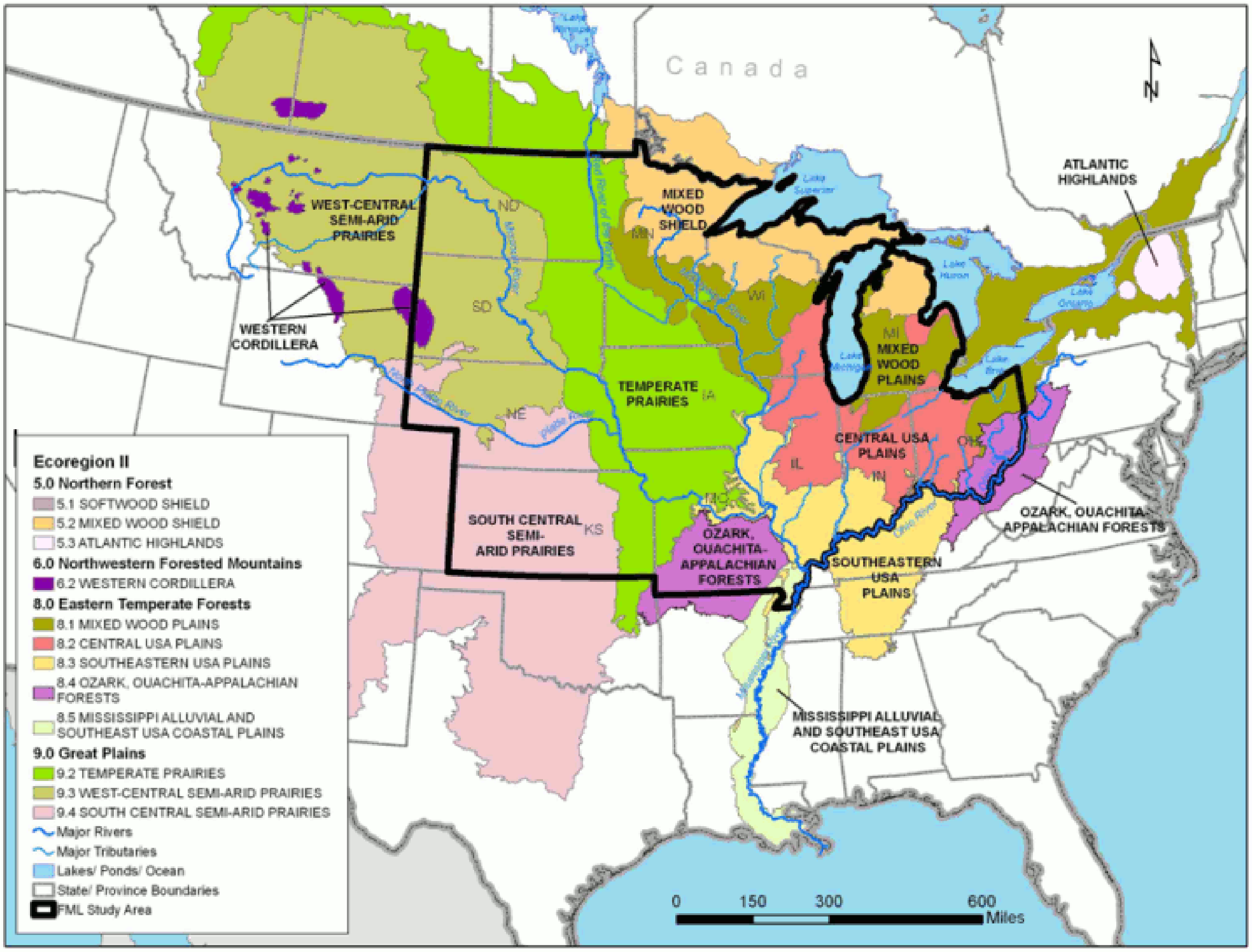


Figure 7-6. Future Midwestern landscapes study area (thick black line) superimposed on the Midwest ecoregions.

Alternative future scenarios will be used to contrast the current path (i.e., the policy-driven ramp-up of biofuel production) with an alternative path, in which hypothetical incentives are directed toward land uses that produce a wider range of services. Conceptual models of these scenarios will be used to explore the nature and magnitude of changes to ecosystems and human well-being expected for each scenario and to set priorities for research. Detailed land use/land cover maps will be constructed for the baseline and alternative future scenarios, and computational models will be employed to simulate the effects of land use changes in terrestrial, atmospheric, and aquatic environments. In addition, a socioeconomic framework and set of indicators will be developed for evaluating the ecological changes in each scenario, in terms of societal well-being.

The FML approach defines a linked-modeling system to address the issues posed by the alternative scenarios. Figure 7-7 illustrates the specific role of AMAD research and model development. In particular, the FML study will examine projected landscape changes and subsequent changes in ecosystem services. This task will make use of advances in CMAQ modeling of land use change (mosaic) and bidirectional ammonia flux to explore the combined impact of land use changes on the deposition of nitrogen to underlying watersheds in the Midwest. Ongoing research will help elucidate the communication of these results in terms that are relevant to ecosystem exposure assessment (e.g., mosaic output and WDT utilization). Planned analyses for the FML include changes in regional ambient concentrations of ozone, oxidized and reduced nitrogen species, sulfur dioxide, sulfate, and fine PM. We also will provide changes in the magnitude and spatial and temporal distributions of ozone and nitrogen flux (emission and deposition) to FML ecosystems defined by NLCD vegetation class.

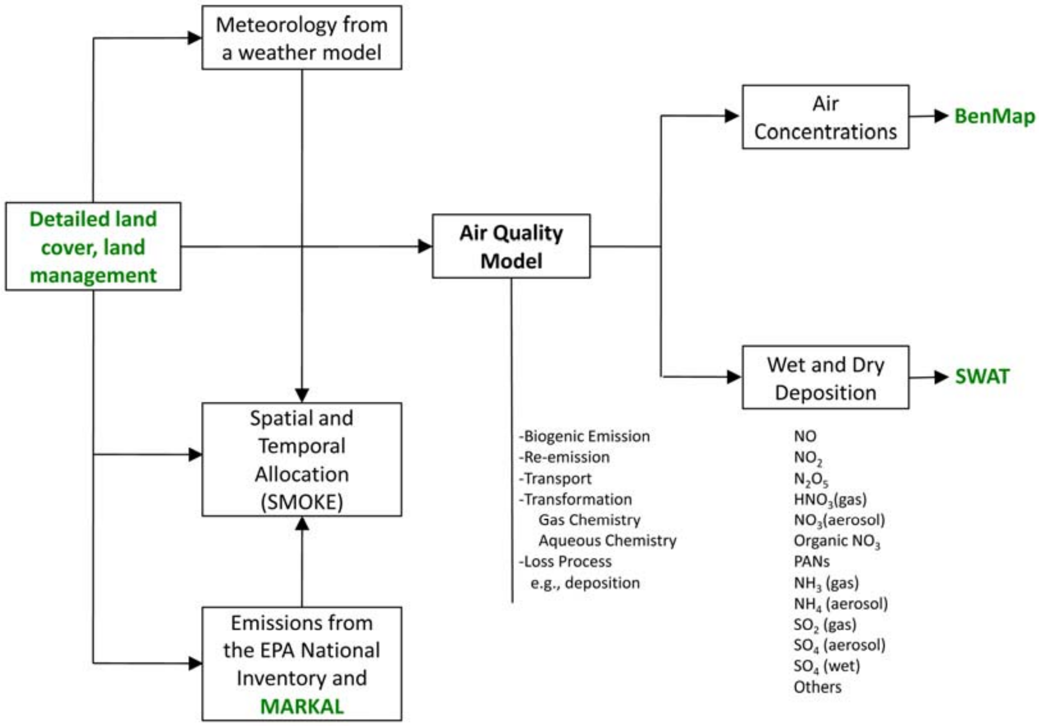


Figure 7-7. Flow chart of AMAD's role in FML model development.

7.3.2 ESRP Nitrogen Pollutant Specific Study

ESRP Pollutant Specific Studies: Nitrogen Regulating Services

The significance of 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 Nr, including the production of plant and animal products (food and fiber) for human consumption and use and the combustion of fuels that supports 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 with smaller scale, regional studies tackling specific problems and ecosystem types.

National Scale Nitrogen Studies

Mapping at the national scale is being developed with an initial focus on selected studies of nitrogen inputs to the landscape. This work is being conducted in a collaborative manner with the ESRP Mapping Team. The ESRP Mapping Team is taking the lead on creating the layers, whereas the Nitrogen Team will provide data and model outputs and will contribute to designing the mapping approach. Three major Nr inputs and transfers have been selected as initial cases for the national mapping: fertilizer input, atmospheric deposition, and nitrogen transfer from land to water.

Nutrient Loading and Atmospheric Deposition

Atmospheric deposition is an important source of nitrogen to terrestrial and aquatic landscapes. There is direct deposition to the landscape and transfer of the deposition from the terrestrial landscape to water bodies. Atmospheric deposition of sulfur, oxidized nitrogen, reduced nitrogen, and ozone will be simulated by CMAQ for a 12-km grid size for the eastern United States and the continental United States. Typical compilations of deposition are monthly and annual accumulated deposition amounts. A base year of 2002 is available to represent current conditions (Figures 7-8 and 7-9). CMAQ simulations for 2006 also may be available. CMAQ projections of deposition for 2020 and 2030 that represent the implementation of nitrogen oxide controls to meet health standards for ozone and $PM_{2.5}$ under the

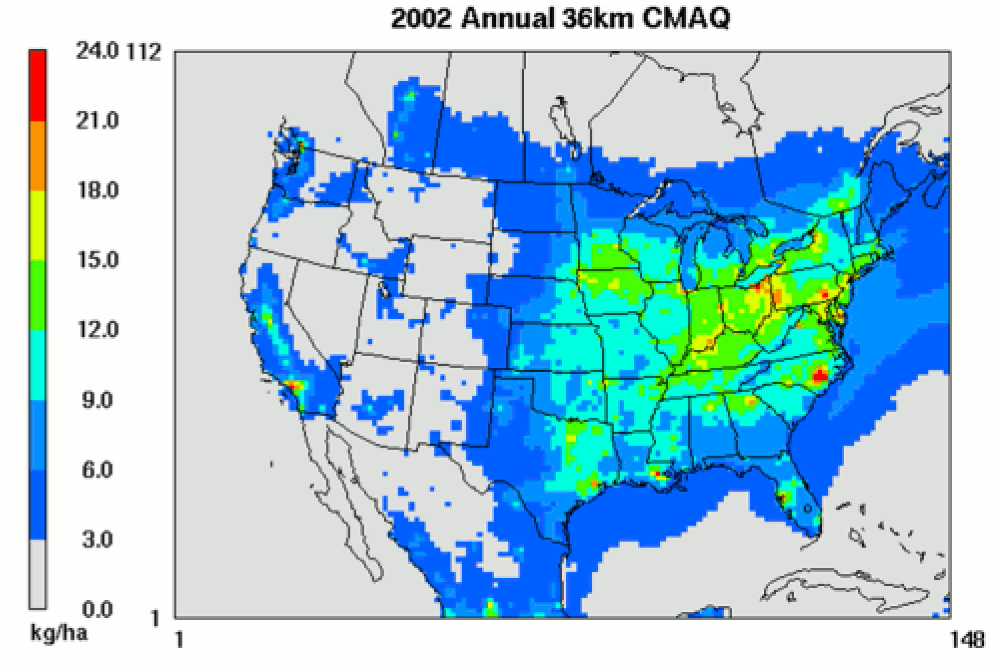


Figure 7-8. 2002 Annual total nitrogen deposition (wet and dry oxidized and reduced species).

