# Report

# on the

# Peer Review

# of the

# Atmospheric Modeling and Analysis Division

# National Exposure Research Laboratory

# Office of Research and Development

# U.S. Environmental Protection Agency

**Research Triangle Park, North Carolina**

**February, 2009**

**Peer Review Panel:**

**David Allen, Chair**
**Douglas Burns**
**David Chock**
**Naresh Kumar**
**Brian Lamb**
**Michael Moran**

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# Executive Summary

## *Introduction and Charge to the Panel*

The National Exposure Research Laboratory (NERL) conducted a peer review of its Atmospheric Modeling and Analysis Division (AMAD), with the goals of assessing the quality of the science being performed within the Division and the responsiveness of the Division to the needs of the Environmental Protection Agency (referred to in this report as EPA, or the Agency).

EPA's Atmospheric Modeling and Analysis Division is one of the largest air-quality model development and evaluation groups in the world. A primary focus of AMAD has been the development, evaluation and application of the CMAQ (Community Multi-scale Air Quality) modeling system, which consists of the CMAQ chemical transport model (CCTM), and its meteorological driver models and pre- and post- processing systems. The CMAQ modeling system provides a quantitative link between emissions of pollutants to the atmosphere and human and ecosystem exposures. This modeling tool supports a wide variety of Agency activities and decision-making processes, and has a wide and deep user base throughout the world.

A review panel, consisting of individuals with air quality modeling research and project management expertise, met with Division staff and management at Research Triangle Park, North Carolina from January 27 through January 29, 2009. Members of the panel were:

Panel Chair
Dr. David Allen, Gertz Regents Professor, University of Texas at Austin

Panel Members
Dr. Douglas Burns, Research Scientist, U.S. Geological Survey
Dr. David Chock, Senior Scientist, Ford Research Laboratory
Dr. Naresh Kumar, Senior Program Manager, Electric Power Research Institute
Dr. Brian Lamb, Professor, Washington State University
Dr. Michael Moran, Research Scientist, Environment Canada

The panel was charged with addressing four primary questions:

1. What is the quality of the scientific research being performed by the Division? (Quality)
2. Is the Division responsive to Agency needs and problems? (Responsiveness)
3. Is the Division's work having impact on Agency decisions? (Impact)
4. Are Division staff leaders in their scientific communities? (Leadership)

Since the Division consists of four existing branches and a fifth, emerging, research area, the charge questions were addressed separately for each of five topical areas. Detailed findings and recommendations for the areas of (1) Model Development, (2) Model Evaluation, (3) Linking Air Quality and Ecosystem Health, (4) Climate Change and Air Quality Interactions, and (5) Linking Air Quality and Human Health are provided in the main body of the report. This summary presents a synthesis of those findings and recommendations for the Division as a whole.

## *Accomplishments and Strengths of the Division*

Before addressing specific charge questions, it is useful to briefly summarize some of the overall accomplishments of the Division. More detailed summaries of the accomplishments associated with specific areas are described in the body of the report. Among the most significant accomplishments of the Division are the following:

- The Division has established the CMAQ models as a leading state-of-the-science regional air quality modeling system, with a large user community.
- The Division has delivered timely and relevant modeling products to EPA and its broader user community.
- The Division has, on its own initiative, developed an independent and on-going external review mechanism for the CMAQ modeling system, and has developed a rigorous internal model evaluation program.
- The Division has developed a balanced portfolio of core research and applied activities in support of EPA needs.
- The Division has established continuing and substantive interactions with the Office of Air Quality Planning and Standards (OAQPS) and other Agency clients and partners.
- The Division has established an effective outreach mechanism to serve the broader user community.
- The Division has aggressively addressed the issue of staff renewal.

The Division had, at the time of the review, 47 current scientific and technical staff. This represents a very significant research commitment to AQ model development, evaluation, and application. A significant expenditure of resources is, however, no guarantee of research productivity, quality, or relevance. The Division's overall success can be attributed in no small part to the talent and experience of its staff, to its forward-looking, thoughtful, and informed management, and to good teamwork and a positive culture. Some specific strengths of the Division include the following:

- A large fraction of the AMAD staff, 42 of 50, hold post-graduate degrees (28 Ph.D., 14 M.Sc.); there is a good mix of complementary disciplines for a numerical modeling program, including several statisticians.

- An organizational arrangement by both research theme and functional team that provides the required mix of skill for different projects and tasks.

- Very close cooperation and coordination between model development and model evaluation that facilitates the identification and prioritization of additional model development tasks.

- Successful ongoing renewal of the Division's staff through its use of ORD's postdoctoral fellowship program and the hiring of a cadre of very able young scientists to fill gaps left by staff turnover (five retirements and four transfers to other divisions or organizations in the past five years).

- Maintenance of close working relationships with key clients, such as regular monthly meetings between AMAD and OAQPS managers and weekly or biweekly meetings between AMAD staff and OAQPS staff working on two key CMAQ inputs, emissions and meteorological modeling.
- Significant attention given to collaborations to improve CMAQ in order to leverage Division resources; collaborators have included other Agency divisions, other government agencies, and university faculty.
- Strategic thinking about future directions, especially in regard to neighborhood-scale modeling to be coupled with human-exposure models, and hemispheric- or global-scale modeling to understand the impact of climate change on air quality.

## *Research Quality*

For each of five theme areas, the panel identified strengths and weaknesses of the research programs and made recommendations. These are summarized in the main body of the report. Summarized here is a synthesis of those findings for the Division.

The panel identified multiple strengths of the research program in regional air quality modeling. The division has developed uniformly strong research teams, with a good balance of skills and good interaction across branches. Extensive interactions across branches of the Division have led to creative development, evaluation and application of modeling tools. The Division has documented its work in the peer-reviewed scientific literature and these publications are cited at rates above the norm for both the Office of Research and Development (ORD) and the general scientific community.

These long-standing research strengths in regional air quality modeling and analysis are now being complemented by a number of new initiatives at global and neighborhood scales. Maintaining the Division's record of excellence as it enters these new areas will pose a number of challenges. Among the most significant of these challenges will be adding the necessary expertise and resources to the Division. Adding expertise and resources may be done in a variety of ways. For example, the Division may form new partnerships (e.g., with NASA on global change), or it might add new staff with targeted expertise, or it might provide significant professional development opportunities for existing staff. All of these alternatives are likely to require significant resources, yet there is a continuing demand for the Division's current activities and it would not be prudent to draw down resources dedicated to existing areas. Unless resources are expanded or some activities are dropped, the Division is unlikely to be able to continue to meet its core regional modeling mission and simultaneously address the new initiatives.

**Recommendation: Preserve the Division's existing resources for regional air quality modeling while responding to new Agency initiatives.** This may necessitate difficult choices regarding which new initiatives the Division is able to pursue.

## *Responsiveness to Agency Needs*

The Division has selected model development activities that address critical and evolving science questions that underlie many of the policy questions facing the Agency and many of the scientific initiatives of ORD. While the activities of the Division are highly relevant to Agency needs, current staffing and resources prevent the Division from addressing all of the topics of interest to the EPA and the broader CMAQ user community. If the Division keeps all CMAQ model development within the Division, it will face difficult choices about which modeling needs merit the use of its limited resources. However, if the Division can mobilize the broad and capable CMAQ user base to promote additional model development, evaluation and application, it may significantly expand the capabilities of CMAQ. Mobilizing the user community in model development, evaluation and application has the added benefits of more deeply engaging the user community and investing them in the continued success of the models. The panel made a series of recommendations that, if implemented, could facilitate greater user contributions to the evolution of CMAQ. The panel noted, however, that user engagement in model evolution must be done carefully, with appropriate quality assurance mechanisms built into the process.

**Recommendation: Develop a public strategic plan, with a 3-5 year time horizon, for the continued development, evaluation and support of the CMAQ model system.** As the Division's own internal plans for model development and evaluation are more widely known, the broader community can identify complementary initiatives.

**Recommendation: Define, as transparently as possible, pathways for users to contribute to the CMAQ modeling system.** Presently, the manner in which the Division identifies scientific results that drive model development initiatives is not widely understood. It is also not clear to the broader user community what types of quality assurance and model evaluation criteria need to be met for user-developed tools to be incorporated into the modeling system. Making these processes transparent will promote user engagement.

**Recommendation: Make available, as possible, inputs and results for selected CMAQ simulations, which can serve as model application and test platforms for the user community.** The Division has invested significant effort in building a variety of long time series simulations (e.g., seasonal, annual, and decadal modeling runs) that have proven very valuable in model performance evaluations within the Division. Making the inputs and results for these simulations broadly available, with appropriate documentation, will facilitate wider model evaluation and analysis activities by the user community. It will also make the model evaluations more straightforward to interpret, since simulations would be based on a consistent set of inputs. These types of "test problems" are common in other modeling communities.

**Recommendation: Seek focused, expert input on Division methodologies, tools and models at critical steps in their development.** The Division has a strong track record of soliciting frequent external peer reviews of the CMAQ modeling system. These reviews have tended to be comprehensive examinations of the modeling system. These should continue, but the Division should add focused teams of external experts that can examine more narrowly defined emerging model system developments (e.g., WRF-CMAQ, inverse emission modeling, or the Carbon apportionment tool). These focused teams should provide input at project initiation, pre-release and other key model development stages.

## *Impact*

The CMAQ modeling system has been used in a large number of Agency decisions and in air quality decisions made by other branches of the federal government, by states, by local governments, other interest groups and other countries. A notable example, and one that suggests a more general recommendation, is the development of a national air quality forecasting system. The Division was instrumental in developing an air quality forecasting system, and as a successful on-going application, its operation has been transferred to another agency. Yet this forecasting capability provided significant model evaluation opportunities (as it was being developed) that should not be lost. In addition, as the CMAQ model continues to evolve, model improvements generated by the Division should be incorporated into the operational forecast model.

**Recommendation: Continue a formal working relationship with air quality forecasting operations.** If this specific relationship is successful, formal methods for integrating operational applications with Division research may become a more general practice.

