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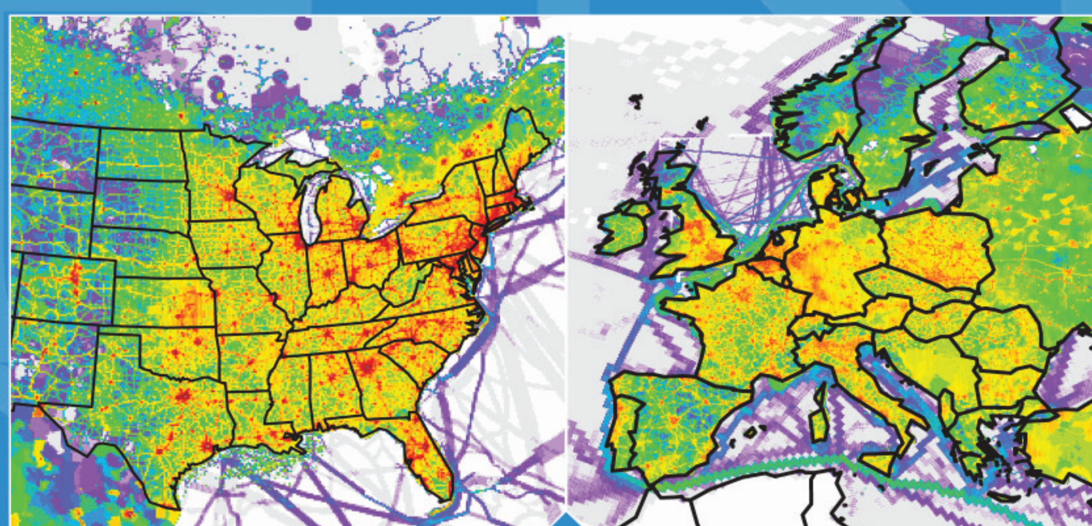
Summary Report of the Atmospheric Modeling and Analysis Division's Research Activities for 2010



Office of Research and Development
National Exposure Research Laboratory

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Summary Report of the Atmospheric Modeling and Analysis Division's Research Activities for 2010

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The information in this document has been funded by the U.S. Environmental Protection Agency. It has been subjected to the Agency's peer and administrative review and has been approved for publication as an EPA document. Mention of trade names or commercial products does not constitute endorsement or recommendation for use.

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 reducing 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 the magnitude of the air pollution problem and 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 framework 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 AMAD for calendar year 2010.

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1.0 Introduction

The research presented here was performed by the Atmospheric Modeling and Analysis Division (AMAD) of the National Exposure Research Laboratory (NERL) in the U.S. Environmental Protection Agency's (EPA's) Office of Research and Development (ORD) in Research Triangle Park, NC. This report summarizes the research and operational activities of the Division for calendar year 2010.

The Division structure includes the following four research branches.

1. Atmospheric Model Development Branch (AMDB)
2. Emissions and Model Evaluation Branch (EMEB)
3. Atmospheric Exposure Integration Branch (AEIB)
4. 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 herein (Appendix E).

The Division's role within the EPA NERL's "Exposure Framework" and 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 four research branches, the Division provides atmospheric sciences expertise, air quality forecasting support, and technical guidance on the meteorological and atmospheric pollution 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 research 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.

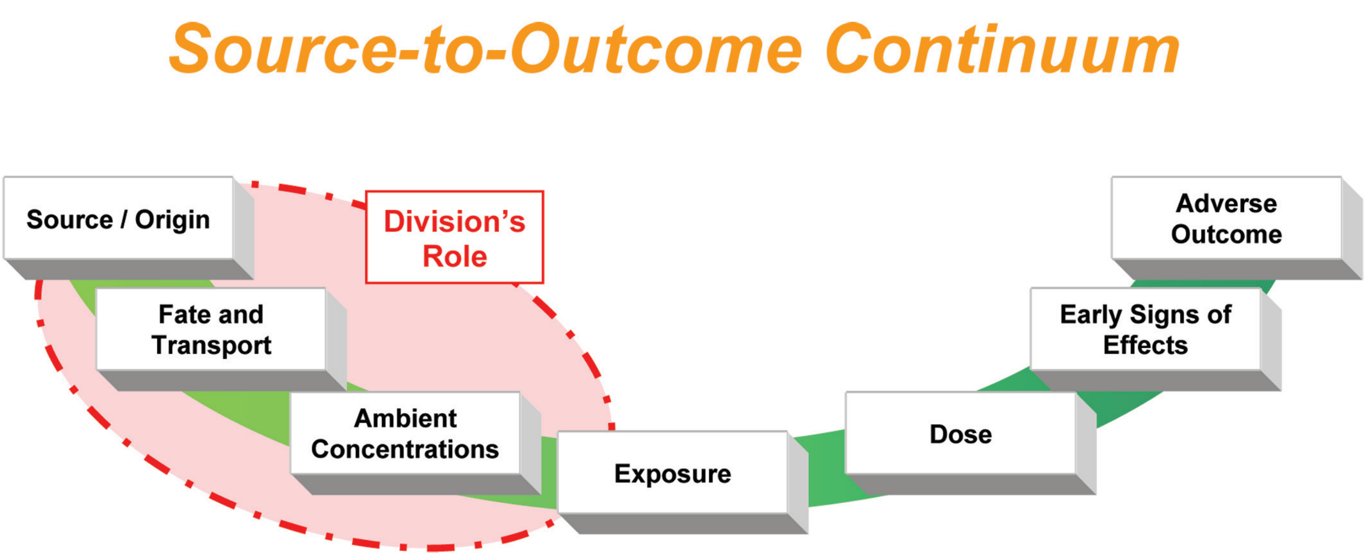

Figure 1-1. AMAD's role in the source-exposure-dose-effects continuum from the atmospheric science perspective. (Adapted from "A Conceptional Framework for U.S. EPA's National Exposure Research Laboratory," EPA/600/R-09/003, January 2009)

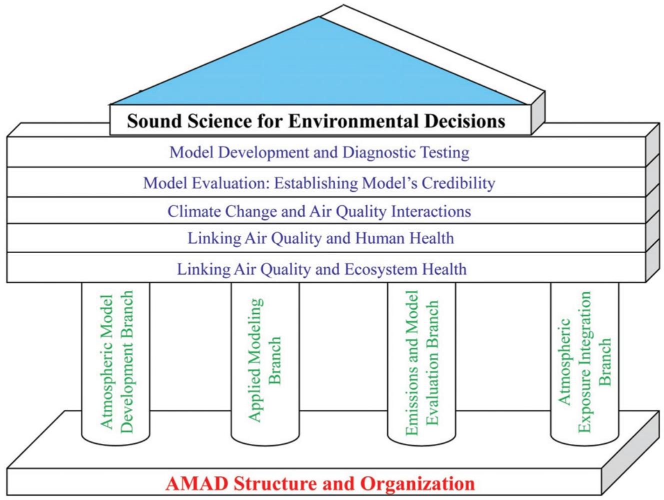

Figure 1-2. AMAD's structure and organization.

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

- Over the next 2 to 3 years, who are the major clients, and what are their needs?
- What research investments are needed to further the science in ways that help the clients? How will we lead or influence the science in this area?
- What personnel expertise, resources, and partners are needed to do this work?
- Does the proposed work fall within the current scope and plans of existing projects, or would personnel resources need to be shifted from other projects to make this happen?

The result is a research strategy for meeting user needs that is built around the 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 2010. The integration of research activities is illustrated in Figure 1-3. This report includes descriptions of research and operational efforts in air pollution meteorology, air quality model development, and 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).

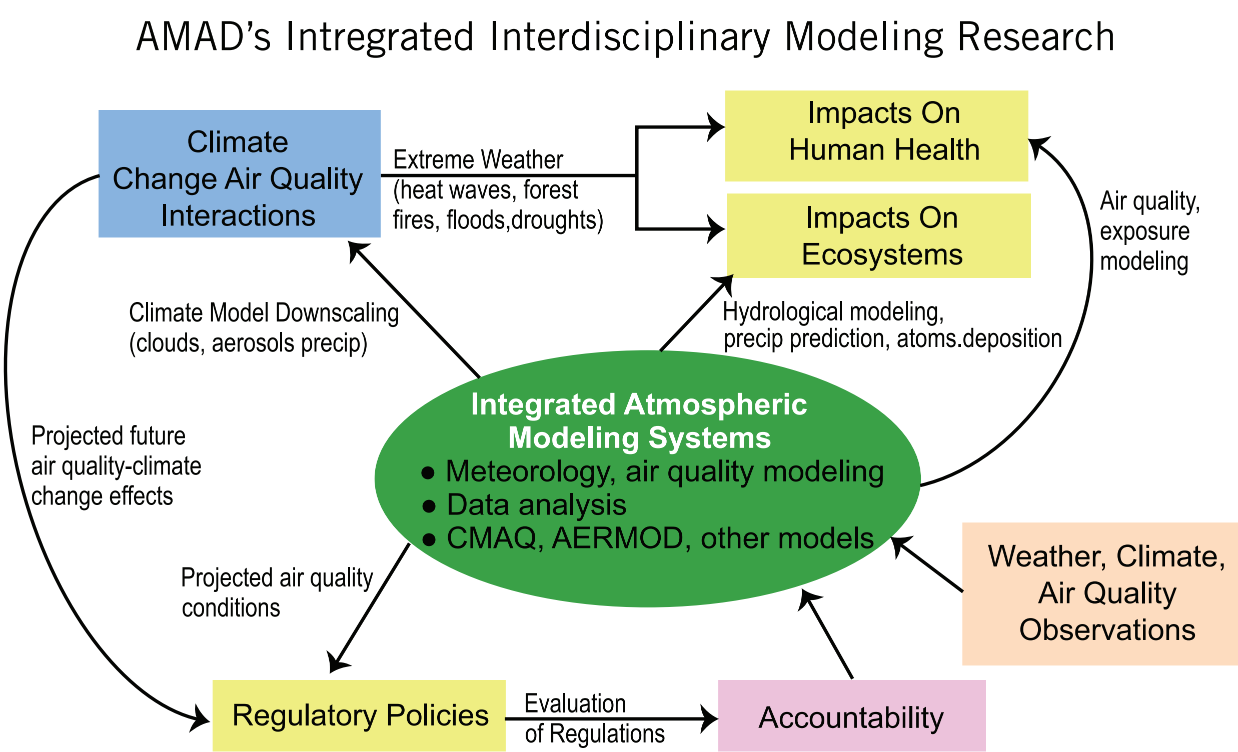

Figure 1-3. AMAD's integrated interdisciplinary modeling research.

2.0 Summary of Accomplishments for the Division

As a summary of and introduction to the annual report for 2010, the following Division accomplishments are highlighted.

2.1 Division-Wide Accomplishments

1. **Issue:** Strategic thinking regarding integrated transdisciplinary approaches to solving environmental problems.

   Accomplishment: Coordination of various articles for the November 2010 issue of the *Air and Waste Management Association's Environmental Manager (EM)* on Integrated Transdisciplinary Research

   Findings: To properly address complex environmental problems, there is growing consensus among the research community that we must move away from the current single-pollutant, single-medium, and single-discipline approach to problem solving with a more integrated transdisciplinary approach. The articles in this issue address the need for integrated transdisciplinary research to solve the environmental problems of tomorrow.

   Impact: This *EM* special issue provides a thought -provoking set of articles for managers to consider integrated transdisciplinary research for problem solving—with examples of complex environmental problems confronting us now (e.g., climate change, transportation fuels in the 21st century, human exposure near roadways and in urban environments).

2. **Issue:** Developing AMAD's strategic research plan

   Accomplishment: A comprehensive Research Strategy was developed outlining the Division's core research in atmospheric model development and evaluation, as well as three major application areas in which air quality models are used for human exposure, ecosystems exposure, and climate change air quality assessments.

   Findings: AMAD's research directions were articulated in three white papers on emerging application areas. These white papers were reviewed by an external panel of experts. The panel's report was complimentary of the Division's proposed research and included constructive comments and suggestions.

   Impact: AMAD's Strategic Plan was made publicly available to promote transparency in the Division's research planning process and facilitate collaborations both within the Laboratory and Agency as well as with external partners. The Strategic Plan positioned AMAD to adapt to emerging research directions within ORD.

3. **Issue:** A key uncertainty in quantification of aerosol radiative effects and their impacts on climate change is the verification of the spatial and temporal variability in its magnitude and directionality and, consequently, its cumulative effect on the radiation balance of the earth-atmosphere system.

   Accomplishment: A research proposal was developed for a comprehensive observational-modeling study to investigate and verify aerosol radiative effects for past air quality conditions (e.g., changes in sulfate burden arising from sulfur dioxide [SO_2] reductions as a result of Title IV of the Clean Air Act [CAA]).

   Findings: Based on a rigorous peer review, the proposal was recommended for funding as a Department of Energy-EPA Interagency Agreement (IAG). This project will support three post doctoral fellows.

   Impact: The successful attainment of the project goals will help quantify the impacts of tropospheric aerosol loading on atmospheric radiation budgets, and also help build confidence in the use of such modeling tools (e.g., the two-way WRF-CMAQ) for climate projection scenarios and emission management options.

4. **Issue:** Systematic intercomparisons and evaluations are needed for regional air quality models over different continental regions.

   Accomplishment: The second Air Quality Model Evaluation International Initiative (AQMEII) Workshop was held September 26 and 27, 2010, in Turin, Italy. The meeting provided a venue for the 50 participants to share and discuss progress on model simulations and data analysis related to this model-intercomparison study.

   Findings: The workshop provided a venue to discuss and finalize activities of the first phase of model intercomparison and evaluation. All participating groups made a commitment to submit their model data to a central site by December. Participants also developed plans for joint publications for a special issue in *Atmospheric Environment*; manuscripts are due in May 2011.

   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.

5. **Issue:** Understanding global air pollution issues to develop sustainable solutions for air quality and climate.

   Accomplishment: Developed a collaborative proposal with N.C. State University (NCSU) and the University of North Carolina-Chapel Hill (UNC-CH) to host a U.S.-India workshop on air quality; the proposal was funded by the National Science Foundation (NSF).

   Findings: The rapid growth of the Indian economy, spurred by industrial and urban expansion, has been accompanied by environmental stresses, particularly in air quality. The current capacity in India in research and operational aspects of air quality forecasting and regulatory management needs further enhancement. A workshop, to be held March 14-24, 2011, with partial support from the NSF and the U.S. Department of Energy, will bring together several experts from the United States and India with a common vision for identifying priority areas of research and development in the air quality and climate area, and a commitment for long-term collaboration.

   Impact: To engage participation by emerging scientists in the field, the workshop will include three days of invited lectures and presentations, followed by a 7-day hands-on training segment. This portion of the workshop will provide training to participants on a publicly available suite of numerical models (i.e., WRF, CMAQ) that are used world wide in a variety of air quality applications, from basic research to local- and regional-level planning and management. The workshop will strive to improve understanding of the emission sources and meteorological conditions that contribute to regional-to-urban-scale air quality and climate issues of relevance to protecting public health and the environment.

6. **Issue:** Supporting international cooperation on air pollution modeling under the North Atlantic Treaty Organization (NATO).

   Accomplishment: Contributed substantially to the organization and program development for the September 27 to October 1, 2010, 31st NATO/Science for Peace and Security (SPS) International Technical Meeting (ITM) on Air Pollution Modeling and its Applications, in Turin, Italy.

   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: More than 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. All papers are subject to peer review by the scientific community and will be published in a book under the NATO banner.

7. **Issue:** Promoting collaboration between U.S. and U.K. scientists on air pollution exposure research.

   Accomplishment: Nearly 50 international experts, including NERL scientists and others from the U.K. Department for Environment, Food, and Rural Affairs, and the Environmental Agency for England and Wales, met during December 6-10, 2010, in London to discuss progress in collaborations to improve and apply air quality models.

   Findings: NERL/AMAD scientists made several presentations at the workshop to promote collaborations in areas of air pollution modeling and its use to guide policy development, local-scale air pollution modeling and analysis, air pollution climate interactions, and air quality human health linkage studies.

   Impact: This collaboration is proposed in recognition of the common concerns for serious health, welfare, and economic impacts of atmospheric pollution. This collaboration recognizes the benefit of defining a research enterprise that involves joint interests and lays the foundation for a co-sponsored program that would improve efficiencies, and avoid redundant research activities and products through the leverage of resources and capabilities within each organization.

2.2 Model Development and Diagnostic Testing

1. **Issue:** Scientifically credible air quality models are needed both for research purposes as well as regulatory applications in the implementation of the National Ambient Air Quality Standards.

   Accomplishment: An interim version of the Community Multiscale Air Quality (CMAQ) modeling system (CMAQv4.7.1) was released publicly.

   Findings: CMAQv4.7.1 incorporated scientific advancements in the representation of 3D advective transport, in numerical solution of the aqueous-phase chemistry, incorporation of tools to assist in diagnostic analysis, and several code fixes recommended by the CMAQ user community.

Impact: CMAQv4.7.1 is being used by the Office of Air Quality Planning and Standards (OAQPS) in the regulatory impact analysis for the Transport Rule, Utility MACT Rule, and the Greenhouse Gas Rule.

2. **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: The CMAQ model was extended to hemispheric scales. Annual simulations for the year 2006 were completed, and model predictions were compared with a variety of measurements from surface, aircraft, and satellite-based platforms.

   Findings: Air quality modeling results for O_3, PM, Hg, and other pollutants over the United States are sensitive to the specification of boundary concentrations. Modeling over the hemispheric domain enables robust examination of modeled processes from an atmospheric budget perspective.

   Impact: CMAQ modeling capability has now 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.

3. **Issue:** The combustion of engineered nanomaterials in diesel fuel can significantly alter ambient exposures to O_3, fine PM, and hazardous air pollutants, with potential health consequences.

   Accomplishment: Completed Annual Performance Measure (APM) 366: Model the local-scale fate and transport of a combusted nanomaterial and its effect on regional-scale air quality.

   Findings: If nanocerium additives receive widespread use, cerium emissions from the United States will increase by a factor of 25. Ambient air concentrations of cerium could exceed 20 ng/m^3 in major cities, representing a 100-fold increase from their current levels.

   Impact: Regulators in the Office of Transportation and Air Quality can now estimate the large-scale consequences of approving versus disapproving these additives in the E211b registration process. In addition, EPA health scientists, who are seeking to develop realistic scenarios for assessing the health impacts of nanocerium additives, now have reasonable estimates of the level to which humans would be exposed in the future if the additives are registered and widely used.

2.3 Air Quality Model Evaluation

1. **Issue:** Despite a reliance on regional air quality models by the international community, methods for evaluating the integrity of these models remain primitive.

   Accomplishment: Under the Air Quality Model International Initiative (AQMEII), an international consortium of model evaluation experts representing 22 countries began to evaluate their models for the North American and European continents. AQMEII accepted an invitation to publish a series of papers in a special issue of *Atmospheric Environment.*

   Findings: Preliminary results on regional air quality model evaluations across North America and Europe were presented at an AQMEII data analysis workshop in Turin, Italy, during September 2010. The importance of boundary conditions on the accuracy of model performance was stressed.

   Impact: AQMEII is facilitating the sharing of improved model evaluation techniques, which will lead to improvements in regional air quality model simulations and characterization of model uncertainties for communication to environmental decisionmakers.

2. **Issue:** Implementing effective emission control strategies to manage the effects of multipollutant mixtures requires air quality models that can predict the response of pollutant levels to changes in emissions and meteorology.

   Accomplishment: Several peer-reviewed articles documenting the dynamic response of the CMAQ model in simulating the weekly and multiannual variations of O_3 precursor emissions were published in the scientific literature.

   Findings: Although the CMAQ modeling system showed skill at replicating the overall response of O_3 and Oxides of Nitrogen (NO_x) concentrations because of changes in emissions and meteorology, potential weaknesses were identified with the characterization of O_3 boundary conditions and the characterization of Volatile Organic Compound (VOC) and NO_x emissions.

   Impact: The research findings are informing the program office regarding the uncertainty of regional air quality models for O_3 attainment demonstrations and are helping shape priorities for model development, particularly in the areas of O_3 boundary conditions and weekly cycles in O_3 precursor emissions.

3. **Issue:** The quantification of uncertainty in air quality modeling results has been an important but elusive goal.

Accomplishment: The Direct Decoupled Method (DDM) was used to provide a probabilistic-based dynamic evaluation of the CMAQ model, and the results were summarized in a manuscript submitted to *Atmospheric Environment*.

Findings: In addition to uncertainties in NO_x emissions, uncertainties in VOC emissions and boundary conditions were identified as areas needing further quantification.

Impact: Characterizing the dynamic response of O_3 to changes in emissions suggests that uncertainties in key inputs, such as emissions and boundary conditions, should be explicitly considered in regional air quality modeling simulations.

4. **Issue:** The public release of CMAQv5.0 needs to be evaluated.

   Accomplishment: The evaluation team began working closely with the development team and has developed a schedule and protocol for model evaluations.

   Findings: Improved communication between CMAQ model developers and evaluators will be accomplished via an internal Wiki site.

   Impact: It is anticipated that a robust model evaluation will be accomplished in an efficient and timely manner to support the release of CMAQv5.0 to the air quality modeling community.

2.4 Air Quality-Global Climate Change

1. **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: Completed APM 284: Test model linkage approaches for downscaling global to regional climate with WRF. WRF downscaling has been tested using both global reanalysis data and output from the Goddard Institute for Space Studies (GISS) Model E Global Climate Model (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 suggests that WRF is able to provide the needed regional texture to a simulated climate, while maintaining fidelity at larger scales to the driving fields. Results are sensitive to the nudging parameters; thus, more testing is needed to determine best configuration for refined climate modeling.

   Impact: AMAD's experiments with data assimilation in the process of downscaling from global to regional climate models 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.

2. **Issue:** The WRF model originally was designed for short-term numerical weather prediction. It was not designed as a regional climate model. Certain aspects of the model, particularly its radiation budget and its treatment of soil heat and moisture fluxes, must be examined and possibly improved for long-term simulations.

   Accomplishment: Two 20-year continuous WRF simulations have been completed using different radiation parameterizations available in WRF. These simulations did not use any nudging.

   Findings: The top-of-atmosphere and surface radiation fields, as well as cloud cover, from these simulations will be compared with 5 years of satellite observations.

   Impact: This work will add confidence to future regional climate simulations conducted by WRF and will facilitate its use as a tool to understand climate-chemistry interactions.

3. **Issue:** Adjoint methods can be used to link the impacts of pollution to sources. Building the adjoint of a complex model like CMAQ requires a wide range of expertise and a community approach.

   Accomplishment: Convened a workshop with international participation on the development of CMAQ-adjoint methods for advanced sensitivity analysis.

   Findings: The CMAQ-adjoint workshop brought together model developers for a intense development session, where the components of the CMAQ-adjoint were assembled together for the first time. Second, a panel discussion was convened. Participants from OAQPS and academia outlined the use of CMAQ-adjoint to address air pollution, ecosystem impact, and climate change mitigation needs.

   Impact: This meeting fostered the community of model developers who are continuing to develop the model to better address air pollution, ecosystem impact, and climate change mitigation needs.

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 quality 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 O_3 feedback on longwave (LW) radiation. Indirect feedback is under development.

Findings: A prototype two-way coupled atmospheric modeling system, based on the WRF and CMAQ models, has been developed and further tested. Direct feedback of aerosols on SW radiation has been successfully implemented. Initial testing suggests that these effects can be large in regions with significant aerosol loading. Comparisons with limited measurements show improvements in simulation skill for SW radiation and 2-m temperature. Inclusion of direct effects leads to suppression of simulated Planetary Boundary Layer (PBL) heights which can then impact simulated air quality.

Impact: The two-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.

2.5 Linking Air Quality to Human Exposure

1. **Issue:** Cohort studies designed to estimate human health effects of exposures to urban pollutants require accurate determination of ambient concentrations to minimize exposure misclassification errors. However, it is often difficult to collect concentration information at each study subject location. In the absence of complete subject-specific measurements, land-use regression (LUR) models frequently have been used for estimating individual levels of exposures to ambient air pollution. The LUR models, however, have several limitations mainly dealing with extensive monitoring data needs and challenges involved in their broader applicability to other locations.

   Accomplishment: Critically evaluated the LUR model being used by the community.

   Findings: A 2010 publication in *Atmospheric Environment* by M. Johnson, V. Isakov, J. Touma, S. Mukerjee, and H. Özkaynak presents the results of evaluation of land use regression models used to predict air quality concentrations in an urban area. Modeled hybrid air quality concentrations of $PM_{2.5}$, NO_x, and benzene in New Haven, CT, were used as pseudo-observations to develop and evaluate the different LUR models. LUR models appeared to perform well in the training datasets. However, when these LUR models were tested against independent hold-out (test) datasets, their performance diminished considerably. This indicated that that complex emissions and atmospheric processes resulting from meteorological, transport, and diffusion and chemical mechanisms can severely limit the predictive power of most LUR-based modeling applications. The paper also provided recommendations on future research to examine best ways to augment basic LUR models with site-specific source-receptor information generated from air quality models and to test how one might transfer LUR model results across different geographical locations or even countries.

   Impact: AMAD's results confirm the challenges facing the LUR community in attempting to fit empirical response surfaces to spatially and temporally varying pollution levels using LUR techniques that are site dependent. These results also illustrate the potential benefits of enhancing basic LUR models by utilizing air quality modeling tools or concepts to improve the models' reliability or transferability. The information derived from this study will be used by EPA as a resource for developing appropriate tools in support of exposure assessments. Through this effort, the Divison has helped advance exposure science.

2. **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 for near-road exposures is needed.

   Accomplishment: For the near-road research program, developed wind tunnel and field study databases to improve model algorithms for urban roadways in support of human exposure and health assessments.

   Findings: A 2009 Journal of the Air & Waste Management Association paper by V. Isakov and co-investigators presents an innovative methodology to link regional- and local-scale air quality models with human exposure models. It shows the presence 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: 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. 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 in the Sierra Club litigation. The Federal Highway Administration requested EPA's guidance and expertise in implementing their near road research requirements as part of this litigation, and an IAG 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. Through this work, the Division has helped to advance exposure science.

3. **Issue:** General consensus exists that populations spending significant amounts of time near major roads face increased risks for several adverse health effects. State and local agencies are interested in considering a roadway design that includes the presence of roadside vegetation as a means of mitigating air pollutant concentrations near roads. However, there are potential advantages and disadvantages of implementing vegetation to mitigate near-road air quality impacts. Vegetation in urban settings can provide numerous benefits beyond air quality improvements, such as ecosystem services, associated with improved physical and mental health and community vitality. Potential disbenefits include pollen production, water demand, channeling of invasive pests and fire into the urban environment, and exacerbation of sprawl by distancing buildings and other land use activities from roadways. Trees also may obstruct visibility on the road and reduce wind speed, cause damage or injury by falling, and create slippery conditions from dropped debris. Ideally, a large suite of costs and benefits should be evaluated in concert to optimize the use of urban vegetation to protect human health and promote sustainable communities. Clearly, more research is needed to assess the role of vegetation in mitigating air quality impacts from traffic emissions.

   Accomplishment: As a first step in evaluating this concept, in April 2010, AMAD scientists in collaboration with scientists from NERL, National Risk Management Research Laboratory (NRMRL), and National Health and Environmental Effects Research Laboratory (NHEERL) organized a workshop on the Role of Vegetation in Mitigating Air Quality Impacts from Traffic Emissions. The workshop included representatives from government agencies, academia, State and local agencies, and nongovernmental environmental organizations with expertise in air quality, urban forestry, ecosystem services, and environmental policy. The participants reviewed the current science and identified future activities in evaluating the potential role of vegetation in mitigating near-road air pollutant concentrations.