1990 CAA Amendments (CAAAs) will be available for mapping as well. Such projections show a significant reduction in oxidized nitrogen deposition across the eastern United States. The 12-km CMAQ grid can be mapped to 12-digit hydrologic unit codes (HUCs) or any other desired set of polygons. The CMAQ data will be augmented by National Acid Deposition Program (NADP) wet deposition data in the mapping exercise. The use of CMAQ dry deposition combined with precipitation-corrected and NADP-augmented CMAQ wet deposition will be examined for the national mapping of nitrogen deposition.

Regional Scale Nitrogen Studies

A regional approach will be pursued for several questions in the ESRP Nr research program that currently cannot be approached nationally. Case studies for the regional approach have been selected that have national significance and for which we desire to develop a national approach. The objective is to extend the regional case studies through a synthesis of methods to be able to encompass a national perspective. CMAQ deposition results will be used in several studies, in particular, the study of tipping points.

Tipping Points in Ecosystem Condition and Services

The critical loads or tipping points approach can provide a useful lens through which to assess the results of current policies and programs and to evaluate the potential ecosystem protection and ecosystem services values of proposed policy options. A major stressor of concern with serious consequences for freshwater aquatic and terrestrial systems is acidification from atmospheric deposition of Nr and sulfur. Several Federal agencies are working together on regional pilot projects across the United States to explore the possible role a critical loads (or tipping points) approach can have in air pollution control policy in the United States. The ESRP Nr research program has selected three of the regional pilot projects that provide an excellent opportunity for the ESRP program to work within and build onto their efforts. They are the Blue Ridge Mountains aquatic systems, the Adirondacks terrestrial systems, and the Rocky Mountain aquatic systems. CMAQ deposition outputs and NADP data will be used to provide deposition inputs to the ecosystem models used in these projects. CMAQ projections to 2020 and beyond of deposition also will be used to assess vulnerable ecosystems. These studies are expected to come to fruition in 2010, after which a synthesis effort will be undertaken to determine how best to create national critical load mapping capabilities for the EPA Office of Air Programs (OAP). Major players in these pilots are EPA, NPS, and the U.S. Forest Service. This research will involve close coordination among ORD (AMAD and the National Health and Environmental Research Laboratory's Western and Atlantic Ecology Divisions), the OAP Clean Air Markets Division, and the Office of Air and Radiation's OAQPS.

7.4 Air-Surface Exchange

The interaction between the atmosphere and the underlying surface increasingly is recognized as important in ecosystem health and in air pollution transport processes. Just as there has been a movement away from assessing human exposure to air pollutants one chemical species at a time toward an integrated one-atmosphere approach, so too should there be an integrated one-atmosphere approach to assessing ecosystems exposure to air pollutants. With this in mind, we propose that now is the time to advance from simply a one-atmosphere to a one-biosphere approach that includes integration across multiple media and biogeochemical processes to more effectively address

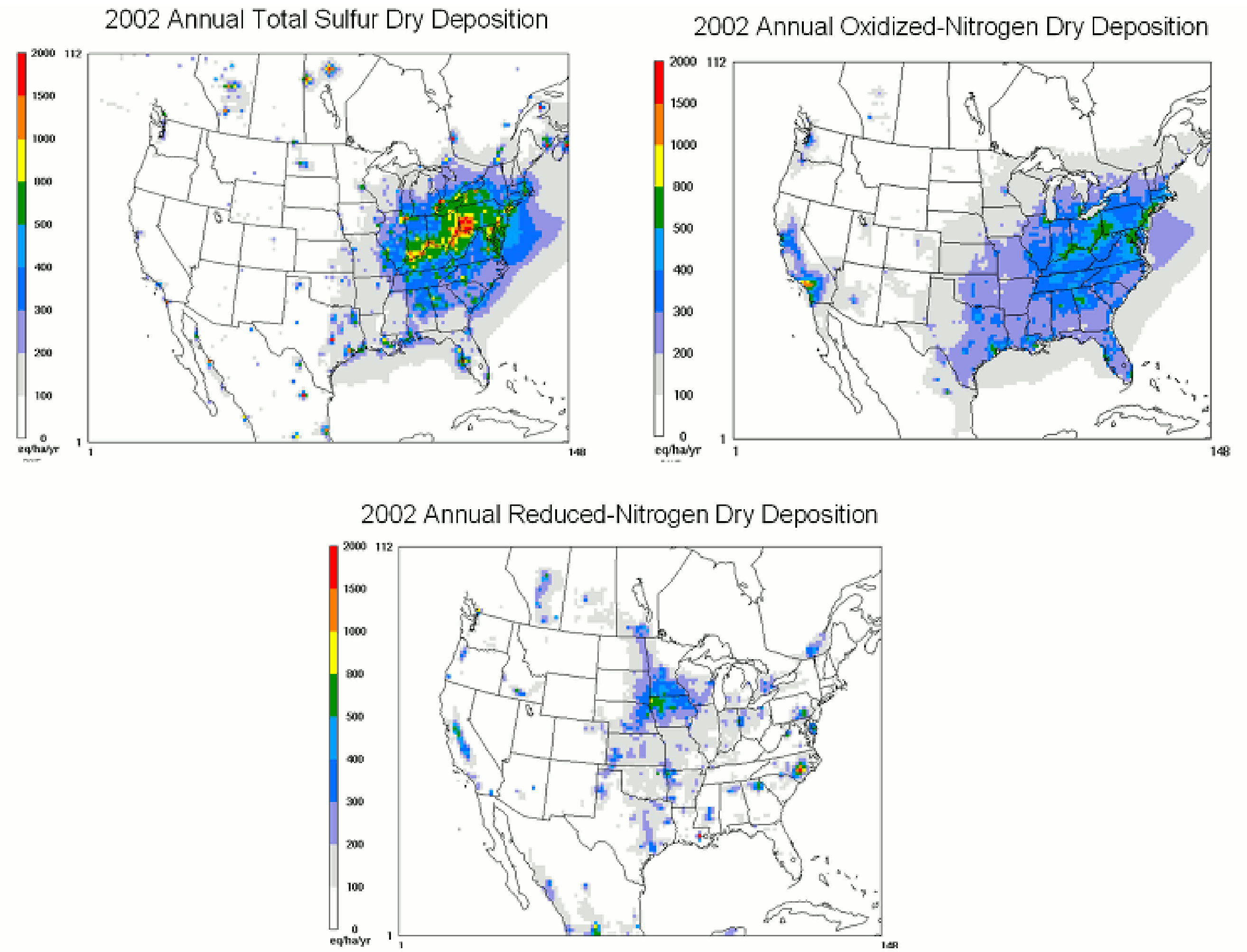


Figure 7-9. 2002 Annual acidifying dry deposition of sulfur and oxidized and reduced nitrogen (eq ha^{-1} year^{-1}).

ecological interactions with the atmosphere as well as human systems.

A deposition-based assessment of the impact of air pollution on ecosystem health is more appropriate than the existing concentration-based standards used to protect human health. However, 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.

Improved Dry Deposition Algorithms for CMAQ

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. A major objective is to reduce uncertainty in deposition/air-surface exchange calculations by discovering and including missing pathways and by creating a more ecosystem-compatible surface-layer link with water quality and terrestrial models (Figure 7-10). Model air-surface exchange uncertainty has led to collaborations with measurement groups and the design of experiments at field campaigns to refine and develop mechanistic air-surface exchange algorithms. This has resulted in the refinement of coarse-mode particulate nitrate aerosol deposition and bidirectional exchange algorithms for NH_3 from soils following fertilizer application and the impact of vegetation canopies on the atmosphere-biosphere exchange.

Improved Dry Deposition for Network Applications

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 (Clarke et al., 1997; Finkelstein et al., 2000; 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.