## *Leadership in the Scientific Community*

The Division has played an important role in developing a regional air quality modeling community directed toward meeting ambient air quality standards, and the Division has established high scientific standards for model development, evaluation and application. The panel's recommendations have addressed how the Division might further strengthen its leadership position in the regional air quality community; however, the Division's community will broaden as CMAQ is used to address air quality issues at smaller scales and at larger scales. The Division's role in leading this expanded community has not yet been articulated and needs to be defined as direction from the Agency emerges.

In conclusion, the panel reiterates its findings that the Division has established the CMAQ models as a leading state-of-the-science regional air quality modeling system, with a large user community; that the Division has delivered timely and relevant modeling products to EPA and its broader user community; and that the Division has developed a balanced portfolio of core research and applied activities in support of EPA needs. The panel also notes that the process for conducting the peer review was well managed and effective, however, in future peer reviews, separate panel meetings with junior staff, in addition to poster sessions and meetings with senior management, would be useful.

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The panel's main findings and recommendations, as described in the Executive Summary, are organized using these four primary questions as a framework. During the review, the Division's work was presented in five major topical areas: (1) Air Quality Model Development, (2) Air Quality Model Evaluation, (3) Linking Air Quality and Human Health, (4) Climate Change and Air Quality Interactions, and (5) Linking Air Quality and Ecosystem Health. For each of these topical areas, the panel was directed, in its charge statement, to organize its findings and recommendations into a framework consisting of three sections:

1. Research
2. Advice and assistance
3. Leadership

NERL requested that both the quality of the Division's work and Division responsiveness to agency needs be addressed in each section. Examples of issues to be addressed in each of these sections, as listed in the charge statement, are given below:

*Research*

| Quality | Responsiveness |
|---|---|
| ***Division's approach to a given environmental problem***<br>Examples:<br>• Has the Division identified major uncertainties and appropriate research priorities?<br>• Are approaches scientifically sound?<br>• In what ways has the Division advanced scientific understanding of the problem? (Has it had an impact?)<br>• Are future directions sound?<br><br>***Division's resources (assume fixed numbers)***<br>Examples:<br>• Are Division's resources effectively and strategically allocated across problems (appropriate depth and breadth)?<br>• Is the skill mix optimized for the scientific direction taken?<br>• Does workforce maintain cutting-edge knowledge and skills?<br><br>***Mechanisms and extent to which findings/products are disseminated to scientific audience in a timely fashion*** | ***Division's responsiveness to Agency needs***<br>Examples:<br>• Is research driven by Agency priorities?<br>• Does the research address the critical issues within EPA's mission?<br>• Is the Agency using the Division's data/products?<br>• Does the Agency adopt approaches or methods developed by the Division?<br>• Does the Division provide information necessary for EPA users to meet statutory requirements or other policy needs?<br>• What problems has the Division solved for the Agency?<br><br>***Balance between core and problem-driven research***<br><br>***Mechanisms and extent to which findings/products are disseminated to Agency in timely fashion*** |

*Advice and Assistance*

| Quality | Responsiveness |
|---|---|
| ***Extent to which Division's assistance is sought by, or provided to, the scientific community***<br>Examples:<br>• Do scientists serve on national/international workgroups, symposia, professional societies, publication boards?<br>• Are they members of research review boards (e.g., study sections) for other organizations?<br>• Do they provide scientific or technical guidance to local, state, tribal and international governments? | ***Extent to which Division's advice/ technical support is sought by the Agency (Program Offices, Regional Offices)***<br>Examples:<br>• Does Division staff participate on major within-Agency workgroups?<br>• Do Division scientists assist the Agency in developing testing guide-lines, interpreting research advances, reviewing Program Office or Regional documents? |

*Leadership*

| Quality | Responsiveness |
|---|---|
| ***Division's leadership role in the scientific community (influence on agendas, decisions, priorities of other researchers/organizations)***<br>Examples:<br>• Do scientists lead collaborative research efforts at the national/international level?<br>• Do they serve on advisory boards of other major agencies/organizations?<br>• Are they invited to chair major committees?<br>• Do they organize major conferences, symposia?<br>• Do they receive awards/honors for scientific contributions? | ***Division's leadership role in the Agency (influence on research planning efforts, decisions, and priorities of the Agency)***<br>Examples:<br>• Does Division staff lead research planning and coordination efforts across Divisions, Agency Labs and Offices?<br>• Do scientists represent ORD/Agency on workshops or workgroups addressing major risk assessment or environmental issues?<br>• Do they receive major Agency awards/honors? |

The following sections of this report describe the panel's assessment of AMAD Research, Advice/Assistance and Leadership in the 5 theme areas of (1) Air Quality Model Development, (2) Air Quality Model Evaluation, (3) Linking Air Quality and Human Health, (4) Climate Change and Air Quality Interactions, and (5) Linking Air Quality and Ecosystem Health.

# Theme 1. Model Development and Diagnostic Testing

## 1A. Introduction

EPA's AMAD division may be the largest air-quality-model development, evaluation, and application group in the world. An important thrust of this NERL division is model development and diagnostic testing. For the past 15 years or more, the primary focus of AMAD's development efforts has been the CMAQ (Community Multiscale Air Quality) modeling system, which now consists of the CMAQ chemical transport model (CCTM), its meteorological driver models (MM5, WRF), emissions processing and emissions modeling systems (SMOKE, BEIS), and other supplemental software and data sets.

The CMAQ numerical modeling system provides a quantitative link between emissions of target pollutants or their precursors to the atmosphere and the resulting ambient air concentrations and dry and wet removal of these pollutants. CMAQ can thus be used to (a) evaluate and assess proposed AQ control measures and management programs, (b) make short-range (i.e., several days) AQ forecasts (c) assess AQ responses to long-term changes (i.e. climate change), (d) provide atmospheric inputs to other models (e.g., water-chemistry and ecosystem models), (e) help design measurement networks, and (f) test scientific hypotheses.

## 1B. Research

AMAD research contributions to AQ model development and testing have been wide-ranging, scientifically sound, and of high quality, and they have contributed significantly both to the AQ modeling community in general and to Agency programs in particular. The development of an operational AQ forecasting system in response to a direct request from Congress is one particularly noteworthy example.

*Accomplishments and Strengths*

In the past five years, the Division has had many significant accomplishments in model development and diagnostic testing, including improvements to the CMAQ CCTM, emissions models, and meteorological models:

- In collaboration with NOAA, development and transition to operation in only four years of a U.S. operational national AQ forecast system for ozone (Eta-CMAQ, then WRF-NMM-CMAQ).
- Release of six public versions of CMAQ (v4.2.2 through v4.7) to the external user community in the 2003-2008 period (see www.cmaq-model.org).
- Development of a multi-pollutant version of CMAQ (v4.7) that can model criteria pollutants ($O_3$, $PM_{2.5}$, $PM_{10}$) and toxic pollutants (Hg plus 40 other species) simultaneously.

- Design and development of AMET and WDT, two post-processing tools to assist client and user communities in making better use of CMAQ results.

- Establishment of a number of targeted collaborations with various other EPA Divisions, other U.S. federal departments and agencies, universities, international organizations, and consulting companies to improve CMAQ. These collaborations have allowed the Division to access complementary external expertise and external facilities. Some examples include the development of the CMAQ sea-salt emissions module, the AMET and WDT post-processing tools, and the CB05 gas-phase chemistry mechanism, the extension of ISORROPIA to base cations, the use of meteorological satellite data to adjust photolysis rates, and various computational efficiency improvements, including parallelization of the CCTM code.

- Initiation of three external peer reviews of the CMAQ modeling system (in 2003, 2005, and 2006) through the CMAS Center to provide critiques and advice on the CMAQ development program, including future directions and priorities (see www.cmaq-model.org).

- Implementation of numerous improvements to the CMAQ modeling system during the 2003-2008 period. Table 1 lists notable new features and upgrades. They include improvements to most aspects of the modeling system, including the specification of input emissions, the meteorological driver, the chemical transport model, and post-processing capabilities. A number of these improvements were made possible by recent advances in understanding of important atmospheric chemical and physical processes.

**Table 1**. Significant developments to the CMAQ modeling system implemented by AMAD during the 2003-2008 time period.

| | |
|---|---|
| 1 | Improved computational efficiency, especially in the aerosol module; |
| 2 | Development of a “side-by-side” two-way-coupled meteorological and chemical transport modeling system (WRF-CMAQ) that can be applied to both AQ-climate studies and to finer spatial scale modeling; |
| 3 | Development of a sectional version of CMAQ; |
| 4 | Significant upgrades to parameterization of secondary organic aerosol (SOA) formation (including contributions of isoprene, sesquiterpenes, benzene, glyoxal, and methylglyoxal precursors and polymerization, acid catalysis, and nox-dependent processes); also required a new release of BEIS (v3.14) to include sesquiterpene emissions; |
| 5 | Roll-out of a new CB05 gas-phase chemistry mechanism, including $Cl_2$ chemistry, and work to implement the SAPRC07 mechanism, an update of SAPRC99; |
| 6 | Implementation of a chemically active PM coarse mode for semi-volatile inorganic ions and elimination of some numerical instabilities in ISORROPIA; |
| 7 | Development of in-line photolysis rate module with aerosol feedback; |
| 8 | Improved treatment of $N_2O_5$ hydrolysis; |
| 9 | Upgrades to HONO emissions and chemistry; |
| 10 | Modifications to representation of cloud mixing in the convective cloud module; |
| 11 | Closer and more consistent connections in treatment of meteorological surface fluxes and dry deposition; |
| 12 | Development of treatment of bi-directional surface fluxes of $NH_3$ and Hg; |
| 13 | Development of a sea-salt emission flux parameterization that considers both open-ocean and surf-zone emissions (relevant for the National Estuary Program); |
| 14 | Development of the Atmospheric Model Evaluation Toolkit (AMET), a meteorological and AQ model evaluation package (released in 2008), and the Watershed Deposition Tool (WDT), a GIS tool to map gridded CMAQ output fields to irregularly-shaped watersheds; |
| 15 | Implementation of an “instrumented” version of CMAQ for process analysis, sensitivity analysis, and source attribution, including sulfur and carbon tracking tools and DDM-3D version; |
| 16 | Modifications to the WRF meteorological model to make it a more suitable and compatible “driver” for the CMAQ CCTM, including incorporation of the Pleim-Xiu land-surface model and “nudging” FDDA; |
| 17 | Development of an improved PBL parameterization (ACM2) that has been implemented in both a meteorological model and an AQ model (CMAQ); |
| 18 | Development of PBL data assimilation techniques; |
| 19 | Development of methodology to build national, model-ready emissions inventory of day-specific daily wildfire and prescribed-burn emissions based on both satellite-remote sensing and surface reports (U.S. wildfire inventories now available for 2002 to 2006 period). |