   Findings: A multidisciplinary group of researchers and policymakers met to discuss the state of the science regarding the potential of roadside vegetation to mitigate near-road air quality impacts. The results are summarized in a journal article in the January 2011 issue of *EM* by Richard Baldauf, Laura Jackson, Gayle Hagler, Vlad Isakov, Greg McPherson, David Nowak, Thomas Cahill, Max Zhang, Rich Cook, Chad Bailey, and Periann Wood.

   Impact: This workshop was a first step in evaluating the potential role of vegetation in mitigating near-road air pollutant concentrations. A multidisciplinary group of researchers and policymakers from government agencies, academia, State and local agencies, and nongovernmental environmental organizations with expertise in air quality, urban forestry, ecosystem services, and environmental policy reviewed the current science and identified future activities to further assess the role of vegetation in mitigating air quality impacts from traffic emissions.

4. **Issue:** In its mission to protect human health and the environment, EPA implemented the NO_x Budget Trading Program (NBP) to reduce the emissions of NO_x and the secondarily formed O_3. These pollutants and their precursors can be transported downwind, contributing to pollutant levels at locations far from the emission sources, potentially impacting human health in downwind areas. This study investigated the health impacts in New York State from exposure to polluted air parcels transported from the Midwest.

   Accomplishment: This study developed and applied a methodology to identify and target the transport of polluted air parcels and demonstrated that the risk for hospital admission resulting from respiratory-related illness was increased in New York State on those days that the air parcel originated over the polluted Ohio River Valley.

   Findings: The results of this analysis indicate that the risk of being hospitalized for respiratory-related illness in New York State is greater on those days when air is transported from the Midwest into New York State as compared to days when air is transported from the North. Using a refined method to examine air parcels moving through a boundary drawn around high-emitting power plants in the midwestern United States resulted in stronger associations across more regions (significant odds ratios ranging from 1.06 to 1.16 for the entire study time period for six of the eight New York State regions). An assessment of temperature and its impact on the odds ratio calculation in the New York City metropolitan region indicates that temperature alone does not explain the increased association between air pollution and respiratory-related hospital admissions.

Impact: This technique is unique in that it examines the health impact of air pollution that can travel hundreds of kilometers downwind of its source region. It is one of the first studies to associate transported air pollution with a health end point in this manner. The approach developed by AMAD can be used as an indicator of exposure from transported air pollution.

2.6 Linking Air Quality and Ecosystems

1. **Issue:** Full implementation of the bi-directional flux approach for ammonia (NH_3) in CMAQ requires grid-level information regarding fertilizer application timing, depth, and amount for each agricultural crop in the model domain. This information needs to be produced in a nationally consistent, process-based manner that can respond to changes in weather/climate, atmospheric deposition, and land use/land cover conditions.

   Accomplishment: The Fertilizer Emission Scenario Tool for CMAQ (FEST-C) and associated agricultural fertilizer modeling system (AFMS) were developed to produce the input information needed for implementation of bi-directional CMAQ (APM 372). FEST-C is the interface that enables the user to identify the combination of preexisting weather, soil, land use/land cover, and agricultural management files that best describe the emissions setting of interest and to execute the programs that estimate the information needed by CMAQ. The tool produces a CMAQ-ready input file for use in bi-directional CMAQ, as well as other supporting variables of interest to Ecological Services Research Program (ESRP) partners that can be read, analyzed, and displayed using the Visualization Environment for Rich Data Interpretation (VERDI) visualization and analysis tool.

   Findings: FEST-C was developed successfully, and a beta version was released in September 2010. The test client set indicated that the current capabilities appear to be adequate. However, the management input files need further improvement and evaluation to fully meet the needs of our ESRP partners and to reduce current emission uncertainties in the CMAQ NH_3 bi-directional model.

   Impact: Development of the FEST-C/AFMS system informed the design and execution of the CMAQ bi-directional NH_3 pilot study completed in FY10. Completion of the beta version of FEST-C/AFMS has laid the foundation for completing the full implementation of bi-directional CMAQ for NH_3 in 2011. Completion of the tool increased the visibility of AMAD within the ESRP, and requests for fertilizer and supplemental variable information have been received from scientists working with the National Atlas, Future Midwest Landscapes, and Albemarle-Pamlico Watershed Study teams to support their nitrogen budget, watershed, and water quality modeling work. A summary of the FEST-C/AFMS system was presented at the 31st International Meeting on Air Pollution Modeling and its Application, September 27 to October 1, 2010, in Turin, Italy.

2. **Issue:** Annual Mercury wet deposition from CMAQ 4.7 multipollutant was biased high when compared with the Mercury Deposition Network (MDN) observations, and, when the CMAQ 4.7 was run at hemispheric scale, mercury was depleted during the period of the run, indicating that the mercury sinks were not balanced by emissions. Oxidized mercury (Hg[II]) is soluble and reactive and removed from the atmosphere much more rapidly than elemental mercury (Hg[0]). The biases in mercury wet deposition and depletion of mercury in the hemispheric runs were the result of the parameterized oxidation rates of Hg[0].

   Accomplishment: Hg[0] has an atmospheric lifetime ranging from 0.5 to 1 year, and Hg[II] has an atmospheric lifetime of days. The relatively slow oxidation rates of Hg[0] to Hg[II] and differences in atmospheric lifetimes required the simulation and evaluation of this chemical mechanism on two scales. A model sensitivity study of mercury oxidation rates was run at the hemispheric and continental United States (CONUS) scales. At the hemispheric scale, the budget of mercury sources and sinks and the model's ability to sustain ambient concentrations near the global background were used to evaluate changes to the mercury oxidation rates. Identical runs were conducted at the CONUS scale and evaluated against MDN and Ambient Mercury Network (AMNet) observations.

   Findings: A controversial gas phase reaction was found to be driving both the depletion of mercury at the hemispheric scale and model deposition biases at the regional scale. The reaction rates in the mercury chemical mechanism in CMAQ and all other chemical transport models remain uncertain and high-quality measurements of mercury oxidation and reduction rates from chamber studies and estimates using computational chemistry are needed to further reduce uncertainty in the model results.

   Impact: This refined chemical mechanism reduced the biases in the modeled wet deposition, improved the hemispheric mercury budget, and better captured the seasonal variation in mercury wet deposition. The mercury chemical mechanism was refined based on the sensitivity study that improved the hemispheric mercury budget and reduced model deposition biases to be included in CMAQ 5.0 and for use in model simulations in support of the EPA's toxics rule.

3. **Issue:** FY10 research published by AMAD scientists suggests that full implementation of the bi-directional flux approach for NH_3 in CMAQ would alter the temporal and spatial simulation of ammonia deposition contributing to excess nutrient deposition to aquatic and terrestrial ecosystems and the formation of fine particulates. The research conclusions were based on a 1-mo simulation, however. Full implementation of this approach into a research version of CMAQ will not be complete until 2011. An eastern U.S. pilot study was developed and executed for an annual simulation to inform the implementation process and to provide initial estimates of the potential value of the investment to incorporate bi-directional exchange of ammonia in CMAQ.

   Accomplishment: A pilot study was designed and executed for the eastern U.S. 12-km CMAQ grid. Preliminary algorithms published in 2010 were added to CMAQ. Parameter time series were estimated offline for the full CMAQ domain and were then combined with these algorithms within CMAQ to estimate ammonia emissions from agricultural soils amended with inorganic nitrogen, canopy uptake, and net flux from the surface.

   Find**ings:** The pilot study suggests that the bi-directional NH_3 flux CMAQ will reduce current unidirectional estimations of nitrogen dry deposition by a factor of two at background sites and by a factor of three for the model domain as a whole. Partitioning of nitrogen to the aerosol phase and wet deposition is increased. Transport of reduced nitrogen out of the modeling domain is increased by about 10%. Precipitation corrected wet deposition and ambient aerosol estimates are improved relative to observations when this approach is used.

   Impact: Numerous "lessons learned" were transferred to the full model implementation process. Findings of the pilot were presented to OAQPS, which now is considering their implications for ongoing rulemaking and the possible contributions of bi-directional CMAQ results to the development of new secondary standards. Four manuscripts are in development, and numerous presentations at professional meetings have been made to begin documenting the new algorithms.

4. **Issue:** To meet total maximum daily load (TMDL) targets to restore water quality, it is necessary to understand the sources of the deposition-driven loading of nitrogen to water bodies, including state and sector-level sources of atmospheric deposition. This requires a sensitivity analysis with an air quality model. "Brute force" sensitivity approaches do not work for pollutants with complex interactions and feedbacks, such as NH_3. The capability to defensibly estimate source attribution for NH_3 deposition has been lacking.

   Accomplishment: Adaptation of the Decoupled Direct Method-3D (DDM-3D) sensitivity technique for atmospheric deposition in CMAQ4.7.1 for reduced nitrogen stemming from NH_3 emissions.

   Findings: The NH_3 deposition from CMAQ could be partitioned successfully to state and sector-level sources of NH_3 emissions. However, the sensitivity algorithms do not consider all NH_3 nonlinearities, so the model sensitivity must be carefully set up to achieve an internally consistent interpretation of the budget partitioning.

   Impact: The foundation has been laid for source attribution analyses that will provide needed NH_3 atmospheric deposition source responsibility estimates to the Chesapeake Bay TMDL process to provide guidance for management to consider to further reduce atmospheric deposition to the watershed and Bay.

3.0
Model Development and Diagnostic Testing

3.1 Overview of Air Quality Model Development

Introduction

AMAD has a primary mission of developing air quality models in a "one-atmosphere" multipollutant paradigm that are based on the current state of the science and directly applicable to EPA's air quality management and policy needs. The first release of the AMAD CMAQ model was in 1998, and AMAD has ongoing responsibilities to further develop, test, and evaluate the CMAQ model in an effort to identify model improvements and advance the science within CMAQ. The AMAD Model Development and Model Evaluation Program elements work closely to carry out these responsibilities.

Within the AMAD Modeling Program, the Model Development Program element is responsible for the continued development, testing, and refinement of the CMAQ model for a variety of spatial (urban through hemispheric) and temporal (days to years) scales and for a variety of pollutants (O_3, PM, air toxics, visibility, and acid deposition). The one-atmosphere model concept enables the interaction of these pollutant regimes within one modeling construct. Through detailed treatment of physical and chemical processes affecting the fate of atmospheric pollutants, these modeling systems provide scientifically sound tools to understand the relationships between sources of air pollution and ambient concentrations over spatial scales ranging from urban to hemispheric and temporal scales ranging from hourly to annual. This is accomplished through an integrated multidisciplinary approach involving physical, chemical, numerical, and computational science to develop a "numerical laboratory," wherein atmospheric physico-chemical interactions can be simulated effectively to guide development of air pollution abatement strategies. Through synthesis of laboratory and field measurements in parameterizations included in the model and diagnostic testing against measurements over wider spatial and temporal scales, the models provide a framework to test and refine hypotheses and process formulations based on limited and controlled data, thereby improving our understanding of key processes regulating the atmospheric fate of pollutants. This comprehensive approach permits the testing of emissions control strategy impacts on the target pollutant, as well as collateral impacts on other pollutants. Model sensitivity and uncertainty tests are conducted to understand the areas of the CMAQ model system that are most in need of developmental focus and where the model response will be greatest. New experimental and theoretical knowledge of important chemical and physical processes in the atmosphere are monitored, analyzed, and incorporated into the model when appropriate. New CMAQ model versions are released for public access on an as needed basis. The Model Evaluation Program conducts evaluations to assess how well the CMAQ model is performing and to better understand the role of the model inputs and model processes in the air quality predictions. This requires comparisons against observational data from a variety of perspectives, where analyses consider different spatial and temporal scales to assess model performance. Interrelationships among different chemical species must also be considered, as well as the influence of uncertainties in meteorological predictions and emission estimates. Model evaluation serves dual purposes: (1) to characterize the accuracy of model predictions and (2) to identify needed improvements in modeled processes within the air quality model or model inputs.

Research Activities and Accomplishments

Several significant scientific and structural updates to the CMAQ modeling system were completed in FY08, resulting in the public release of CMAQv4.7. CMAQ v4.7 features a new aerosol module, that contains substantial scientific improvements over the aerosol modules released in previous versions of CMAQ.

New pathways for secondary organic aerosol (SOA) formation from precursors, including isoprene, sesquiterpenes, benzene, glyoxal, and methylglyoxal, were incorporated to improve the model's ability to represent the contribution of organic carbon (OC) to airborne fine PM. The model was updated to represent sea-salt emissions from wave-breaking in the coastal surf zone. A new parameterization to represent the heterogeneous dinitrogen pentoxide (N_2O_5) hydrolysis on particle surfaces, which includes dependence on temperature, relative humidity, inorganic PM composition, and phase state, was developed and incorporated in CMAQ. Modifications to the treatment of gas-phase chemistry in CMAQv4.7 were directed at improving the partitioning of airborne oxidized nitrogen, as well as providing a consistent treatment for multipollutant applications (O_3, PM, air toxics, and mercury).

In FY10, an interim version of CMAQ (v4.7.1) was released publicly and included the following features:

- Instrumented versions of CMAQ (including the sulfur tracking model, the primary carbon source apportionment model, and the direct decoupled sensitivity analysis method) to aid in diagnostic investigations
- Updates to the vertical advection scheme to reduce numerical diffusion associated with the original scheme

- Updates to the numerical solver for aqueous chemistry to improve robustness and mass conservation characteristics
- An on-line photolysis rate module that incorporates the radiative impacts of aerosol loading simulated by the model has been included; this enhancement enables investigation of potentially important impacts of scattering and absorbing aerosols in modulating photolysis rates and atmospheric photochemistry regulating the formation of secondary air pollutants.

A prototype of a new modeling system that couples the meteorological model (based on the WRF) and chemistry-transport (CMAQ) calculations within a single executable, following a two-way coupled modeling paradigm, was developed successfully.

Efforts to expand the applicability of the CMAQ modeling system to hemispheric scales were pursued. An annual simulation for 2006 and numerous sensitivity runs were conducted over a domain encompassing the Northern Hemisphere. Model predictions of O_3, $PM_{2.5}$ and constituents, and precursor species were compared with a variety of measurements from surface, aloft, and remote sensing platforms.

A new chemical mechanism, SAPRC-07TB, was developed and incorporated into CMAQ. This version was customized for EPA to include an explicit description of reactive HAPs and high-emissions O_3 and PM precursors. In this mechanism, CMAQ uses an efficient operator technique to reduce the number of equations representing low-NO_x chemistry, which speeds up the run time while allowing more detail in the chemistry.

Many chemical reactions in the atmosphere are initiated by the photo-dissociation of trace gases. These reactions are responsible for most of the smog buildup, which is detrimental to humans, animals, plant life, and materials. To accurately model and predict the effects of air pollution, good photo-dissociation reaction rate (or photolysis rate) estimates must be made. The CMAQv4.7 release included an optional inline photolysis rate module. This module allows for feedbacks of modeled atmospheric pollutants in the radiative transfer calculations. Several refinements are planned for the inline photolysis module in preparation for the FY11 CMAQ release, including: (1) specification of the O_3 column, (2) cloud attenuation effects, (3) incorporation of temperature (and possibly pressure) dependencies on the absorption cross sections/quantum yields, and (4) improvement to the surface albedo (including snow albedo and sea ice effects). In addition to these refinements, the module may be refined structurally to accomplish the following: (1) move cross-sections and quantum yields for photolysis rates from the module's source code to an input file, (2) use a preprocessor program to create the input file, and (3) enable photolysis rates to be shared with other CMAQ modules (e.g., the cloud module).

Next Steps

Two APMs related to CMAQ development are required for FY11.

1. Improved CMAQ modeling system for use in urban-scale residual nonattainment
2. An operational two-way coupled WRF-CMAQ modeling system will be publicly released.

Collectively, these require exploration of novel modeling methodologies to extend the CMAQ modeling system to address emerging environmental problems at scales different from traditional CMAQ applications. Model applications to date have demonstrated clearly the continued need to account for and to improve the representation of interactions of atmospheric processes occurring at the various spatial and temporal scales. Model simulations over annual cycles have pointed to the need for more robust methods for specifying lateral boundary conditions. Although linking with global scale atmospheric chemistry models has been pursued and will continue to be investigated, it is also recognized that biases in the global model can propagate and influence regional CMAQ calculations and often confound the interpretation of regional model results. The specifications of the lateral boundary conditions, to a large extent, dictate the simulated variability in the free troposphere, which in turn can impact the simulated surface-level background values for a variety of trace species. The tightening of the NAAQS to lower threshold values (e.g., the recent revisions to the O_3 NAAQS) places additional requirements on the ability of atmospheric chemistry transport models to accurately represent the entire spectrum of ambient concentrations, including the background values. Expansion of the modeling system to hemispheric scales provides opportunities to consistently represent processes at all scales and will improve the characterization of long-lived pollutants (e.g., mercury). The extension also supports future applications to study the linkage and interactions between global climate and air quality. On the other end of the spectrum, emerging Agency problems focusing on air quality-human exposure linkage will require application of the model at significantly finer resolutions to capture variability in ambient concentrations of a number of pollutants (O_3, PM, and air toxics) and resultant human exposure. These extensions will require further development and enhancement of various physical and chemical process modules/algorithms included in the modeling system.

The two-way coupled WRF-CMAQ system will be essential for high resolution modeling because of the very high-frequency of meteorology data needed for air quality modeling at urban scale resolutions. Many other aspects of modeling science and techniques also need further development for urban-scale applications. Although both meteorology and air quality models have been applied at grid cell sizes down to 1 km and even less, there are science issues at these fine scales that need further development and analysis. For example, meteorology simulations at these scales have been shown to better capture local dynamical effects caused by complex terrain and coastal circulations; however, current mesoscale models need considerable modifications to realistically capture the effects of urban environments on local wind fields, temperature and humidity, boundary layer dynamics, and local atmospheric dispersion. Also, there are scale limitations for Eulerian grid models. For example, the subgrid scale assumption of PBL models begins to break down as grid cell size is reduced toward 1 km because size of the largest eddies in the convective boundary layer are on the order of the PBL depth, which approaches or exceeds the 1-km grid scale. Wind field modeling in urban areas also presents a scale issue where the urban buildings, which are treated as roughness elements at larger grid resolutions, become obstacles to the flow at finer resolutions. What happens to pollutants emitted in such an environment is the key question.

An alternate photolysis module is planned for the FY11 release. This module will use a radiance module to calculate actinic flux at 27 wavelength bins (from 290nm to 800nm) at all altitudes within the troposphere. The radiance model will incorporate the independent variables of solar zenith angle, earth-sun distance as a function of Julian day, surface elevation, surface reflectance, cloud attenuation and reflectance, integrated aerosol optical depth, modulation of stratospheric aerosol depth, aerosol single scattering albedo and scattering phase function, and a latitude and season-specific model of atmospheric gases and season-specific dependence for aerosol vertical profile. The radiance model is expected to reproduce the accuracy of a 64 stream calculation with a computational speed that is faster than a two-stream calculation. The radiance model will be coupled with a photochemistry model that will incorporate temperature and pressure dependencies in the cross-sections and quantum yields of currently modeled photochemical reactions. The coupled radiance and photochemistry models then will comprise a complete photolysis module.

Clouds cover about 60% of the earth's surface and provide a means to efficiently transport constituents from the polluted boundary layer to the free troposphere, with substantial implications for long-range pollution transport and climate. Although CMAQ has hundreds of explicit or semi-explicit kinetic expressions to describe gas-phase chemistry, the aqueous chemical mechanism is limited to only a few (about seven) oxidation reactions. A more accurate and flexible solver for aqueous chemistry will be developed for the CMAQ model, which will enable changing the reactions within the aqueous mechanism. The new solver will be benchmarked against the original by using box model and CMAQ simulations. Through collaborations with investigators at Rutgers University, new nitrogen-related chemistry will be added to the aqueous module. The new chemistry will be evaluated with nitrogen deposition data collected during special studies (e.g., Bay Regional Atmospheric Chemistry Experiment [BRACE]) prior to public release.

3.2 CMAQ Aerosol Module

Introduction

The treatment of aerosol chemistry and physics is a critical component of the CMAQ modeling system. Ambient particles contain a mixture of numerous chemical species that originate from primary particle emissions and from secondary formation pathways linked to gaseous precursors. Representation of this chemical diversity is an ongoing modeling challenge that requires the simulation of mass transfer between the gas and particle phases via condensation and evaporation, heterogeneous reactions of gaseous molecules on the particle surfaces, reactions that occur within the condensed particle phase, and homogeneous nucleation of particles from low-vapor-pressure gaseous precursors. In addition to those processes, our ability to predict the ambient concentration, composition, and size distribution of atmospheric PM is dependent on the accuracy of emission inventories, the numerical representation of aqueous-phase cloud and fog processes, and an accurate treatment of particle deposition. A correct simulation of atmospheric aerosol properties is vital for the prediction of $PM_{2.5}$ concentration changes resulting from emission reductions and for calculations of regional haze. Two emerging priorities in the FY10-FY11 time period will be (1) to accurately simulate the mass concentration and composition of coarse particles (PM_{Coarse}), for which a new NAAQS is anticipated, and (2) to simulate exceedances of the new 24-h $PM_{2.5}$ NAAQS (35 µg m^{-3}), which occur predominantly in urban areas.

Recent evaluation studies have revealed that the largest biases in CMAQ $PM_{2.5}$ results are driven by overpredictions of the unspeciated $PM_{2.5}$ (Appel et al., 2008; Mathur et al., 2008), referred to hereafter as $PM_{Other.}$ Observations of PM_{Other} are obtained from the gravimetric $PM_{2.5}$ mass measurement minus the sum of several chemically-speciated measurements (sulfate[SO_3], NO_3, ammonium, OC, and elemental carbon[EC]). Model predictions of PM_{Other} consist of unspeciated primary $PM_{2.5}$ plus any noncarbonaceous material (e.g., oxygen and hydrogen atoms) associated with the organic aerosol. In FY09-FY11, three efforts will be undertaken to mitigate the incommensurability in PM_{Other} evaluations and improve model performance for this important quantity.

Research Activities and Accomplishments

As new configurations have been added to the CMAQ modeling system (e.g., CMAQ-MP, CMAQ-TX, CMAQ-Hg, CMAQ-DDM, sulfate tracking, carbon apportionment), it has become increasingly difficult to maintain the code archive because of some subtle inefficiencies in the aerosol module architecture.

In FY10-FY11, problematic portions of the aerosol code will be incrementally updated and tested with a goal of removing the most egregious inefficiencies before the FY11 release of CMAQ.

In FY10, the new secondary organic aerosol (SOA) treatment released in CMAQ v4.7 was described in a journal publication by Carlton et al. (in press). In FY10-FY11, the precursor-specific SOA results will be evaluated against organic-tracer-based measurements collected by HEASD in Research Triangle Park, the Midwest (LADCO sites), and Southeast (SEARCH sites). Based on our findings from those evaluations and reports from any ongoing National Center for Environmental Research (NCER)-funded extramural research, we will refine the model treatment of biogenic SOA. In FY10, HEASD delivered an APM summarizing their new experimental findings on anthropogenic SOA. Based on their report, combined with the results of ongoing extramural research, the anthropogenic SOA formation pathways in CMAQ will be overhauled in FY11-FY12. Specifically, we expect to revise the treatment of alkane SOA and add new SOA formation pathways from light-weight PAHs (e.g., naphthalene, alkyl napthalenes).

Coordinating with investigators from ENVIRON and the Electric Power Research Institute (EPRI), a new SOA module using the volatility basis set (VBS) will be implemented in CMAQ and tested against the base SOA module in CMAQ. If those tests are successful, we will strive to release the VBS code as a user-specified option in FY11. In the future, after sufficient testing, this may become the default option.

A major focus of the FY11 APM for CMAQ model development is improved $PM_{2.5}$ predictions in "residual" nonattainment areas, several dozen counties which are forecasted to remain in nonattainment of the NAAQS even after all of the national-scale emission control programs (e.g., Clean Air Interstate Rule [CAIR], NO_X SIP Call, diesel retrofit, etc.) have taken effect. The vast majority of these residual problems are likely to be dominated by primary $PM_{2.5}$. Thus, a detailed examination of the emission sources contributing to primary $PM_{2.5}$ will be critical. In FY10, the primary carbon source apportionment module that has been released with the past three public releases of CMAQ will be upgraded to CMAQ v4.7 and released to the public. In FY10-FY11, the source apportionment capability in CMAQ will be extended to treat other primary $PM_{2.5}$ species, such as the trace metals emitted from industrial facilities. The resulting instrumented model will be used to assess and improve $PM_{2.5}$ emission inventories in residual nonattainment areas.

In CMAQ, gas/particle equilibrium for inorganic species has been computed using the ISORROPIA module since the release of CMAQ v4.2 in 2002. The current version of that module, ISORROPIA v1.7, treats the SO_4^{2-}/NO_3-/Cl-/NH_4+/Na+/H_2O system in a computationally efficient manner, but it suffers from numerical instabilities under certain extreme conditions. Over the past several years, three new thermodynamic modules have been developed as promising alternatives to ISORROPIA. Through a National Oceanic and Atmospheric Administration (NOAA)-funded contract with the Georgia Institute of Technology, ISORROPIA v2.0 was developed and released in FY09. The main advancement in ISORROPIA v2.0 is that it treats three additional species that are abundant in sea salt and soil dust: (1) Ca_2+, (2) K+, and (3) Mg_2+. In FY11, we will implement the latest ISORROPIA module in the FY11 release of CMAQ.

Next Steps

A new CMAQ subroutine will be developed to produce model estimates of total $PM_{2.5}$. At present, model users who seek $PM_{2.5}$ predictions from CMAQ must perform a linear combination of several dozen species in the model output. Inconsistencies in the postprocessing methodology can lead to discrepancies in the model results reported by different users, even when the exact same CMAQ configuration is applied to identical inputs. In addition to bringing consistency to the method of summing individual chemical components, the new subroutine will simulate changes in mass (i.e., artifacts) that occur when ambient $PM_{2.5}$ is sampled and analyzed by the Federal Reference Method (FRM). The measurement artifacts to be simulated are volatilization losses of ammonium nitrate during sampling, adsorption of semi-volatile organic gases during sampling, and retention of particle-phase water during gravimetric analysis of the filters (with consultation from Neil Frank [OAQPS]). The main output of this new subroutine will be gridded and time-resolved mass concentrations of $PM_{2.5\ FRM}$ which, for the first time, can be compared directly with the large surface network of FRM monitors (i.e., State and Local Air Monitoring Stations [SLAMS]). Once the key measurement artifacts are incorporated into the CMAQ calculations, the final modeled values of $PM_{2.5\ FRM}$ can be used without hesitation in data fusion efforts (e.g., for CDC-PHASE). The SLAMS data are the basis for NAAQS attainment demonstrations so the modeled $PM_{2.5\ FRM}$ output values should prove very useful to OAQPS, EPA regions, and the States.