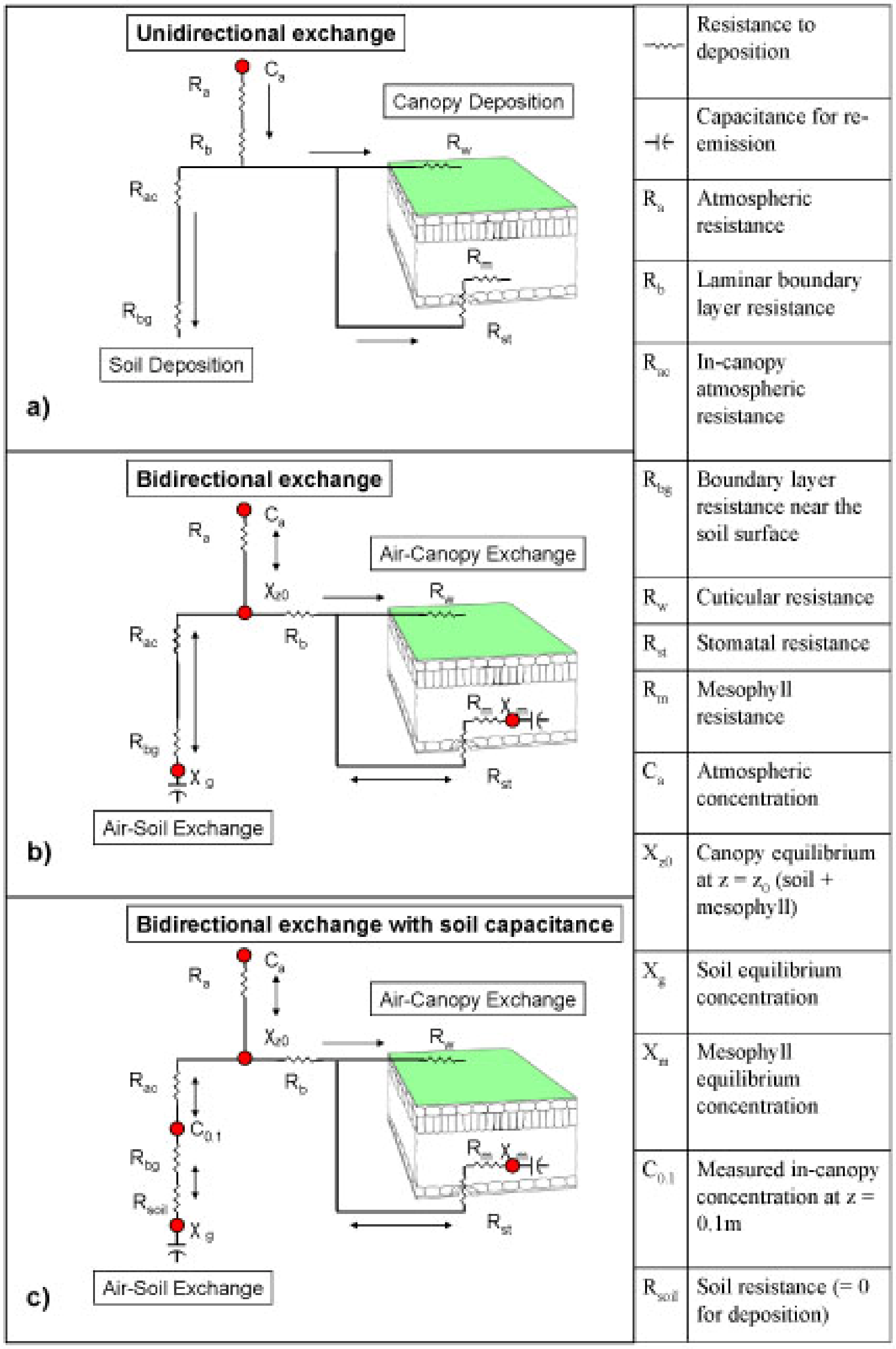


Figure 7-10. Air-surface exchange resistance diagrams of unidirectional exchange (a), bidirectional exchange of ammonia (b), and bidirectional exchange of mercury and ammonia using the FEST-C tool (c).

7.4.1 Nitrogen Surface Exchange

Excessive loading of nitrogen from atmospheric nitrate and ammonia deposition to ecosystems can lead to soil acidification, nutrient imbalances, and eutrophication. Accurate nitrogen deposition 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, creating these estimates is a high priority for water and soil chemistry modeling of nutrient loading, soil acidification, and eutrophication.

In collaboration with the atmospheric measurement community, we have conducted work to advance nitrogen air-surface exchange (dry deposition and evasion from soil and vegetation surfaces), modeling of ammonia, and the treatment of coarse-mode nitrate chemistry in the CMAQ model. This process has included the following steps.

(1) Develop testable hypotheses from the literature in the form of new modules or routines for CMAQ
(2) Assist in the design of the field campaign needed to collect measurements of the parameters required to further develop these algorithms and to conduct robust evaluations of them
(3) Use the resulting field measurements to refine and evaluate the model algorithms for the development of an operational model (Figure 7-11)

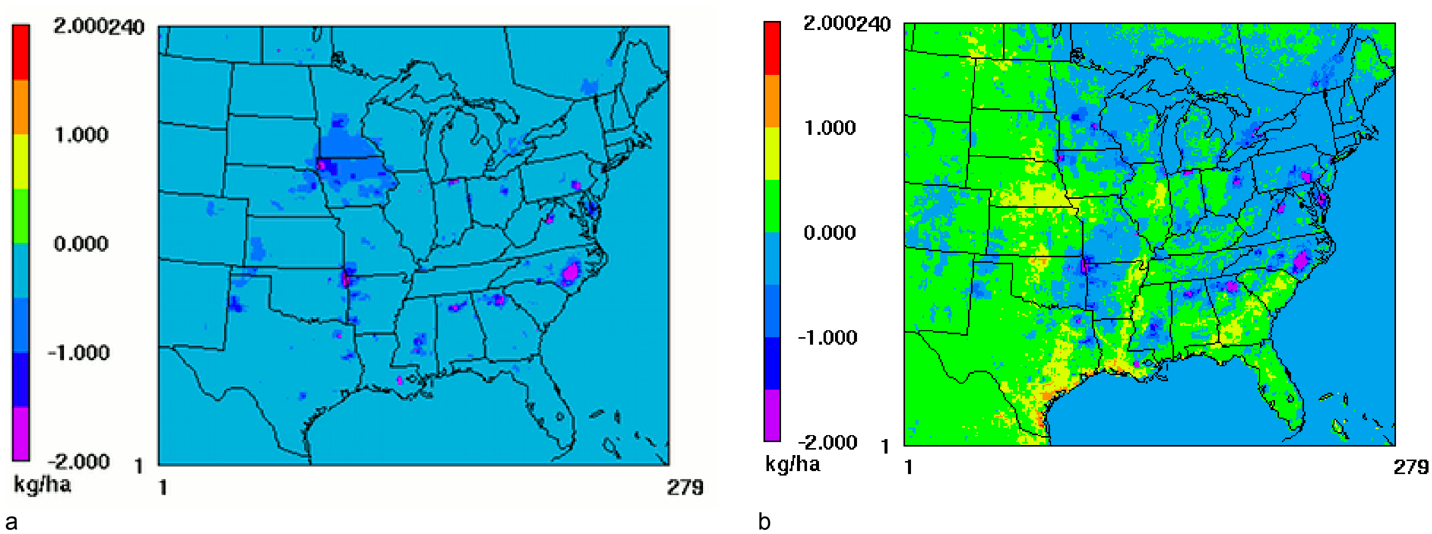


Figure 7-11. Mean air-surface exchange of NH_3 for the month of July estimated by CMAQ v4.7 using MM5 with the PX land surface scheme for (a) unidirectional exchange of NH_3 and (b) bidirectional exchange of NH_3 (positive values indicate net evasion and negative values indicate net deposition).

The development of the bidirectional ammonia 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 enhance the credibility of the CMAQ nitrogen budget for ecosystem assessments. Results from the bidirectional ammonia exchange model helped prioritize current and future measurement needs in field experiments.

7.4.2 Soil NH_3 Emissions

CMAQ representation of the regional nitrogen budget is limited by its treatment of NH_3 soil emission from and deposition to underlying surfaces as independent rather than tightly coupled processes and by its reliance on soil emission estimates that do not respond to variable meteorology and ambient chemical conditions. The present study identifies an approach that addresses these limitations, lends itself to regional application, and will better position CMAQ to meet future assessment challenges. These goals were met through the integration of the resistance-based flux model of Nemitz et al. (2001) with elements of the U.S. Department of Agriculture Environmental Policy Integrated Climate (EPIC) model. Model integration centers on the estimation of ammonium and hydrogen ion concentrations in the soil required to estimate soil NH_3 flux. The EPIC model was calibrated using data collected in collaboration with NRMRL and N.C. State University during an intensive 2007 field study in Lillington, NC. A simplified process model based on the nitrification portion of EPIC was developed and evaluated. It then was combined with the Nemitz et al. (2001) model and measurements of near-surface NH_3 concentrations to simulate soil NH_3 flux at the field site. Finally, the integrated flux (emission) results were scaled upward and compared to recent national ammonia emission inventory estimates. The integrated model results are shown to be more temporally resolved (daily), while maintaining good agreement with established soil emission estimates at longer time scales (monthly) (Figure 7-12). Although results are presented for a single field study, the process-based nature of this approach and NEI comparison suggest that inclusion of this flux model in a regional application should produce useful assessment results if nationally consistent sources of soil and agricultural management information are identified.

Fertilizer Scenario Tool for CMAQ (FEST-C)

Enhancements to the CMAQ bidirectional flux model require additional, nationally consistent information regarding fertilizer application timing, amount, and mode of application, as well as soil characteristics and surface losses in runoff. Research (Cooter et al., 2010) has demonstrated that a well-vetted agricultural management model can provide this information. A work assignment has been drafted for the development of a nationally consistent version of this model, designed to run either in stand-alone mode for independent analyses or in

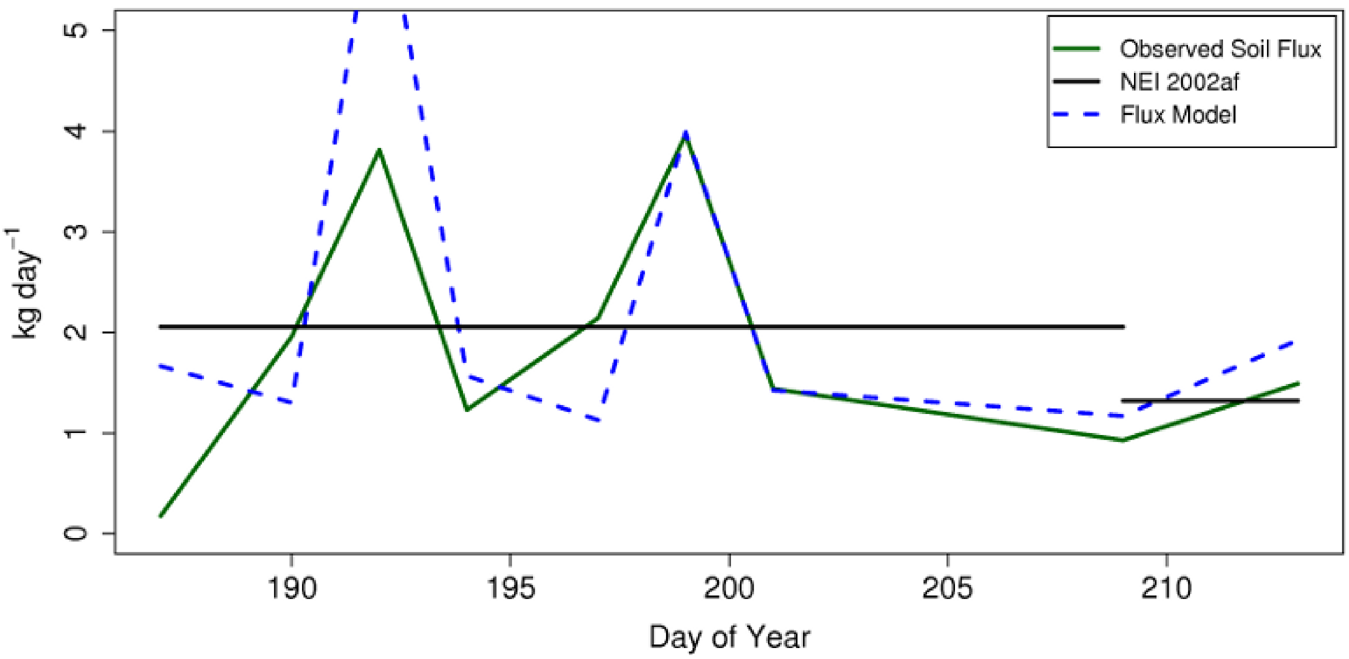


Figure 7-12. Daily Harnet County, NC, NEI soil emission estimates and simplified process model estimates plotted with Lillington, NC, observations.

conjunction with SMOKE to produce CMAQ-ready input information to address "what-if" questions associated with current and alternative land use, land cover, and air quality changes in response to population growth, bio-energy, and air quality regulatory policy and climate change. The stand-alone version of the model will output files that can be displayed and analyzed using the VERDI visualization tool.