- Associated with all of these model developments and improvements have been ongoing evaluation studies and diagnostic testing using data from major field programs. Field studies can provide (for short periods) detailed sets of measurements of a broad set of chemical species with high time resolution and sometimes high spatial resolution and above-surface measurements. AMAD made use of short-term data sets from the following programs and field studies during the 2003-2008 period to advance CMAQ development:
    - 2004-08 NOAA-EPA AQ forecast system evaluation for a wide range of seasonal and synoptic conditions;
    - analysis of carbonaceous aerosol vs. SEARCH network daily measurements using new process analysis tools in CMAQ;
    - 2001 Northeast Oxidant and Particle Study (NEOPS) field campaign;
    - 2002 Northeastern AQ Study (NEAQS) field program;
    - 2002 Bay Regional Air Chemistry Experiment (BRACE) field study in Tampa Bay, Florida and interactions of gas-phase species and coarse PM;
    - 2004 ICARTT northeast U.S. field program and vertical profiles of CMAQ;
    - 2006 TexAQS field campaign.

*Limitations*

- The Division is in danger of trying to cover too much ground with too few resources, especially in relation to future model development plans to extend the scale of CMAQ to the neighborhood scale and the hemispheric scale. Note that this same concern was raised in 2003 by the 1st CMAQ external peer review panel that was organized by CMAS.

*Future Directions*

Plans for future directions presented to the review panel by AMAD included the following:

- improved treatment of chemical lateral boundary conditions;
- increase of maximum CMAQ domain size from continental to hemispheric scale;
- further development of modeling system to handle finer grid resolutions;
- improvements to chemical interactions between gas-aerosol-aqueous phases;
- improvements to the chemical mechanisms;
- improvements to model performance during cold seasons;
- improvements for optical and radiative properties, especially for AQ-climate applications;
- continued effort to characterize unspeciated $PM_{2.5}$;
- implementation of wind-blown dust emissions module and treatment of chemical interactions between crustal base cations and gases;
- development of a parameterization for lightning NOx emissions, a source of nitrogen that is currently missing from the model;
- transition from BEIS to the MEGAN biogenics emissions module (benefits should include better treatment of vegetation phenology, more up-to-date emission factors, applicability to other continents);
- investigation of use of non-traditional upper air data in meteorological data assimilation;

- use of National Land Cover Dataset (NLCD) in calculation of land-surface fluxes and dry deposition;
- improvements to treatment of stable boundary layers, including nighttime and winter conditions; and
- continued development of coupled WRF-CMAQ system for both AQ-climate and fine-scale modeling (key to two FY11 Annual Performance Measures).

All of the above future directions should contribute to improved simulation for one or more of the primary CMAQ applications, but some of these model improvements will be harder to achieve than others due to limitations in data availability or current scientific understanding. For example, being able to model wind-blown dust emissions will improve short-term PM and visibility simulations and also long-term acid deposition estimates. However, modeling wind-blown dust requires information about some soil properties that are not typically available, information about seasonal variations in vegetation cover, and accurate predictions of soil moisture. Stable boundary layers are a common occurrence but the parameterization of stable boundary layers in AQ models has not advanced significantly in the last three or four decades. Improvements here would be very beneficial but are likely to be hard-won.

*Suggestions for Improvement*

There are a few other emerging issues that were not raised by AMAD during the on-site review. The Division might also consider addressing the following issues, with the understanding that the future directions discussed above may take precedence depending upon Agency needs:

- PM number density and the ultrafine mass fraction. These aspects of PM have been raised by some in the health community as being more closely linked to health impacts, including by studies of near-roadway PM exposure. Modeling these aspects of PM, however, will place new demands on the development of emissions inventories and on the numerical treatment of the PM size distribution in order to conserve both number and mass simultaneously;
- Hemispheric AQ modeling. Moving to this spatial scale requires improvements to both model inputs and the model itself, including the specification of hemispheric emissions (i.e., Asian and European anthropogenic emissions, biogenic emissions), hemispheric meteorological modeling and data assimilation from a wide range of data sources, including satellites, aircraft, buoys, and ships, the treatment of background chemistry and emissions (e.g., DMS, $CH_4$), and the treatment of upper boundary conditions and stratosphere-troposphere exchange;
- Possibility that semi-volatile VOC emissions from vehicular and other sources are not accounted for in current emission inventories and AQ models. Work by the group at Carnegie-Mellon, for example, suggests that these emissions may be a missing organic PM source;
- Data fusion techniques. There have been some efforts to combine AQ model predictions and AQ and other measurements (e.g., precipitation, cloud cover) by various approaches, including kriging, model output statistics, objective analysis, and model-space and observation-space methods in data assimilation, but further improvements and applications of such techniques to CMAQ are likely possible.

- Development of a 2-way nested domain capability or the use of a non-uniform grid system that would provide higher resolution in specific areas of interest within larger domain simulations. Such a capability is fairly common in meteorological modeling and would be useful for modeling situations where chemical feedbacks from a high-resolution domain would have significant impacts on the coarser scale as well. One example might be AQ modeling for mega-cities, where a realistic treatment of small-scale chemistry and dispersion in the urban core and urban plume could conceivably change the predicted regional-scale impacts.
- A more in-depth study of horizontal physical diffusivity and its parameterization for different grid scales is in order. Presently, numerical diffusion is often lumped together with physical diffusion, and the true impact of this lumping is often unknown. What is known though is that the errors would tend to be large near the peak concentration regions and regions with large concentration gradients.

## *1C. Advice and Assistance*

As demonstrated by the following examples, AMAD's model development research has had a significant impact in supporting EPA's policy, planning, and priorities.

- Application of CMAQ by the Agency (OAQPS) to provide technical foundations and benefit assessments for a number of Agency regulations, including:
    - Clean Air Interstate Rule (CAIR)
    - Clean Air Mercury Rule (CAMR)
    - Revised $O_3$ NAAQS final rule
    - Locomotive and Commercial Marine final rulemaking
    - NOx/SOx secondary NAAQS review (underway)
    - Renewable Fuels Standards Act-2 rulemaking (upcoming)
- Contributions to Agency science assessments (e.g., 5-year NAAQS reviews, incorporation of CIRAQ results in ORD interim national AQ assessment)
- Application of CMAQ to State Implementation Plans (SIPs) by U.S. regional planning organizations (RPOs), individual states, and consultants
- Establishment of the Community Modeling and Analysis System (CMAS) Center at the University of North Carolina, which provides support to the large external CMAQ community of users (~1000), has organized a series of seven regional AQ modeling conferences focused on CMAQ, and offers courses on using CMAQ and its emissions, meteorological, AQ, and post-processing components; the external community in turn has authored more than 25 CMAQ publications (e.g., see weblink http://www.cmascenter.org/resources/bibliography.cfm?temp_id=99999#CMAQ_DEV)
- Improvements to the comprehensiveness of U.S. national emission inventories through the development of methodologies to estimate emissions from non-traditional sources (e.g., biogenics, wildfires, ocean wave-breaking)

Work on model improvements has been prioritized based on relevance to Agency issues (i.e., application needs) and expected impact.

- Significant internal recognition of AMAD'S contributions to EPA itself appears strong, as suggested by significant number of intra-agency awards
- Dec. 2008 memo from AQAD director (Richard Wayland) is very supportive overall of AMAD contributions to Agency programs (see Section 14 of *Peer Review Support Document*)
- Large number of research collaborations with groups inside Agency (Table 11.4 of *Peer Review Support Document*)
- Participation in and contributions to ORD and NERL planning activities
- AMAD has also been responsive to recommendations from past external reviews. For example, it was noted in both the 2nd and 3rd CMAQ External Peer Review reports (see weblink http://www.cmaq-model.org/) that AMAD had already made significant responses to a number of the recommendations contained in the 1st and 2nd CMAQ External Peer Review reports, respectively.

The division has provided additional advice and assistance both to the Agency and to outside organizations and groups, including the following examples:

- The Division has worked with the National Park Service to assess air concentration and deposition at Shenandoah National Park;
- The Division has provided assistance to the Chesapeake Bay Program since 1992 and more recently to the Tampa Bay Estuary Program;
- The Division has worked with the New York Department of Environmental Conservation to establish a state-level AQ forecasting program;

## *1D. Leadership*

AMAD has been actively engaged with the rest of the Agency and with the external science community during the 2003-2008 period, providing leadership within these communities in a number of ways.

- development of a state-of-the-science regional AQ modeling system
- transfer of EPA-developed meteorological parameterizations to NCAR's Weather Research Forecast (WRF) meteorological model
- choice of research problems as an example to the larger scientific community
- large number of research collaborations with groups inside and outside the Agency (cf. Table 11.4 of the *Peer Review Support Document*)
- strong publishing record: 50 AMAD staff (including some now retired or transferred) contributed to 161 journal articles published during 2003-2008 period, including 104 first-authored publications (i.e., > 25 articles per year)

- Division staff hold 5 adjunct professorships, sit on 7 journal editorial boards, and serve as officers in 3 professional societies and as committee members in 4 professional societies
- Division staff have mentored ~8 post-doctoral fellows and students
- creation of CMAS to provide support to the external community of CMAQ users
- organization of conferences, workshops, and special issues (e.g., 2005 NOAA-EPA Golden Anniversary modeling conference, 2006 special issue of *Atmospheric Environment* on model evaluation, 2007 AMS-EPA regional AQ model evaluation workshop, 2009 AQMEII model evaluation workshop)

## 1E. Summary and Recommendations

**Findings:**

- The Division has developed CMAQ, a leading state-of-the-science regional air quality modeling system, and has continued to innovate in improving the model science.