$PM_{2.5}$ emission inputs will be augmented to explicitly speciate a number of chemical components that are currently part of PM_{Other}. At present, the Sparse Matrix Operator Kernel Emissions (SMOKE) processor generates gridded files that include $PM_{2.5}$ emissions of sulfate (SO_4^{2-}), (NO_{3-}), OC, and EC, where as all of the remaining mass is lumped together as PM_{Other}. The PM_{Other} component constitutes over half of the National Emission Inventory (NEI) for $PM_{2.5}$. Using detailed speciation profiles derived from our previous work (Reff et al., 2009), we will modify the SMOKE processor to subdivide the emissions of PM_{Other} into primary ammonium (NH_4+), sodium (Na+), chloride (Cl-), selected trace elements (magnesium[Mg], aluminum[Al], silicon [Si], potassium[K], calium [Ca], titanium [Ti], manganese [Mn], and iron [Fe]), non-carbon organic mass (NCOM), and a greatly-reduced quantity of PM_{Other}. The CMAQ code will be modified to read these new species from the emission files and incorporate them into the chemistry and transport operators.

The CMAQ aerosol module will be enhanced to treat the oxidation of OC that occurs in the atmosphere. It has been shown that OC oxidation increases NCOM (Turpin and Lim, 2001), thereby enhancing ambient $PM_{2.5}$ mass concentrations. Our preliminary analyses of ambient data indicate that NCOM constitutes 10%–25% of $PM_{2.5}$. However, the oxidation of secondary OC is treated very crudely in CMAQ v4.7 (using a zeroth order oligomerization rate constant) and the oxidation of primary OC is neglected entirely (a constant OM/OC ratio of 1.2 is assumed for all sources of OC). These shortcomings will be addressed in FY11, and the resulting model predictions of NCOM will be evaluated against measurement-based estimates of the same quantity.

The net result of the research described above will be 10 newly predicted quantities from the CMAQ model ($PM_{2.5\ FRM}$ and fine-particle Mg, Al, Si, K, Ca, Ti, Mn, Fe, and NCOM) and more accurate predictions of NH4+, Na+, and Cl- (because their direct emissions from anthropogenic sources will be accounted). When the total modeled concentrations of individual $PM_{2.5}$ species (i.e., SO_4^{2-}, NO_3, NH4+, EC, and OC) are subtracted from the new model estimates of $PM_{2.5\ FRM}$, we will obtain model results for PM_{Other} that are commensurate with the difference-based observations of PM_{Other} collected across the Interagency Monitoring of Protected Visual Environment Network (IMPROVE) and Chemical Speciation Networks. We then will be equipped to assess and address the CMAQ model biases for PM_{Other} in a rigorous manner.

Building on the findings published in FY08 (Davis et al., 2008) plus recent experimental evidence from researchers at NOAA, the University of Washington, and the University of Illinois, CMAQ model treatment of the heterogeneous reaction between N_2O_5 and particle surfaces will be updated in FY11-FY12 to account for the influence of organic content and/or organic coatings.

EPA is considering a new ambient standard for PM_{Coarse}, defined as PM_{10} minus $PM_{2.5}$. The largest sources of PM_{Coarse} are sea salt, fugitive dust from anthropogenic activities (e.g., road traffic, agricultural tilling, construction), and windblown dust from arid land. All of these sources are treated in CMAQ except for natural windblown dust. In FY11, efforts will be made to incorporate new algorithms for estimating windblown dust emissions (Tong et al., in preparation) directly into the CMAQ model and incorporate those new species into the chemistry and transport operators. With these advancements, the model infrastructure will be in place to numerically predict PM_{Coarse} concentrations at various times and locations.

CMAQ does a reasonably good job of predicting fine particle mass concentrations (e.g., $PM_{2.5}$), but a much poorer job representing the number concentration of atmospheric particles. In FY11, we will coordinate with members of the external CMAQ user community to improve the treatment of nucleation and primary particle emissions in the FY11 release of CMAQ. These two updates will be the first steps toward refining CMAQ predictions particle number.

3.3 CMAQ Gas-Phase Chemistry

Introduction

The treatment of gas-phase chemistry, including the production of gas-phase pollutants; production of semi-volatile components, which can form aerosols; and the associated gas-phase chemistry solvers, will always be at the core of any advanced air quality model, particularly those that are formulated with the one-atmosphere, multipollutant concept. As such, periodic revisions to the representation of atmospheric chemistry in air quality models are needed to incorporate new scientific findings as they become available and to address emerging air pollution issues that may arise. Also, it is often necessary to revise existing chemical mechanisms and solvers to be consistent with changes that are made in other parts of the modeling system to enhance computational performance, ease of use, and functionality. This is an ongoing process that is necessary to keep advanced air quality models, such as the CMAQ model, accurate, scientifically relevant, and fully operational.

In the past, gas-phase chemical mechanism development focused on single-pollutant issues, but since largely it has become clear that it is more appropriate to treat chemistry in an integrated, multiphase, multipollutant manner. The general goal of our research in this area is to develop, refine, and implement the gas-phase chemical mechanisms for use in the CMAQ model to accomplish the following objectives:

- Ensure that CMAQ and other models that are used for regulatory and research purposes have scientifically justifiable gas-phase 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-phase chemistry and the chemistry occurring in aqueous- and particle-phases are accounted for adequately, so that we can truly 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

Research Activities and Accomplishments

In FY10, we completed the incorporation of one new, state-of-the-science atmospheric chemical mechanism into CMAQ, the SAPRC-07TB mechanism, and initiated incorporation of the Regional Atmospheric Chemistry Mechanism, version 2 (RACM2).

The RACM2 mechanism is an updated and expanded version of RACM and includes more detailed aromatic and isoprene chemistry. RACM2 was developed in 2007 and contains 349 chemical reactions. One hallmark of RACM2 is its detailed representation of peroxy radical chemistry in rural and remote environments. By implementing RACM2 in CMAQ, we will provide a computational laboratory for examining the influence of gas and aerosol production in these types of environments and their influence on air quality. This quality of RACM2 also may provide a basis for future extensions to hemispheric simulations.

The SAPRC-07 mechanism is an updated version of the SAPRC-99 mechanism, which has been used widely in CMAQ and other air quality models for many years. In FY10, we have completed the incorporation of a customized, multipollutant version of this mechanism, SAPRC-07TB, which provides an explicit description of the most important species and reactions for a number of current EPA applications. SAPRC-07TB enables criteria, HAPs, and multipollutant applications to give consistent results. In addition, the detailed organic chemistry in the original version of SAPRC-07 provides the capacity for changing the way that individual VOCs are represented by our version of the mechanism. In the coming fiscal year, we will complete our analyses of the behavior of SAPRC-07TB in CMAQ and incorporate any updates in inorganic and organic reactions. In addition, as we improve our ability to describe important SOA and cloud chemistry, we can use this information to develop more explicit versions of SAPRC-07TB that include these details.

The CB05 mechanism will continue to be a major mechanism used in regulatory applications where many simulations are performed and for research studies done over long time periods. This mechanism uses structural lumping techniques to provide a highly compact representation, which makes it the most computationally efficient mechanism currently available for use in CMAQ multipollutant studies. Recent published updates to the aromatic chemistry (in specific the toluene chemistry) were incorporated in the CB05 mechanisms, and extensive testing of the impacts of the update on O_3 and PM predictions was conducted. We will monitor research in atmospheric chemistry and perform periodic, limited updates to CB05 as appropriate, with a particular emphasis on CBO6.

Next Steps

In the next 3 years, we will finalize inclusion of RACM2. We will make additional updates and improvements to the standard versions of these mechanisms to make them consistent with the latest research findings and provide details needed by the aqueous and aerosol computations, thus ensuring that the gas, aqueous, and aerosol chemistries are correctly integrated.

More importantly, we will start looking beyond the standard, fixed-species, fixed-coefficients mechanism suite to determine the best methodology for representing atmospheric chemistry in the future. Given the rapidly changing research discoveries in atmospheric chemistry, we will examine whether a more flexible approach to mechanism creation is compatible with EPA's current modeling applications. We will explore collaborations with groups in the United Kingdom, in particular the Master Chemical Mechanism (MCM) developers. This mechanism suite will allow CMAQ users to better match the type of application with an appropriate mechanism. In addition to these "base" mechanisms, we also are developing extended versions for both special research purposes, and versions which will include the chemistry of additional HAPs for use in full, multipollutant analyses, described in section 3.8 (Air Toxics). Research versions of the SAPRC-07TB and CB05 mechanisms also will be constructed for special studies. Two versions, in particular (see just below), will be important components of our work during over the next few years:

1. SAPRC-07TB with detailed primary pollutants for reactivity studies—Current government-industry joint efforts to study VOC reactivity have identified the derivation of new reactivity scales as the most important need to improve the scientific basis of reactivity-based VOC regulations. To address this need, we are initiating efforts to rederive reactivity scales using CMAQ with the decoupled direct method (DDM). This is a large effort, which requires incrementally adding the more than 800 detailed species in SAPRC-07, in groups of 20 to 50, to a condensed version of SAPRC-07TB. The sensitivities for each VOC then will be used to calculate a wide variety of metrics that quantify potential contributions of individual VOCs to O_3 formation across the United States. The results of these simulations will be used by States, local air pollution agencies, and EPA to develop SIPs that better address the role of VOCs in O_3 formation.
2. SAPRC-07TB with detailed, updated isoprene chemistry—Isoprene is one of the most widespread VOCs emitted in most of the world. A robust and justifiable representation of isoprene chemistry and its effect on hydroxyl and hydroperoxy radical formation, on cycling of nitrogen oxides and on production of formaldehyde are all essential to have confidence that we adequately are representing O_3 and organic aerosol formation and sensitivity. Groups within AMAD are collaborating are reexamining and potentially revising the treatment of isoprene

in SAPRC-07TB. Both a detailed and a condensed update to the current isoprene chemistry will be examined for potential inclusion in CMAQ-MP.

All new and modified mechanisms will continue to be compatible with improved chemical representations for SOA modeling being developed within HEASD and will be linked closely with work performed under other AMAD tasks.

The development of flexible, in-house chemical mechanisms will be one area that we will begin explore in FY11. Under the U.S.-U.K. collaborative agreement, we will study the feasibility of incorporating condensed representative versions of the MCM into a format appropriate for CMAQ applications. With this approach, we hope to more quickly incorporate new ground-breaking science into the mechanisms without the long time lag (6 to 10 years) between official fixed mechanism versions. We will monitor the scientific community for any new methods for representing gas-phase chemistry with an increased emphasis on interactions with aerosol formation and greater accuracy of condensations. These new methods are at the frontiers of practice in the atmospheric chemistry modeling community. We will keep up to date with developments in this area and initiate efforts in the later years of this task to implement advanced chemistry representations in CMAQ.

3.4 Planetary Boundary Layer Modeling

Introduction

Air quality modeling systems are essential tools for air quality regulation and research. These systems are based on Eulerian grid models for both meteorology and atmospheric chemistry and transport. They are used for a range of scales from continental to urban. A key process in both meteorology and air quality models is the treatment of subgrid-scale turbulent vertical transport and mixing of meteorological and chemical species. The most turbulent part of the atmosphere is the PBL, which extends from the ground up to about 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 realistically convective conditions. Simple nonlocal-closure PBL models, such as the Blackadar convective model that has been a mainstay PBL option in Fifth-Pennsylvania State University (PSU) National Center Atmospheric Research (NCAR) 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 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 supergrid-scale and subgrid-scale components of turbulent transport in the CBL. Testing ACM2 in one-dimensional form and comparing with large-eddy simulations (LES) and field data from the second and third Global Energy and Water Cycle Experiment (GEWEX) Atmospheric Boundary Layer Study, known as the GABLS2 (CASES-99) and GABLS3 (Cabauw, NL) experiments, demonstrate that the new scheme accurately simulates PBL heights, profiles of fluxes and mean quantities, and surface-level values. The ACM2 performs equally well for both meteorological parameters (e.g., potential temperature, moisture variables, winds) and trace chemical concentrations, which is an advantage over eddy diffusion models that include a nonlocal term in the form of a gradient adjustment.

Research Activities and Accomplishments

The development and application of ACM2 in both WRF and CMAQ now has achieved consistent PBL treatment for meteorological and chemical species. Therefore, we will pursue further development of the ACM2, particularly for stable conditions. Very high concentrations of aerosols have been observed in areas of winter cold pools. Many western North American cities are located in basins where cold air can collect, resulting in extremely stable inversion layers that trap locally emitted pollutants. Current meteorology and air quality models have insufficient vertical resolution and incomplete physical representations to accurately simulate these conditions. In FY09 and FY10, AMAD was involved in a Regional Applied Research Effect (RARE) project to model winter air pollution episodes in Fairbanks, AK, where extreme surface inversion layers can result in very high concentrations of $PM_{2.5}$. This modeling study uses a series of nests with horizontal grid resolutions of 12, 4, and 1.33 km and very high vertical resolution, with the lowest layers of 4-m thickness. We will continue to use the Fairbanks modeling as a testbed for SBL model development.

We have continuing involvement with the GEWEX GABLS. The ACM2 model was a participant in the GABLS2 experiment that was a comparison of single-column PBL models for a 2-day period of the CASES99 field experiment (Svensson, and Holtslag, 2006). The ACM2 was also a participant in the GABLS3 experiment which is a single diurnal cycle at the Cabauw meteorological tower in the Netherlands. The results of the GABLS3 experiment will be published soon in *Boundary Layer Meteorology.* We have used the GABLS3 experiment and the LES data created for GABLS1, which was a SBL case over sea ice in the arctic, to develop a new SBL model that was presented to the 19th Symposium on Boundary Layers and Turbulence in August 2010. The new SBL scheme also has been tested in WRF and evaluated for its simulation of low-level nocturnal jets.

Next Steps

AMAD will have continued involvement in the Fairbanks project through FY11, in particular, an analysis of the results of the air quality simulations. Also, an evaluation of the new SBL scheme in WRF will continue in FY11 and be extended to testing in CMAQ and the coupled WRF-CMAQ.

3.5 Meteorology Modeling for Air Quality

Introduction

Meteorology models are very important components of air quality modeling systems because they describe the physical, dynamic, and thermodynamic state of the atmosphere. The Division, therefore, has a vested interest in developing components and capabilities that are needed for air quality applications based on existing meteorology models. For example, the Division has been instrumental in the development of nudging-based four dimensional data assimilation (FDDA) in MM5 and more recently, in WRF Model. FDDA has been shown to significantly decrease the errors and biases of modeled meteorology that is a direct input to air quality models. We also have developed a land-surface model (LSM) and PBL schemes for MM5 and transferred them to WRF for better simulations of the PBL depth and surface fluxes and temperature, humidity, and wind within the PBL, which are also critical for air quality modeling fidelity. MM5 has served as the Division's primary source of meteorologically modeled input to the air quality model for more than a decade, but, although MM5-based meteorology is still being used in some limited research, the Division now has transitioned fully to WRF for all of our new model developments and applications.

Research Activities and Accomplishments

From FY10 and into FY11, a total of five annual WRF simulations of the CONUS at 12 km will be completed for various CMAQ applications, which represent the official transition away from MM5, as well as a transition from 36-km CONUS to a more refined 12-km scale.

Land-use and vegetation data are important for (1) land surface modeling within the meteorology model (WRF), (2) dry deposition and bidirectional surface flux modeling, and (3) modeling biogenic emissions of photochemically active chemical species. Thus, we have been working to upgrade and update the land-use/vegetation data used in our modeling systems. We already have accomplished the first stage of this effort by integrating higher quality and higher resolution land-use databases, the National Land Cover Database (NLCD) for the United States and the Moderate Resolution Imaging Spectroradiometer (MODIS) land-use data for outside the United States, into WRF to improve modeling of air-surface exchange processes. The NLCD is based on 30-m resolution L-enhanced thematic mapping classified into 30 land use categories. The MODIS data has 20 land-use categories at 1 km resolution. The NLCD and MODIS datasets have been combined such that the higher resolution NLCD is used preferentially where available, with MODIS being used elsewhere. The Pleim-Xiu LSM in WRF and the M3dry dry deposition model in CMAQ have been modified to conform to this new hybrid land-use dataset. We have tested the new NLCD and MODIS data in a variety of applications in FY10 and will continue to analyze the result in FY11. Although significant differences in model performance between simulations with NLCD and the old U.S. Geological Survey (USGS) were not apparent in terms of surface meteorological variables and precipitation at the 12-km scale, some modest improvements were noted as the model grid scale is decreased to 4 km and 1 km. We now have moved almost exclusively to using NLCD (MODIS outside the United States) for almost all modeling applications.

Another related area of research is the development of a new vegetation dataset for biogenic emission modeling also based on the NLCD/MODIS. The land-use data will be combined with forest inventory data (FIA) and agricultural data from the National Agricultural Statistical Service (NASS) to create a high resolution dataset that contains accurate information on tree species groups and crop types that could be used by the Model of Emissions of Gases and Aerosols from Nature (MEGAN) and Biogenic Emission Inventor System (BEIS) biogenic emission models. After testing and refinement of the parameterizations in WRF and CMAQ that depend on land-use, the capability to use the hybrid NLCD/MODIS land-use database will be released to the WRF and CMAQ communities.

Another research area concerns the improvement and application of data assimilation methods in the meteorological model. Data assimilation is used in the meteorology model to constrain the natural error growth in the meteorology and air-quality simulations. Typically for air-quality modeling, a nudging-based FDDA is applied throughout the simulation period to create dynamic analyses. We are testing new FDDA techniques, including the utilization of both nonstandard surface and upper air observations that, in theory, will reduce the uncertainty of the analyses used to drive the FDDA and soil nudging. These observation platforms include radar wind profilers, aircraft, satellite wind, satellite sea surface temperature, and a more dense set of surface observations from the numerous mesonet sites around the country. Furthermore, we have begun to explore using the 3D Variational Analysis (3DVar) in the WRF system, which has the potential to assimilate remotely sensed data (e.g., satellite radiance, Doppler precipitation estimates). We are aggressively pursuing the testing of techniques begining in mid-FY10, and are analyzing the results, which will be published in late 2011. The results, thus, far are encouraging in that systematic biases in transport wind are reduced through the use of some of these observational datasets.

Next Steps

The meteorological model fields are processed into the CMAQ modeling system using the Meteorology-Chemistry Interface Processor (MCIP). MCIP prepares the meteorological fields in space and time for the emissions processing and the chemistry transport model (CTM). MCIP performs horizontal and vertical transformations, diagnoses additional fields, and produces the output in a format that is compatible with the CMAQ system. The community release of MCIP supports model output from MM5 and WRF-ARW. In FY11, MCIP will be updated on an as-needed basis to support internal Division modeling needs, as well as the CMAQ community. In particular, scientific changes to MCIP have been completed to support the NLCD/MODIS land-use, but further upgrades will be required especially for the more detailed vegetation work yet to be done. Furthermore, MCIP may need to be modified to support the urban canopy parameterizations in WRF, to remove the dry deposition velocity calculations, and to support upgrades to the Geostationary Operational Environmental Satellites (GOES) processing. Releases of MCIP will occur in conjunction with major CMAQ releases and intermittently, as needed.

A few projects in which analysis will continue through FY11 are Northern Hemisphere annual simulations at a 108 km grid scale. We also are using the high-resolution NLCD at 4 km and 1 km over Houston, Cleveland and Atlanta. In FY11, we also will complete annual 2009 and 2010 CONUS 12-km CMAQ simulations.

New guidelines for FDDA-based meteorological simulations used for air quality models are expected to be released as a result of this 2010-2011 research. We will rerun some of the longer term simulations to ensure the results of the limited 4-day test case hold for seasonal and annual simulations. Journal articles will document how the simulations of meteorology and regional transport were improved, which will build confidence in the inputs for CMAQ.

Our meteorological modeling research program also focuses on improving finer scale meteorological modeling simulations. The Division has embarked on a methodical study of the efficacy of meso-gamma scale meteorological modeling simulations to address the suitability of the resultant fields for air quality modeling. Several simulations at fine scales have been or will be generated in FY11. We have executed a base simulation that uses a very similar configuration as our 12-km scale simulations in terms of the way surface processes are handled (PX LSM and ACM2 PBL schemes). We also have begun and will complete several simulations that use a new and much more advanced treatment of the urban canopy using the same modeling domain as the base 1 km. The urban canopy parameterization uses highly resolved urban morphology data, like building height, building to surface fraction, urban fraction, and building area fraction, to represent a number of influences cities have on atmospheric flow. Not only will the meteorology of the simulations be compared with the base simulation, but equivalent CMAQ simulations will be executed to determine whether the air quality predictions are improved. A seasonal Atlanta area 1-km simulation is also another urban-related task for 2011. The air quality simulations driven by this urban meteorology will be used in a new technique to link air quality with human exposure. The outcome of this research will contribute toward the FY11 APM "Improved CMAQ modeling system for use in urban-scale residual non-attainment," as well as toward improving linkages with human exposure models within the Laboratory. This research also will help define a practical (horizontal scale) limit of predictability for deterministic meteorological models to be used for air quality modeling.

3.6 Integrated Meteorology-Chemistry Modeling

Introduction

Traditionally, 3-D CTMs that are used for air quality research and regulation are driven by 3-D meteorology fields provided by a priori runs of a meteorology model. Historically, the CTMs and meteorology models developed over several decades along independent tracks with little regard for computational, numerical, or even scientific consistency between the two systems. In recent years, however, there have been several efforts to combine meteorology and chemical transport models into single interactive systems. A primary driver for this trend has been the need to include the direct and indirect feedback effects of gases and aerosols on radiative forcing. Although effects are mainly important for climate applications, it is becoming evident that they have substantial affects on local meteorology and air quality in regions of extreme air pollution. Zhang (2008) has provided an overview of several coupled meteorology-chemistry models including the WRF/chem (Grell, 2005) model in which chemistry has been added into the WRF model (Skamarock, 2008) at the science process level. Another approach is to couple historically independent meteorology and chemical transport models into a single executable. Advantages of this approach include maintaining consistency with existing separate sequential meteorology-chemistry systems that are being continuously and extensively applied and evaluated. Furthermore, the numerical and computational techniques employed in meteorology models and CTMs differ considerably because of the greater need for strict mass conservation and positive-definiteness of transported scalars in the CTM. Also, CTMs generally use fractional integration of various processes, wheras meteorology models use generally integrate all prognostic variables and parameterizations each main time step. Because of these and other reasons we have coupled the WRF meteorology model and the CMAQ model to create a coupled modeling system with two-way interactions between chemistry and meteorology.

Research Activities and Accomplishments

A two-way meteorological and air quality coupled modeling system, WRF-CMAQ, has been developed in FY10 to enhance model accuracy by eliminating excessive interpolation of hourly meteorological data and by incorporating aerosol feedback information from the air quality model to the meteorological model. The two-way coupled system consists of three components: (1) WRF, (2) CMAQ, and (3) the coupler. The coupler is encapsulated in Fortran 90 modules, so the details of the two-way coupling system are transparent to the users. This design enables WRF or CMAQ to be detached from the system easily and executed in standalone mode. The single-source coding approach makes code maintenance less complicated.

Next Steps

Extensive testing of the two-way coupled WRF-CMAQ is underway and will continue into FY11. The testing includes a wild fire episode in California in June 2008, where emitted smoke was concentrated enough in the central valley that SW radiation levels were much lower than normal. Initial tests show the model with SW feedback had lower radiation and daytime temperatures that agreed much better with observations than did the model with no feedbacks. Other tests are being done on a hemispheric scale. A manuscript that documents these efforts is being prepared and will be published in FY11-2012.

3.7 Mercury Modeling

Introduction

As methods to measure mercury in the laboratory and in the atmosphere continue to be developed, and as further experimentation is performed, the basic scientific understanding of atmospheric mercury behavior continues to improve. As new information becomes available from the peer-reviewed scientific literature, improved formulations for simulating atmospheric mercury behavior will be added to the CMAQ model. This likely will involve the addition of new physicochemical species to the CMAQ model that are found to have important reaction with atmospheric mercury. Mercury is emitted to air from a variety of environmental and industrial sources. Industrial sources will continue to be treated using model input data from emission inventories. However, treating environmental sources of mercury will require a multimedia modeling approach, where entirely new modeling structures are added to simulate media other than the atmosphere, such as water bodies, soils, and vegetation. It is assumed that atmospheric mercury model development will be aided by the deployment of new ambient mercury concentration monitors, and that dry deposition will be added as a measured parameter of the Mercury Deposition Network.

Research Activities and Accomplishments

Parameterizations were implemented that estimate the surface water mercury oxidation and reduction reactions, vegetation uptake of elemental mercury (Hg0), and reduction of soil-bound mercury to estimate the emission potential of the natural surfaces. This allows CMAQ to parameterize the air-surface water concentration gradient dependence on the elemental mercury flux (Foley et al., 2010), the recycling of recently deposited divalent mercury, and the enrichment of elemental mercury concentrations in vegetation, soil, and surface waters that have been documented recently in the literature (Bash and Miller, 2009). These improvements capture observed pulses of emissions following precipitation in arid environments during measurement campaigns and are an inline estimation of natural mercury emissions that remains consistent with changes in modeled chemical mechanisms and boundary conditions, changes that would require updates to offline natural emission estimates (Bash, 2010).

Next Steps

The following are improvements and issues being considered for the FY11 CMAQ release.

- Chemical kinetics information—Kinetic rate constants for gaseous and aqueous mercury reactions will be updated as new information becomes available for reactions of mercury with any other chemical species included in the model provided there is sufficient time to test the updated model before release.
- Multimedia treatment for air-surface exchanges of elemental mercury—The CMAQ model will be enhanced to include dry deposition and emission of mercury to soils and vegetation (in addition to water bodies) based on bi-directional flux treatments where dry deposition and emission are treated as a combined process with either an upward or downward net flux. This modeling advance will be based on new scientific information on the behavior of mercury within those new media.

3.8 Air Toxics

Introduction

In the past, chemical mechanism and air quality development have focused on O_3 and primary inorganic PM; we are expanding the scope of the atmospheric photochemistry in CMAQ to include predictions for a large number of HAPs.

Research Activities and Accomplishments

We have expanded the base mechanisms of CB05 and SAPRC-07, as described in the previous section, to characterize the production and decay of approximately 40 additional HAPs, including VOCs, inorganics, and metals. These mechanisms are used by the Agency to develop full, multipollutant analyses that examine the consequences of emission control strategies on multiple types of pollutants: O_3, PM, HAPs, visibility, acid deposition, etc. Developing the chemistry for these HAPs includes appropriately accounting for compounds with a wide range of atmospheric reactivity and source types, in all phases (gas, aerosol, and aqueous).

Next Steps

In the next 3 years, further efforts in this area will overlap with the developments in the base mechanism but with an emphasis on HAPs. We anticipate that, over the next few years, the following efforts will be made.