7.4.3 Canopy NH_3 Exchange

Regional and global estimates of the impact of ammonia emissions on climate change, air-quality, and human and ecosystem health must be scaled up with air quality models. The effect of soil emission processes and in-canopy sources and sinks on the net ecosystem flux need further quantification (Sutton et al., 2007). Scientists from AMAD have collaborated with field scientists from NRMRL and Duke University to estimate in-canopy and soil ammonia exchange processes based on field measurements and modeling theory and have designed experiments to elucidate a better process level understanding of the biological, chemical, and mechanical processes influencing the soil-vegetation-atmosphere exchange of nitrogen over managed and natural ecosystems. An analytical in-canopy scalar transport closure model based on the mixing length theory developed by Prandtl (1925) that estimates in-canopy sources and sinks by using measured concentration and wind speed profiles was developed. In-canopy sources and sinks were estimated, and above-canopy micrometeorological fluxes, 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. Ammonia concentrations were measured at four heights in the canopy and at one height above the canopy using manually collected denuders in addition to three collocated above-canopy continuous Ammonia Measurement by Annular Denuder with Online Analysis (AMANDA) concentration. Vertical profiles of wind speed, heat, and momentum fluxes were made from inside the canopy to a height of 10 m using an array of 3D sonic anemometers. Ancillary vertical profiles of temperature were measured using copper/constantan thermocouples for model evaluation.

Modeled ammonia and sensible heat fluxes agreed well with above-canopy micrometeorological flux measurements. The soil at this site was found to be a consistent emission source, whereas the vegetation canopy was typically a net ammonia sink with the lower portion of the canopy being a constant sink (Figure 7-13). The upper portion of the canopy was dynamic, exhibiting periods of local deposition and evasion. The use of simple Eulerian-based, in-canopy exchange estimates allowed for a physically descriptive partitioning of atmospheric-soil and atmospheric-vegetation exchange of measured scalars. These detailed source and sink estimates are being used to constrain NH_3 soil emission estimates and the influence of the vegetation canopy on the net flux for managed agricultural land types in CMAQ.

A goal is also to harmonize the local ecosystem scale (tens of square kilometers) with the regional airshed scale (thousands to millions of square kilometers). Surface NH_3 concentrations were measured beginning early in the 2009 fiscal year along transects in

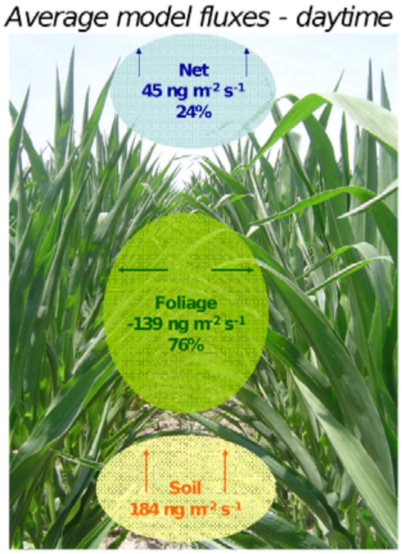


Figure 7-13. Ammonia exchange budget estimated from the annalytical closure model.

North Carolina and with NASA Tropospheric Emission Spectrometer (TES) retrievals to collect data on a regional scale to evaluate the regional application of these local mechanistic models (Figure 7-14). These observations and observations from monitoring networks will develop a new continental-scale ammonia emission inventory using model inversion techniques for CMAQ with and without ammonia bidirectional surface exchange. NH_3 bidirectional model parameters, soil and vegetation emission potentials (Γ), and point sources will be optimized in the bidirectional model inversion.

7.5 CMAQ Ecosystem Exposure Studies

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, causing acidification of lakes and streams and eutrophication of coastal systems. Reductions in atmospheric deposition of sulfur and oxidized nitrogen resulting from regulations in the 1990 CAAAs 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 just from measurements. The goal is to bring air quality into ecosystem management through regional air quality modeling and to facilitate the air-ecosystem linkage.

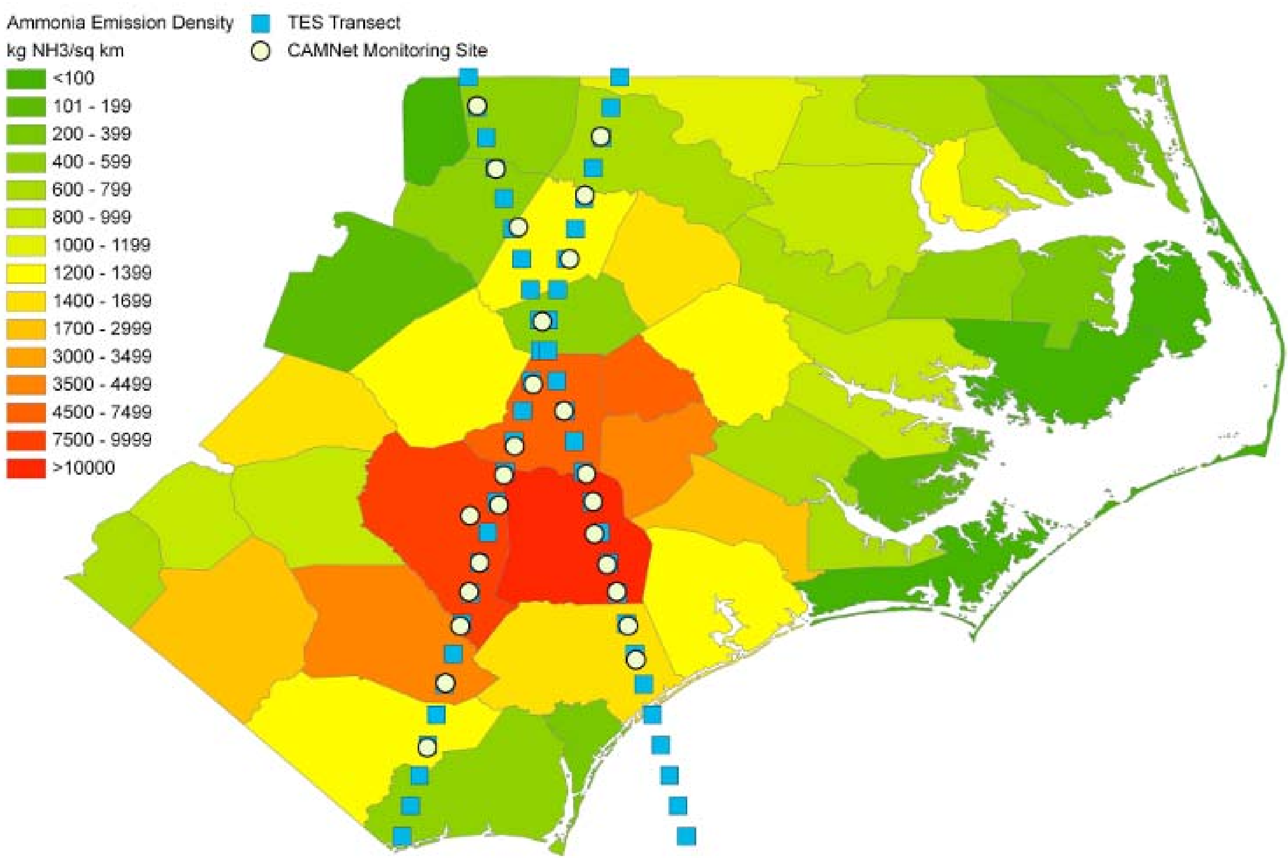


Figure 7-14. TES transect locations and surface observations overlaid on a map of the estimated NH_3 emission density in Eastern North Carolina.

Through identification of basic management questions, we define what research and tool developments for the air quality modeling system are needed to make the linkage functional and the air-ecosystem modeling applicable and useful.

Our 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. We develop an understanding of the needs of the 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? Which anthropogenic or natural source is responsible for and where is the deposition from? How much will deposition change because of air quality regulations and population and/or economic growth? Guidance on several fronts has been developed; for example,

- a combination of local emission sources and long-range transport of pollutants requires both local and regional approaches,
- the uncertainty in ammonia emissions and concentrations is very important, and
- CAAA reductions have been significant.

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 total maximum daily load (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-SO_x 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. Although zeroing out this conversion reduces HNO_3 and NO_3^- deposition by 18% and 26%, respectively, total oxidized nitrogen is reduced by only 6% (Figure 7-15).

7.5.1 Airsheds

Long-Range Transport

Airsheds typically have a larger spatial extent than estuaries, watersheds, and National Parks. For NO_x emissions, the range of influence is multi-State, leading to airsheds that are multi-State in size. This is also true for NH_3 emissions, which is counter to conventional wisdom in the ecological community. The airshed is defined as the domain from which emissions would account for a significant majority of the deposition to the receptor watershed.