- The Division has generally been responsive to the needs of CMAQ users in developing and providing updated versions of the model. This includes a concerted effort to improve the model's computational efficiency as well as its science.

**Recommendations:**

- Develop a public strategic plan, with a 3-5 year time horizon, for the continued development, evaluation and support of the CMAQ modeling system. It is clear that the Division has identified a set of future directions and formulated a development plan for CMAQ, but these are not widely known outside of the Division. As the Division's own internal plans for model development and evaluation become more widely known, the broader CMAQ community can identify complementary initiatives and avoid duplicative research.

- Define, as transparently as possible, pathways for users to contribute to the CMAQ modeling system. Presently, the manner in which the Division identifies scientific results that drive model development initiatives is not widely understood. It is also not clear to the broader user community what types of quality assurance and model evaluation criteria need to be met for user-developed tools to be incorporated into the modeling system. Making these processes transparent will promote user engagement and may in turn benefit the Division.

  We note that a related concern was raised in the 2nd CMAQ External Peer Review report (p. 12), where the suggestion was made by that review panel that extramural improvements to CMAQ such as CMAQ-MADRID should be brought into the core model version so that the code changes would not need to be "migrated" into each new CMAQ release. AMAD responded that this suggestion could be very time-consuming, although it was noted that CMAS had set up and maintains a multi-version repository of research versions of CMAQ. This response was re-iterated by AMAD during the 3rd

CMAQ External Peer Review (see p. 8), but it was also noted by AMAD that some modules developed outside of the EPA have been incorporated into the core model (e.g., ISORROPIA, UCD sectional PM version, DDM-3D). It was suggested that the existence of an active collaboration between AMAD and the external developers made this transfer more likely to happen.

In view of AMAD's efforts to encourage the development of an external CMAQ community, it would be worthwhile for AMAD to communicate its position on this subject to the community and to describe the minimum requirements that should be met.

- Establish a process to communicate and consult with the external user community before features are removed from CMAQ and provide a rationale for such removals when a new model version is released. Many new features and improvements have typically been introduced in each CMAQ release, but before version 4.7 was released in Sept. 2008, very few existing features had been removed (the RADM2 gas-phase chemistry mechanism was dropped in version 4.5). When CMAQ version 4.7 was released, however, five CMAQ options were dropped: plume-in-grid (PinG); CB4 gas-phase chemistry mechanism; AERO3 module and AE3 mechanism; RADM cloud module; and the stand-alone mercury version of CMAQ. The loss of support for selected model features means a loss of backward compatibility. It would be helpful to the larger CMAQ user community if advance warning of such decisions were given and an opportunity to comment was made available. It would also be informative as part of the release of a new model version to provide reasons for the removal of any features.

  For this panel, the loss of support for the CMAQ PinG module in version 4.7 was the most surprising. AMAD's response to the 2nd CMAQ External Peer Review report (p. 4) stated that new research and development on the PinG module was to be phased out after 2005 and a reason was given, but the PinG module was then upgraded in CMAQ version 4.6 before being phased out in version 4.7. Others in the CMAQ user community might have been similarly surprised.

- Seek focused, expert input on Division methodologies, tools and models at critical steps in their development. The Division has a strong track record of soliciting frequent external peer reviews of the CMAQ modeling system. These reviews have tended to be comprehensive examinations of the modeling system. These should continue, but the Division should add focused teams that can examine more narrowly defined emerging model system developments (e.g., coupled models and WRF-CMAQ, hemispheric CMAQ, inverse emission modeling, or the Carbon apportionment tool). These focused teams should provide input at project initiation, pre-release, and other key model development stages.

**Finding:**

- In collaboration with NOAA, AMAD was responsible for the development and transition to operation in a short time (four years) of the first U.S. operational national AQ forecast system for ozone. In 2003 the EPA and NOAA signed a Memorandum of Agreement to collaborate on the design, development, evaluation, and implementation of an operational daily AQ forecast system. The resulting operational air-quality forecast model (AQFM) was based in large part on the CMAQ CCTM and other key components of the CMAQ modeling system. The Division has suggested (see *Peer Review Support Document*, p. 4-11) that this collaboration was concluded successfully at the end of FY08 with "the transfer of AMAD's models and modeling guidance to NOAA's operational arm" at the same time that the NOAA staff seconded to the EPA were formally transferred to EPA/NERL/AMAD. However, two of the original design goals for the AQFM have not yet been met: (1) that the AQFM forecast domain should include all 50 U.S. states, including Alaska and Hawaii; and (2) that the AQFM forecasts include both ozone and $PM_{2.5}$ forecasts. At the present time the AQFM forecast domain only includes the contiguous 48 states and $PM_{2.5}$ forecasts are not yet operational.

**Recommendation:**

- AMAD should continue a formal working relationship with NOAA on operational AQ forecasting. Maintaining such a relationship would benefit both parties. NOAA would continue to have a formal mechanism to access AMAD expertise during the transition to a larger forecast domain that supports AQ forecasts for Alaska and Hawaii and to operational $PM_{2.5}$ forecasting. This agreement would also institutionalize NOAA's access to the EPA's latest anthropogenic emission inventories, to AMAD's models and methodologies to estimate natural emissions, and to the near-real-time provision of continent-wide $O_3$ and $PM_{2.5}$ measurements via the EPA's AIRNow meta-network. AMAD in turn would continue to learn from having CMAQ applied 24/7 over a continental-scale domain using a different meteorological driver (WRF-NMM) with advanced meteorological data assimilation techniques to forecast both gas and aerosol species. Such an agreement would also provide EPA with a formal procedure to provide NOAA with newer versions of CMAQ, thus supporting an ongoing transition of research advances to the operational arena and avoiding a divergence of AQ forecasts being made by the EPA for policy purposes with those being made by NOAA for short-term guidance. If this specific relationship is successful, formal methods for integrating operational applications with Division research may become a more general practice.

**Finding:**

- AMAD's model development research has had a significant impact in supporting EPA's policy, planning, and priorities. The CMAQ modeling system has been used to provide analysis and benefits assessment underlying such Agency regulations as the Clean Air Interstate Rule, the Clean Air Mercury Rule, the revised $O_3$ NAAQS Final Rule, and the Locomotive and Commercial Marine Final Rule. It has also been used by the states in preparing State Implementation Plans for submission to the Agency.

**Recommendation:**

- When required, the Division's core activities should be expanded in order to maintain any Division capabilities that are not currently required to support Agency policy activities but which have been required in the past and are likely to be needed again in the near future. A significant investment is usually required to build the scientific expertise and modeling tools needed to bring leading-edge science to support policy development. In a research environment where science continues to evolve at a rapid pace, both expertise and models must also be updated on an ongoing basis to be of most use. For example, CMAQ mercury modeling has contributed to Agency policy in the recent past and will almost certainly be needed in the future. Efforts should be made by the Division to maintain this capability.

# Theme 2. Model Evaluation: Establishing Model's Credibility

## 2A. Introduction

A Long-Term Goal of the Office of Research and Development's Clean Air Research Multiyear Plan is to reduce uncertainty in standard setting and air quality management decisions. Model evaluation is a key component of the AMAD activities that allow the ORD to move toward this goal. Confidence in the model predictions can only be increased if the model describes the chemical and meteorological processes reliably, has reliable emissions, boundary and initial conditions as input, and has an accurate computational methodology. An evaluation of all these components and the model as a whole also requires reliable observational data for comparison purposes. However, because of the very wide range of the temporal and spatial scales of the processes involved, and the fact that most of the processes can only be studied through observation rather than experimentation, model evaluation becomes a very challenging task.

Model evaluation helps identify and potentially improve weaknesses in the model or its components, and can also help improve the design of data collection and measurement processes. The AMAD has a rather elaborate and comprehensive framework to evaluate CMAQ. The evaluation framework consists of four different components: operational, diagnostic, dynamic, and probabilistic. Operational evaluation compares model-predicted and routinely measured concentrations of the end-point pollutants of interest. Diagnostic evaluation attempts to identify areas where improvement is needed, and is tied directly to model development activities of AMAD. Dynamic evaluation is concerned with how model predictions respond to changes in meteorology and/or emissions. Probabilistic evaluation attempts to incorporate model and input uncertainties in the characterization of model predictions and to capture the stochastic nature of the atmospheric processes through the judicious usage of deterministic-model runs.

## 2B. Research

*Accomplishments and Strengths*

- An outstanding strength of the AMAD in research is the team work and spirit of the staff. In particular, members of the Model Development and Diagnostic Testing Team and the Model Evaluation Team have collaborated closely to help facilitate model improvement.
- The AMAD places eight full-time equivalents of scientists on model evaluation. This indicates the high priority AMAD places on this activity. The AMAD's strong support and the positive attitudes of the scientists help assure the high quality of the research.
- To facilitate and standardize the model evaluation effort, the AMAD has developed the Atmospheric Model Evaluation Toolkit (AMET), which is a package of data analysis and graphical tools for use by both the model developers and users. This tool has been enthusiastically received by practitioners and is a great asset for model improvement.
- As noted in the review of Theme 1, to evaluate the direct relevance and usefulness of CMAQ for 24-hour real-time forecasting operations, the AMAD formed a partnership with

NOAA to develop the National Air Quality Forecast System (NAQFS). This partnership has the advantage of both supporting the air quality forecasting operation and helping identify shortcomings in the model.