- Characterization of explicit PAHs—This class of compounds includes a large number of organics with multiple benzene rings, possessing a wide range of vapor pressures, toxicity, and reactivity. Because some PAHs and their by-products can be highly carcinogenic and/or produce SOA, we are initiating efforts to include their chemistry in upcoming releases of CMAQ-MP.
- Description of arsenic compounds—Arsenic is a major contributor to national air toxics assessments but has potentially complex chemistry involving aqueous transformations. We are initiating efforts to better predict the complex transport and transformations of arsenic in CMAQ.
- Mechanism improvements for the most toxic air pollutants—We will continue to monitor the scientific literature and refine our representation of HAPs chemistry in CMAQ-MP. We work closely with EPA, the Office of Air and Radiation (OAR), and OAQPS to identify those compounds that pose the largest risks for acute and chronic health effects to the United States population, and we will focus on refining our chemical representation of these compounds. This will help us to ensure that the chemistry and transport of these important pollutants is characterized appropriately. In SAPRC-07TB, we have incorporated additional pathways for highly toxic acrolein formation that were not available in previous chemical mechanisms. In the next planning cycle, we will incorporate information from current research studies on aromatic chemistry to help us to refine our treatment of aromatic HAPs and their toxic by products.
- Description of new, emerging toxic air pollutants—There is increasing evidence that a large number of species, beyond those HAPs listed in the Clean Air Act 112(b), also can cause serious, adverse health effects. For example, multifunctional carbonyl compounds, formed as secondary pollutants from a wide variety of nontoxic VOCs, may provide sources of additional toxicity in atmospheric mixtures. As more details on the exact structures of compounds that can cause inflammatory responses to urban smog are discovered, we will initiate efforts to better represent these classes of compounds in CMAQ-MP.
- Incorporation of persistent organic pollutants, pesticides and hydrofluorocarbons—There are many other pollutants that are either toxic per se or have the potential to cause toxic effects in aquatic systems, and understanding the lifetime and distributions of these compounds is of worldwide concern. CMAQ has been used in past studies of two of these compounds (atrazine and tetrafluoropropene), and we anticipate that, as new information on emerging pollutants becomes available, CMAQ-MP will provide an ideal basis for studying these types of toxic pollutants.

Our efforts in air toxics modeling will continue to be closely coordinated with other gas, aqueous, and aerosol chemistry being performed by AMAD, as described in other sections of this report, as well as other efforts in NERL/HEASD and in OAQPS.

3.9 Nanoparticles Modeling

As industrial production of nanomaterials increases, a capability to accurately simulate the transport and fate of these materials has risen to a high priority. As an initial case study of nanomaterials, we are investigating air quality effects of doping diesel fuel with nanoparticulate cerium oxide ($nCeO_2$). $nCeO_2$ is used as a diesel fuel combustion catalyst to reduce fuel consumption and reduce emissions of greenhouse gases and PM. In FY09, we assembled a database of diesel-engine dynamometer studies that have been conducted with and without $nCeO_2$ in the fuel.

Research Activities and Accomplishments

In FY10, we used the just-mentioned database to develop a national emission scenario in which diesel fuel across the United States has been doped with a $nCeO_2$ additive. Those emission estimates were used to assess the additive's effect on regional-scale air quality using CMAQ.

Next Steps

In FY11, we will simulate the dynamics of the particle population emitted in diesel exhaust (with and without $nCeO_2$) near a major roadway to gain a detailed understanding about the atmospheric transport and fate of nanomaterials. Results from this 3-year effort will be presented to clients in the Office of Transportation and Air Quality (OTAQ) during FY11.

3.10 Emissions Modeling Research

Introduction

Emissions are among the most important drivers of the CMAQ modeling system. However, their estimates are subject to a large degree of uncertainty related to limited knowledge on sources, processes, chemistry, locations, and temporal variability. The NARSTO Emission Inventory Assessment (www.narsto.org/section.src?SID=8) affirms the large degree of uncertainty in emission inventories, particularly for precursors of airborne fine PM and for sources of OC, EC, and NH_3. Most anthropogenic emissions used in the CMAQ system are derived from EPA's National Emission Inventory (NEI) (www.epa.gov/ttn/chief/eiinformation.html).

AMAD's emission modeling research 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 from the NEI. As such, our research includes the development, evaluation, and implementation of emission models for biomass burning, fugitive dust, lightning, and biogenic sources. These sources emit O_3 precursors (VOC_s and nitrogen oxides), particulate matter, and some air toxins. Work performed in this area also supports the Division's efforts in the Air Quality Model Evaluation International Initiative (AQMEII), nanoparticles, and the Fairbanks, AK, EPA RARE project.

Research Activities and Accomplishments

During 2010, the Division focused on biomass burning, biogenics, fugitive dust, and improved speciation.

- Biomass burning—After working with EPA's OAQPS in helping the release of an operational satellite-based biomass burning emission estimation system for the NEI, the Division turned its attention to evaluating the emissions from this system in the context of air quality modeling and in working with other researchers on improving areas of greatest uncertainty. Collaborations with the National Aeronautics and Space Administration (NASA) as well as with researchers at Michigan Technological University and the University of Kentucky, continued under a NASA-funded grant. A 2-day workshop was held to continue the study of plume heights and agricultural burning emission estimates. Annual emission estimates being in 2003 have been provided by our collaborator, collaborators at the University of Louisville. These emission estimates are being evaluated for inclusion in future versions of the NEI.
- Biogenic emissions—For the 2011 release of CMAQ, we plan to offer two alternatives for biogenic emissions: NCAR's MEGAN and the BEIS version 3.14. Both models are now in the modeling system, and emissions from each have been compared. In concert with the Division's ecosystems-related research, we worked with UNC's Center for Environmental Programs (CEP) to incorporate updated agricultural data and information from the 30-m resolved National Land Cover Database (NLCD). We plan to create an update to the Biogenic Emission Landcover Database (BELD) that is based on the NLCD. Under a NASA-ROSES-funded grant with the University of Maryland, we collaborated on the use of satellite imagery to evaluate soil NO_x emissions (see presentation by H. Plata, "Soil NO_x model/satellite measurement intercomparisons," at http://www.cmascenter.org/conference/2010/agenda.cfm).
- Lightning NOx—Via a collaboration with NASA and the University of Maryland, the Division 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. 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 NOx is included in the model.
- Wind-blown and fugitive dust—The Division continued to interact with scientists in 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). A wind-blown dust module is being incorporated into the 2011 CMAQ release. For fugitive dust from anthropogenic sources, we have revised the methodology and improved the speciation of these emission sources. Specifically, we have included the speciation of trace metals from all anthropogenic sources to better understand the emission inventory and available measurements. We have revised the transportable fraction applied to the fugitive dust emission inventory to be consistent across the entire inventory and have incorporated temporal allocation adjustments to better account for variations in the emission inventory. Finally, we have included rain and snow events into the emission processing to account for meteorological effects on dust in the emissions processing. Two of presentations on this research were given at the 2010 Community Modeling and Analysis System (CMAS) conference: H. Simon et al., "Modeling the trace-elemental composition of $PM_{2.5}$ in CMAQ," and (2) G. Pouliot et al., "Assessing the anthropogenic fugitive dust emission inventory and temporal allocation using an updated speciation of particulate matter." Both presentations may be viewed at http://www.cmascenter.org/conference/2010/agenda.cfm.
- Speciated emissions—The Division continued to work with partners within EPA to improve the SPECIATE database, which is central to the speciation of VOC and PM gas and aerosols for emissions used in the CMAQ modeling system. Portions of this work are summarized in Simon et al. (2010) and were presented by Simon and colleagues at the 2010 CMAS conference.

Next Steps

The Division plans to continue improving and evaluating those components of the emission modeling system used in CMAQ and areas in which other organizations, such as OAQPS, are able to provide support.

The Division's research is organized around several model evaluation studies addressing O_3 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 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 SMOKE modeling system. SMOKE was developed to provide emission data to CMAQ. The emission modeling advances are in direct support of the major update of CMAQ planned for FY11.

Biomass burning—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. We plan to prepare one or more publications for submittal to a peer-reviewed journal related to this effort.

We also plan to continue our collaboration with scientists at NASA Langley, 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 emissions—We plan to continue work with 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 release the next version of CMAQ with MEGAN and BEISv3.14.

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 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 after the fall 2011 release of CMAQ.

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. NASA has indicated that a draft journal article on this work is in preparation. We plan to incorporate the lightning algorithm into the fall 2011 release of CMAQ.

Geogenic dust—As time permits, we will continue to interact with NOAA's air quality modeling forecast research team to prepare a publication and to include an algorithm for improved estimates of fugitive dust to 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 inline wind-sblown fugitive dust emission algorithm in the CMAQ code.

4.0 Air Quality Model Evaluation

4.1 Introduction

To ensure the integrity of regional air quality models for environmental decision-making, the Division conducts extensive evaluation studies to rigorously assess air quality model performance in simulating the spatial and temporal features embedded in air quality observations. We analyze the performance of meteorology, emissions, and chemical transport models to characterize model performance and also to identify what model improvements (inputs or processes) are needed. Thus, the Division's model evaluation efforts are tied tightly to its model development research activities.

Our evaluations seek to answer four fundamental questions: (1) Is the model getting the right answer? (2) Is the model getting the right answer for the right reasons? (3) How well does the model respond to changes in emissions and/or meteorology? and (4) What is the uncertainty associated with the performance of the model? We have used these questions to construct a model evaluation framework (Dennis et al., 2010) consisting of operational, diagnostic, dynamic, and probabilistic techniques. 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 (Foley et al., 2010). Diagnostic evaluation

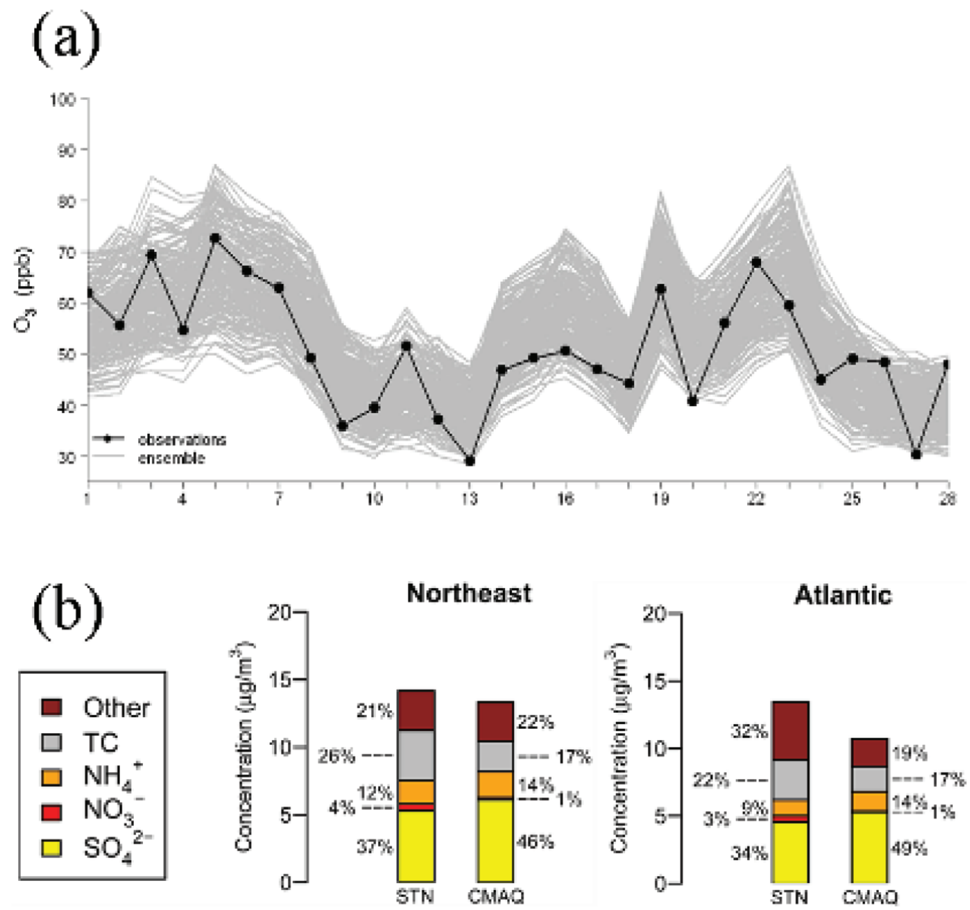

Figure 4-1. Examples of two types of model evaluation techniques: (a) probabilistic—time series of daily maximum 8-h O_3 concentrations from a 200-member CMAQ model ensemble at a monitoring site in an urban location; and (b) diagnostic—percent contribution of individual aerosol species comprising the total average regional $PM_{2.5}$ mass concentrations predicted by CMAQ and measured by the Speciated Trends Network (STN) sites.

investigates the processes and input drivers that affect model performance (Bhave et al., 2007, see Figure4-1b below). 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 (Godowitch et al., 2010). 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" (Pinder et al., 2009, see Figure 4-1a). Because these four types of model evaluation are not necessarily mutually exclusive, the Division's model evaluation studies often incorporate aspects from more than one technique of evaluation.

Information on selected aspects of the Division's model evaluation research program follows just below.

4.2 Atmosphepheric Model Evaluation Tool

Introduction

To conduct and communicate model evaluation requires the availability of statistical and graphical software. Over the past several years, the Division has been working on the development and application of the Atmospheric Model Evaluation Tool (AMET). AMET is an open-source software package designed to aid in the evaluation of meteorological and air quality models. AMET is a combination of several publically available software packages: specifically, the MySQL database software, PERL, and R statistical software. The database is used to store observed and modeled data, whereas the R software is used to perform various statistical analyses and create a number of different statistical plots. An example of AMET's capability is shown above in Figure 4-1b.

Research Activities

Recent activities have focused on communicating and releasing the software to the air quality modeling community.

Accomplishments

Appel et al. (2011) reported on the design and public release of AMET. AMETv1.1 was made available through the CMAS center Website at www.cmascenter.org.

Next Steps

Work is ongoing to create AMETv2.0, which should include enhancements to the database and analysis codes to provide greater support of new data sources (e.g., satellite data). It is likely that the next release of AMET will occur in late 2011 or early 2012.

4.3 Air Quality Model Evaluation Initiative

Introduction

The Air Quality Model Evaluation International Initiative (AQMEII) is a joint research project between air quality modeling groups in North America (U.S. and Canada) and Europe (numerous European modeling groups from various countries). AQMEII aims to promote research on regional air quality model evaluation across the European and North American atmospheric modeling communities through the exchange of information on practices, the realization of intercommunity activities and the identification of research priorities, keeping policy needs in focus. The activity is organized around the concept of Operational, diagnostic, dynamic, and probabilistic evaluation defined and discussed at the joint EPA/American Meteorological Society workshop in Research Triangle Park in 2007 and the first AQMEII workshop in Stresa, Italy, in 2009. AQMEII is coordinated by two co-chairs, Dr. Rao from AMAD and Dr. Galmarini from the European Union's Joint Research Center in Italy. In addition, Environment Canada serves as a regional focal point with the U.S. and Europe. The results of AQMEII will be available to the scientific community in general at academic, institutional, and private sector levels.

Research Activities

The Division is responsible for performing and evaluating the CMAQ model simulation for North America. As one of the coordinating members of AQMEII, AMAD has been responsible for coordinating the availability of the input data (e.g., meteorology, emissions) that were used for the modeling applications for North America.

Recent activities have focused on communicating and releasing the software to the air quality modeling community.

Accomplishments

Over the course of the year, Division scientists have been working closely with groups in Canada and Europe to compare the results of their modeling efforts and identify the strengths and weakness of each air quality model, with the ultimate goal of the research project being to learn how to improve those models and the methods of evaluating results from air quality models. By the end of 2010, the Division had completed the CMAQ modeling for North America and submitted all output data to the European Union's Joint Research Center for further analysis.

Next Steps

A special issue of *Atmospheric Environment* will be dedicated to results from the AQMEII project, and AMAD has committed to submitting a number of manuscripts to the special issue on topics ranging from meteorology, emissions, and boundary conditions to analyses of the operational performance of the AQMEII CMAQ modeling results to principal component analysis (PCA) of the modeling results. All of these papers are joint research projects with many international groups contributing to each of the manuscripts. Submission of manuscripts to the special issue of *Atmospheric Environment* is due in May 2011. In addition, results from the AQMEII project will be presented at the 2011 CMAS conference and the AQMEII workshop to be held in Chapel Hill, NC, in October 2011.

4.4 Diagnostic Evaluation

Introduction

Diagnostic evaluation research during the year examined the interaction of meteorology on chemical transport modeling.

Research Activities

Our focus has been on photochemical O_3 formation and horizontal transport processes because they strongly influence the temporal evolution and spatial variability of the simulated 3-D O_3 distribution within the lower troposphere. Results from the CMAQ with the Carbon Bond CB05 chemical mechanism are being evaluated against surface-based routine measurements, as well as upper air profile measurements obtained by research aircraft during intensive field studies from three summer months in 2002, when several high-O_3 episodes occurred in the eastern United States. Net O_3 production efficiency (OPE) results suggested photochemical O_3 formation was comparable between the model and observations, with OPE values of 6.7 and 7.6, respectively, within the afternoon PBL. Evaluation of wind profiles revealed wind speeds generated by the WRF model with the FDDA base approach displayed greater underestimation of observed speeds in the nocturnal residual layer aloft. During a multiday O_3 episode, when a low-level jet occurred nightly in the Mid-Atlantic region, modeled results with the base FDDA underestimated the maximum jet speed by up to 3 m/s (Figure 4-2), and wind directions exhibited a southerly bias of 20˚ or more relative to observed directions. Trajectory analysis demonstrated that these differences in winds can introduce large spatial displacements in modeled and observed O_3 patterns within the region. A follow-up sensitivity study with the WRF meteorological model has been performed with different FDDA options, which also included the use of additional available wind profile data (i.e., boundary layer wind profiler measurements and Doppler radar wind profiles). Results demonstrated that model simulation of the Mid-Atlantic nocturnal low-level jet winds was improved when more observed wind profiles were assimilated.

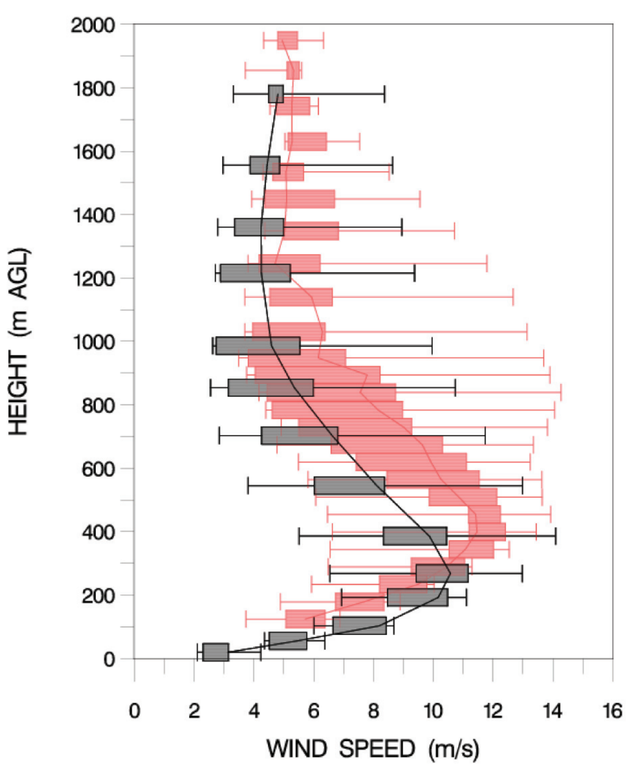

Figure 4-2. Modeled (gray) and observed (rose) wind speed profiles averaged over the nocturnal periods of August 11-15, 2002, at Ft. Meade, MD. Boxes span the 25th to 75th percentiles, and whiskers extend from the 10th to 90th percentiles.

Accomplishments

More accurate transport patterns based on these findings are expected to lead to model improvement in estimating air quality concentrations because wind fields generated by the WRF model are directly applied in the CMAQ chemical transport model simulations for retrospective periods.

Next Steps

Journal manuscripts presenting results of this diagnostic evaluation study and WRF/FDDA sensitivity effort are being prepared for journal submission in 2011.

4.5 Dynamic Evaluation

Introduction

Dynamic evaluation examines a model's concentration response caused by changes in emissions and/or meteorology through comparisons to observed concentration change. Therefore, historical periods must be identified that provide observable changes in pollutant concentrations that can be related closely to known and appreciable changes in emissions and/or meteorology. The time period spanning EPA's NO_x SIP call program provides a valuable test of model response using the dynamic evaluation approach since substantial reductions in NO_x emissions occurred in the major point source sector during 2003-2004. Gégo et al. (2007) and U.S. EPA (2007) show examples of how observed O_3 levels exhibited notable decreases after implementation of the NO_x SIP Call. Gilliland et al. (2008) documented the results of an initial dynamic evaluation study based on CMAQ model simulations with three different chemical mechanisms to assess maximum 8-h O_3 changes between summer 2002 (pre-NO_x SIP Call) and summers 2004 and 2005 (post-NO_x SIP Call).

Recognizing the large reduction in anthropogenic activity that naturally occurs on weekends relative to weekdays, we performed a dynamic evaluation of CMAQ modeling system for the so-called "weekend O_3 effect" to determine if observed changes in O_3 because of weekday-to-weekend (WDWE) reductions in precursor emissions could be accurately simulated. The weekend O_3 effect offered another opportunity for dynamic evaluation, as it is a widely documented historical phenomenon that has persisted since the 1970s.

Research Activities

During the past year, the Division expanded on the NO_x-SIP Call analysis by assessing the changes in maximum 8-h O_3 concentrations (≥ 95th%) from CMAQ simulations spanning five consecutive summer periods (2002 to 2006) against concentration changes at the rural-based Clean Air Status and Trends Network (CASTNET) sites. Figure 4-3 below depicts variations in the modeled and observed O_3 changes for each summer period relative to 5-year mean values. The modeled results track the observed changes rather closely, and considerable overlap exists during most periods. However, the largest differences between the modeled and observed values occur for the summer 2002 period, which are attributable to the notable model underestimates of maximum O_3 levels during several high O_3 episodes. A diagnostic study has been underway to investigate horizontal transport and O_3 chemical formation to examine whether either of these processes is contributing to the underestimation. In addition,

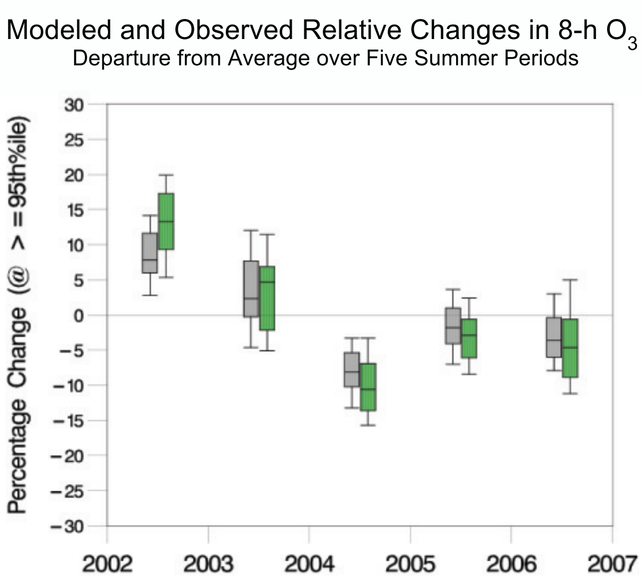

Figure 4-3. Box/whisker plot of the percentage change in modeled (gray) and observed (green) maximum 8-h O_3 concentrations (>95th percentile) for each summer period relative to a 5-year mean at the CASTNET monitoring sites in the eastern United States. The boxes span the 25th to 75th percentiles and whiskers extend from the 10th to 90th percentiles.

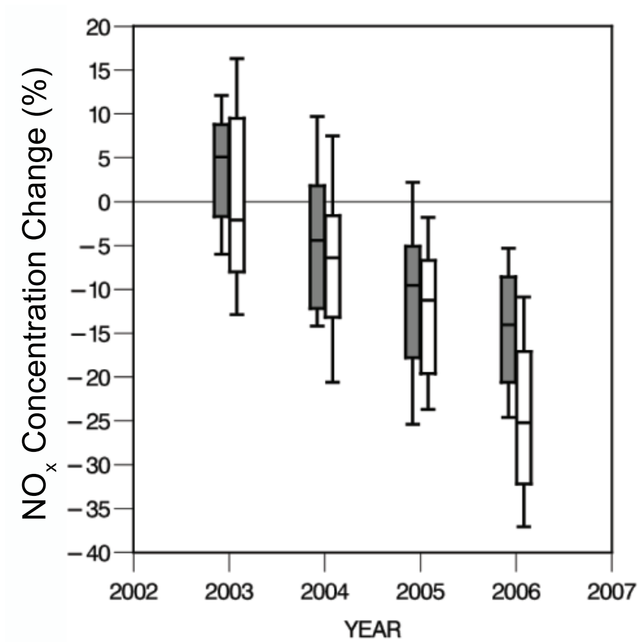

Figure 4-4. Change in weekday 3-h average morning NO_x concentrations. Model results (gray) and observations (white) are based on 42 urban sites. Each box/whisker plot shows the median values (line inside boxes). Boxes span the 25th to 75th percentiles, and whiskers extend from the 10th to the 90th percentiles of the concentration distributions.

analyses are proceeding with modeled and observed O_3 profiles over multiple summers to determine the extent of concentration change aloft.

Another dynamic model evaluation effort examined weekday morning (high-traffic period) concentrations of NO_x to assess changes in modeled and observed NOx levels that could be attributable to mobile emission changes over this multi-year period. Although modeled mobile emissions dropped by 25% over this period, CMAQ results were governed by the 15% decrease evident in total NO_x emissions, which also include notable contributions from area, nonroad, and the minor point-source sectors.

Using 18 years (1988 to 2005) of observed and modeled O_3 and temperature data across the northeastern United States, we reexamined the long-term trends in the weekend effect and confounding factors that could complicate the interpretation of this trend and explored whether CMAQ could replicate the temporal features of the observed weekend effect. This work was performed in collaboration with researchers from the State University of New York and the University of Idaho.

Accomplishments

Three journal articles on dynamic evaluation were published during 2010. Godowitch and Rao (2010) revealed that spatial patterns of percentage decreases in O_3 between 2002 and 2006 showed strong similarities between the modeled and observed results, although the modeled changes were somewhat less than observed changes. Godowitch et al. (2010) reported that observed urban NO_x concentrations decreased by nearly 25%, whereas modeled concentrations declined by about 15% from 2002 to 2006 (see Figure 4-4). Pierce et al. (2010) reported that CMAQ could replicate the decrease in amplitudes of the weekly O_3 cycle that occurred during an 18-year period. However, similar to the two other dynamic evaluation studies, the modeled response of O_3 to weekday-weekend differences in emissions was somewhat less than that observed. These studies suggest that more attention should be given toprobing uncertainties in emission estimates, reducing the grid cell size in the lowest layer of CMAQ, and using time-dependent and more realistic boundary conditions for the CMAQ simulations.

4.6 Probabilistic Model Evaluation

Introduction

Most model evaluation studies have focused on assessing the performance of a single set of deterministic modeling results. However, it is well known that air quality predictions are sensitive to uncertainties in meteorology, emissions, and processes represented within the chemical transport model itself.

Research Activities

To support probabilistic model evaluations and the application of air quality models in a probabilistic manner, research is underway to achieve the following accomplishments.