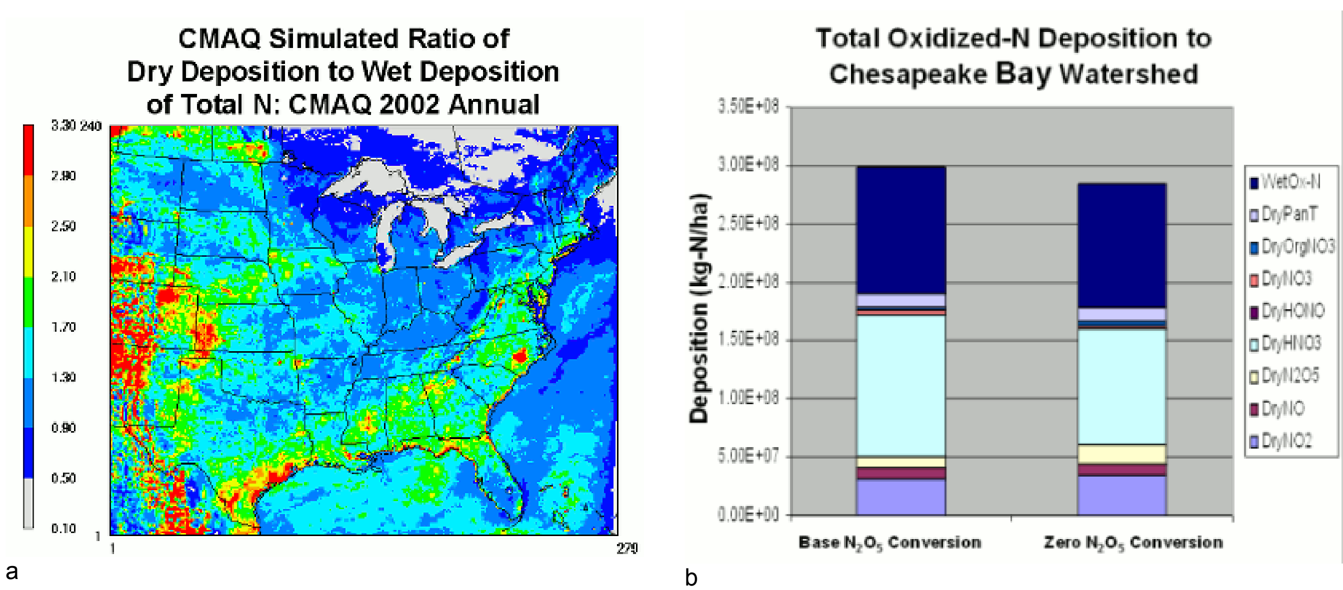


Figure 7-15. CMAQ is a source of data for ecosystem managers that is not available in routine monitoring data, such as (a) complete dry and wet deposition estimates, and (b) the "one atmosphere" concept of CMAQ is needed to understand the balance between uncertainties in atmospheric reaction rates and deposition pathways.

Airsheds: Oxidized-Nitrogen Deposition into Coastal Estuaries

Using the procedure developed for the Chesapeake Bay and outlined in Dennis (1997), airsheds for 20 coastal watersheds along the East and Gulf Coasts were developed. Examples of oxidized nitrogen airsheds are seen in Figure 7-16.

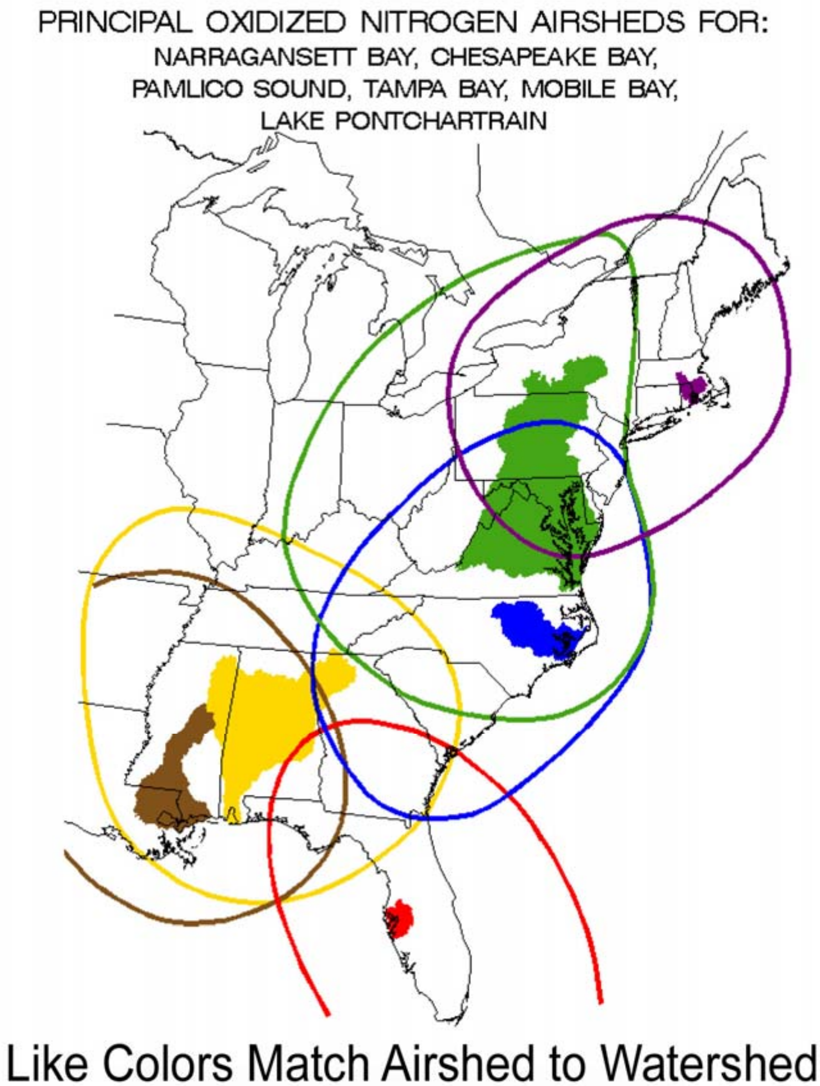


Figure 7-16. Air sheds (solid lines) and watershed (solid areas) for Narragansett Bay (purple), Chesapeake Bay (green), Pamlico Sound (blue), Mobile Bay (yellow), Lake Pontchartrain (brown), and Tampa Bay (red).

7.5.2 Chesapeake Bay Restoration

Chesapeake Bay is the largest estuary in the United States and was the Nation's first estuary targeted by Congress for restoration. Reversal of the rapid loss of living resources resulting from excess nutrients (mainly nitrogen), and restoration of the quality of the Bay has been the goal of the Chesapeake Bay Program since its inception in 1983. Atmospheric deposition of nitrogen to the Chesapeake Bay watershed and Bay surface is a major contributor to the Bay nitrogen load, affecting current conditions and needing to be addressed in Bay restoration efforts. The atmosphere is estimated to contribute a quarter of the total nitrogen load delivered from the watershed to the Bay. Direct atmospheric deposition to the Bay's tidal waters increases the fraction of the total load of nitrogen to the Bay from atmospheric deposition by approximately a third. Chesapeake Bay has been placed on EPA's list of impaired waters, with a TMDL plan required in 2011. To provide the best modeling science for the TMDL plan, a major upgrade of the Chesapeake Bay Watershed model v5.1 is being used, as well as CMAQ v4.7. This atmospheric modeling will be a major update from the earlier use of the extended Regional Acid Deposition Model (RADM). The grid size is 12 km, better resolving the Bay, and the effect of sea salt is included. The CMAQ modeling for the Chesapeake Bay TMDL planning has the following three major foci.

(1) Development of scenarios estimating the deposition reductions expected by 2010 and 2020 because of CAA regulations, such as the CAIR (as further modified as the result of court actions [Figure 7-17])

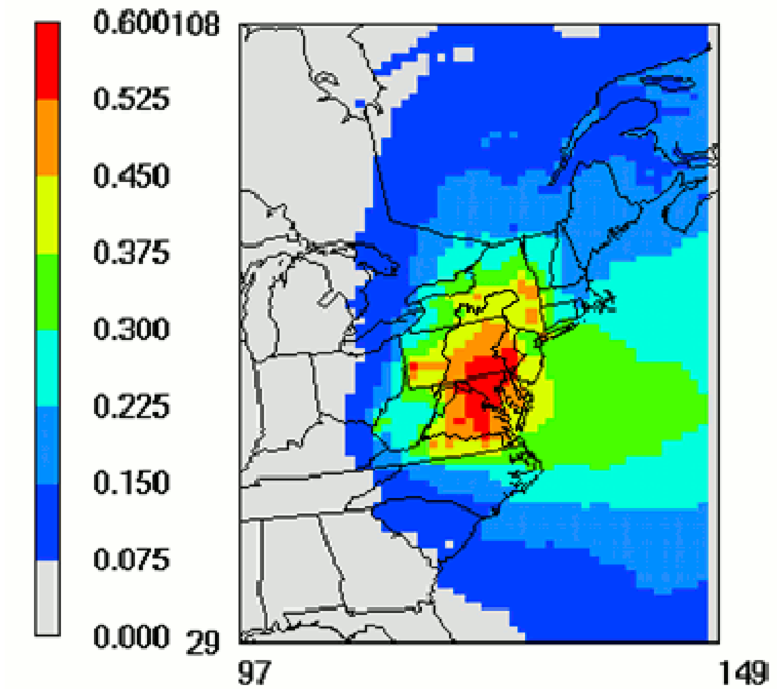


Figure 7-17. Model-predicted contributions of six Bay States account for 50% of the 2020 oxidized nitrogen deposition to the Chesapeake Bay Watershed.

(2) A new NH_3 budget analysis at 12 km, using a prototype CMAQ with NH_3 bidirectional air-surface exchange incorporated, showed that incorporating bidirectional exchange of ammonia will have an important impact of reducing the local dry deposition and an impact on the estimates of the range of influence of ammonia emissions, almost doubling the range.

(3) Estimation of the relative contribution the NO_x emissions from the six Bay States make to the atmospheric deposition of oxidized nitrogen to the Bay watershed and Bay surface after implementation of (CAIR). The State allocation data form the basis for a management decision rule for allocating State emission reductions that are beyond the national rules to watershed deposition reductions that can count as State allocation reduction credits.

7.5.3 Tampa Bay

The Tampa Bay Estuary Program (TBEP) set restoration of underwater seagrasses, an indicator of overall Bay health, as a long-term natural resource goal. Water quality targets and associated nitrogen loading goals have been developed and adopted to support attainment and maintenance of the seagrass restoration goal. Atmospheric deposition of nitrogen is the largest source type contributing to nitrogen loading to Tampa Bay. Direct deposition to Tampa Bay is central and is estimated to be second only to storm water runoff, but a portion of storm water runoff is caused by atmospheric deposition (wet and dry). Tampa is an excellent example of a coastal bay where the existence of sea salt is a significant factor in the rate of local nitrogen dry deposition. Tampa Bay is unusual in that a large portion of the watershed is urbanized and a major fraction of the oxidized nitrogen deposition to Tampa Bay is estimated to come from local sources (40% to 50%). Two of the largest utility emitters of NO_x emissions in the country in 2000 are located at the edge of Tampa Bay. They have, through a consent decree, agreed to reduce their NO_x emissions by up to 95% by 2010. A research beta version of CMAQ, CMAQ-UCD, incorporates sea salt. The Florida Department of Environmental Protection (FDEP) organized, with ORD help, the Bay Regional Air Chemistry Experiment (BRACE) field study that took place in Tampa during May 2002. One key objective of BRACE is to provide field data to evaluate CMAQ-UCD. The four major thrusts of the Tampa Bay Model Evaluation and Application study are

(1) to evaluate CMAQ-UCD against the BRACE May 2002 data and make any model refinements that may be required;

(2) to assess the relative contributions from the different emissions sectors, particularly mobile sources and utilities, to the annual oxidized nitrogen deposition to Tampa Bay;

(3) to 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 (Figure 7-18); and

(4) to assess the change in annual deposition to Tampa Bay that could be attributed to mobile source and utility reductions under the CAIR in 2010.