- In a remarkably short time frame, the AMAD updated the meteorological model in NAQFS (WRF-NMM). The subsequent spatial and temporal evaluations of the NAQFS show that the WRF-NMM-CMAQ model generally performs well but with some regional systematic errors and biases. Overall, the WRF-NMM-CMAQ has great potential to improve both the science and applicability of the model.
- The AMAD has explored and developed post-processing bias-adjustment techniques. One of these, based on the Kalman Filter, can significantly reduce model bias and should help improve air quality forecasting even though it is not designed to identify model shortfalls.
- The Division has statisticians as members of the staff. This is a remarkable asset to the Division. By using block kriging, they help illustrate the role of spatial correlation structure in understanding the incommensurability issue between grid-averaged concentrations and point measurements. The methodology implicitly highlights the need to adjust model grid size to reduce incommensurability. Application of this methodology can be very helpful in human exposure studies for pollutants of different spatial and temporal scales.
- The AMAD researchers use instrumented models for diagnostic evaluations to investigate how the model responds to perturbations in various model parameters. Three such models are considered: the Direct Decoupled Method (CMAQ-DDM-3D), carbon apportionment (CMAQ-CA), and sulfur tracking (CMAQ-ST). The CMAQ-DDM-3D is used to estimate the impact of precursor-emission changes on ozone, quantify uncertainties in model outputs when model structural and/or parametric uncertainties are explicitly considered, and estimate emissions via inverse modeling. CMAQ-CA is designed to track the size, composition and sources of primary carbonaceous aerosol. This activity has led to improvement in the National Emissions Inventory. CMAQ-ST tracks emitted sulfur through its different chemical and physical pathways. The usefulness of these instrumented models has been well demonstrated. If the emissions and emission changes are reliable, these tracking tools can also be an excellent test for model performance.
- Emissions are among the largest sources of uncertainty in air quality modeling. The AMAD has used inverse modeling to reconstruct emissions for seasonal agricultural ammonia emissions and urban NOx emissions. The resulting ammonia seasonal emission estimates have been incorporated directly into the SMOKE emission system. In the NOx study, satellite $NO_2$ information was used to help reveal a NOx bias in the free troposphere. Whether the bias is a chemistry issue, a transport issue, or both needs to be investigated.
- In dynamic model evaluation, AMAD has performed a ground-breaking study to compare the model-predicted changes and observed changes in ozone concentrations during the summer months in the Eastern US as a result of NOx emission reductions dictated by the NOx SIP call. The AMAD had an elaborate modeling design with different combinations of emission changes, meteorological changes, and changes in chemical mechanism. The years selected for the study were 2002 (pre-NOx-SIP call), and 2004 and 2005 (post-NOx-SIP call). This project allowed the EPA to conclude that there was a general underprediction of ozone reductions compared to observations, and that CB05 with updated emission inventories appears to perform better in predicting ozone response to NOx reduction. There was also a significant underprediction of ozone and NOx at altitudes above 2000 m. The AMAD plans to conduct diagnostic analyses of modeled and

observed vertical concentration and wind profiles to assess transport and vertical mixing processes. Dynamic model evaluation is a critical area of activity for the evaluation of the applicability of air-quality models for policy-related simulations and AMAD has done an outstanding job in undertaking this activity.

- The AMAD has also undertaken probabilistic model evaluation. Bayesian model averaging has been used to construct a probability distribution function of ozone concentration at a specific location and time. The distribution function is in turn an observation-calibrated weighted average of model-prediction distributions generated by allowing for structural and parametric uncertainties in the model. This approach would be very useful if the weights, which are the posterior models' probabilities for inclusion in the averaging process, are relatively stable under a relatively wide range of environmental conditions. Probabilistic model evaluation is a new activity at AMAD and in the air-quality modeling community in general. It allows the use of results from deterministic models like CMAQ in a stochastic context. And it also conveys the degree of confidence in the range of model-predicted concentrations in describing actual observations. This valuable activity would not have been effectively undertaken in a timely manner had the Division not brought well-trained statisticians on board.

*Limitations*

- In inverse modeling, use of only one set of the DDM sensitivity coefficients can impose substantial restrictions on the outcome of the emission estimates. For example, if the sensitivity is with respect to an emission-change factor applied to the emission profile, then the basic temporal and spatial variations of the emission profile has been implicitly adopted, which may or may not match reality.
- The AMAD model evaluation effort has largely been confined to CMAQ, although the mercury version of CMAQ was included in two model inter-comparisons. Accordingly, opportunities for new insights gained by evaluating non-CMAQ models are not available.
- The AMAD is expanding its neighborhood-scale modeling capability and concurrently plans to greatly enhance its modeling capability at the global and/or hemispheric scale, and global-to-regional downscaling. All these efforts are likely to pose a severe challenge to resource allocation, and perhaps constrain some of the model evaluation efforts.

*Future Directions*

- Further interaction between AMAD and the NAQFS group would be a mutually beneficial collaboration. Such a collaboration would allow for the potential incorporation of the post-processing, bias-adjustment technique based on the Kalman Filter or the Bayesian model averaging method to provide confidence-level estimates of the air quality forecast. This is a highly valuable approach for health protection.
- The AMAD intends to continue to update and expand the suite of instrumented models. In particular, the AMAD is exploring developing in-house capabilities in adjoint modeling. This is a worthwhile approach to understand how a perturbation or sensitivity coefficient of a given species concentration can be traced back to its origin at an earlier time according to a given model like CMAQ. Within the limit of its applicability, the approach can help

identify potential areas for improvement in CMAQ when predicted changes in emissions can be compared with the actual changes.

- Use of highly-resolved $NO_2$ satellite data coupled with improved model chemistry, once available, is strongly encouraged for inverse modeling of NOx emissions. There may be a grid scale problem for inverse modeling of carbon monoxide, especially in the regions of interest, in the microenvironments near the emission sources. For elemental carbon, such a study may be useful if the concern is the regional transport of the pollutant. In this connection, a hemispheric or global model may be more suitable because elemental carbon, and many other pollutants and pollutant precursors can be transported long range.
- Applying dynamic model evaluation to the most current CMAQ version is recommended especially when there are sufficient and significant changes from the version used in the earlier evaluation. To evaluate the ability of MOBILE6 (and possibly link-based mobile emissions) to actually capture the NOx emission changes may necessitate a smaller-scale model, with a 2x2 $km^2$ or at most 4x4 $km^2$ grids. The 12x12 $km^2$ grid may be less useful because the NOx emissions are rather granular spatially in an urban environment, and beyond an urban area where the larger grid may be useful, interferences from other emission sources, chemical and physical processes may blur the signals of the mobile-source NOx emission changes.
- The AMAD intends to better characterize the model uncertainty by improving the uncertainty estimates of sector emissions. It also intends to incorporate the $NO_2$ data in addition to the ozone data to help weight ensemble members in Bayesian model averaging. These are useful efforts to improve the robustness of the weights. Applying the methodology to $PM_{2.5}$ is perhaps worthwhile, but characterizing model uncertainties is more challenging because of the added complexity and uncertainty of aerosol chemistry. Applying the methodology to regional downscaling is much less useful presently because of the huge uncertainty associated with regional climate predictions from existing general circulation models, and there are no bona fide observations for comparison purposes.

*Suggestions for Improvement*

- It is recommended that AMAD take advantage of information and data gained from the NAQFS to develop an in-depth and systematic model evaluation of episodic air quality events for different parts of the country. This could be conducted in close collaboration with the NCEP NAQFS group.
- Air quality models contain structural, parametric (including emissions) and numerical uncertainties. In inverse modeling, it would be helpful to ascertain how some of the non-emission uncertainties in the model are translated into uncertainties in the emission estimates. This is especially important because the emission profile leading to good agreement between observation and model prediction is simply an outcome of a closed-loop iterative effort driven by the least-squares assumption in inverse modeling, not an indication that the derived emissions are more reliable.
- To minimize profile presumptions on the emissions, it would be useful in the inverse modeling approach to look into the use of Kalman filter with an explicit transfer matrix linking emissions to concentrations (instead of a Jacobian based on the sensitivity coefficients) for time-dependent inversions to construct some relatively granular temporally and spatially dependent emission profiles.

- The validity of the sensitivity coefficients beyond say, a 10-20% emission perturbation can become an issue for pollutants undergoing nonlinear processes. So if the converged emissions are significantly different from those of the initial emissions assumed by inverse modeling, what is the potential implication? This issue needs to be investigated. The AMAD has been careful in the choice of species or species groups for study in this regard.
- In assessing the transport and vertical mixing processes in the model study of the NOx-SIP Call, it is also necessary to assess the reliability of the horizontal transport and mixing processes in the model. The notorious numerical problems associated with advection should not be ignored.
- The model-predicted ozone changes due to emission changes like the NOx-SIP Call is most certainly grid-size dependent. An investigation of this issue would be helpful but challenging. This issue is also tied to the issue of subgrid parameterization of chemistry, which can be quite intractable. Simply reducing the grid size and re-running the model does not fully address the problem.
- It would be worthwhile to compare the performance of CMAQ and non-CMAQ models like CAMx. Considerable insight would be gained in such a comparison, leading to subsequent model improvement. Also, it would be worthwhile to look into the incorporation of non-CMAQ models in Bayesian model averaging.

## *2C. Advice/Assistance*

- Through CMAS, the AMAD has played a major role in advising and assisting the user community, including members of federal, state, tribal and regional regulatory agencies, and international governmental agencies.
- The implementation of AMET is another clear indication of the responsiveness of AMAD to the needs of the user community.
- Members of the AMAD have worked closely with members of the Air Quality Assessment Division (AQAD), keeping the latter informed on the science and process issues as the new version of CMAQ (v4.7) was being developed and evaluated. The same is true in the development of the coupled WRF-CMAQ system.
- Members of the AMAD have also served on EPA review panels on grants proposals.

## *2D. Leadership*

- Because the AMAD has a very high concentration of expertise over a wide spectrum of air quality issues, its leadership role in the scientific research communities is unchallenged. The long record of awards/honors received by members of the AMAD bears this out.
- Many members of the AMAD are invited speakers and/or chairs or organizers of many national and international conferences, workshops, and symposia. Many also serve on professional societies and publication review boards, and some are on the faculties of universities.

## *2E. Summary and Recommendations*

**Findings:**

- Overall, the AMAD has done an outstanding job in model evaluation. The research quality is high, and the effort is responsive to the needs of the Agency.
- The Division has worked closely with AQAD to inform, deliver and help implement as necessary new versions of CMAQ for applications.
- The Division has taken the role of assisting the user community. Many of the members are also playing a leadership role in air quality modeling research.
- There is tremendous value to be gained if the heretofore fruitful NAQFS partnership between AMAD and NOAA could be re-affirmed and institutionalized.