- Estimate the sensitivity of O_3 and aerosol predictions to different model configurations and inputs (an AQMEII activity)
- Develop methods to assess the uncertainty in CMAQ predictions of O_3 and aerosols using an ensemble of model configurations and input sets
- Apply these methods to assess the uncertainty in CMAQ-predicted changes in O_3 and aerosols resulting from emission changes
- Use statistical methods to postprocess the ensemble of model runs based on observed pollutant levels
- Use the uncertainty information to help prioritize key model development needs

In previous years, this work was based on a 12-member ensemble of CMAQ simulations that included six different MM5 configurations and two different chemical mechanisms. We expanded the membership of the ensemble to include uncertainty from emissions by using the CMAQ-DDM-3D to generate large member ensembles, while avoiding the major computational cost of running a regional air quality model multiple times. The resulting ensemble of CMAQ-estimated O_3 concentrations was used to fit a probability distribution function, and the quality of the ensemble-derived pdf was assessed using observations and parametric (confidence interval) and nonparametric (ranked-histogram) methods. A journal article of this work was published in *Environmental Science and Technology* (Pinder et al., 2009)

Accomplishments

During 2010, we began exploring statistical postprocessing methods to weight the ensemble members and improve estimates of model uncertainty. We applied a Bayesian model averaging (BMA) technique to calibrate the ensemble predictions by weighting each individual ensemble member based on how closely it matches observed O_3 values. We evaluated these methods based

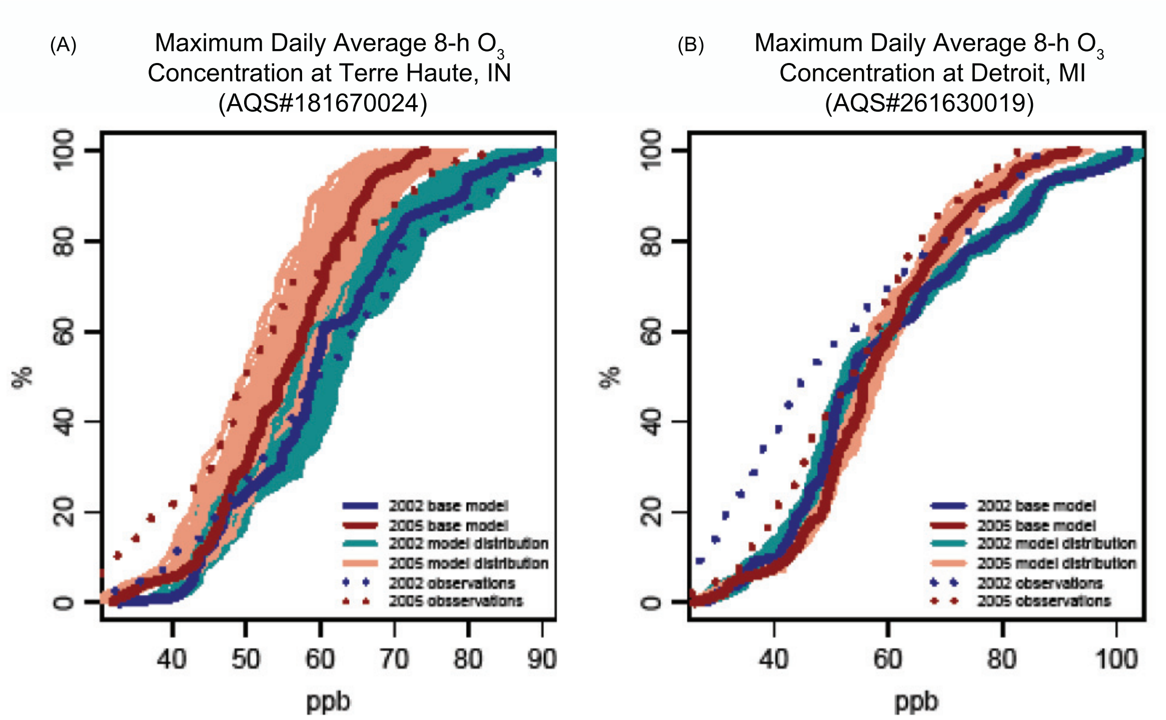

Figure 4-5. Base model, observational, and model ensemble empirical cumulative distributions of maximum daily average 8-h O_3 concentrations for 2002 and 2005 at two AQS sites: (a) Terre Haute, IN; and (b) Detroit, MI. All ensembles were constructed based on ±50% uncertainty in emissions of area and mobile NO_x and ±3% uncertainty in emissions of point NO_x. The wide spread of the ensemble at the Terre Haute site indicates greater sensitivity to NO_x emissions in comparison with the site in Detroit.

on observed O_3 in the Southeast in the summer of 2005. A manuscript describing these results currently is being drafted and is expected to be submitted for journal review in 2011. As we continue to develop and improve these methods for creating probabilistic model outputs, we are also investigating how these tools can be used in policy-relevant applications. Specifically, we are combining probabilistic evaluation techniques with dynamic evaluation of model-predicted O_3 concentrations. Using DDM-produced sensitivity coefficients and building on our previous model evaluation efforts, we estimated the dynamic response of the model because of NO_x reductions between 2002 and 2006, while accounting for uncertainties in NOx emission inputs (Figure 4-5). This work has been described in a journal article accepted for publication by Napelenok et al. (2011).

Next Steps

We currently are collaborating with Rice University and N.C. State University to explore other Bayesian estimation techniques for quantifying the uncertainty in model inputs and outputs. In addition, we are collaborating with OAQPS on a pilot project to compare a DDM-based approach for examining emission control options with response surface modeling methods that have been developed and used by the regulatory community for the past several years. This project will enable us to explore the strengths and weaknesses of different probabilistic approaches for supporting EPA's air quality management and policy needs.

5.0
Climate and Air Quality Interactions

5.1 Introduction

Energy generation from fossil fuels contributes to global warming and degrades air quality, both of which profoundly impact human and ecosystem health. Atmospheric levels of carbon dioxide (CO_2) and other GHGs have increased dramatically since the Industrial Revolution, and emissions from fossil fuel combustion have been linked to human disease since the London smog event in 1952. The Intergovernmental Panel on Climate Change (IPCC) Fourth Assessment Report (AR4) (Solomon et al., 2007) concluded that the continued rise in GHGs from human activity is the primary cause of the temperature increases observed over the 20th century, and that global warming is likely to continue over the next century even with significant mitigation of greenhouse gas emissions. These temperature increases also lead to changes in other climatic conditions, such as changes in precipitation intensity and duration. Extreme weather conditions could become more frequent, which, in turn, can affect adversely human and ecosystem health. Emissions from anthropogenic combustion sources are also the largest sources of PM, O_3, CO, and NO_x and sulfur. These pollutants are known to contribute to respiratory and cardiovascular effects in human populations, as well as ecological effects to aquatic (acidification and eutrophication) and terrestrial ecosystems (damage to agricultural and other vegetation).

The scientific issues of global climate change have been studied for decades. However, in response to the 2007 U.S. Supreme Court decision in Massachusetts vs. EPA and the EPA Administrator's recent Endangerment Finding under the CAA Act (U.S. EPA, 2009), the EPA must rapidly prepare for rulemaking regarding control of emissions. Additionally, the EPA Office of Air and Radiation (OAR) recognizes that some "traditional" pollutants regulated under the Clean Air Act also have radiative forcing properties (e.g., the black carbon component of $PM_{2.5}$, O_3) that impact climate. The Agency has a need for integrated policy approaches to both mitigate climate change and manage air quality.

The urgency also has increased greatly to understand the implications of climate change on local and regional scales, given the numerous anticipated impacts on environmental protection and regulatory responsibilities of the Agency. For example, research already has demonstrated that future climate conditions very likely will increase air quality risks and decrease the effectiveness of emission control efforts (e.g., Nolte et al., 2008; Weaver et al., 2009). In addition to enhanced photochemical production in a generally warmer environment, greater frequency of stagnation events could exacerbate air quality problems. It also is anticipated that increases in extreme precipitation events could lead to additional water-borne disease outbreaks and degradation of water quality conditions. Anticipated damages to aquatic and terrestrial ecosystems could include impacts such as encroachment by invasive species and biome migration.

The Agency's needs fall into two broad questions from the air, climate, and energy integrated transdisciplinary research (ITR) plan that will be used to organize and focus AMAD research activities described in this chapter. The first regards risk assessment and adaptation: How will climate change impact air and water quality, water availability, and ecosystems? Then, there is risk mitigation: How can the Agency best contribute to climate change mitigation through U.S. controls of both long-lived GHGs and short-lived pollutants?

Accomplishments

Because this research area represents a significant broadening of scope beyond AMAD's traditional domain of air quality, a white paper, "Integration of air quality and climate change—modeling connections from global to regional scales," was undertaken to help plan and guide the research. This white paper, together with white papers on interactions between air quality and human health and between air quality and ecosystems, was reviewed by an external panel in March 2010. The white papers contributed to the development of AMAD's 5-year Strategic Plan and were published on the Division's Web site in October 2010.

5.2 Regional Climate Modeling: Dynamical Downscaling

Introduction

Global climate models (GCMs) are used to simulate gridded climate conditions with worldwide coverage. Because GCMs often are run for multicentury simulations, GCMs typically generate output at fairly coarse temporal (e.g., monthly or daily) and spatial (e.g., 2° latitude × 2.5° longitude or 1° latitude × 1° longitude) intervals. To investigate and understand regional effects of climate change (and particularly to capture extreme events), higher temporal and spatial frequency of the gridded fields is required. One broad category of methods to create regional climate fields that are influenced by GCM simulations is "downscaling." Downscaling involves using the fields from a GCM, in combination with additional information about the regional scale (e.g., topography, land use, historical regional climate data) and physical, mathematical, and/or statistical models, to extend the GCM simulation to finer spatial and temporal granularity. With increased horizontal texture, the downscaled fields are more sensitive than the GCMs to local spatial heterogeneities in weather and climate that result from topographical changes, land/water interfaces, vegetation, and population. Downscaled climate fields can then be used to simulate the regional impacts of climate change on water quality and availability, agriculture, ecosystems, human health, air quality resulting from emissions control strategies, and energy demand.

Dynamical downscaling involves using a regional climate model (RCM), where the initial and lateral boundary conditions are obtained from a GCM. Dynamical downscaling is fundamentally similar to regional weather forecasting, except that a GCM is used for lateral boundary conditions; there are no observations to assimilate, and simulation periods are years or decades rather than days or weeks. Furthermore, rather than evaluating the model based on its skill in representing day-to-day weather observations, the model's performance is evaluated in terms of how well it represents climatic features, such as seasonal means, the magnitude of extremes, or the frequency of events exceeding some threshold.

Research Activities

For AMAD's dynamical downscaling, the WRF model is being used as an RCM. Initial work is using coarse-scale reanalysis fields (i.e., 2.5° × 2.5°) as input, which is comparable in resolution to the GCM that will be used for downscaling future climate. Focusing first on reanalysis data enables comparison of the RCM output to a wide variety of observational data, including both gridded data at smaller spatial scale and point observations, to examine the extent to which the RCM added value over the coarse-scale input data.

Simulations over the continental United States have been conducted using grid cells that are 36-km x 36-km in size. A key goal of this research is to develop optimal techniques for downscaling the large-scale forcing resolved by coarse grid global data while allowing effective small-scale forcing and dynamical response to be well represented by the RCM. Comparative analysis of scale-selective techniques for data assimilation (nudging) and boundary condition specification are important aspects of this research. Thus, modeling experiments will compare the effects of using no nudging (other than through the lateral boundaries), analysis nudging, and spectral nudging. Evaluation is planned against means and extremes of near-surface fields, cloud and radiation fields, and spectra.

Accomplishments

During 2010, AMAD completed an initial study on the use of WRF as an RCM. Three simulations of the year 1988 were conducted, and the results obtained using analysis nudging, spectral nudging, and without any nudging were compared to each other and to data from the North American Regional Reanalysis (NARR) product. A manuscript describing this study (Bowden et al., 2011) has been completed and will be submitted for publication in 2011.

Also during 2010, AMAD created its first continuous, multidecadal WRF simulations. Simulations were as described above but covered the period from 1988 to 2007. These simulations will be used for several evaluation studies that are planned for 2011.

Concurrent with the RCM simulations conducted using reanalysis data, we have developed a dynamical downscaling linkage between WRF and the NASA GISS Model E GCM. A 6-year test dataset was acquired from collaborators at GISS to establish the logistical connections between Model E and WRF (i.e., vertical coordinates, state variables, linkage of surface fields) and to test the downscaling techniques.

Next Steps

Evaluation of the 20-year WRF simulations is in progress. In addition to analyzing how well WRF represents mean climatic variables, such as surface temperature, precipitation, and radiation fields, we will focus on the effect of analysis and spectral nudging on those mean variables and on the simulated atmospheric circulation. In addition, we plan to examine the ability of WRF to capture the frequency of extreme events, such as droughts and floods.

As GISS develops Model E fields for the IPCC AR5, those data will be made available at high temporal frequency (i.e., three-hourly or six-hourly) for "time slice intervals" (i.e., approximately decadal subsets) of the GCM simulation. Using knowledge gained from the reanalysis testing, evaluated dynamical downscaling techniques will be employed to create regional downscaled climate fields from current and future decadal time slices that will be used to analyze high-resolution regional climate change effects.

Several aspects of dynamical downscaling need to be refined to adapt WRF, which is a numerical weather prediction model, to regional climate applications. For example, the model must be able to realistically simulate the surface energy budget over multidecadal simulations. Initial testing with different radiation schemes in WRF has shown a persistent underprediction of cloud cover that results in overheating of the land surface. Clearly, improvements in the cloud and radiation physics components of WRF are needed for regional climate applications. In 2011, we will be evaluating the modeled radiation fields from the 20-year retrospective WRF simulations against satellite retrievals from the Clouds and Earth's Radiant Energy System (CERES) and MODIS instruments, which are both aboard the Aqua and Terra satellites, and against observations taken at the Department of Energy's Atmospheric Radiation Measurement (ARM) Climate Research Facility. These efforts to evaluate and improve the cloud and radiation budgets in WRF are being coordinated with research to implement indirect aerosol radiative forcing in the WRF-CMAQ system (described below and in Chapter 3), which also involves evaluation using CERES and MODIS data. These 20-year WRF simulations also will help with understanding how well extremes and variability are simulated by WRF, helping build confidence in future-year estimates of extreme events and variability under climate change conditions.

5.3 Regional Climate Modeling: Statistical Downscaling

Introduction

Statistical downscaling methods use correlations among historically observed and modeled meteorological variables under current climate conditions to predict future regional and/or local patterns and events from 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 to gain a better understanding of fine-scale variability, even down to point locations, given high-resolution training data.

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 can be 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). (See Schmith, 2008, for more discussion.) However, statistical downscaling does make this "stationarity" assumption as it extrapolates to future conditions.

Research Activities

During the past year, AMAD has been reviewing, improving, and testing statistical downscaling methods, with an emphasis on evaluation and calibration. Most of this research is being done using a regression-based downscaling technique proposed by Hoar and Nychka (2008), which models the response variable (i.e., surface temperature) as a function of fine-scale temperature estimates obtained by applying a thin-plate spline interpolation technique to the output of a GCM (or other coarse-resolution model). This enables us to bypass the difficulties associated with predictor selection (a difficult issue with many regression-based methods), so that we can focus on issues associated with calibration, training period selection, and quality and quantity of training data. If the efficiency and accuracy of this method proves suitable, this method could be adapted to use different response variables or different predictors.

Accomplishments

In the past year, AMAD has implemented a regression-based statistical downscaling method proposed by Hoar and Nychka (2008). We currently are finishing a period of extensive testing, with a particular focus on understanding the impact of such assumptions as stationarity and temporal correlation. The downscaling method has been applied for temperature and has been trained and evaluated using fine-scale output from the PRISM model, encompassing the continental United States during the period, 1907 to 1996.

In tests with simulated data, we found that temporal correlation does have an impact on the downscaling estimates and should be accounted for in the downscaling model. Two statistical techniques to aid in detecting and estimating temporal correlation, the Durbin-Watson test and restricted maximum likelihood (REML), performed well in our simulation studies. With these adjustments, the Hoar and Nychka method produced confidence intervals for future years' temperature that were well calibrated, with only a small loss in efficiency because of the autocorrelation. These simulation studies provided benchmarks of how well we could expect the method to perform in "ideal" circumstances, in which stationarity and type of correlation structure can be assumed.

AMAD also applied the downcaling technique to the PRISM temperature data. With a 30-year training period (1907 to 1936), the method was used to obtain temperature estimates for individual years (1937, 1996) and interval averages (1937 to 1966 and 1967 to 1996). In contrast to the simulated cases, the confidence intervals generated by the technique were calibrated poorly. The magnitude of this discrepancy (between simulated cases and cases using PRISM) suggests that there are fundamental problems with the assumptions of the method when applied to "real-world" cases and, particularly, with the assumption that the statistical associations remain constant over time. Work is currently underway to determine whether this problem can be ameliorated (e.g., additional covariates, other data sources, etc.).

Next Steps

AMAD is planning future work to better understand the relative strengths and weaknesses of statistical and dynamical downscaling for various applications. Research questions of particular interest include those that follow.

- Developing at least a basic understanding of how the uncertainty may change when applied to future-year GCM simulations
- Identifying the relative strengths/weaknesses of the dynamical and statistical approaches to downscaling
- Determining whether hybrid downscaling approaches may be able to capitalize on the strengths of both dynamical and statistical methods

5.4 Development of Coupled Regional Climate and Chemistry Modeling System

Introduction

Climate change is influenced by long-lived GHG and also by short-lived radiatively active gases and aerosols that typically are modeled by regional-scale air quality models such as the CMAQ model. The direct and indirect feedback effects of gases and aerosols on radiative forcing and cloud microphysics have important climate impacts, particularly at regional scales. Thus, both GCM and RCM components of the climate modeling system need to include these air quality feedback effects. Therefore, AMAD is developing a coupled regional climate and chemistry modeling (RCCM) system that can downscale climate and chemistry from the GCM through a series of nested grids from hemispheric to continental to local scales.

Research Activities

A two-way coupled WRF-CMAQ modeling system is being developed and tested for air quality and climate applications at scales ranging from hemispheric to local. There are several advantages to an integrated meteorology and chemistry modeling approach, including more frequent data exchange for high-resolution modeling; better integration of physical processes, such as cloud-chemistry interactions; and feedback effects of gases and aerosols on radiation and cloud microphysics. Thus, the WRF-CMAQ system is an important development for air quality research and assessment over multiple scales and regional climate modeling, where direct and indirect feedbacks on radiation, clouds, aerosols, and precipitation are important.

Further research and development of more comprehensive treatments of direct and indirect feedback of short-lived gases and aerosols on radiation and cloud properties are needed. WRF-CMAQ currently includes direct feedback of aerosols, accounting for size distribution and chemical composition, on SW radiation in the Community Atmospheric Model (CAM) radiation scheme and the Rapid Radiative Transfer Model for GCMs (RRTMG) SW scheme (Iacono et al., 2008). The direct effects of tropospheric O_3 on LW radiation in the CAM and RRTMG LW schemes also have been implemented. Some initial evaluation studies have shown an expected response to these direct feedback effects for both typical summer conditions in the eastern United States and for an outbreak of multiple wildfires in California in June 2008. Aerosol direct radiative effects associated with scattering and absorption of incoming radiation result in a reduction of SW radiation reaching the surface, which then translates to reduction in temperature at the surface, as well as a reduction in PBL height. For moderate pollution levels, such as during typical summer conditions in the eastern United States, impacts on SW reduction and subsequent suppression in PBL heights are relatively modest. Significantly, larger changes in simulated surface radiation were seen for the California wildfire case where smoke from the wildfires resulted in much higher aerosol loading. The reduced SW radiation caused much cooler surface air temperatures (up to 4 to 5 K in the smoke plumes), lower PBL heights (up to 400 m), and significantly higher ground level concentrations of O_3 and $PM_{2.5}$ (Mathur et al., 2009). Evaluation of direct aerosol forcing is continuing in 2011 by extending the initial 10-day test case for the eastern United States to the full month of August 2006 using the RRTMG radiation scheme and the current versions of both WRF (v3.2) and CMAQ (v5.0). The California wildfire case also is being updated with the latest model versions and improved estimates of wild fire emissions.

New research aimed at improved modeling of aerosol mixing state and optical properties has been initiated through collaboration with UNC. The work will lead to more accurate direct radiative effects of mixed composition aerosols, particularly involving black carbon aerosol, in the RRTMG SW scheme. Through this collaborative research, we also are investigating the feedback effects of aerosols on LW radiation. It is hypothesized that some aerosols, especially black carbon, may absorb LW radiation as well as does SW radiation.

Aerosols also affect radiation through their role as cloud condensation nuclei (CCN). Greater concentrations of CCN lead to a greater number of smaller cloud droplets, causing greater SW cloud albedo. Activation of aerosols as CCN alters cloud microphysics such that warm rain processes are less efficient, thereby extending cloud lifetime. These effects of increased aerosol concentrations on clouds are known as the first and second indirect effects, respectively.

Development and evaluation of the direct and indirect feedback processes in the two-way coupled WRF-CMAQ modeling system, and eventually the RCCM, will advance through comparison with the latest release version of the online coupled WRF/Chem model. WRF/Chem currently simulates aerosol, cloud, and radiative interactions when employing its CBM-Z photochemical mechanism and MOSAIC aerosol scheme (Chapman et al., 2009). Sensitivity tests using present-day and future emission scenarios oriented toward climate change studies will be conducted with both the WRF/Chem and the two-way WRF-CMAQ modeling systems, and subsequent simulation results will be analyzed to evaluate their feedback processes.

Recent forecasting and retrospective CMAQ applications over continental scales and for annual cycles have pointed to the need for more robust methods to specify chemical lateral boundary conditions (LBC). Although linking with global-scale atmospheric chemistry models has been pursued, it also is recognized that biases in the global model can propagate and influence regional CMAQ calculations and often confound interpretation of model results. The successful extension of CMAQ to hemispheric scales would provide several advantages: (1) consistent LBCs for regional calculations focusing on air quality issues in the United States (i.e., the biases arising from process formulations are consistent at all scales); (2) opportunities to explore emerging challenges related to the processes regulating "background" levels (The recent revisions to the O_3 NAAQS and possible further reductions in the O_3 standard make the accurate representation of background O_3 in the model even more imperative than before); (3) lay the foundation for future applications of the integrated WRF-CMAQ model to explore radiative impacts of aerosols and radiatively active gases, such as O_3, on the earth's energy budget and the indirect feedbacks of aerosols on cloud microphysics; and (4) a framework for assessing uncertainties in modeling regional distributions of long-lived HAPs and toxics (e.g., mercury). When the WRF-CMAQ model is configured for climate studies, the hemispheric grid domain will be an important link between the global climate model and the regional nested grids over North America and local areas.

Accomplishments

During 2010, an initial implementation of aerosol indirect effects using the CCN activation scheme from the two-way, or online, coupled WRF/Chem model (Abdul-Razzak and Ghan, 2000) was adapted to WRF-CMAQ.

Initial testing of the WRF-CMAQ over the Northern Hemisphere has shown realistic ground-level concentration distributions over the major emissions regions and realistic aerosol optical depth (AOD) compared with MODIS satellite retrievals. Preliminary analysis of the hemispheric simulation for March 2006 showed remarkably good agreement of modeled AOD with AERONET observations in Beijing and Greenbelt, MD.

The proposal, "Development of a Next-Generation Comprehensive Global Environmental Modeling System for Assessing Air and Water Quality in Current and Future Climates," was selected for funding as one of the initial EPA ORD Pathfinder Innovation Projects. The proposal is to extend CMAQ to the global scale by coupling it to the Ocean-Land-Atmosphere Model (OLAM) GCM. OLAM uses a telescopic finite-volume discretization scheme that divides the globe into regular polygons of arbitrary size. It has the capability to provide greater spatial resolution over areas of interest, while simulating the entire globe

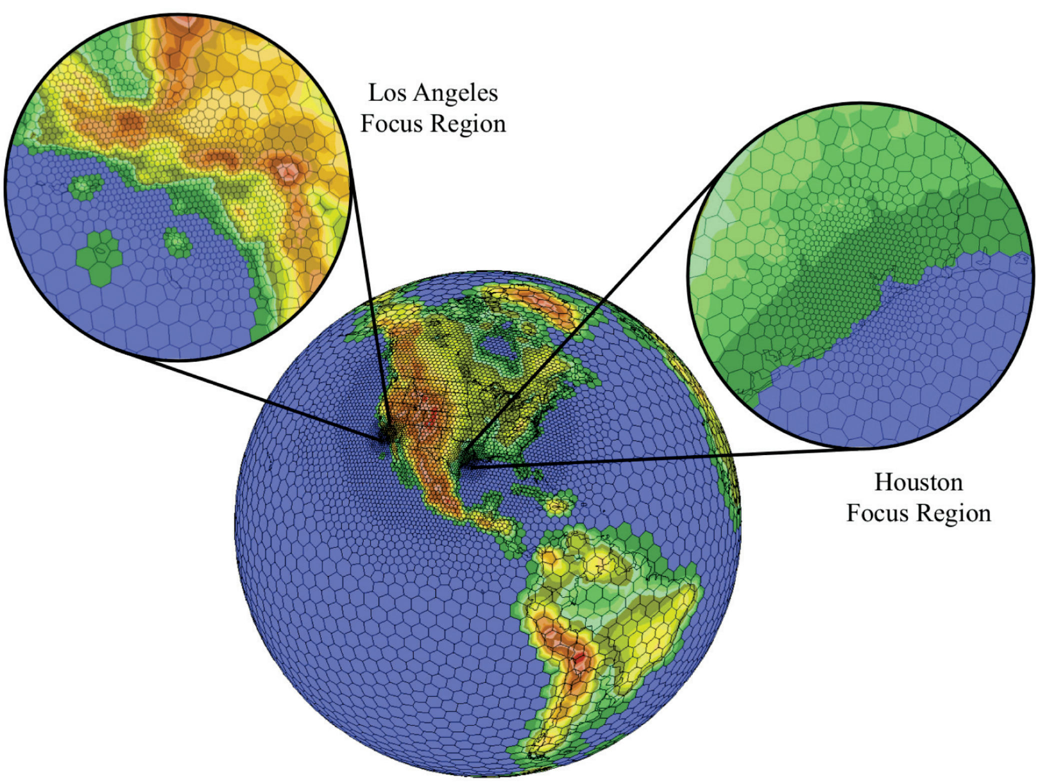

Figure 5-1. Example global telescoping grid structure.

(see Figure 5-1). Simulating the entire globe at once would avoid problems that can arise in downscaling a GCM with an RCM, such as poor temporal resolution of lateral boundary conditions, inconsistent physics treatments between different modeling platforms, and the inability of the RCM to feed back on the GCM solution.

3-year collaborative project with the Department of Energy (DOE) entitled: Evaluation of the Interactions Among Tropospheric Aerosol Loading, Radiative Balance, Clouds, and Precipitation. This observational-modeling study aims to address this issue by systematically investigating changes in anthropogenic emissions of SO_2 and NO_x over the past two decades in the United States, their impacts on anthropogenic aerosol loading over the North American troposphere, and subsequent impacts on regional radiation budgets. The DOE funding of this interagency agreement will be used to support three new postdoctoral fellows to work on this project.

5.5 Decision Support Tools for Managing Air Quality and Mitigating Climate Change

Introduction

Emissions of long-lived and short-lived GHGs and aerosols have a substantial impact on both climate and air quality. The goal of this effort is to develop an integrated suite of models to examine the impacts and understand the key uncertainties of emission mitigation strategies on both climate and air quality. Ultimately, the goal is to answer the question: What is the impact of U.S. emission control strategies on air quality and climate? Figure 5-2 describes the two classifications of decision-support tools. On the left side of the diagram are screening tools to enable decisionmakers to rapidly identify emission scenarios and policy options of interest. On the right is the series of models, spanning global and regional scales, needed to fully assess the impacts of a given policy option. The screening tools can be used to identify a narrow but critical subset of emission scenarios or policy options that then can serve as input to the more complete models. The work in this section describes AMAD efforts relevant to the screening tools and the Atmosphere-Ocean General Circulation Modeling.