The Tampa Bay assessment is being conducted in concert with FDEP and TBEP, using grid sizes of 8 km over Florida and 2 km over the Tampa region. The

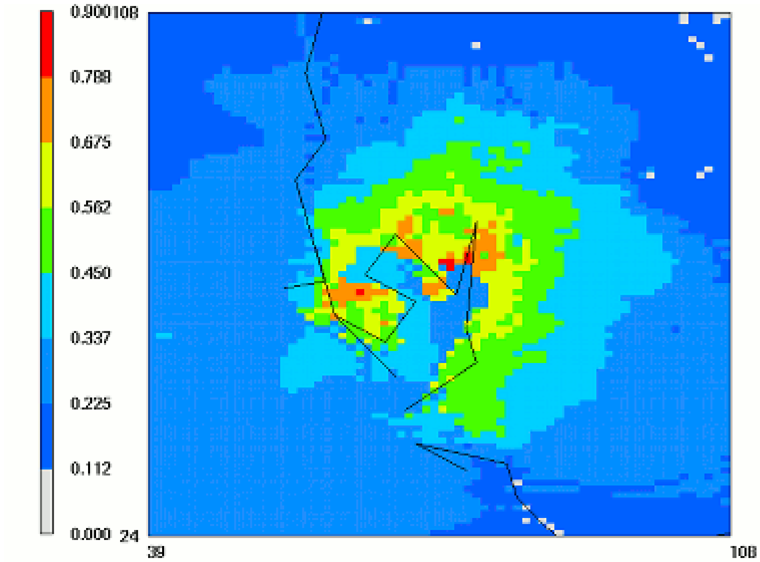


Figure 7-18. Fraction of total oxidized nitrogen deposition to Tampa Bay explained by local emission in the watershed.

CMAQ-UCD also has been used as a benchmark model for the development of the dynamic sea salt parameterization in the 2008 CMAQ v4.7.

7.6 Software Tool Development

Linking air quality and ecosystems is inherently transdisciplinary. Significant effort often is required to analyze observations and model results and provide them in a form required to support management decisions. Most off-the-shelf tools do not address the specialized needs or applications encountered in analyzing data from a multimedia perspective, making it more difficult than is necessary to link elements of the multimedia components together. As such, it is necessary to provide the larger ecosystem modeling and management communities with tools designed to utilize air quality modeling data. This primarily takes the form of tools used to convert air quality model output to formats used by ecologists and ecosystem managers and tools to visualize and analyze model output. The need for specialized tools is especially pertinent to bringing atmospheric components together with watershed components for multimedia management analyses.

7.6.1 Visualization Environment for Rich Data Interpretaion (VERDI)

VERDI is a flexible, modular, Java-based program for visualizing multivariate gridded meteorology, emissions, and air quality modeling data created by environmental modeling systems such as the CMAQ model and the WRF model. VERDI offers a range of options for viewing data, including 2D tile plots, vertical cross-sections, scatter plots, line and bar time series plots, contour plots, vector plots, and vector-tile plots. Scripting capability in VERDI provides a powerful interface for automating the production of graphics for analyzing data (Figure 7-19).

VERDI was developed for EPA by Argonne National Laboratory and currently is supported by the Community Modeling and Analysis System (CMAS) Center, which is hosted by the Institute for the Environment (IE) at the University of North Carolina at Chapel Hill (UNC-CH) and can be downloaded from the CMAS VERDI website (http://www.verdi-tool.org/). VERDI is an open source program, and community involvement in further development is encouraged. VERDI is licensed under the Gnu Public License (GPL) v3, and the source code is available through SourceForge (http://verdi.sourceforge.net/). In 2008 and 2009, additional capabilities were added to VERDI, including an alternate tile plot routine, an areal interpolation plot that provides the capability of the Watershed Deposition Tool, and the ability to display CMAQ data in polar stereographic and lat-long projections.

7.6.2 Watershed Deposition Tool

Background. Atmospheric wet and dry deposition can be important contributors to total pollutant loadings in watersheds. Because deposition can be expensive to monitor over an entire watershed, estimates of deposition often are obtained from regional-scale air quality models, such as the EPA's regional-scale, multipollutant CMAQ. CMAQ can be used to estimate deposition resulting from a number of scenarios, including current conditions and future emissions reductions that are expected because of rules, such as CAIR and Clean Air Mercury Rule. CMAQ produces gridded output with typical grid sizes of 36, 12, and 4 km. Because watersheds do not conform to the grid layout of CMAQ, additional tools must be used to map the results from CMAQ to the watersheds to provide the linkage between air and water needed for TMDL and related nonpoint-source watershed analyses. This linkage then enables water quality management plans to include the reductions in atmospheric deposition produced by the air regulatory community in their calculation of loadings to the watershed.

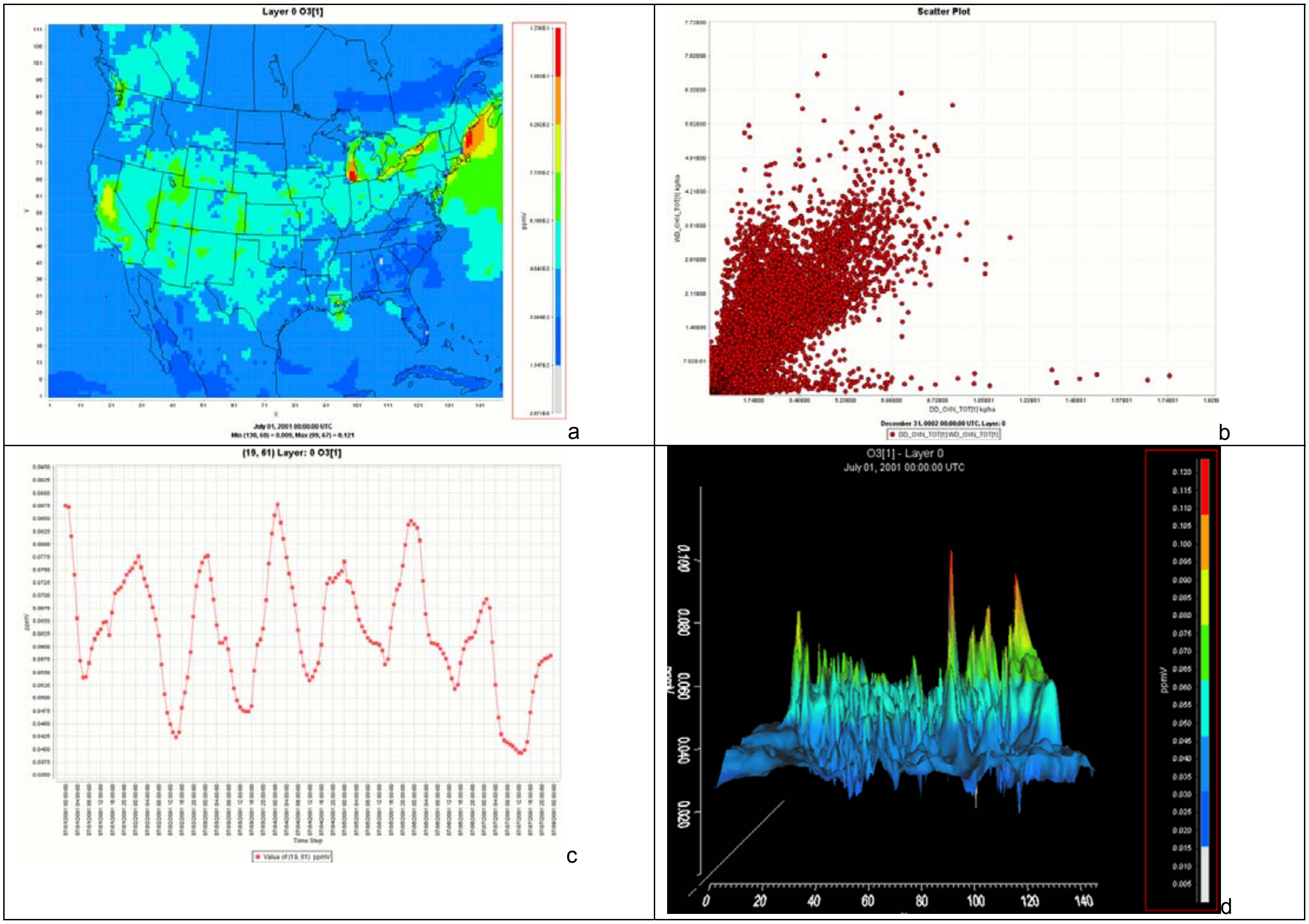


Figure 7-19. Examples of VERDI used to visualize and evaluate CMAQ output: (a) VERDI tile plot of hourly surface ozone, (b) VERDI scatter plot of annual oxidized nitrogen wet deposition versus oxidized nitrogen dry deposition, (c) VERDI time series plot of hourly surface ozone for a selected cell, and (d) VERDI contour plot of hourly surface level ozone.

Overview of the Watershed Deposition Tool. The Watershed Deposition Tool (WDT) was developed by the AMAD 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 TMDL and related nonpoint-source watershed analyses. This software tool takes gridded atmospheric deposition estimates from EPA's regional, multipollutant air quality model, CMAQ, and allocates them to 8-digit HUCs of rivers and streams within a watershed, State, or Region (Figure 7-20). The WDT can calculate the weighted average CMAQ atmospheric deposition (wet, dry, and wet + dry) across a selected HUC or a set of selected HUCs for a given scenario. The WDT also can calculate the average change in air deposition across an HUC between two different air deposition simulations. Calculations can be exported to comma-separated values files. For experienced geographic information system (GIS) users, the WDT also can export GIS shapefiles of the CMAQ gridded outputs. The tool is designed to work under the Microsoft Windows system.