**Recommendations:**

- As the Division takes on new areas of activities in climate-change impact on air quality, prioritization of projects becomes necessary. Prioritization ought to be based on the direct practical relevance of the project and its ability to improve understanding and/or to truly reduce uncertainty.
- The AMAD is encouraged to work with non-CMAQ model developers to gain from each others' insights and modeling experience.
- In considering air quality modeling of the neighborhood scale and hemispheric scale, it would be useful if AMAD could lay out potential revisions and new emphasis in the approaches for model evaluation. For example, in the case of hemispheric modeling and multi-year simulation, a pertinent issue would be how to handle emissions that contribute to long-range transport and formation of target pollutants like ozone. In the neighborhood scale, one issue would be the extent of the spatial and temporal granularity of the pollutants of interest compared to the resolution of the model.
- Diagnostic analyses of modeled and observed vertical concentrations and wind profiles to assess transport and vertical mixing processes are not only necessary, but long overdue. The role of physical transport has generally been taken for granted and assumed to be taken care of by mass adjustment and artificial diffusion in the numerical methods. This is unfortunate. A careful evaluation of the dispersion characteristics, both vertical and horizontal, within and above the planetary boundary layer is strongly encouraged. Past and planned (if any) field studies with tracer releases should be useful for this purpose.

# Theme 3. Linking Air Quality and Human Health

## 3A. Introduction

The goal of this research theme is to reduce uncertainties in linking air pollution sources and health exposure. The AMAD attempts to achieve this by combining grid-based, regional-scale models with urban-scale, dispersion models to provide spatially and temporally resolved air pollution concentrations. The ultimate goal is to use these high resolution air quality model predictions in exposure modeling as compared to using measured pollution concentrations, because measurements are lacking in spatial coverage in most cases. The three main projects under this research area are:

- Developing a hybrid modeling approach by combining results from a regional scale model (CMAQ) and a dispersion model (AERMOD).
- Improving the near-road component of AERMOD to better assess the spatial variability of air quality near roadways.
- Evaluating the effectiveness of regulatory actions by investigating the relationships among emissions, ambient pollutant concentrations, human exposures and health outcomes.

## 3B. Research

*Accomplishments and Strengths*

- AMAD has coupled the CMAQ model with the AERMOD model, thereby developing an approach that can be used to simulate local impacts from pollution sources. This approach provides spatially resolved ambient concentration estimates at the census block group level; this information can be input to human exposure models. This approach could serve as a good tool to assess the relative changes in local air quality from different pollution control measures.
- The Division is one of the few groups conducting research on improving the understanding of the impacts of traffic pollution on local air quality and exposures. Some of the laboratory and field measurements, including use of a mobile sampling platform for pollutant and air toxic measurements, conducted by the Division should help in developing better algorithms for and evaluating parameterizations of near-roadway dispersion models.
- The Division explored the use of the linked hybrid air quality and exposure modeling results as part of a feasibility study to assess public health impacts of emission reduction activities in New Haven, CT.
- EPA's meteorological wind tunnel is an important tool for examining near-road dispersion, and the Division has used that resource to examine flow and dispersion around roadways with different configurations (e.g., barriers, road cuts).

- Based on previous wind tunnel studies, the Division has developed an algorithm for inclusion into AERMOD for simulating the influence of depressed roadways.
- The Division has conducted significant research to assess various statistical methods to combine observed and modeled pollutant concentrations to provide improved air quality surfaces for use in exposure modeling and health studies. Currently, 5 summers of combined daily ozone surfaces are being used in exposure modeling, and 9 years of combined ozone surfaces are being used in an epidemiology study.

*Limitations*

- The AMAD has correctly identified the problem of few ambient observations to provide metrics of exposure in epidemiological studies. These sparse measurements fail to capture the large spatial variability in air pollutant concentrations found near roadways or major industrial sources. AMAD has developed an approach to use data obtained from air quality models coupled with high resolution data from local scale dispersion models and their research direction is focused towards improving this modeling approach. The one major limitation of this approach is that although the coupled model results are highly resolved, they cannot be assumed to be better than a single point measurement until the performance of the fine spatial scale model is assessed. Improving the algorithms in dispersion models (such as better simulation of near-roadway conditions) is worthwhile; however a more real problem that needs to be addressed is the lack of available fine-scale meteorological data when running these dispersion models and fine scale concentration measurements to assess the performance of the models. AMAD's future research aims to better evaluate the dispersion models by using data from special studies, but unless these models are evaluated when they are applied in new settings, their applicability will be questionable.
- It seems AMAD is also planning to use the hybrid approach to provide air quality data for use in epidemiological studies to determine relationships between air quality and health effects. There is a critical need to establish the adequacy of using model predicted air quality concentrations in epidemiological studies before using this technique for that purpose. Although it may fall outside the scope of AMAD, there should also be a focus on developing interpolation techniques to better estimate ambient air quality population-weighted exposure metrics when relatively higher numbers of measurements are available in an urban area. It would be instructive to compare the results of epidemiological studies obtained using interpolation of observed air quality data versus using the air quality data obtained from air quality models.
- It is not clear why AMAD has decided to use a regulatory model like AERMOD for linking with CMAQ to develop the hybrid modeling approach. There are other dispersion models in the public domain (such as SCICHEM) that could be good candidates for coupling with CMAQ. In fact, SCICHEM has already been interfaced with CMAQ by other researchers for simulating the short-term chemistry of power plant plumes.
- AMAD is also examining the effectiveness of regulatory actions by investigating the relationship among emissions reductions, air quality changes, and exposure. A more comprehensive approach to evaluate the effectiveness of regulatory actions would be to determine if the observed health effects have decreased over time and if those decreases

in adverse effects can be attributed to a reduction in exposure to pollutants controlled via various regulatory actions. AMAD may need to work with other divisions to fully evaluate these relationships.

*Future Directions*

- AMAD is planning to continue to improve the near-road component of AERMOD as part of the hybrid modeling approach. Improving the capabilities to simulate near-road concentrations is a worthwhile exercise, as health studies point to a relationship between health effects and pollution from traffic sources. A major part of this future work should focus on evaluating any new parameterizations that are developed for near-road treatment in AERMOD. Moreover, a guidance document should be developed that clearly delineates the conditions under which the hybrid approaches can be used with a high degree of confidence.
- AMAD is also planning to conduct further wind tunnel studies to examine additional roadway configurations and different atmospheric stability conditions. These studies should provide data that can be used to improve not only AERMOD, but other dispersion models as well.
- AMAD intends to conduct computational fluid dynamics modeling of near-road dispersion. This is an exciting area of research but it is also resource intensive, especially when a three-dimensional system with potentially complex geometry is used. Many two-dimensional systems have been developed in the past, but their applicability is rather limited
- AMAD is also planning to collaborate with other EPA laboratories and the FHWA on conducting field campaigns in different cities (Las Vegas, Detroit, and Raleigh) to better understand the relationship between traffic emissions and roadway-related air pollution concentration gradients. This is another worthwhile activity that should help advance the basic science in understanding the impact of traffic-related emissions on ambient concentrations at local scales.
- A future direction in this research theme is to investigate the ability to embed hybrid fine-scale modeling within the CMAQ grid structure. This is a very good idea provided that there is also a fine-scale emission inventory upwind of the area of interest to enhance the granularity of the model predictions. Nested models have been used by others and it would be a good idea to take advantage of insights and experience that are already available to speed up the effort.
- AMAD is planning to develop an approach for assessing the effectiveness of future regulations to include metrics (predictions of changes associated with promulgation of a rule) and indicators (actual levels of the same or closely related parameters observed during implementation) established *a priori*. This is certainly a worthwhile exercise and it is hoped that the Division will draw upon the latest NARSTO assessment on multi-pollutants and accountability.

*Suggestions for Improvement*

- There is a critical need to develop better techniques to provide high resolution data for exposure models and for epidemiological studies. AMAD is to be commended in its efforts to improve dispersion models by providing high resolution data at local scales. It is recommended that AMAD convene a workshop with experts from the health and exposure sciences and the air quality community to critically examine the approach selected by the Division and to consider alternative methodologies.

- Whatever approach is deemed appropriate, it is recommended that AMAD develop a guidance document on the use of these new approaches to link air quality and exposure models with an emphasis on the limitations of these approaches.
- AMAD should explore the use of other dispersion models or at a minimum describe the rationale for using AERMOD as the model of choice. Familiarity with the model should not be a sufficient criterion.
- To explore the interface of air quality models and exposure estimates, the Division could conduct a study where different metrics of exposure (derived from nearest measurements, interpolated concentration surfaces, and model simulations) are used to examine how epidemiological results may differ depending on the source of exposure data.

## *3C. Advice/Assistance*

- The Division's research under this theme directly addresses the agency's mission of protecting public health by examining the link between air quality and health. As mentioned earlier, the Division may need to expand its research scope to fully resolve the accountability issue.
- AMAD's research in improving the hybrid approach is leading to improvements in models like AERMOD that are used by other groups at EPA and beyond.
- The coupled urban/regional modeling system can be a good tool to assess the impact of various control measures by projecting future air quality and exposures at urban and local scales.
- Division scientists are active in the national and international scientific community and openly share their expertise and scientific products with other scientists and other government agencies. They serve on various national and international workgroups, professional societies, and editorial boards of scientific publications.
- Division scientists actively participate in various collaborations with other governmental agencies (state, local, tribal, and international) and various cross-disciplinary workgroups within the agency.

## *3D. Leadership*

- Division scientists are actively seeking leadership positions in various capacities at the national and international level. Senior staff of the division lead collaborative research efforts at different levels. Most of the scientists are active in scientific conferences/workshops in various capacities (conference chairs; session chairs; invited speakers).
- Many of the division scientists have received awards/honors for their scientific contributions.

- Division scientists play many leadership roles in leading research planning and coordination efforts across other divisions and labs within the agency. They participate as agency representatives in addressing major environmental issues at national and international levels.
- Division staff have received major agency awards for their contributions.