This schematic describes the models and linkages from changes in policy decisions to changes in SLCF, GHG, and CAPs, and their local impacts on human health and ecosystems.

Research Activities

Decision support tools for scenario analysis. A key finding of the Climate Impacts on Regional Air Quality (CIRAQ) project is that future air quality largely is driven by changes in future emissions. Forecasting emission changes over decades is impossible, so decision-makers rely on scenarios to help guide their choices. However, scenarios are comprised of many assumptions. Discovering policy options that deliver robust results across a range of assumptions requires investigating many scenarios. Unfortunately, state-of-the-science global and regional climate models require tremendous computational resources. Exploring more than a handful of scenarios is not tenable. Decisionmakers need approximation tools that can be used to rapidly screen the costs and benefits of climate mitigation strategies.

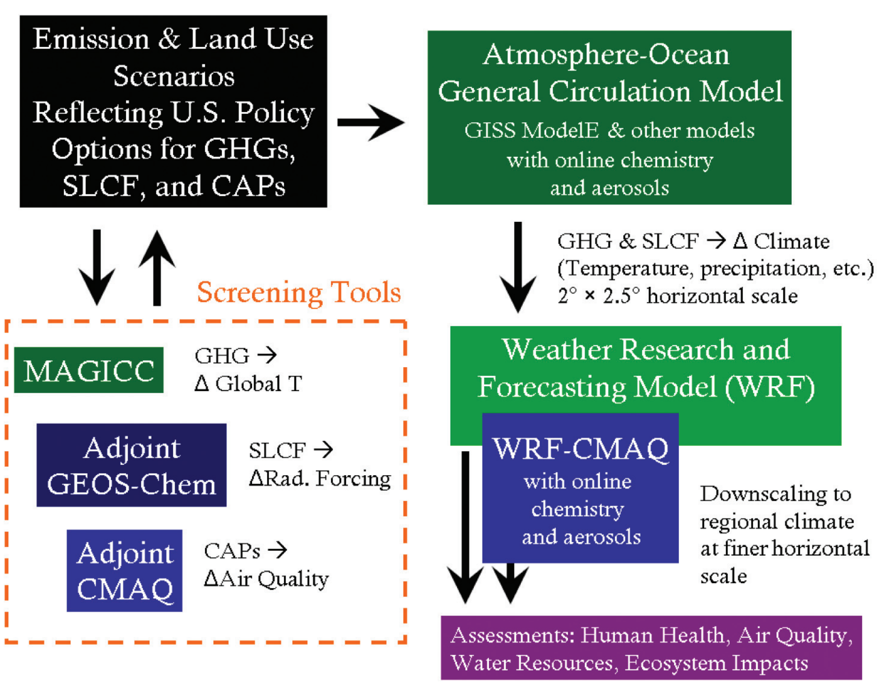

Figure 5-2. Schematic describing model linkages.

For long-lived GHGs, the emissions are proportional to the climate impacts. However, short-lived climate-forcing gases and aerosols undergo chemical and physical transformations that substantially change their climate impacts. Radiative forcing can be used as an approximate surrogate for the impact of these species on climate. We are developing an integrated assessment model composed of four parts: (1) the GEOS-Chem global chemical transport model, (2) the LIDORT radiative transfer model, (3) the adjoint of these two models coupled together, and (4) the market allocation (MARKAL) model. This project is named GLIMPSE.

GEOS-Chem and LIDORT can estimate the impact of emissions, chemical fate, and transport on direct radiative forcing. The adjoint of these models can be used to build a reduced form model that can rapidly assess the impacts of a change in emissions on radiative forcing. Finally, MARKAL connects technologies and energy demands to emissions. With GLIMPSE it is possible to examine combined constraints of GHG emissions, short-lived species radiative forcing, and relative cost to examine the trade-offs between different policy options.

This tool is being developed in collaboration with our colleagues in NRMRL who are extending MARKAL to include more sources of short-lived, radiatively active gases and aerosols. This is in collaboration with University of Colorado professor Daven Henze, who is the original developer of GEOS-Chem Adjoint,. Finally, successful completion will require frequent interaction with our colleagues in the EPA program offices to match the decision-support tool to their needs.

The first application of the tool will be to examine impacts of emission reductions from black carbon and sulfate. Next, it will be extended to include radiative forcing and chemical precursor emissions for O_3. Finally, the adjoint version of CMAQ will be included as part of GLIMPSE to simultaneously assess air quality and radiative forcing.

Global modeling of U.S. Emission control strategies; impacts of short-lived, radiatively active gases and aerosols. Although greenhouse gas emissions and short-lived species radiative forcing are useful approximations, they do not fully prescribe the change in climate. Scenarios and policy options that merit further consideration will be used as input to the global climate model for a complete assessment of the global climate impacts of U.S. climate mitigation strategies.

The first phase of this work will use the GISS ModelE simulations prepared for the regional climate downscaling task. These climate simulations simulate present day and future climate under multiple Representative Concentration Pathways (RCPs), the scenarios under development for the IPCC AR5. GISS Model E simulations will provide detailed diagnostic information for 10-year timeslices, beginning in 1980, 2000, 2030, and 2100.

In the second phase, a few scenarios informed by policy options developed using GLIMPSE will be used as input to additional climate simulations using GISS Model E coupled with online chemistry to resolve the climate impacts of U.S. emission control strategies on global climate. A key purpose of these simulations is to contrast the relative impact of GHG mitigation with emission reductions of short-lived climate-forcing species. The results from these simulations will be used with the regional downscaling methods described in Task AMAD11-108 to determine the regional climate impacts of U.S. emission changes.

Accomplishments

We have developed a prototype of the GLIMPSE system, presented the results at scientific meetings and conferences, met with stakeholders in the program offices, and incorporated their feedback.

Next Steps

In 2011, we will use GLIMPSE as a tool to analyze the impacts of U.S. emission control strategies on concentrations and global radiative forcing of short-lived, radiatively active aerosols, including SO_4, black carbon, and OC and to assess the impact of possible climate change mitigation policies on radiative forcing and air quality.

Also in 2011, we will conduct a review of proposed feedback mechanism to assess the impacts of reactive nitrogen emissions on climate change, and we will conduct a bounding study using models and observations to examine the extent to which anthropogenic emissions enhance O_3 in the upper troposphere.

5.6 Biosphere-Atmosphere Interactions: Improving the Treatment of Isoprene Oxidation

Introduction

The scenarios described above characterize emissions trajectories for sources that can be controlled directly. However, climate and land management changes are likely to impact future emissions of VOCs as well. With warming temperatures and increased CO_2, isoprene emissions are expected to increase. A review of the NCER STAR-funded projects on climate and air quality identified a key uncertainty in the future O_3 production efficiency as the chemical treatment of isoprene and the formation of isoprene nitrate compounds.

Isoprene is emitted naturally by many species of trees and shrubs. With the exception of methane, which reacts much more slowly in the atmosphere, isoprene is the most highly emitted VOC, both worldwide and within the United States. It is an important precursor for O_3 formation and is thought to be a substantial contributor to SOA. These species are critical for understanding interactions between air quality and climate for two reasons. First, in the future, we expect there to be much more isoprene relative to NO_x. As demonstrated by recent field measurements, the isoprene, chemistry and formation of O_3 under these conditions is highly uncertain. Second, unlike the rest of the United States, the climate in the Southeast has not warmed. To what extent have light-scattering aerosols from isoprene contributed to this trend?

We are partnering with collaborators making field measurements and conducting laboratory studies to improve our understanding of isoprene oxidation and to assess the relative impacts of uncertainties in isoprene emissions, chemical mechanism and reaction rates, and dry and wet deposition rates.

Research Activities

Recent laboratory and theoretical studies have provided new insight into the oxidation of isoprene, including more detailed understanding of the formation and fate of isoprene nitrates (INs; Paulot et al., 2009), formation of epoxides under low-NO_x conditions, and reformation of HO_x via isomerization reactions. We have incorporated these reactions into the SAPRC07 chemical mechanism and simulated the time period of the INTEX-NA field campaign to investigate the impact of INs on O_3 production and the oxidized nitrogen budget.

Accomplishments

The new scheme has been evaluated against smog chamber experiments from three different laboratories. The results show improved predictions of O_3 for the experiments with the lowest NO_x concentrations. We also have implemented the new scheme into the CMAQ model and have conducted simulations for the INTEX-NA field campaign period during summer 2004. When compared with ambient measurements, we find this updated chemistry provides a more accurate simulation of the isoprene oxidation products methacrolein, methyl vinyl ketone, and alkyl nitrates. Including limited HO_x radical regeneration in the oxidation of isoprene improves simulated hydroxy radical (OH) concentrations, especially when isoprene concentrations are high. Over the southeastern United States, a region of high isoprene emissions, simulations including this chemistry show a 2 to 4-ppb increase in O_3 (see Figure 5-3) and 30% increase in SOA.

Next Steps

We now are testing updates to the nitrate radical oxidation pathway for isoprene, as well as experiments to examine the sensitivity of simulated O_3 concentrations to key reaction rates in the chemical mechanism. A follow-on study is planned for 2011 that will focus on assessing the relative impact of chemical mechanism uncertainties with uncertainties in emissions and deposition rates on simulated O_3 concentrations.

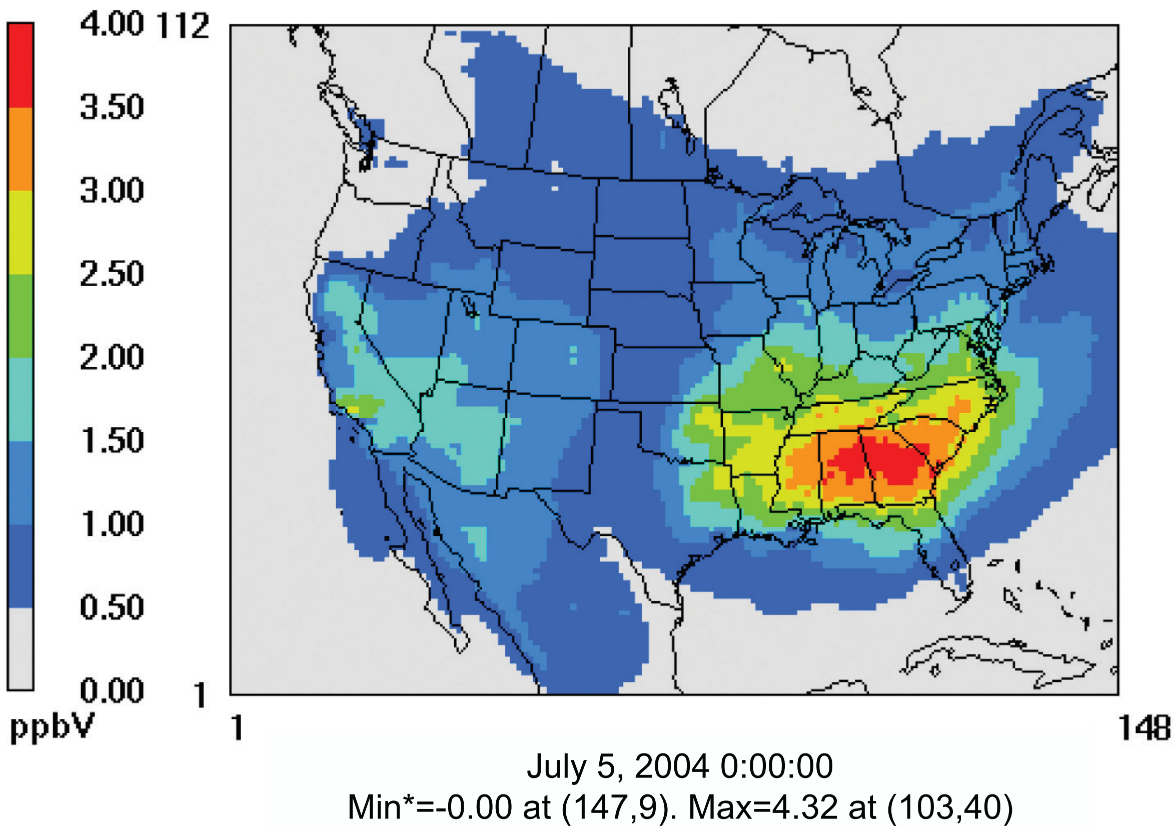

Figure 5-3: Change in simulated mean surface-level O_3 concentration because of updated chemical mechanism.

6.0
Linking Air Quality to Human Health

6.1 Introduction

The need for improved dispersion models to support human exposure assessments in urban areas has led to a significant effort to design and build a new modeling construct to efficiently provide near-field concentration estimates to support exposure and health related studies. Included in this effort is the ongoing near-roadway research program that has been working toward improving the urban-scale line-source (mobile source) dispersion algorithms. Additionally, this task involves development and application of model evaluation techniques and acquiring, assessing, and processing databases for model development and evaluation purposes. The new modeling system will be applied in ongoing exposure and health studies in collaboration with clients within and outside of EPA.

Along with the need for better models is the need to understand the optimal accuracy and precision in exposure estimates needed to conduct human exposure and health studies. In the absence of personal exposure measurements, epidemiology studies traditionally have relied on imperfect surrogates of personal exposures, such as area-wide ambient air pollution levels based on readily available outdoor concentrations from central monitoring sites. The direct use of monitoring data inherently assumes that they are representative of the air quality over a broad area. However, there is increasing evidence that the current monitoring network is not capturing the sharp gradients in exposure caused by high concentrations near, for example, major roadways. Yet, providing more detailed exposure information can be resource intensive and may result in greater (or undefined) uncertainty. Research in the Division has focused on improving the understanding of the optimal level of accuracy and precision for use in exposure estimates.

6.2. Research Description

EPA's Clean Air Research multiyear plan increases the emphasis on research to better understand the linkages between sources and health outcomes. This research area is focused on the critical modeling link between sources of air pollutants in urban areas and health outcomes. Modeling the wide variety of pollutant sources in the meteorologically and topographically complex urban environment will require the development of an improved modeling system that is both complete in its handling of the urban setting yet computationally efficient because of the hundreds and possibly thousands of sources that are considered in exposure analyses. Additionally, model development and evaluation databases and model evaluation techniques will be developed to accomplish this task. The EPA Fluid Modeling Facility is uniquely designed for conducting laboratory studies characterizing the often steep concentration gradients expected in urban areas and is a major source of development and evaluation data.

The new dispersion modeling system will be based in a significant way on the previous development of the American Meteorological Sociey/EPA Regulatory Model (AERMOD) urban-scale dispersion model. Although AERMOD is designed for a wide variety of regulatory applications, the new model will benefit from the science and algorithm basis of AERMOD without the computational burden often required for regulatory analyses. The new model will be an integral part of a hybrid modeling system that links observations with both regional- and urban-scale modeled concentrations to provide the necessary concentration distributions required for human exposure modeling and associated health risk assessments. Although the new dispersion model is not expected to account for complex chemistry, it is anticipated that, for selected pollutants (e.g., NO), near-field chemistry may be accounted for with simple parameterizations.

In urban areas, mobile sources are a significant contributor to air pollution exposure. This research area includes an effort to further understand the atmospheric transport and dispersion of mobile source pollutants within the first few hundred meters of the roadway, a region often characterized by complex flow (e.g., vehicle-induced turbulence, noise barriers, road cuts, buildings, vegetation). Examination of traffic emissions and potential population exposures near roadways includes field and laboratory measurements of concentration distributions near simulated roadways. This task involves the investigation of near-road dispersion through numerical, wind tunnel, and tracer studies, with the goal of characterizing the near-road spatial distribution of mobile source pollutants and the development of improved modeling algorithms within the new urban-scale dispersion model.

Research in the Atmospheric Exposure Integration Branch (AEIB) also includes a project to compile the results of a suite of tiered exposure studies to capture the critical elements relevant to characterizing exposure (e.g., variability of pollutant, health study design), common findings resulting from the studies, and remaining challenges. This work requires close coordination across NERL's air quality modeling and measurement groups (AMAD and HEASD) to tap their collective knowledge of the chemistry and physical processes involved with the spatial and temporal properties of multiple pollutants. In addition, close collaboration with the epidemiology community (HEASD, the National Center for Environmental Assessmant [NCEA], NHEERL and academia) is critical in understanding the different demands of the various health study designs and to demonstrate the impact of the tiered exposure definitions on the health effect measure. This research provides critical information on the level of spatial and temporal data needed to support human exposure and health studies. It will result in greater efficiencies as more refined exposure information can require more resources, yet result in more (or undefined) uncertainty.

6.3. Accomplishments

Wind Tunnel Modeling of Flow and Dispersion near Roadways

A series of physical modeling experiments was performed in the Division's Meteorological Wind Tunnel, investigating 14 common roadway configurations, including a flat roadway with no surrounding obstacles (base case), noise barriers of varied height and distance from the roadway, two different porous barriers intended to simulate the dispersive effects of roadside vegetation, and depressed and elevated roadways. Results show that the configuration of the roadway can have a substantial effect on the concentrations both on and downwind of the roadway (Heist et al., 2009a). The results are being used to develop algorithms for inclusion in dispersion models to account for these effects.

As part of the EPA and FHA field study of mobile source pollutant dispersion near Interstate 15 in Las Vegas, NV, a laboratory study was conducted in the Meteorological Wind Tunnel on a 1:200 scale model of the study area to examine the effect of the road depression associated with a railroad overpass at the field site and to explicitly define the flow and concentration fields surrounding this major roadway (Figure 6-1). Wind tunnel data show that the roadway depression (of about 5.5 m maximum depth) results in a decrease in maximum ground-level concentration of about 25% over that observed with a flat roadway (Heist et al., 2009b).

Dispersion Model Algorithm Development

A new line-source algorithm (AERLINE) has been developed that efficiently computes dispersion from sources, such as roadways, considering multiple lanes of traffic, low wind, meander conditions and varying wind directions (including those parallel to the traffic flow) (Venkatram et al., 2009). Comparison of AERLINE against the Raleigh 2006 highway field study for both downwind and upwind concentrations is in progress. A draft algorithm formulation was developed that accounts for the influence of roadways that are depressed below grade. This algorithm is currently undergoing evaluation against wind tunnel data and will be included in AERLINE in FY11.

Analysis of the Raleigh 2006 Pilot Field Study

The 2006 Raleigh field study, conducted in the summer 2006, was designed to provide data to characterize the influence of traffic-generated emissions in the near-road environment, especially to help assess the impact on air quality and particle toxicity near a heavily traveled highway. Pollutant measurements were synchronized with real-time traffic and meteorological monitoring devices

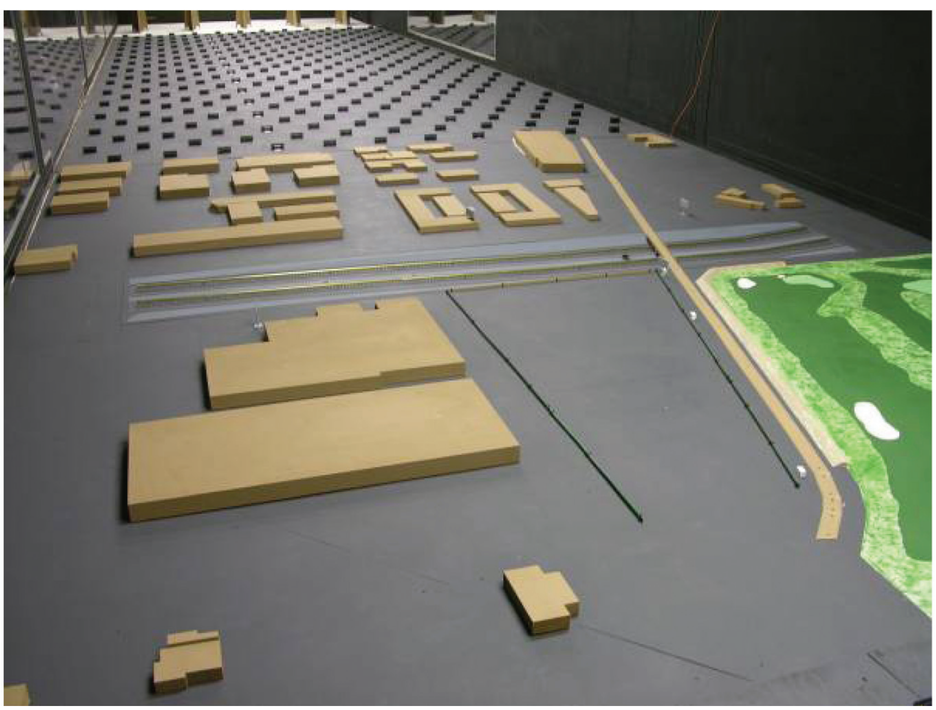

Figure 6-1. Wind tunnel model of Las Vegas field study area built at 1:200 scale.

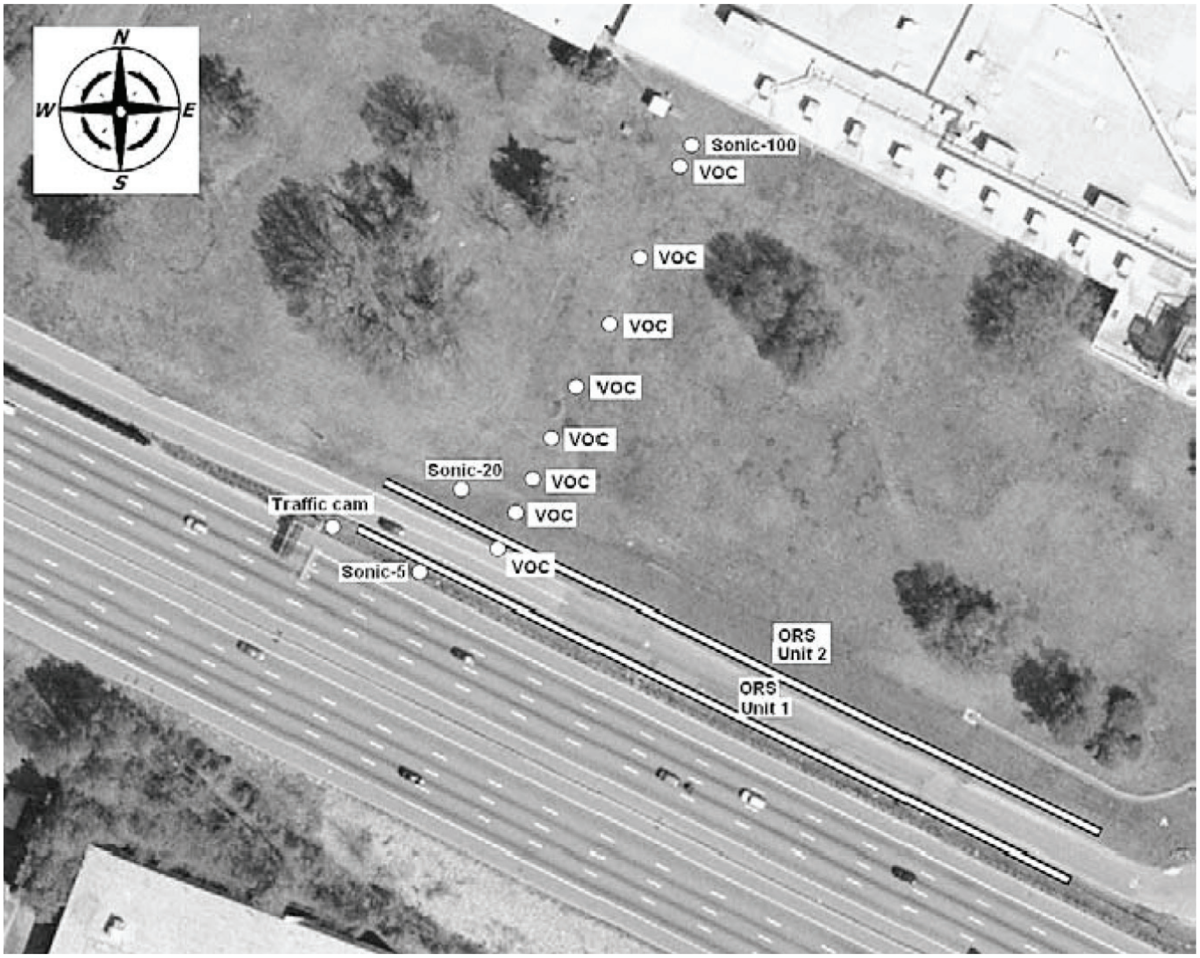

Figure 6-2. Aerial photograph of study location in Raleigh, NC.

to provide continuous and integrated assessments of the variation of near-road pollutant concentrations and particle toxicity with changing traffic and environmental conditions, as well as distance from the road (Figure 6-2). This research helped to demonstrate the temporal and spatial impact of traffic emissions on near-road air quality (Isakov et al., 2007; Venkatram et al., 2007).

Tracer Field Study of Flow and Dispersion near Roadway Noise Barriers

An interagency agreement was developed between NERL and NOAA's Field Research Laboratory to conduct a field study in Idaho Falls of flow fields and tracer dispersion from a line source (simulating roadway emissions) immediately upwind of a 6-m-high barrier (typical of near-road noise barriers found in urban and suburban areas) (Figure 6-3). Simultaneous line-source tracer release and measurements were conducted without the barrier. The results currently are being analyzed to be used for model algorithm development to account for the effects of noise barriers in AERLINE. Unlike the associated wind tunnel studies, which are limited to neutral conditions, the tracer studies were designed to examine dispersion for all atmospheric stabilities (Finn et al., 2010).

Computational Fluid Dynamics (CFD) Modeling of Near-Road Configurations

To complement the wind tunnel and tracer studies of near-road dispersion, a series of CFD simulations has been initiated in collaboration between NERL (AMAD and HEASD) and NRMRL. In FY09, the FLUENT CFD code was used to simulate the six-lane flat roadway scenario, with conditions identical to the wind tunnel study. The wind tunnel results were used to suggest the most appropriate on-road initial dispersion conditions and the most appropriate turbulence parameterization, as well as other flow parameters to be used for other roadway scenarios.

Gulf of Mexico Oil Fire Plume Modeling

During remediation efforts following the British Petroleum oil spill, more than 400 separate controlled burns were conducted over a 2-m period, resulting in the removal of approximately 11 million gallons of crude oil from the Gulf (see Figure 6-4). AEIB scientists co-authored a journal article describing a risk assessment of the airborne dioxin that was a by-product of these controlled burns (Schaum et al., 2010). The paper describes a screening-level assessment of the exposure and potential cancer risk to nearby workers and residents potentially exposed

Figure 6-3. Photograph of bag samplers and anemometers downwind of a simulated noise barrier at the Idaho Falls field site.

to dioxin via inhalation. The authors also examined the potential for this population to be exposed to dioxins in fish harvested for consumption. Using available information about the size and rate of each burn, meteorology from nearby buoys, and the NOAA North American meso-meteorological model, scientists determined that the worst case concentrations occurred within 50 m of burns when wind speeds were at their highest, (10 m per s). These dispersion modeling results and the limited on-site monitoring provided critical input to the dioxin risk assessment. The estimated cancer risks from the predicted air concentrations and deposition were found to be lower than the EPA's typical range when consideration is given to require additional actions, such as cleanup or the establishment of regulatory policy.