Deposition Components Available from CMAQ

•Nitrogen
- Dry Oxidized Nitrogen
- Wet Oxidized Nitrogen
- Total (Wet + Dry) Oxidized Nitrogen
- Dry Reduced Nitrogen
- Wet Reduced Nitrogen
- Total (Wet + Dry) Reduced Nitrogen
- Total Dry (Reduced + Oxidized) Nitrogen
- Total Wet (Reduced + Oxidized) Nitrogen
- Total (Reduced + Oxidized) Nitrogen

Sulfur
- Total Wet Sulfur
- Total Dry Sulfur
- Total (Wet + Dry) Sulfur

•Mercury
- Total Wet Mercury
- Total Dry Mercury

Total (Wet + Dry)Mercury

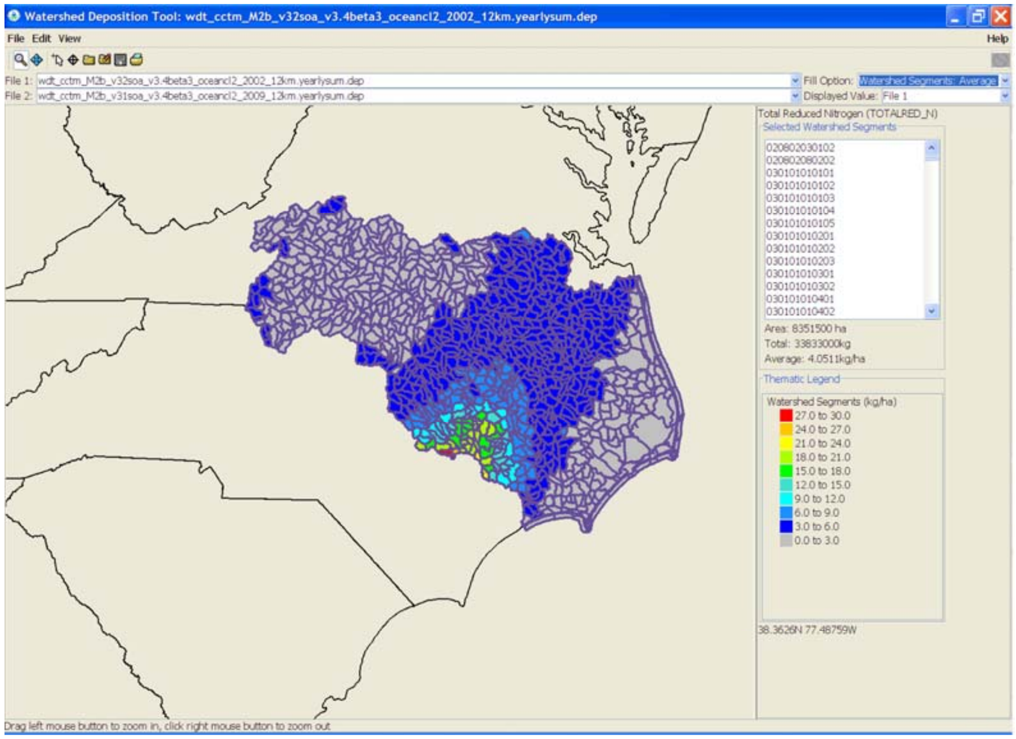


Figure 7-20. Screen shot of the 2002 annual CMAQ total reduced nitrogen deposition mapped to watersheds draining into the Albemarle-Pamlico Sound displayed in GIS mapping software.

7.6.3 Spatial Allocator

The Spatial Allocator was developed by the IE at UNC-CH for EPA to provide tools that could be used by the air quality modeling community to perform commonly needed spatial tasks without requiring the use of a commercial GIS (Figure 7-21). There are three components to the Spatial Allocator.

(1) Vector tools: These tools process vector GIS data to perform functions such as mapping data from counties to grids and visa versa.

(2) Raster tools: These tools process raster data to perform functions such as converting NLCD land-use data into gridded land use.

(3) Surrogate tools: These tools use the Vector Tools and additional Java tools to help manage the creation and manipulation of spatial surrogates used in emissions modeling.

The Spatial Allocator and associated documentation is available for downloading from the CMAS Center (http://www.ie.unc.edu/cempd/projects/mims/spatial/), which is hosted by the IE at UNC-CH.

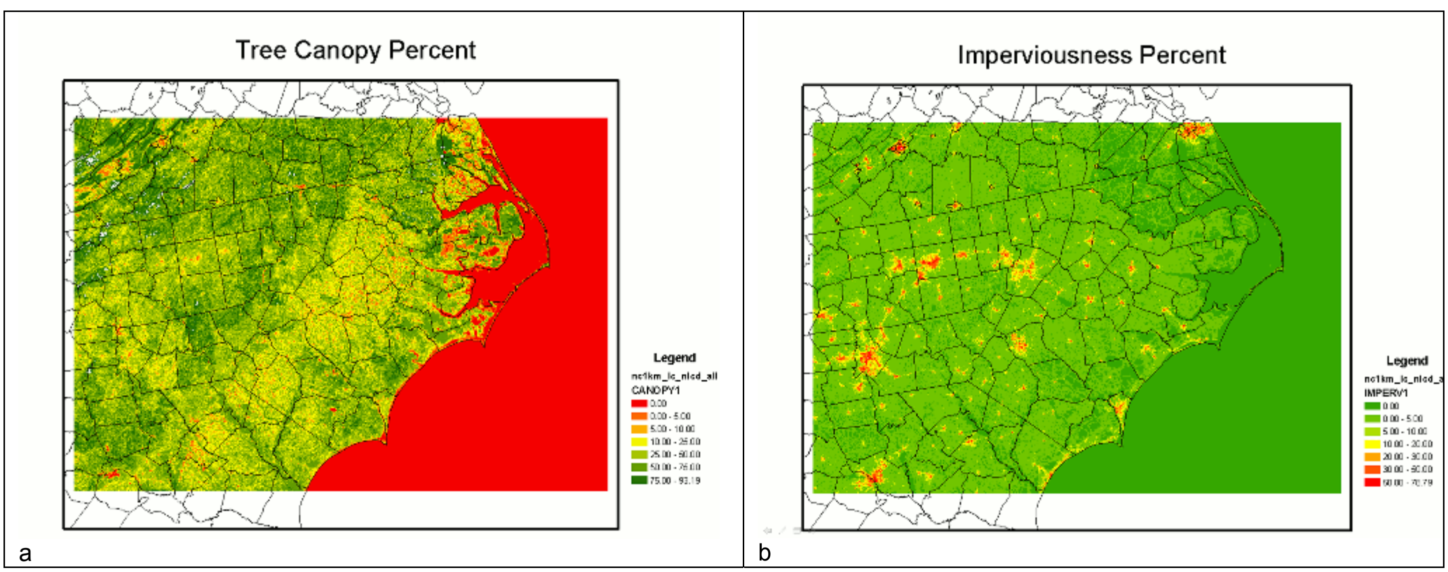


Figure 7-21. Spatial Allocator output from raster tools on North Carolina 1-km grids for fractional tree canopy coverage (a) and impervious surfaces (b) from NLCD data.

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APPENDIX A

Atmospheric Modeling and Analysis Division Staff Roster

(As of December 31, 2009)

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S.T. Rao, Director
David Mobley, Deputy Director
Patricia McGhee, Assistant to the Director
Sherry Brown
Wanda Payne (SEEP[1])
Ken Schere, Science Advisor
Gary Walter, IT Manager
Jeff West, QA Manager

Emissions and Model Evaluation Branch
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Wyat Appel
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Kristen Foley
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Atmospheric Exposure Integration Branch
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Jesse Bash
Jason Ching
Jim Crooks (Postdoctoral Fellow)
Robin Dennis
Val Garcia
Megan Gore (Contractor)
Vlad Isakov
Donna Schwede
Joe Touma
Myrto Valari (NRC[2] Postdoctoral Fellow)
David Heist, Fluid Modeling Facility
Ashok Patel (SEEP), Fluid Modeling Facility
Steve Perry, Fluid Modeling Facility
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Shawn Roselle
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Farhan Akhtar (ORISE[3] Postdoctoral Fellow)
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Russ Bullock
Barron Henderson (ORISE[3])
Jerry Herwehe
Chris Nolte
Tanya Otte
Rob Pinder
Jenise Swall
Ben Wells (Contractor)
Ying Xie (NRC[2] Postdoctoral Fellow)

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[1]SEEP - Senior Environmental Employee Program
[2]NRC – National Research Council
[3]ORISE – Oak Ridge Science and Education Program

APPENDIX B

Division and Branch Descriptions

Atmospheric Modeling Analysis Division

The 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.

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. AMDB 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.

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 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.

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 the 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.

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, 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 to 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

2009 Awards and Recognition

EPA Bronze Medal

Alice Gilliland, William Hutzell, Deborah Luecken, Rohit Mathur, Sergey Napelenok, Christopher Nolte, Tanya Otte, Thomas Pierce, Robert Pinder, Jonathan Pleim, George Pouliot, Shawn Roselle, Golam Sarwar, Kenneth Schere, Donna Schwede, David Wong, and Jeffrey Young – CMAQ Multi-Pollutant Model Team

ORD Technical Assistance to the Regions or Program Offices Award

Scientific and Technological Achievement Awards Winners

Deborah Luecken and William Hutzell – Development and analysis of air quality modeling simulations for HAPs

Scientific and Technological Achievement Awards Honorable Mention

Prakash Bhave – Receptor modeling of ambient PM data using positive matrix factorization: Review of existing methods

Golam Sarwar and Prakash Bhave – Modeling the effect of chlorine emissions on ozone levels over the eastern United States

Joe Touma – Modeling population exposures to outdoor sources of HAPs

Joe Touma – Impact of underestimating the effects of cold temperature on motor vehicle start emissions of air toxics in the United States

NERL Special Achievement Award

S.T. Rao – Goal 3: Leader in the Environmental Research Community

Ellen Cooter, Robin Dennis, Vlad Isakov, Thomas Pierce, Donna Schwede, and Joe Touma – Goal 4: Integrate Environmental Science and Technology to Solve Environmental Problems

Robert Gilliam, Alice Gilliland, Rohit Mathur, Christopher Nolte, Tanya Otte, Jonathan Pleim, Shawn Roselle, David Wong, and Jeffrey Young – Goal 5: Anticipate Future Environmental Issues

AMAD Awards

Best Paper: Alice Gilliland, Kristen Foley, Robert Pinder, S.T. Rao, and Jim Godowitch – Dynamic evaluation of regional air quality models: Assessing the changes in ozone stemming from changes in emissions and meteorology

Second Best Paper: Russ Bullock – The North American Mercury Intercomparison Study (NAMMIS): Comparisons of OC predications with measurements

Third Best Paper: AnnMarie Carlton, Rohit Mathur, and Shawn Roselle – CMAQ model performance enhanced when in-cloud secondary organic aerosol is included: Comparisons of OC predications with measurements

Teamwork Award: Steve Howard – Demonstrating the quality of unselfish teamwork within the Division to promote scientific research, as well as external and internal collaborations

Leadership Award: Prakash Bhave – Demonstrating leadership abilities in scientific research, external and internal collaborations, mentorship, and project management

APPENDIX D

2009 Publications

(Division authors are in bold.)