## *3E. Summary and Recommendations*

**Findings:**

- Overall, AMAD has identified a key gap in exposure modeling, i.e., the lack of high resolution spatial and temporal ambient data to use in exposure models and epidemiological studies. The approach selected by AMAD to address this issue relies heavily on model simulated data, however it remains to be seen how robust this approach may be in real applications.
- AMAD is advancing the science to better characterize near-road variability in pollutant concentrations. The basic research results obtained through field and laboratory measurements could be used to advance the algorithms in various dispersion models.
- AMAD's goal to address the issue of accountability is commendable, but it is very challenging to determine if a change in health effects is a result of changes in air quality or some other factors. A simple use of exposure models to determine the change in exposures may not be sufficient to answer the accountability question.

**Recommendations:**

- AMAD should explore convening a workshop with experts from health and exposure sciences and air quality community to critically examine the hybrid approach selected by the Division and to consider alternative methodologies. Different approaches may be appropriate for different needs.
- Whatever approach is deemed appropriate, it is recommended that AMAD develop a guidance document on the use of these new approaches to link air quality and exposure models with emphasis on limitations of these approaches.

# Theme 4. Climate Change and Air Quality Interactions

## *4A. Introduction*

Beginning in 2002, EPA initiated a significant effort to assess the impact of global change on future air quality. A number of extramural projects were funded via the EPA STAR grant program, while AMAD undertook a parallel effort within the agency. Results from a number of these studies, including the AMAD work, were integrated in an interim assessment report in 2007. Also in 2007, the focus on linkages between air quality and climate underwent a significant change when the Supreme Court ruled that EPA consider $CO_2$ as an air pollutant under the Clean Air Act. Subsequent events provided an injection of funds into AMAD, and the AMAD research direction has been modified to include investigation of feedbacks between air pollutants and regional climate. In this review, elements from the initial assessment and initial work addressing greenhouse gas (GHG) emissions and feedback on regional climate are addressed.

## *4B. Research*

To approach an assessment of the impact of global change on air quality, the agency held a workshop on the topic and used this as a starting point for the extramural grant program and for AMAD work. The general approach was to focus on comparisons between current conditions and projected conditions in the year 2050 and to apply a variety of modeling methods to conduct the assessment. Many of the individual groups employed output from global circulation and chemistry models to set meteorological and chemical boundary conditions for continental and regional scale simulations for current and future conditions. In most cases, the downscaling involved using MM5 to simulate current and future weather conditions, and a separate chemical transport model (such as CMAQ) to simulate current and future air quality conditions. Within AMAD, this approach was employed where the GISS II' global model output was used with MM5 and global chemical conditions were obtained from GEOS-Chem to provide BC for CMAQ simulations. Both were global runs for the IPCC A1B scenario.

In the second area of work, AMAD has initiated the linkage of WRF-CMAQ as a coupled, online system. This step was taken primarily to provide a tool to address questions related to feedback of aerosol pollutant levels on regional climate.

*Accomplishments and Strengths*

- The pilot project on climate downscaling has been completed. AMAD has focused on evaluation of the current regional climate and chemical transport simulations and comparing these with air quality under future weather conditions while keeping US emissions constant in all cases. This approach provides information about the effects of climate change upon air quality and avoids the uncertainties in the projected land use change and global or US pollutant emission changes. Thus, the strength of this approach is that it can provide relatively unambiguous information about climate change effects on air quality.

- A new WRF-CMAQ prototype has been developed and evaluated. Given the popularity of WRF-CHEM, the development of WRF-CMAQ is a welcome addition to the field and provides a second avenue for investigation of climate/aerosol feedbacks. There is a large CMAQ user community that has invested considerable resources in learning to use and helping to improve CMAQ. There is an extensive infrastructure associated with CMAQ in terms of emissions processing which is largely missing for WRF-CHEM. In addition, CMAQ has capabilities that are not readily available in WRF-CHEM in terms of chemical mechanism options, diagnostic modeling codes (process analysis, etc), and other features. Thus, it is understandable and desirable that WRF-CMAQ as a coupled system be developed and made available to the community.
- The climate change/air quality assessment team appears to have a good mix of expertise. The level of effort for the climate assessment with AMAD has been at a relatively low level, but this is magnified since it is part of the larger EPA extramural climate assessment program.
- The division has established good collaborations with global modeling groups in order to access the appropriate global modeling expertise and results. This will be a key advantage in terms of future work.

*Limitations*

- The AMAD group has served as one of the ensemble of EPA climate/air quality assessment groups, but AMAD is in a position to provide more leadership to promote greater collaboration and sharing of datasets, tools, and results among the extramural research groups.
- The development of WRF-CMAQ has not involved the community to any large extent, and the panel believes there would be benefits from greater community participation in this effort.
- So far, attention has been paid to the impact of temperature increase. The AMAD may also want to look into the impact of drought on the biosphere and its subsequent emissions and air quality. An increase in drought intensity and/or occurrence can also increase the incidents of forest fires and shorten the lifespan of trees. The resulting impacts on air quality are issues worthy of further investigation.
- If changes in future anthropogenic emissions are to be included in the climate-change study, it will be necessary to also consider the emission impact of changes in land use/land cover due to potential changes in agricultural practice and likely expansion of arable and marginal lands for renewable fuel production, and substantial shifts in emissions and emission sources due to the likely increased use of other clean fuels like low-carbon electricity, nuclear energy, and other factors.

*Future Directions*

- The group is well poised to continue to expand the work on downscaling of global change and investigation of the effects of global change on air quality. However, it will be important to strategically choose future simulations to create a small ensemble that covers the range of uncertainties in future projections. An important aspect will be the need to review the directions being pursued within the NCER grants program to fill gaps and to optimize the mix of modeling approaches. In this regard, the AMAD group could play a key coordination role among the NCER research projects.

- The investigation of alternative downscaling techniques coupled with the use of different advanced general circulation models, and completion of a series of downscaled climate simulations will provide a foundation for a wide range of global change impact investigations that go far beyond air quality. The AMAD group is in a position to partner with other EPA divisions and with outside groups to provide these simulations and expertise for applications related to water quality, human and ecosystem health, and other climate issues.
- Investigation of greenhouse-gas mitigation strategies is another arena of climate change where the AMAD group can play a large role. For example, what is the impact of biofuels on air quality and climate change or what is the impact of an all electric mobile fleet upon air quality and climate change? Also, as the role of methane is better recognized in transcontinental ozone formation, its emissions, both natural and anthropogenic, are in need of an in-depth study. These issues could provide a separate, but related area of investigation, which will require strategic decisions regarding resources.
- It would be very worthwhile to conduct parallel WRF-CMAQ and WRF-CHEM simulations for a range of conditions to help evaluate both systems and to provide both communities with some degree of confidence in these coupled systems. In this regard, special attention is needed to evaluate the coupled system to determine whether the coupling correctly treats aerosol feedbacks to the meteorology. Evaluation methods that go beyond the normal paired meteorological and air pollutant concentrations will be required, and these evaluations may require special field programs and datasets.

## *4C. Advice/Assistance*

The pilot project, establishment of partnerships with the global modeling community, and development of the WRF-CMAQ prototype are each very positive steps taken by AMAD in response to the agency need to address the interactions of climate change and air quality.

- The pilot project, together with the NCER grant results, can be formulated in a way to provide guidelines to regions and states about how to account for climate change effects for incorporation into control strategy planning. The interim assessment document is the first step in this process. An important aspect of this approach is the requirement that the regional downscaling of climate conditions be fully evaluated and essentially demonstrated as correct. AMAD found that for the global model employed, the regional climate simulations were biased to warmer temperatures and lower precipitation compared to current conditions. Further work using other global models and the WRF met model is needed to correct this deficiency.
- The AMAD results fit well within the overall climate and air quality research program and AMAD has helped advance our understanding of the impact of climate change on future air quality. Within the context of the larger collection of EPA funded projects, some groups followed a similar path of constant emissions, while others addressed the

effects of land use and emission changes. The net result is that information is now available that provides insight into the relative importance of climate change versus land use and emission changes. In addition, information is available that helps document the uncertainties associated with using different models, different model configurations, and different IPCC global scenarios.

- The AMAD research specifically targeted the climate effects portion of the assessment and results from this will be valuable for establishing guidelines and tools for regional and state planning with regard to climate effects.
- The AMAD provided data used in the current interim EPA assessment document; this is the primary product provided to states and regions from the AMAD climate assessment work.
- Development of WRF-CMAQ is a very positive contribution both in terms of linking the models in a way that addresses time step and mass consistency issues and in terms of providing a tool to investigate aerosol /climate interactions at the regional scale
- It does not appear that any more specific guidance or products have been developed for regional or state use. At the same time, it seems clear that agencies and states are beginning to ask how climate effects should be addressed. However, the timeline associated with these requests is usually aimed at 2020 or 2030 as opposed to 2050. A key question is whether the AMAD and the larger agency effort can be used to provide guidance for these shorter timelines. In addition, the regions and states are interested in results that address climate effects as well as changing atmospheric composition (background levels) over these same timelines. In this regard, how is AMAD connected to the EPA long range transport program? Collaboration with this group would be quite useful for addressing boundary conditions questions. Further work will be required to address these needs.

## *4D. Leadership*

- Within the climate change/air quality effort, AMAD scientists have made presentations at a number of national and international meetings, results have been published in the peer reviewed literature, and the scientists have been active as journal reviewers.
- AMAD scientists have played a significant role in all of the workshops and meetings associated with the agency climate change/air quality program. In addition, most of the staff are involved in a wide range of other agency activities and appear to participate in a number of different workgroups.
- As indicated above, the AMAD scientists have been involved in the agency climate change/air quality program which is the only national program addressing this topic. Staff serve on the CMAS external advisory board and have received agency awards for their work.
- Beyond these contributions, it is difficult to judge whether there is much involvement in other outside activities such as membership on societal committees. There is no evidence, positive or negative, for their role in providing guidance to state or local agencies or tribes.

## *4E. Summary and Recommendations*

**Findings:**

- Overall, the AMAD climate change/air quality research program fits well within the larger EPA program and AMAD scientists are making valuable contributions to our understanding of the effects of global change on air quality. These contributions are in line with the level of resources previously available and similar in scope to those from the extramural climate assessment grants.
- The research directly addresses Agency priorities and has the potential to provide valuable guidance to states and regions for air quality planning needs.