Accountability Indicators Project

In its mission to protect human health and the environment, the EPA implemented the NO_x Budget Trading Program (NBP) to reduce the emissions of NO_x and secondarily formed O_3. These pollutants and their precursors can be transported downwind, contributing to pollutant levels at locations much farther from the emission sources, potentially impacting human health in downwind areas. In this study, we investigated the health impacts in New York State from exposure to polluted air parcels transported from the Midwest. We developed and applied a methodology to identify and target the transport of polluted air parcels and demonstrated that the risk for hospital admission because of respiratory-related illness was increased in New York State on those days that the air parcel originated over the Ohio River Valley, where several high-emitting power plants are located (Figure 6-5). More specifically, we examined air parcels moving through a boundary drawn around high-emitting power plants in the Midwest using back-trajectories and found significant associations with these transported air parcels (risk estimates ranged from 1.06 to 1.16 for the entire study time period) for six of the eight New York State regions). The approach developed by this research can be used as an indicator of exposure for transported air pollution.

6.4. Next Steps

Model Development

AEIB will focus on the design and development of a new urban-scale modeling construct that is similar in nature to AERMOD but without the regulatory structure. Instead, the new model will address the specific needs of human exposure and health analyses. The overall model design will emphasize computational efficiency, user friendliness, use of readily available inputs, and the characterization of uncertainty, and it will make use of existing model algorithms in existing dispersion models. Wind tunnel and field studies will feed into the development and testing of near-road algorithms in relation to atmospheric stability, wind direction, and vehicle-induced turbulence.

Model Evaluation

The new dispersion model will be the air quality core of the human exposure modeling system (including observations and regional modeling) in the approach to link urban sources and human exposure assessments and human health outcomes. Evaluation of both individual model algorithms and the overall modeling approach in human exposure and health-related scenarios is needed.

Figure 6-4. Example of a controlled burn of spilt oil in the Gulf of Mexico.

Databases for use in model evaluation will include the MESA AIR (Baltimore) study, the NEXUS (Detroit) study, Urban 2003 (Oklahoma City), and the California Energy Commission urban tracer study (Southern California). In addition, wind tunnel study data and the Idaho Falls tracer study also can serve in an evaluation capacity, particularly for individual model algorithms. Through collaboration with U.K. scientists, the DAPPLE urban study data-base in London also will be considered for the evaluations.

Applications of New Modeling System and Client Collaboration

Once the new modeling system has been developed and tested, inclusion of it or its components will be considered in the HEASD's Community and Environmental Justice modeling effort (i.e., C-FERST/STREETS software). Additionally the new dispersion model will be used to support the design and interpretation of the air quality and health study planned for the Research Triangle Park, area in 2013 or 2014. Collaboration with the Federal Aviation Administration on the development of specific applications at airports will be initiated because of the significance of these urban source areas. Finally, collaborations with the Office of Transportation and Air Quality and the FHA relative to characterization of mobile source emissions and the FHA/EPA field studies will continue.

A large part of AEIB's local-scale modeling application efforts will be focused on characterizing the concentration distributions related to the NEXUS research project currently underway 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. Exposure metrics developed in this project will be coupled with the Childhood Health Effects from Roadway and Urban Pollutant Burden Study (CHERUBS). Modeled and monitored air quality and exposure data will be coupled with assessments of respiratory effects to investigate the relationships between traffic-related exposures and observed health effects. Air quality modeling is being conducted with the current AERMOD dispersion model for a screening level analysis. AERLINE and the new dispersion model will be used in a refined analysis once actual measurements of traffic and air quality are available from the study.

Synthesis Analysis

Various levels of air pollution characterization (e.g., statistical combination of observed and modeled values, hybrid modeling approaches) will be provided for several tiered exposure studies, including the Cooperative Agreements with the University of Washington, Rutgers University, and Emory University, and the collaborative effort with the New York State Department of Health. A synthesis analysis will be conducted to summarize the results from the tiered studies described above, as well as other studies, to document the findings in a systematic way. The analysis will identify the spatial and temporal resolution needed for the various human exposure and health study designs commonly used, the characteristics of the various air pollutants of concern (e.g., variability, reactivity), and our current knowledge regarding the state-of-science estimates that currently can be provided and the uncertainty surrounding these estimates.

Demonstration Project

The concepts summarized and examined in the synthesis analysis will be incorporated into a dispersion model being developed specifically for use in human exposure and health studies. For example, pollutants that must be characterized at finer spatial resolutions also might need simple chemistry (e.g., NO_2), as well as line-source capability. Thus, such approaches will be integrated into the new model and applied in studies such as NEXUS through C-FERST. C-FERST is a framework developed for use by communities and individuals to estimate human exposure to toxic substances and to identify and prioritize risks from these substances.

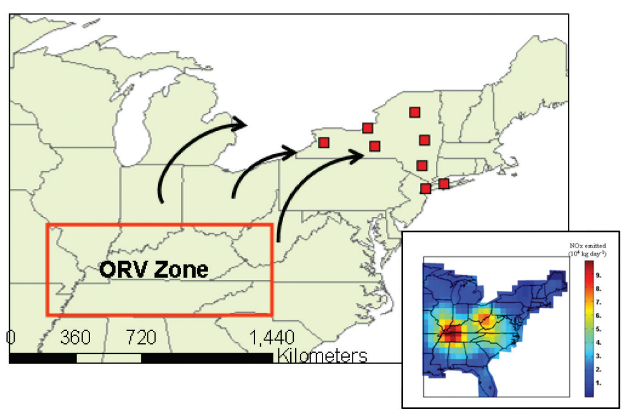

Figure 6-5. Graphic on left shows high NO_x emissions in Midwest (July 1997) and graphic on right shows transport of pollution from Midwest into New York State. Red squares are locations from which back-trajectories were initiated.

7.0
Linking Air Quality and Ecosystem

7.1 Introduction

EPA is charged with protecting the health and welfare of the Nation. The CAA definition of welfare effects includes, but is not limited to, effects on soils, water, wildlife, vegetation, visibility, weather, and climate. Terrestrial and aquatic ecosystems represent an integration of all these factors. Atmospheric deposition is an important nonpoint source of pollution impacting ecosystems. Deposition of both nitrogen and sulfur is the main source of acidification of fresh water and terrestrial ecosystems. Atmospheric deposition of nitrogen is a contributor to nitrogen-nutrient enrichment affecting Western ecosystems and eutrophication affecting estuaries. From 15% to 40% of the nitrogen load to coastal estuaries is estimated to come from atmospheric deposition. Atmospheric deposition is a major source of mercury that is methylated and subsequently bio-accumulated in food chains, affecting wildlife and humans.

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 square kilometers) with the regional airshed scale (thousands to millions of square 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.

Achieving these goals requires a coordinated research strategy covering a variety of activities to best use AMAD's limited resources. The strategy involves: (1) improvements in CMAQ's bi-directional and uni-directional air-surface exchange characterizations, (2) improvements in the WRF/CMAQ land surface characterizations and air-surface exchange in complex terrain, (3) improvements in precipitation fields, (4) linkage of hydrologic models with WRF/CMAQ to provide a consistent connection between precipitation and hydrology for a system-consistent linkage to ecosystem models, and (5) application of expanded model capability to support assessments of management scenarios The research is organized into three interrelated tasks.

1. Air Deposition and Ecosystem Services Assessments
2. Air-Ecosystem Linkage Studies
3. Model and Tool Development

Relevance. The National Research Council (NRC) and the Clean Air Act Advisory Committee (CAAAC) have urged EPA to pay increased attention to ecosystem protection and develop its capacity in this direction. In response, the Agency has undertaken a joint review of the existing secondary (welfare-based) NAAQS for O_3, NO_X and sulfur oxides (SOX). This is the first time secondary standards have been addressed separately from the primary standards. The secondary NAAQS review is focused on ecological effects from exposure to O_3 concentrations and from atmospheric deposition associated with acidification sulfur and nitrogen and nutrient enrichment nitrogen. Because the CAA stipulates that the NAAQS are for ambient air concentrations, not deposition, the air quality models serve a critical function to connect air quality and deposition to support the secondary NAAQS. In addition, the NRC and CAAAC recommended that EPA explore the use of critical loads in the development of the secondary NAAQS. The Office of Air Programs (OAP) is exploring the use of critical loads (associated with atmospheric deposition) as a management tool. In addition, a multiagency group on critical loads as an approach to ecosystem management for land management agencies has been established. The agencies are the National Park Service (NPS), the United States Forest Service (USFS), USGS, and EPA. Modeling of critical loads by these agencies is focusing in the eastern United States on acidification and is focusing on acidification in the eastern United States and on nitrogen nutrient enrichment nationally, but with a focus on the western United States on nitrogen nutrient enrichment.

The climate change research program at EPA has begun to be equally concerned about ecosystem response, as well as air quality and human health. The goal is to identify and evaluate mitigation and adaptation strategies that will sustain or improve current ecosystem functioning and provision of services. This requires that changes in climate and land use are expressed in ways that can be translated by models to changes in such ecosystem functions and services. EPA's climate change program also puts a priority on assessing and predicting water quality, not just water quantity. Using models to investigate alternative future scenarios facilitates comparing and contrasting the effects of land use change with the effects of climate change on air-surface exchange of nutrients and pollutants and, ultimately, ecosystem health.

In parallel, EPA's ESRP has a focus on ecosystem services and their relationship to human health and well-being. The overarching ESRP research questions are; What are the effects of multiple stressors on ecosystem services, at multiple scales, over time; and What is the impact of different plausible changes in these services on human well-being and on the value of the services. Land use change and climate change are considered to be two important drivers to be addressed in the context of changing ecosystem services. Tansdisciplinary research programs that explore interactions between air, water, and land are central to addressing these questions and developing the science and modeling tools necessary to simulate alternative future scenarios and mitigation strategies.

The objective of the ecology theme research is to advance the development and application of state-of-the-science atmospheric tools to determine the exposure of ecosystem receptors to atmospheric pollution causing and contributing to ecological and ecosystem service degradation. The intent is to provide an improved ability to connect forecasts of the effect of air management actions on future atmospheric deposition to ecosystem models. The air-ecosystem research within AMAD aims to provide better atmospheric connections for three major ecosystem assessment areas described below.

1. Atmospheric deposition that better supports SO_x-NO_x welfare standards and critical load assessments and determinations
2. Air-ecosystem exposure linkage of atmospheric stressors to ecosystem models to support ecosystem assessments coupled with air management drivers, including the assessment of ecosystem services
3. Atmospheric/meteorological-ecosystem exposure linkage to support ecosystem impact assessment of climate change

7.2 Air Deposition and Ecosystem Services Assessments

7.2.1 Introduction

The thrust of this research is to define, develop and investigate targeted CMAQ linkage applications for study and learning and to develop guidance on how to best establish chemical and meteorological linkages with ecosystem models, including improvement of linkages to address climate impacts on ecosystems. Three major areas of research are (1) connection of WRF precipitation to consistent surface hydrology, (2) linkage to water quality/watershed models, and (3) linkage to ecosystem welfare and critical load models. Target ecological end points include fresh water aquatic, estuarine aquatic, and terrestrial systems. A key focal point is to develop a model representation of the hydrologic overland flow with other agency partners that is consistent with the precipitation from WRF/CMAQ. This focal point addresses a critical issue identified by the most recent linkage research. The thrust of linkage to water quality model research is to address air-water model cross-media (linkage/ coupling) connection issues and develop approaches to reconcile space-time mismatches for management support. Development of guidance for critical load estimation is the third part of the research thrust. Accuracy requirements for effective model-to-model communication are explored and defined and approaches are developed to more effectively provide atmospheric deposition to ecosystem models for stressor relationships for critical load management support.

7.2.2 Research Direction

The objectives of this research are: (1) to develop a linkage between meteorological-model-produced precipitation and associated modeled surface hydrology to address air-water paradigm mismatches and support ecosystem exposure and loading estimates under climate change, (2) to actively use the CMAQ model to research and explore climate and air-ecosystem linkage issues to develop guidance on how to improve the linkage, (3) to illuminate model functioning and examine areas of model uncertainty to identify areas for further model development, and (4) to improve CMAQ and tool development and inform application approaches in support of multimedia modeling and ecosystem management. Primary attention is focused on the elements of the hydrological cycle that impact ecosystem loading and exposure to atmospheric pollutants. Two focal areas are the NO_x-SO_x air quality standard review and the study of critical loads (deposition-based tipping points). Aspects of weather and climate beyond that can combine with the hydrological cycle to impact ecosystem loading and exposure to atmospheric pollutants also will be explored. The lessons are to be synthesized to inform research planning for linkage research, CMAQ and ecosystem model development (including ecosystem services assessment), and integrated multimedia model development and application.

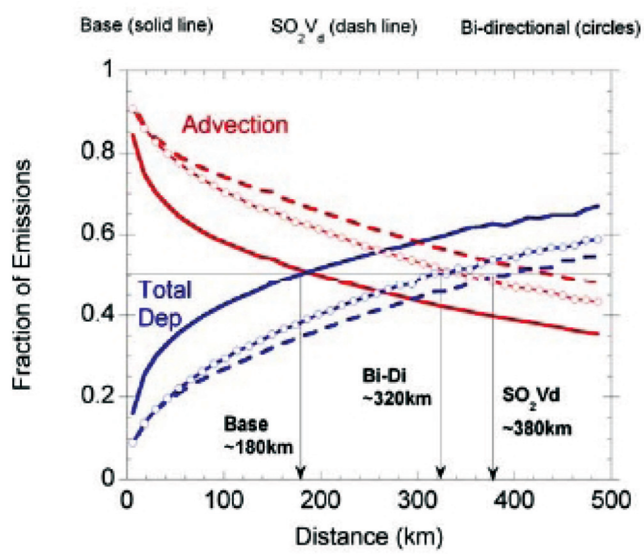

Figure 7-1. Range of influence of NH_3 emissions from a single, isolated Sampson County, NC cell in 2002 CMAQ simulations using unidirectional, the deposition velocity as a surrogate, and bidirectional NH_3 surface exchange parameterizations, Dennis et al. (2010)

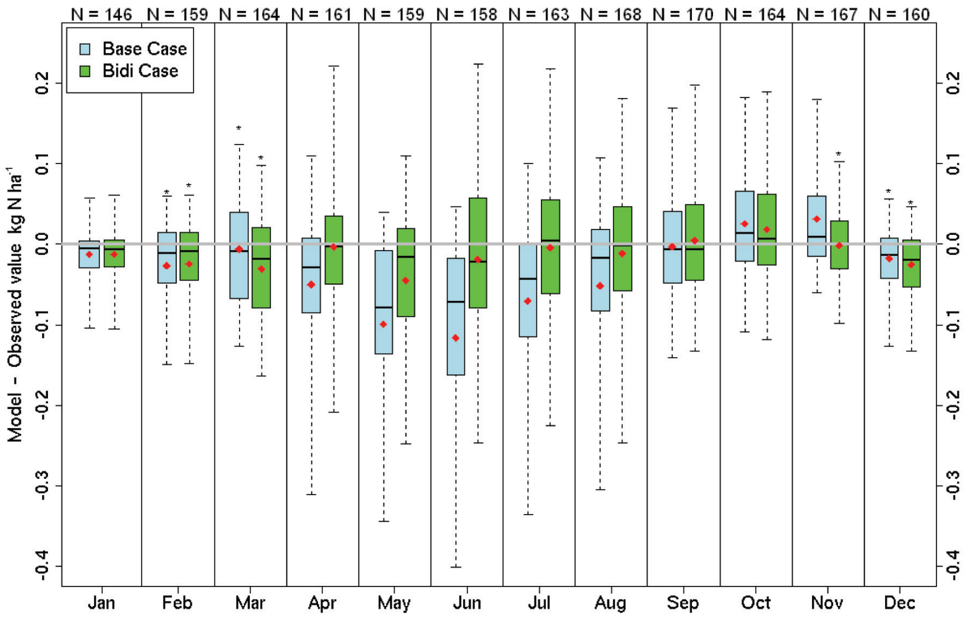

Figure 7-2. Monthly NH_4 wet deposition bias when compared to NADP deposition for an annual 2002 simulation for a base case unidirectional exchange and a bidi case with bidirectional NH_3 exchange. The red diamond in the box plot represents the mean monthly deposition bias. Monthly adjustments to precipitation biases have been applied where precipitation errors significantly correlate with deposition error; a star above the box plot indicates that this correction was not applied.

7.2.3 Accomplishments

CMAQ sensitivity runs for Chesapeake Bay with the new DDM-3D capability for NO_y deposition were completed for an emissions sector analysis and a six-Bay-State relative-contribution analysis for the 2020 CAIR scenario. The Chesapeake Bay Modeling Subcommittee was briefed on the results. Using the DDM-3D corrected earlier problems with the brute-force approach.

A new NH_3 budget analysis at 12 km, using a prototype CMAQ with NH_3 bi-directional air-surface exchange incorporated, showed that incorporating bi-directional exchange of NH_3 will have an important impact of reducing the local dry deposition and an impact on the estimates of the range of influence of NH_3 emissions, almost doubling the range (Figure 7-1). These results underline the importance of incorporating NH_3 bi-directional exchange in CMAQ (Dennis et al., 2010).

WRF meteorology for 12-km CONUS domain for 2002 was completed in FY10 for ESRP and general use. Preliminary annual CMAQ runs with inline lightning NO_x algorithm simulations were completed in FY10 for 2002 using WRF 12-km CONUS 2002 meteorology.

A pilot simulation of the bi-directional CMAQ was completed to show proof of capability to meet the FY11 deliverable to the Nitrogen Team of bidirectional CMAQ total nitrogen deposition fields. Preliminary evaluation against limited ambient NH3 observations and NADP wet deposition estimates suggests that the changes from the unidirectional CMAQ are reasonable and result in reduced CMAQ simulation bias (Figure 7-2).

Preliminary estimates of county-level nitrogen-fertilizer input uncertainty, expressed as a coefficient of variation and preliminary FEST-C denitrification estimates were shared with Nitrogen Team members assembling an N-input meta-database.

7.2.4 Next Steps

The objectives of future research in multimedia modeling for air-ecosystem linkages and ecosystem service assessments are: (1) to study and improve the connection between meteorological and atmospheric models and ecosystem models to address air-water paradigm mismatches; (2) to actively use the CMAQ model to research and explore climate and air-ecosystem linkage issues to develop guidance on how to improve transdisciplinary modeling; (3) to illuminate model functioning and examine areas of model uncertainty to identify areas for further model development to inform future research focusing on the development and evaluation of future modeling techniques and tools for CMAQ; and (4) to improve the capacity of CMAQ to address drivers of change of particular interest to the ESRP assessments of ecosystem services, such as land use and land cover change in response to population growth or bio-energy policy and climate change in support of transdisciplinary modeling and ecosystem management. Two focal areas are the NO_x-SO_x secondary air quality standard review and the study of critical loads (deposition-based tipping points). The lessons are to be synthesized to inform research planning for CMAQ and ecosystem model development and for integrated transdisciplinary model development and application. The final objective is to provide atmospheric inputs (e.g., wet and dry deposition of nitrogen and ambient particulate concentrations) to the ESRP national and place-based research teams to support overall ecosystem service assessment activities.

7.3 Air-Ecosystem Linkage Studies

7.3.1 Introduction

The thrust of this research is to develop CMAQ modeling research and applications in multimedia modeling assessments associated with ESRP, using CMAQ as a laboratory. The ESRP teams with which AMAD is interacting most are: the Future Midwest Landscapes (FML) place-based team, the Nitrogen Team involving national and regional assessments, the Mapping Team involving provision of deposition-related data layers, and the Coastal Carolinas place-based team. Provision of CMAQ physical and chemical outputs to link to ecosystem models for scenarios representing current and future conditions are major objectives.

7.3.2 Research Direction

An underlying objective is to identify and to elucidate atmosphere-ecosystem services of relevance to the ESRP, in collaboration with OAQPS. The role of these services is then communicated to the broader ecosystem community through participation in national and place-based ESRP teams, research planning committees, and peer reviewed publications. A fundamental objective is to assess the relevance and capacity of CMAQ to address and respond to drivers of change of particular interest to ESRP, such as land use and land cover change in response to population growth or bio-energy policy and climate change. Coupled with this is the objective to provide atmospheric inputs (e.g., wet and dry deposition of nitrogen and ambient particulate) concentrations to the ESRP national and place-based research teams to support overall ecosystem service assessment activities. A final objective is to develop the capacity of CMAQ to address secondary welfare NAAQS for SO_2 and NO_x.

7.3.3 Accomplishments

Activities in FY10 focused on continued development of the APWS implementation plan and coordination with watershed model development for the Cape Fear basin. Planning focused on extending the coordination of air-water linkage testing with air-water/terrestrial research being performed for the Cape Fear basin with the Ecosystem Research Division (ERD).

A beta version of FEST-C was completed and was transferred to the ESRP Nitrogen, mapping, and FML Team scientists (Cooter et al., 2010). We continued to interact with FML SPARROW, SWAT, and BMP modelers regarding their use of CMAQ deposition and FEST-C Nitrogen budget estimates. We participated in regular research planning conference calls and coordinated FEST-C output plans with FML modelers.

The FML was identified by AMAD as a pilot for improved cross-divisional cooperation. A NERL pool postdoctoral position was developed with ESD to explore the more effective use of their planned and on-going field Nitrogen and landuse/landcover research in CMAQ model development and evaluation for the ESRP.

Chesapeake Bay place-based research activities were aimed at contributing to an overall understanding of Chesapeake Bay nitrogen issues for development of a Bay implementation plan.

7.3.4 Next Steps

Several research topics are planned for the future research in multimedia modeling for air-ecosystem linkages and ecosystem service assessments organized under the three headings below.

1. Multimedia Linkage and Transdisciplinary Studies
   - Linking to water quality and terrestrial models
   - Linking to ecosystem welfare and tipping points
   - Linking hydrology model to WRF/CMAQ system
   - Linking climate, air quality and ecosystem services
2. Using CMAQ as a Laboratory for Deposition Research
   - Gulf hypoxia and regional watershed modeling with SPARROW
   - Chesapeake Bay TMDL and presidential directive
   - Secondary NAAQS-driven research
3. Ecosystem Services Research Program
   - National pollutant-driven research (Nitrogen Team)
   - Place-based driven research
   - FML
   - Albemarle-Pamlico Watershed and Estuary Study (APWES)
   - Chesapeake Bay ESRP research

7.4 Model and Tool Development

7.4.1 Introduction

The thrust of this research area is to further develop and advance CMAQ and supporting tools for ecosystem applications. The research is subdivided into five key areas: (1) to improve the parameterizations of the air-surface exchange of atmospheric pollutants, both bi-directional and unidirectional for aquatic and terrestrial landscapes; (2) to develop subgrid scale land-use-specific deposition estimates and to develop parameterizations of subgrid variation in dry deposition because of complex terrain; (3) to advance the WRF/CMAQ land surface parameterizations and leaf area index (LAI) estimates to improve connections to ecosystem models; (4) in coordination with the model development team, to improve the modeling of the amount, location, and duration of precipitation by WRF to reduce the error in wet deposition estimates from CMAQ as well as to extend WRF precipitation predictions to finer grid scales in complex terrain; and, finally, (5) to develop and advance tools to facilitate the linkage of CMAQ with ecosystem.

7.4.2 Research Direction

A major objective is to improve unidirectional and bi-directional exchange process descriptions in CMAQ, with an emphasis on incorporation of bi-directional exchange algorithms in CMAQ for NH_3 and mercury. This objective also includes evaluation of CMAQ deposition predictions to test improvements; to suggest further model improvements, including the search for missing pathways in CMAQ; and to reduce uncertainty in deposition calculations. A second major objective is also to develop subgrid-scale approaches to better represent dry deposition variability within a grid. The third major objective is to advance the land surface parameterizations used by WRF/CMAQ. A final major objective is identification, development, and enhancement of air-surface interfaces and tools needed to facilitate the use of CMAQ deposition outputs by analysts and researchers not familiar with the atmospheric deposition model and enable CMAQ to better support ecosystem studies and support CMAQ process enhancements.

7.4.3 Accomplishments

To improve the understanding of bidirectional exchange processes, AMAD collaborated with field scientists from EPA/NRMRL and the NOAA ARL in planning and conducting a field campaign where NH_3 surface exchange was measured over corn, unfertilized grassland, and forest canopies. Data from the field studies have been used in several model development efforts, during including first-order and simplified-first-order closure models for flux from a vegetative canopy (Bash et al., 2010) and a process-based soil NH_3 emissions model (Cooter et al., 2010). A bi-directional flux pilot study for the eastern United States was conducted by Robin Dennis, Ellen Cooter, Megan Gore (NCSU graduate student), Viney Aneja (graduate students supervising professor), and Jon Pleim. The purpose of the pilot is to facilitate the step-wise implementation of the new bi-directional flux algorithms developed and constrained by observations collected in collaboration with NRMRL and NOAA into CMAQ. As a first step, the new canopy model and emission potential from the soil emission model were incorporated into CMAQ 4.7.1. Testing and evaluation began in 2010, and several manuscripts are being prepared for submission in 2011.

The CMAQ deposition model was changed to enable mercury-specific deposition processes. Consideration of the mesophyll resistance was added, which is important for modeling elemental mercury. For reactive gaseous mercury (RGM), the chemical parameters were changed to be consistent with HgC_{l2}. Previously, RGM had been modeled using HNO_3 as a surrogate. This enables CMAQ to parameterize the air-surface water concentration gradient dependence on the elemental mercury flux (Foley et al., 2010), the recycling of recently deposited divalent mercury, and the enrichment of elemental mercury concentrations in vegetation, soil, and surface waters that have been documented recently in the literature (Bash and Miller 2009). These improvements capture pulses of emissions observed following precipitation in arid environments observed during measurement campaigns and are an inline estimation of natural mercury emissions that remains consistent with changes in modeled chemical mechanisms and boundary conditions, changes that would require updates to offline natural emission estimates (Bash 2010).

AMAD scientists are collaborating with USDA to build CMAQ modeling capability to simulate pesticide transport in a project that was initiated in FY10. CMAQ with pesticide fate and transport capability will be evaluated with special observations collected by the U.S. Department of Agriculture (USDA). A coordination meeting was held in March 9, 2010, in Research Triangle Park among the USDA Principal Investigators (Cathleen Hapeman and Laura McConnell), the USDA postdoctoral fellow assigned to the project (Cody Howard), and interested AMAD scientists. The first phase of the project was to design a field study to be conducted during spring/summer 2011. Dr. Howard was provided Pesticide Emissions Model (PEM) code by AMAD which he is now using on USDA machines. He completed both the SMOKE and CMAQ training offered by CMAS. Subsequent to training, he requested and was provided AAA connection to the HPCC to facilitate his continued exploration of CMAQ.

Unidirectional Exchange

In FY09, as part of a collaborative effort with NRMRL, deposition velocity estimates from CMAQ for ultrafine particles were compared against field measurements taken over a loblolly pine forest stand in FY06 and FY07. The results were presented at the 2009 NADP meeting.

In FY09-10, staff collaborated with scientists from the United States and Canada on a study of sulfur budgets of watersheds in Southeastern Canada and the Northeastern United States Wet deposition is measured at these sites, but dry deposition estimates are not available. A number of approaches for estimating the contribution of dry deposition were investigated.

The wet deposition results and ambient NH_4 concentrations from CMAQ version 4.7.1, with the changes made during implementation of the NH_3 bi-directional exchange pilot project were evaluated against network observations.