Journal Articles

Brixley, L., J. Richmond-Bryant, **D. Heist**, **G.E. Bowker**, **S.G. Perry**, and R.W. Wiener. The Effect of a Tall Tower on Flow and Dispersion Throught a Model Urban Neighborhood: Part 2. Pollutant Dispersion. *Journal of Environmental Monitoring*. Royal Society of Chemistry, Cambridge, UK, 11(12):2171-2179 (2009).

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APPENDIX E

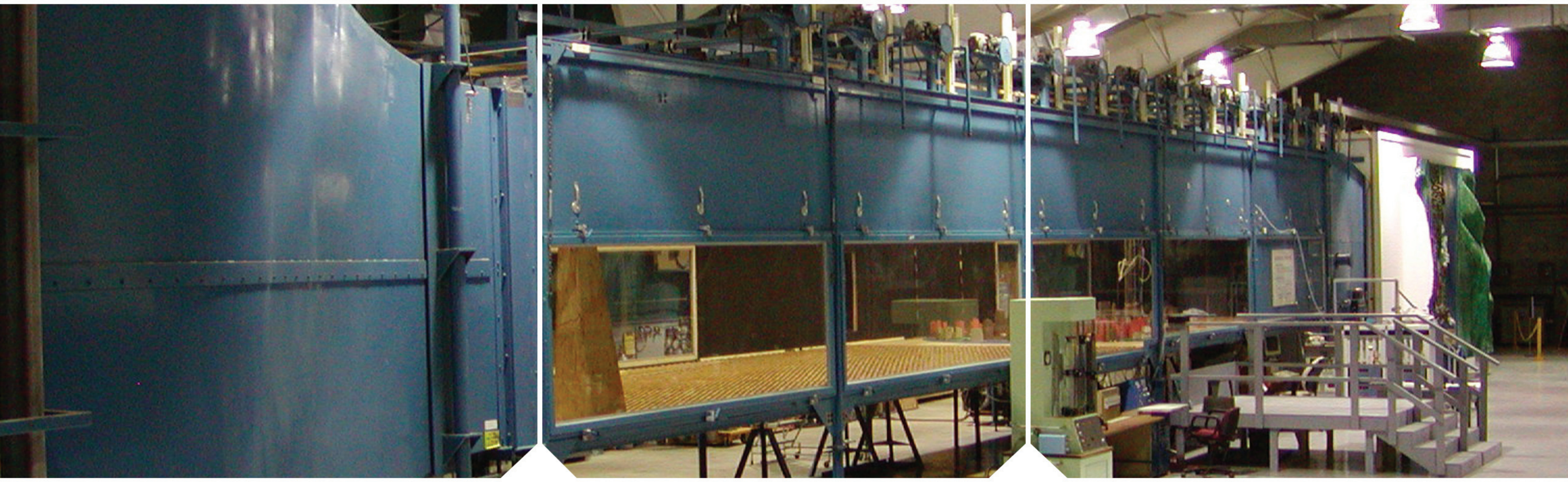
Acronyms and Abbreviations

ACM	Asymmetric Convective Model
AEIB	Atmospheric Exposure Integration Branch
AERMOD	American Meteorological Society/EPA Regulatory Model
AMAD	Atmospheric Modeling and Analysis Division
AMB	Applied Modeling Branch
AMDB	Atmospheric Model Development Branch
AMET	Atmospheric Model Evaluation Tool
AMS	American Meteorological Society
APM	Annual Performance Measure
APMB	Air-Surface Processes Modeling Branch
AQI	air quality index
AQMEII	Air Quality Model Evaluation International Initiative
ARL	Air Resources Laboratory
ASMD	Atmospheric Sciences and Modeling Division
BEIS	Biogenic Emission Inventory System
BELD3	Biogenic Emissions Land Cover Database, v3
BOSC	Board of Scientific Counselors
BRACE	Bay Regional Atmospheric Chemistry Experiment
CAA	Clean Air Act
CAAAs	Clean Air Act Amendments
CAIR	Clean Air Interstate Rule
CASTNET	EPA's Clean Air Status and Trends Network
CBL	convective boundary layer
CCSP	Climate Change Science Program
CCTM	CMAQ Chemistry-Transport Model
CDC	Centers for Disease Control and Prevention
CEM	Continuous Emission Monitoring
CHERUBS	Childhood Health Effects from Roadway and Urban Pollutant Burden Study
CIRAQ	Climate Impacts on Regional Air Quality
CIYA	Cash in Your Account
CMAQ	Community Multiscale Air Quality Model
CMAQ-TX	Community Multiscale Air Quality Model-Texas
CMAQ-UCD	University of California Davis aerosol module coupled to the Community Multiscale Air Quality Model
CMAS	Community Modeling and Analysis System
CO	carbon monoxide
CTM	Chemical Transport Model for Mercury
DDM	Decoupled Direct Method
DDM-3D	Decoupled Direct Method-3D
DEM	digital evaluation model
DOC	U.S. Department of Commerce
DTM	digital terrain model
EC	elemental carbon
EGU	electric generating units
EMEB	Emissions and Model Evaluation Branch
EMEP	European Monitoring and Evaluation Programme
EPA	U.S. Environmental Protection Agency
EPIC	Environmental Policy Integrated Climate Model
ESRP	Ecological Services Research Program
FDDA	4D data assimilation
FDEP	Florida Department of Environmental Protection
FEST-C	Fertilizer Emissions Scenario Tool for CMAQ
FHA	Federal Highway Administration
FMF	Fluid Modeling Facility
FML	Future Midwestern Landscapes
FRD	NOAA's Field Research Division
GBMM	Grid Based Mercury Model
GCM	global climate model
GFDL	Geophysical Fluid Dynamics Laboratory
GHG	greenhouse gas
GIS	geographic information system
GISS	Goddard Institute for Space Studies
GLIMPSE	Geos-CHEM LIDORT Integrated with MARKAL for the Purpose of Scenario Exploration
GPL	Gnu Public License
HAP	Hazardous Air Pollutant
HAPEM	Hazardous Air Pollutant Exposure Model
HEASD	Human Exposure and Atmospheric Sciences Division
HNO_3	nitric acid
HONO	nitrous acid
HO_2	hydroperoxyl radical
H_2O_2	hydrogen peroxide
HUC	hydrologic unit code
IC/BC	initial condition and boundary condition

ICARTT	International Consortium for Atmospheric Research on Transport and Transformation
IE	Institute for the Environment (UNC-CH)
IMPROVE	Interagency Monitoring of Protected Visual Environment Network
INTEX	Intercontinental Chemical Transport Experiment
INTEX-NA	Intercontinental Chemical Transport Experiment-North America
IPCC	International Panel on Climate Change
ISORROPIA	thermodynamics partitioning module
ITM	International Technical Meeting
LBC	lateral boundary condition
LES	large-eddy simulations
LIDAR	Light Detection and Ranging
LIDORT	Linearized Discreet Ordinate Radiative Transfer
LSM	land surface model
LW	longwave
MAE	mean absolute error
MCIP	Meteorology-Chemistry Interface Processor
MDA	maximum daily average
MDN	Mercury Deposition Network
MEGAN	Model of Emissions of Gases and Aerosols from Nature
MLBC	multilayer biochemical model
MM5	fifth generation of the Penn State/UCAR Mesoscale Model
MPI	message passing interface
MYSQL	open source database software
NAAQS	National Ambient Air Quality Standard
NADP	National Acid Deposition Program
NAM	North American Mesoscale
NAMMIS	North American Mercury Model Intercomparison Study
NARSTO	formerly the North American Research Strategy for Tropospheric Ozone
NAS	National Academy of Sciences
NASA	National Aeronautics and Space Administration
NATO	North Atlantic Treaty Organization
NBP	NO_x Budget Trading Program
NCAR	National Center for Atmospheric Research
NEI	National Emission Inventory
NERL	National Exposure Research Laboratory
NGA	National Geospatial Agency
NH_3	ammonia
NLCD	National Land Cover Data
NMM	Nonhydrostatic Mesoscale Model
NO	nitrogen oxide
NO_2	nitrogen dioxide
NO_3	nitrate
N_2O_5	dinitrogen pentoxide
NO_x	oxides of nitrogen
NO_y	oxidized nitrogen
NOAA	National Oceanic and Atmospheric Administration
NOAH	NOAA's land surface model
NPS	National Park Service
Nr	reactive nitrogen
NRMRL	National Risk Management Research Laboratory
NUDAPT	National Urban Database and Access Portal Tool
O_3	ozone
OAP	Office of Air Programs
OAQPS	Office of Air Quality Planning and Standards
OC	organic carbon
OH	hydroxy radical
ORD	Office of Research and Development
PAH	polycyclic aromatic hydrocarbon
PAN	Peroxyacyl nitrate
PBL	planetary boundary layer
PM	particulate matter
PMML	Predictive Model Markup Language
PRISM	Parameter-Elevation Regressions on Independent Slopes Model
PX LSM	Pleim-Xiu Land Surface Model
QUIC	Quick Urban Industrial Complex
Qv	Water vapor mixing ratio
RCM	Regional Climate Model
RELMAP	Regional Lagranian of Air Pollution
REMSAD	Regional Modeling System for Aerosols and Deposition
RMSE	root mean squared error
SCIAMACHY	Scanning Imaging Absorption Spectrometer for Atmospheric Cartography
SEARCH	SouthEastern Aerosol Research and Characterization Study
SGV	subgrid variability
SHEDS	Stochastic Human Exposure and Dose Simulation
SIP	State Implementation Plans
SMOKE	Sparse Matrix Operator Kernel Emissions
SO_2	sulfur dioxide
SO_4	sulfate
SOA	secondary organic aerosol
SOA_{cld}	secondary organic aerosol formed in clouds
SPS	Science for Peace and Security
STAR	Science To Achieve Results
STENEX	Stencil Exchange
STN	Speciated Trends Network
SW	shortwave
TBEP	Tampa Bay Estuary Program
TEAM	Trace Element Analysis Model
TES	Tropospheric Emission Spectrometer

TexAQS	Texas Air Quality Study
TM	Thematic Mapper
TMDL	total maximum daily load
UCP	urban canopy parameter
UNC-CH	University of North Carolina at Chapel Hill
USGS	U.S. Geological Survey

VERDI	Visualization Environment for Rich Data Interpretation
VOC	volatile organic compound
WDT	Watershed Deposition Tool
WRF	weather research and forecasting
WSOC	water soluble organic compound
YSU	Yonsei University



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