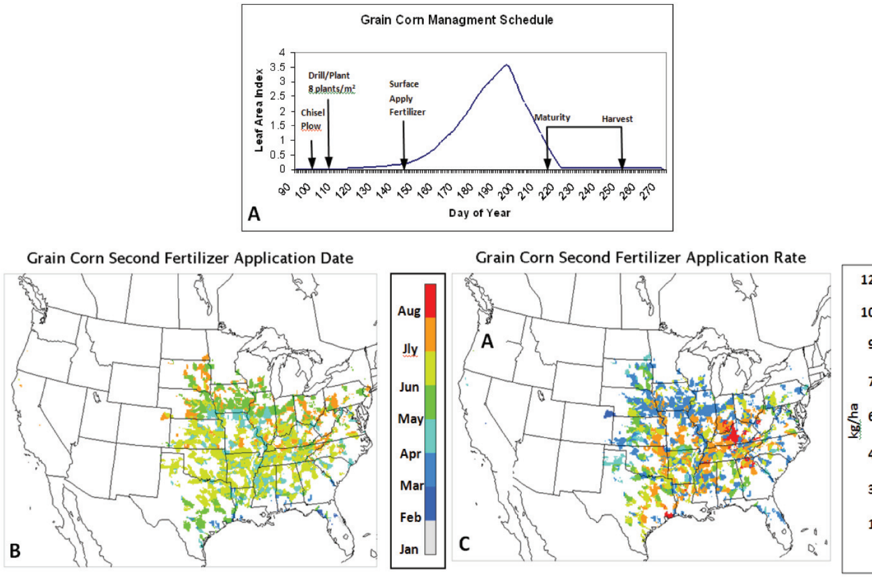

Figure 7-3, Rainfed grain corn (A) example management schedule, (B) second fertilizer application date, and (C) second first fertilizer application rate.

Subgrid-Scale Variability

In FY07, work was begun on implementing the capability in CMAQ to output land-use-category specific deposition velocities (referred to as the mosaic approach) to examine the effects of subgrid-scale variability in land use on calculated deposition fluxes. Initial efforts focused on disaggregating the CMAQ deposition velocities by accounting for the effects of subgrid-scale surface roughness. In FY08, a prototype of the mosaic approach was put into the full CMAQ model for further testing and analysis. This prototype was expanded in FY09, and the CMAQ mosaic was run for a 2-week period in May 2002 to test the capability of the code to capture the temporal trend in leaf area index and deposition velocity. A subset of the results from this analysis was presented at the 2009 NADP meeting. In FY10, the mosaic approach was further adapted to enable output of stomatal flux for each land use category. This new capability is being utilized in a study of O_3 exposure.

Modeling for CASTNet

Concerns about the comparability of deposition estimates between the U.S. CASTNET and the Canadian monitoring network, CAPMoN, have been raised, and a comparison of the deposition velocity model approaches was done in FY07-09. A manuscript describing this analysis has been submitted to *Atmospheric Environment* for publication. Data gaps in the meteorological data collected at the CASTNET sites result in missing values for the predicted deposition velocity and, therefore, the flux. In FY09-10, a study was done to design a method for imputing missing flux values to provide a more complete historical dataset. A manuscript describing this study has been submitted to *Water, Air, and Soil Pollution*.

Fertilizer Emission Scenario Tool

During FY09, a work assignment was initiated and a formal work plan was developed and approved for development of the Fertilizer Emission Scenario Tool (FEST-C). FEST-C provides information on fertilizer application timing, amount, and mode of application, as well as soil characteristics and surface losses in runoff for use by CMAQ (Figure 7-3). During FY10, a beta version of FEST-C was delivered as part of APM372. Contractor code was transferred from the AMAD CMAS vehicle to the OAQPS emissions modeling contract. As part of this delivery, a briefing seminar was given and access and training was provided to OAQPS and ESRP/mapping and FML theme scientists. Quality Assurance (QA) of initial FEST-C results was initiated, and a code outline for full implementation in bi-directional CMAQ was developed. An overview of FEST-C was presented at the 2010 CMAS meeting. Additionally, the Spatial Allocator tool was enhanced to process data produced by the FEST-C tool and the Environmental Policy Integrated Climate (EPIC) for CMAQ NH_3 bi-directional flux modeling. This includes handling of transformed WRF input weather files, as well as EPIC output files. A poster describing this effort was presented at the 2010 CMAS meeting.

Updated Land Cover Data

A new land cover data-set was developed for use with CMAQ that consists of information from the National Land Cover Dataset (NLCD) for the United States and MODIS data for Mexico and Canada. The Spatial Allocator tool was revised to include raster tools for converting NLCD data to the gridded format required for CMAQ modeling. During FY10, MCIP was modified to accept 2001 NLCD as land cover input, and a test case of the bi-directional CMAQ pilot was run using NLCD.

During FY09, 2002 USDA county-level crop data were assembled and provided to the contractor (UNC) for update of BEIS agricultural crop fractions. This work was a collaborative effort with the emissions modeling team. Results of the updated crop information have been QA'd and accepted. During FY10, the updated BELD agricultural data was used to distribute crop area in the beta version of the FEST-C tool, and issues were identified that will be resolved during FY11. Work plan delays have pushed completion of the BELD update (BELD 4.0) into FY11.

Watershed Deposition Tool

The Watershed Deposition Tool (WDT) was developed 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 (total maximum daily load) and related nonpoint-source watershed analyses. This software tool takes gridded atmospheric deposition estimates from NOAA/EPA's regional, multipollutant air quality model, CMAQ, and allocates them to 8-digit HUCs (hydrologic cataloging units of rivers and streams) within a watershed, State, or region. WDT was delivered to AMAD in FY07 and released to the public via the AMAD Web site at http://www.epa.gov/asmdnerl/EcoExposure/depositionMapping.html. The software and sample CMAQ data files can be downloaded from the Web site. In FY08, the WDT was updated and continues to be used widely by the community to map CMAQ deposition estimates to watershed delineations, (Figure 7-4). The WDT was developed by Argonne National Laboratory and contains proprietary code. In keeping with EPA's efforts to provide open source products to the extent possible, the capabilities of the WDT were migrated into the Visualization Environment for Rich Data Interpretation (VERDI) during FY08 and FY09. A description of the WDT and example application of the tool was published in Schwede et al. (2009). In FY10, files for 2002-2006 from the CDC PHASE study were made available for download and use with the WDT.

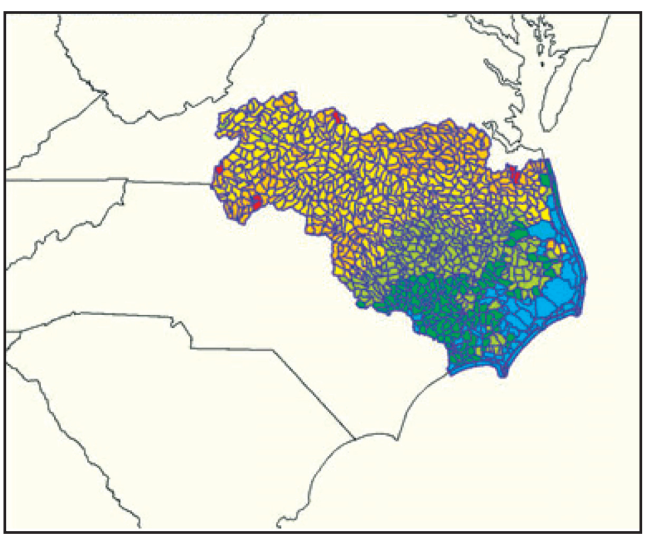

Figure 7-4. Watershed deposition tool output showing the average (per unit area) annual total (wet+dry) oxidized nitrogen deposition (kg-H/ha) estimated for each 12-digit HUC in the Albemarle-Pamlico Basin for 2002.

Visualization Environment for Rich Data Interpretation

In FY07, the initial version of VERDI was delivered to AMAD. VERDI is an open source Java tool for visualizing CMAQ and other environmental data. It is designed as an update/replacement for the Package for Analysis and Visualization of Environmental Data (PAVE), which currently is used for visualizing CMAQ data. An initial version of the VERDI was released formally to the public in FY08 for use in visualizing CMAQ output. The software and associated documentation are available from http://verdi-tool.org. The distribution of the tool is managed by CMAS. In FY08-09, additional capabilities were added to VERDI, including an alternate tile plot routine, an areal interpolation plot that provides the capability of the WDT, and the ability to display CMAQ data in polar stereographic and lat-long projections. A demonstration of this enhanced version of VERDI was given at the 2009 CMAS meeting. Numerous enhancements were made to VERDI in FY10, including improving the scripting capability and overlay capabilities, adding a remote file browser, and adding the capability to export shapefiles. A poster describing the enhancements was presented at the 2010 CMAS meeting.

Spatial Allocator

The Spatial Allocator tool was revised to include raster tools for converting NLCD data to the gridded format required for CMAQ modeling and to process data produced by the FEST-C tool.

7.4.4 Next Steps

The objectives in air-surface exchange model and tool development is to further improve and advance CMAQ and supporting tools for ecosystem applications. The research is subdivided into six key areas: (1) to improve the parameterizations of the air-surface exchange of atmospheric pollutants, both bi-directional and unidirectional for aquatic and terrestrial landscapes; (2) to develop subgrid-scale land-use-specific deposition estimates, to develop parameterizations of subgrid variation in dry deposition because of complex terrain, and to develop techniques to account for deposition of pollutants via cloud water deposition; (3) to advance and modernize the WRF/CMAQ land surface parameterizations to improve connections to ecosystem models; (4) to develop a model representation of the hydrologic overland flow, with other Agency partners that is consistent with the precipitation from WRF/CMAQ; (5) in coordination with the model development team, to improve the modeling of amount, location, and duration of precipitation by WRF to reduce the error in wet deposition estimates from CMAQ as well as to extend WRF precipitation predictions to finer grid scales in complex terrain; and, finally, (6) to develop and advance tools to facilitate the linkage of CMAQ, with ecosystem models based on lessons learned from the model applications.

Several research topics are planned for the future research in the air-surface exchange and model tool development organized under the two headings below.

1. Air-Surface Exchange
   - Bi-directional exchange
     - NH_3
     - Mercury
     - Pesticides
   - Unidirectional exchange
     - NO_y
     - SO_2
   - Subgrid variability
     - Land use variability
     - Terrain variability and occult deposition
2. Data and Tool Development
   - Fertilizer Emissions Scenario Tool for CMAQ (FEST-C)
   - Watershed Deposition Tool (WDT)
   - Visualization Environment for Rich Data Interpretation (VERDI)

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APPENDIX A

Atmospheric Modeling and Analysis Division Staff Roster (as of December 31, 2010)

Office of the Director
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

Emissions and Model Evaluation Branch
Tom Pierce, Chief
Wyat Appel
Brian Eder
Kristen Foley
Jim Godowitch
Steve Howard
Roger Kwok (NRC[2] Postdoctoral Fellow)
Sergey Napelenok
George Pouliot
Havala Pye (ORISE[3] Postdoctoral Fellow)
Alfreida Torian

Atmospheric Exposure Integration Branch
Val Garcia, Chief
Jesse Bash
Jason Ching
Jim Crooks (Postdoctoral Fellow)
Robin Dennis
Megan Gore (Contractor)
Vlad Isakov
Gill-Ran Jeong (Visiting Scientist)
Donna Schwede
Myrto Valari (NRC[2] Postdoctoral Fellow)
David Heist, Fluid Modeling Facility
Ashok Patel (SEEP[1]), Fluid Modeling Facility
Steve Perry, Fluid Modeling Facility
Bill Petersen (Contractor), Fluid Modeling Facility
John Rose (SEEP[1]), Fluid Modeling Facility

Atmospheric Model Development Branch
Rohit Mathur, Chief
Shirley Long (SEEP[1]), Secretary
Prakash Bhave
Garnet Erdakos (NRC[2] Postdoctoral Fellow)
Rob Gilliam
Bill Hutzell
Deborah Luecken
Martin Otte (Postdoctoral Fellow)
Shawn Roselle
Golam Sarwar
John Streicher
David Wong
Jeff Young
Shaocai Yu (Postdoctoral Fellow)

Applied Modeling Branch
Jon Pleim, Acting Chief
Melanie Ratteray (SEEP[1]), Secretary
Farhan Akhtar (ORISE[3] Postdoctoral Fellow)
Bill Benjey
Jared Bowden (NRC[2] Postdoctoral Fellow)
Russ Bullock
Dan Cohan (Visiting Scientist)
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 the magnitude of the air pollution problem and 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
2010 Awards and Recognition

EPA Gold Medal
William Benjey, Ellen Cooter, Alice Gilland, and Robert Gilliam—Climate Change and Air Quality Assessment Team

ORD Bronze Medal
Vlad Isakov, Joe Touma and others—Cummulative Air Accountability Team

ORD Bronze Medal
Prakash Bhave, Ann Carlton, Rohit Mathur, Sergey Napelenok, Robert Pinder, George Pouliot, Golam Sarwar, and others–Organic Aerosol Science Team

ORD Technical Organic Assistance to the Regions or Program Offices Award
Kenneth Schere, Jonathan Pleim, Rohit Mathur, George Pouliot, Rogert Gilliam, and Thomas Pierce—Fairbanks Modeling Team

ORD Diversity Leadership Award
Prakash Bhave—For recognition of his various approaches to model diversity ideals and for his active support of diversity programs

NERL Special Achievement Award
Wyat Appel and Robert Gilliam—Goal 1, Support the Agency's Mission: Developing the Atmospheric Model Evaluation Tool (AMET) and overseeing its successful transfer to the meteorological and air quality modeling community

S.T. Rao and David Mobley—Goal 2, Be a High Performing Organization: Efforts to improve integration and coordination of research across HEASD

Jonathan Pleim—Goal 3, Be a Leader in the Environmental Research Community: Demonstrating excellence in advancing the state of the science in atmospheric modeling

Prakash Bhave, Ann Carlton, Deborah Luecken, Rohit Mathur and Golam Sarwar–Goal 4, Integrate *Environmental Science and Technology* to Solve Environmental Problems: Recognizing NERL's Atmospheric Chemistry and Modeling Team, who effectively integrated research across research disciplines and organizations

Kristen Foley—Meritorious Research Support Award: Providing much needed statistical and programming support toward the advancement of credible air quality models

Ken Schere, Alice Gilliland and others—Teamwork Award: Modeling Linkage Team

David Heist and Steven Perry—Blue Ribbon Paper Award: The Effect of a Tall Tower on Flow and Dispersion Through a Model Urban Neighborhood. Part 1: Flow Characteristics and Part 2: Pollutant Dispersion

Robert Pinder, Robert Gilliam, Wyat Appel, Sergey Napelenok, Kristen Foley, and Alice Gilliland – Blue Ribbon Paper Award: Efficient Probabilistic Estimates of Surface Ozone Concentration Using an Ensemble of Model Configurations and Direct Sensitivity Calculation

Prakash Bhave, Heather Simon, George Pouliot, and David Mobley – Blue Ribbon Paper Award: Emissions Inventory of $PM_{2.5}$ Trace Elements Across the U.S.

Shawn Roselle—Leadership Award: Demonstrating leadership and assembly of various CMAQ versions and for providing enthusiastic support of its use by the program offices, contract staff, and internal division staff

Bill Hutzell—Collaboration Award: Essential role in the improvement and maintenance of the computer code for the Community Multiscale Air Quality Model

AMAD Awards
Blue Ribbon Paper: David K. Heist and Steven Perry—Effect of a Tall Tower On Flow and Dispersion Through a Model Urban Neighborhood. Part 1: Flow Characteristics and Part 2: Pollutant Dispersion

Blue Ribbon Paper: Robert Pinder, Robert Gilliam, Wyat Appel, Sergey Napelenok, Kristen Foley, and Alice Gilliland—Efficient Probalisitic Estimates of Surface Ozone Concentration Using an Ensemble of Model Configurations and Direct Sensitivity Calculation

Blue Ribbon Paper: Prakash V. Bhave, Heather Simon, George A. Pouliot, and David Mobley—Emissions Inventory $PM_{2.5}$ Trace Elements Across the United States.

Leadership Award: Shawn Roselle—Demonstrating leadership in coordinating the development and assembly of various CMAQ versions and for providing enthusiastic support of its use by the program offices, contract staff, and internal division staff.

Collaboration Award: Bill Hutzell. For his essential role in the improvement and maintenance of the computer code for the Community Multiscale Air Quality Model

APPENDIX D

2010 Publications(Division authors are in bold.)

Journal Articles

Appel, W., S.J. Roselle, R.C. Gilliam, J.E. Pleim and **R.C. Gilliam**. Sensitivity of the Community Multiscale Air Quality (CMAQ) Model v4.7 Results for the Eastern United States to MM5 and WRF Meteorological Drivers. *Geoscientific Model Development*, Copernicus Publications, Katlenburg-Lindau, Germany, 3(1):169-188, (2009).

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Dennie, R.L., T. Fox, M. Fuentes, A. Gilliland, S. Hanna, C. Hogrefe, J. Irwin, **S.T. Rao**, R. Scheffe, **K.L. Schere**, D. Steyn and A. Venkatram. A Framework for Evaluating Regional-Scale Numerical Photochemical Modeling Systems . *Environmental Fluid Mechanics*, Springer, New York, NY, 10(4):471-489, (2010).

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Foley, K., S.J. Roselle, W. Appel, P. Bhave, J.E. Pleim, T.L. Otte, R. Mathur, G. Sarwar, J.O. Young, R.C. Gilliam, C.G. Nolte, J. T. Kelly, A. Gilliland and J.O. Bash. Incremental Testing of the Community Multiscale Air Quality (CMAQ) Modeling System Version 4.7. *Geoscientific Model Development*, Copernicus Publications, Katlenburg-Lindau, Germany, 3(1):205-226, (2010).

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Horton, R., C. Rosenzweig, R. Ramaswamy, P.L. Kinney, **R. Mathur** and **J.E. Pleim**. Integrated Climate Change Information for Resilient Adaptation Planning. *EM: Air and Waste Management Associations Magazine for Environmental Managers,* Air & Waste Management Association, Pittsburgh, PA, (11):14-25, (2010).

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APPENDIX E
Acronyms and Abbreviations

3D	3-Dimensional
4D	4-Dimensional
AAA	Authentication Authorization Audit
ACM	Asymmetric Convective Model
AEIB	Atmospheric Exposure Integration Branch
AERLINE	
AERMOD	American Meteorological Society/EPA Regulatory Model
AERDNET	AErosol RObotic NETwork
AFMS	Agricultural fertilizer modeling system
AMAD	Atmospheric Modeling and Analysis Division
AMB	Applied Modeling Branch
AMDB	Atmospheric Model Development Branch
AMET	Atmospheric Model Evaluation Tool
AMNet	Ambient Mercury Network
AOD	Aerosol Optical Depth
APM	Annual Performance Measure
APWS	Albemarle-Pamlico Water Shed
AQMEII	Air Quality Model Evaluation International Initiative
AQS	Air Quality System
AR4	Fourth Assessment Report
AR5	Fifth Assessment Report
ARL	Air Resources Laboratory
ARM	Atmospheric Radiation Measurement
BEIS	Biogenic Emission Inventory System
BELD	Biogenic Emissions Landuse Data
Bidi	Bidirectional
BMA	Bayesian Model Averaging
BMP	Best Management Practice
BRACE	Bay Regional Atmospheric Chemistry Experiment
C-FERST/ STREETS	Community-Focused Exposure and Risk Screening Tool / Screening Tool for Roadway Emissions and Exposure to Toxics
CAA	Clean Air Act
CAAAC	Clean Air Act Advisory Committee
CAIR	Clean Air Interstate Rule
CAM	Community Atmospheric Model
CMAQ-MP	
CAP	Criteria Air Pollutants
CAPMON	Canadian Air and Precipitation Monitoring Network
CASTNET	EPA's Clean Air Status and Trends Network

CBO5	Carbon Bond 2005
CBL	Convective Boundary Layer
CBM-Z	Carbon Bond Mechanism-Zaveri
CCN	Clouds and the Earth's Radiant Energy System
CDC	Centers for Disease Control and Prevention
CEP	UNC's Center for Environmental Programs
CERES	Clouds and Earth's Radiant Energy System
CFD	Computational Fluid Dynamics
CHERUBS	Childhood Health Effects from Roadway and Urban Pollutant Burden Study
CIRAQ	Climate Impacts on Regional Air Quality
CMAQ	Community Multiscale Air Quality Model
CMAQ-TX	Community Multiscale Air Quality Model-Texas
CMAS	Community Modeling and Analysis System
CO	Carbon Monoxide
CO_2	Carbon Dioxide
CONUS	Continental US
CTM	Chemical Transport Model
DAPPLE	Dispersion of Air Pollution and Penetration into the Local Environment
DDM	Decoupled Direct Method
DOE	Department of Energy
DDM-3D	Decoupled Direct Method-3D
EC	elemental carbon
EMEB	Emissions and Model Evaluation Branch
EPA	U.S. Environmental Protection Agency
EPIC	Environmental Policy Integrated Climate Model
EPRI	Electric Power Research Institute
ERD	Ecosystem Research Division
ESD	Environmental Sciences Division
ESRP	Ecological Services Research Program
FDDA	4D Data Assimilation
FEST-C	Fertilizer Emissions Scenario Tool for CMAQ
FIA	Forest Inventory Data
FLUENT	Computational Fluid Dynamics Sofware produced by ANSYS, Inc. (its not an acronym, just the name of the software)
FML	Future Midwestern Landscapes
FRM	Federal Reference Method
FY	Fiscal Year
GCM	Global Climate Model

GABLS	GEWEX Atmospheric Boundary Layer Study
GEOS-Chem	Global 3-D chemical transport model (CTM) for atmospheric composition driven by meteorological input from the Goddard Earth Observing System (GEOS) of the NASA Global Modeling and Assimilation Office
GEWEX	Global Energy and Water Cycle Experiment
GHG	Greenhouse Gas
GISS	Goddard Institute for Space Studies
GLIMPSE	Geos-CHEM LIDORT Integrated with MARKAL for the Purpose of Scenario Exploration
GEOS	Goddard Earth Observing System
HAP	Hazardous Air Pollutant
HEASD	Human Exposure & Atmospheric Sciences Division
Hg[II]	Oxidized Mercury
HgC_{12}	Mercuric Chloride
Hg[O]	Elemental Mercury
HNO_3	Nitric Acid
HONO	Nitrous Acid
HO_2	Hydroperoxyl Radical
H_2O_2	Hydrogen Peroxide
HUC	Hydrologic Unit Code
HPCC	High Performance Computers and Communication
IAG	Interagency Agreement
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
INs	Isoprene Nitrates
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
ITR	Integrated Transdisciplinary Research
LADCO	Lake Michigan Air Directors Consortium
LAI	Leaf Area Index
LBC	Lateral Boundary Condition
LES	Large-Eddy Simulations
LIDAR	Light Detection And Ranging
LIDORT	Linearized Discreet Ordinate Radiative Transfer
LSM	Land Surface Model
Lur	Land-Use Regression
LW	Longwave
M3dry	Models 3 Dry Deposition Model
MACT	Maximum Achievable Control Technology
MAE	Mean Absolute Error
MCIP	Meteorology-Chemistry Interface Processor
MARKAL	Maximum Achievable Control Technology
MCM	Master Chemical Mechanism
MDA	Maximum Daily Average
MDN	Mercury Deposition Network
MEGAN	Model Of Emissions Of Gases And Aerosols From Nature
MESA AIR	Multi-Ethnic Study of Atherosclerosis and Air Pollution
MLBC	Multilayer Biochemical Model
MM5	Fifth Generation Of The Penn State/Ucar Mesoscale Model
MODIS	Moderate Resolution Imaging Spectroradiometer
MOSAIC	Model for Simulating Aerosol Interactions and Chemistry
MP	Multipollutant
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
NARR	North American Regional Reanalysis
NARSTO	Formerly the North American Research Strategy for Tropospheric Ozone
NAS	National Academy of Sciences
NASA	National Aeronautics and Space Administration
NASS	National Agricultural Statistical Service
NATO	North Atlantic Treaty Organization
NBP	NO Budget Trading Program
NCAR	National Center for Atmospheric Research
NCEA	National Center for Environmental Assessment
$nCeO_2$	Nanoparticulate Cerium Oxide
NCER	National Center for Environmental Research
NCOM	Graphically Reduced Carbon Organic Mass
NCSU	North Carolina State University
NEI	National Emission Inventory
NERL	National Exposure Research Laboratory
NEXUS	Near-road EXposure to Urban air pollutants Study
NGA	National Geospatial Agency
NH_3	Ammonia

NH_4	Ammonium
NHEERL	National Health & Environmental Effects Research Laboratory
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
NRC	National Research Council
NRMRL	National Risk Management Research Laboratory
NSF	National Science Foundation
NUDAPT	National Urban Database And Access Portal Tool
O_3	Ozone
OAP	Office Of Air Programs
OAQPS	Office Of Air Quality Planning And Standards
OAR	Office Of Air & Radiation
OC	Organic Carbon
OH	Hydroxy Radical
OLAM	Ocean-Land-Atmosphere Model
OM	Organic Mass
OPE	ozone production efficiency
ORD	Office of Research and Development
OTAQ	Office of Transportation and Air Quality
PAH	Polycyclic Aromatic Hydrocarbon
PAN	Peroxyacyl Nitrate
PAVE	Package For Analysis And Visualization Of Environmental Data
PBL	Planetary Boundary Layer
PCA	Principal Component Analysis
PEM	Pesticides Emissions Model
PM	Particulate Matter
$PM_{2.5}$	Particulate Matter Smaller Than 2.5 Microns In Diameter
$PM_{2.5FRM}$	$PM_{2.5}$ is defined above and FRM is: Federal Reference Method
PM_{10}	Particulate Matter Smaller Than 10 Microns In Diameter
PM_{COARSE}	Particulate Matter Between 2.5 And 10 Microns In Diameter
PM_{OTHER}	Model Species Representing $Pm_{2.5}$ That Is Not Chemically Speciated
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
RACM2	Regional Atmospheric Chemistry Mechanism, version 2
RARE	Regional Applied Research Effort
RCCM	Regional Climate and Chemistry Modeling System
RCM	Regional Climate Model
RCP	Representative Concentration Pathways
RELMAP	Regional Lagranian of Air Pollution
REML	Durbin-WatsDon test and restricted maximum likelihood
REMSAD	Regional Modeling System for Aerosols and Deposition
RGM	reactive gaseous mercury
RMSE	root mean squared error
ROSES	Research Opportunities in Space and Earth Sciences
RRTMG	Rapid Radiative Transfer Model for GCMs
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 Plan
SLAMS	State or Local Air Monitoring Station
SLCF	short-lived climate forcers
SMOKE	Sparse Matrix Operator Kernel Emissions
SO_2	sulfur dioxide
SO_4	sulfate
SO_X	sulfur oxides
SOA	secondary organic aerosol
SOA_{cld}	secondary organic aerosol formed in clouds
SPARROW	Spatially Referenced Regressions on Watershed Attributes
SPS	Science for Peace and Security
SST	Sea Surface Temperature
STAR	Science To Achieve Results
STENEX	Stencil Exchange
STN	Speciated Trends Network
SW	Shortwave
SWAT	Soil & Water Assessment Tool
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
USDA	United States Department of Agriculture
USFS	United States Forest Service
USGS	U.S. Geological Survey
VBS	Volatility Basis Set
VERDI	Visualization Environment For Rich Data Interpretation
VOC	Volatile Organic Compound
WDT	Watershed Deposition Tool
WDWE	Weekday-To-Weekend
WRF	Weather Research And Forecasting
WSOC	Water Soluble Organic Compound
YSU	Yonsei University

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