**Recommendations:**

- Guidance to the states is not yet available and feedback should be solicited, in collaboration with OAQPS, from the regions and states as to the type of information needed. There is currently a void in terms of how states and regions account for climate and global changes effects in air quality planning projects.
- Attention should be given in further downscaling simulations for documenting the range of results for potential land use and emission changes.

**Finding:**

- The development of WRF-CMAQ as a coupled system is a welcome addition for the CMAQ modeling community

**Recommendations:**

- Further work is warranted to complete the initial development of WRF-CMAQ and make it available to the community.
- Evaluation of the coupled system will require new thinking about how to evaluate the coupled aspect of the model and to demonstrate its utility. This should include some careful comparisons with WRF-CHEM simulations for a range of conditions.

**Finding:**

- The division has a good publication rate and in the area of global change, papers are beginning to appear in the literature.

**Recommendation:**

- Dissemination of these research results should continue to emphasize peer reviewed journals. Global change work would be very appropriate for high impact journals, including the Journal of Geophysical Research, Environmental Science and Technology, and Atmospheric Chemistry and Physics, and this is encouraged.

**Finding:**

- The AMAD scientists working in this area are all involved in a number of coordinated research projects outside of this effort and seem to contribute to agency workgroups across a range of topics. The scientists are active in terms of peer reviewed publications and presentations at a variety of technical meetings. There is less evidence for their role at the national or international level in terms of non-Agency organizations and programs.

**Recommendation:**

- As the Division extends its work to continental and hemispheric scales, new expertise should be added to the Division. Adding expertise and resources may be done in a variety of ways. For example, the Division may form new partnerships (e.g., with NASA on global change), or it might add new staff with targeted expertise, or it might provide significant professional development opportunities for existing staff.

# Theme 5. Linking Air Quality and Ecosystem Health

## 5A. Introduction

The research in this theme focuses on ecosystem exposure through wet and dry atmospheric deposition inputs as predicted by CMAQ and its meteorological driver model. The principal focus over the past several years has been on nitrogen and mercury. The work on nitrogen deposition has had a principal emphasis on deposition to estuarine ecosystems---first the Chesapeake Bay, and later Tampa Bay. The principal application for mercury deposition was in support of the Clean Air Mercury Rule. The inclusion of sea salt effects on dry deposition of nitrate, completed as part of the BRACE Tampa Bay study, was a key model development. Another model development that will greatly assist ecosystem effects work is the inclusion of bi-directional exchange of mercury and ammonia in the latest version of CMAQ. New directions for ecosystem work include greater emphasis on the issue of ecosystem acidification and development of the ability to better link CMAQ to watershed and ecosystem models through development of the Watershed Deposition Tool (WDT). This tool should encourage greater collaboration between AMAD scientists, CMAQ, and applied ecosystem modeling work such as critical loads studies.

## 5B. Research

*Accomplishments and Strengths*

- No current measurement networks account for all of the atmospheric deposition of nitrogen, which makes the CMAQ model an important ecosystem tool because it accounts for many unmeasured species.
- Assistance provided to the Chesapeake Bay and Tampa Bay Programs in terms of providing those groups with modeled nitrogen deposition estimates is to be commended and represents a significant accomplishment. AMAD scientists have a long and successful history of working with these programs, especially the Chesapeake Program. AMAD accomplishments and contributions were noted by two support letters from leaders of each of these estuary programs.
- The development of the Watershed Deposition Tool represents an important step in reaching out to watershed modelers in support of critical loads, TMDL, and acidification studies. The tool is an attempt to overcome the issue of applying gridded CMAQ output to the irregular grids used by various watershed and ecosystem models. It will be interesting to see how widely this tool is used in the future, and whether it helps to form a bridge between AMAD and terrestrial and aquatic scientists. The WDT is in an advanced beta test at the moment, and the program can be obtained by contacting a member of the AMAD staff. Follow through to make this an open source tool available through the AMAD web site or through CMAS is planned and is encouraged by the peer panel.
- The continued development of the CMAQ mercury model is noted. In addition to the bidirectional exchange of mercury, some updated chemical reactions have been added to

the model. The work on model inter-comparisons at the North American and global scales is important given our rapidly evolving knowledge of controls on the mercury cycle.

- Involvement by AMAD personnel in the Ad-Hoc Critical Loads Subcommittee (CLAD) of the National Atmospheric Deposition Program is commendable and provides a good link to investigators doing critical loads studies. CLAD provides a good forum for AMAD to feature CMAQ capability to support critical loads studies as well as an opportunity to identify potential collaborators and new users of CMAQ.

*Limitations*

- Some limitations in applying CMAQ to critical loads studies were noted, including the current inability to simulate base cation deposition in CMAQ. This limitation was discussed with AMAD staff at the review, and limitations with natural dust emissions in the current emissions inventory were noted. Plans call for updates that may allow base cation deposition to be modeled in the future. There are also some limitations in applying CMAQ at many of the long-term watershed study sites such as those in the EPA LTM/TIME program where critical loads estimates are needed. Many of these sites have watersheds that drain only a few square kilometers, whereas CMAQ national domain simulations use either a 36 km or 12 km grid-cell size. This limitation was discussed with AMAD staff at the review, and an ability to simulate at the 4 km grid scale was noted as well as early attempts to utilize orographic precipitation databases such as PRISM. An ability to simulate orographic precipitation enhancement at as fine a spatial scale as possible, would vastly improve the ability to apply CMAQ to critical loads studies at many long-term sites where data are available.
- The panel noted the curious lack of any modeling efforts related to ozone effects on terrestrial ecosystems. This seems to be a result of a decision by the EPA Ecological Research Program to focus on aquatic rather than terrestrial resources as stated on page 3-17 of the Peer Review Support Document. This criticism applies equally to the acidification issue as well because recovery of aquatic biota, while strictly an aquatic problem, depends on recovery within terrestrial ecosystem compartments such as the soil.
- The inability of the CMAQ model to account for the deposition of organic nitrogen is recognized, and was discussed with pertinent staff at the review. Current scientific knowledge does not seem to allow accurate modeling of organic nitrogen deposition, but this area should be monitored for possible inclusion in future versions of CMAQ.

*Suggestions for Improvement*

- Incorporate base cation deposition into CMAQ once emissions inventory updates and modeling of wind-blown dust allow reliable estimates.
- Continue improving ability to link CMAQ with watershed studies, TMDL studies, and critical loads studies by further reducing spatial scale for modeling and further exploring ability to simulate enhancement of wet deposition through orographic effects.
- Include consideration of ozone deposition results in tandem with other deposition studies.
- Continue adding new or updated reactions of mercury chemistry, including the halogen reactions, as our knowledge in that area is improving.

## 5C. Advice/Assistance

- This group has done an admirable job advising EPA on likely outcomes of CAIR and CAMR.
- AMAD has been successful in helping to stimulate the development of a nascent effort within the National Atmospheric Deposition Program to measure ammonia using passive sample collection techniques. This information will not only help improve ammonia deposition modeling within CMAQ, but will help to close the gap in terms of unmeasured nitrogen deposition species.
- One can argue that the Agency failed to adequately foresee that the Acid Rain Program within the Clean Air Act Amendments of 1990 would not stimulate widespread ecosystem recovery in many impacted areas. We are not certain of the role AMAD may have played in this process, but it is clear that ecosystem compartments such as soils were not adequately considered (e.g., calcium depletion), and the time lags involved in migration of biota to extirpated locations may not have been fully considered within EPA. This possible oversight appears to now be the topic of some concern as evidenced by what appears to be a commitment to use CMAQ to address critical ecosystem loads, and to make the model easily available to others with similar interests.
- AMAD modelers appear to have used the model to describe to the Agency the unintended consequences of clean air legislation such as the effects of reducing sulfur dioxide emissions on increasing ammonium deposition based on the representation of atmospheric chemistry in the model.

## 5D. Leadership

- The staff generally publishes at a good rate in the peer-reviewed literature, is actively involved in national and international collaborative research efforts, and is active in working committees within professional societies and with other groups. Overall, the staff appears to be leaders among their scientific peers and within EPA.
- Several of the AMAD staff who work on ecosystems effects studies have received various awards from EPA such as the Bronze Medal. The awarding of these medals points to the leadership role of these modelers within the Agency.
- Participation in international and continental mercury model comparisons efforts is noteworthy, and will help in further refining the CMAQ mercury model.
- Involvement and activities within the Chesapeake and Tampa Bay Programs has established AMAD's leadership role in use of CMAQ to model the role of atmospheric N deposition in estuarine nitrogen budgets. It appears that the model is being used by estuarine programs in Connecticut and other locations.

## 5E. Summary and Recommendations

**Findings:**

- Although the ecosystem work represents a small part of the overall effort within AMAD, this work is important in developing links to the ecosystem/watershed research community, supporting EPA policy efforts such as CAIR, and further expanding the CMAQ user community.
- Development of the Watershed Deposition Tool represents a positive step by providing an opportunity for ecosystem and watershed modelers to more easily use CMAQ output in their models.
- Future climate change work within EPA may present opportunities for the ecosystem effects modeling group within AMAD.
- The CMAQ mercury deposition model successfully informed EPA about the expected effects of CAMR on mercury deposition.
- Mercury modeling with CMAQ in support of CAMR highlights the likely limited benefit and limited geographic area where improvements in mercury bioaccumulation would be expected. These results highlight the global nature of the mercury problem.

**Recommendations:**

- AMAD should continue to support ecosystem effects work utilizing CMAQ.
- Continued development of the Watershed Deposition Tool is encouraged. Future developments should consider a process to further reduce the grid scale size of output so that the model can more easily be applied to small watersheds, and incorporation of orographic precipitation effects which greatly influence deposition in complex terrain. Continued development of the Tool should further enlarge the CMAQ modeling community and highlight the usefulness of CMAQ as an ecosystem effects/watershed modeling tool.
- Depending on the direction of future climate change research within EPA, opportunities may arise to link AMAD work with ecosystem change studies. This type of work would provide another avenue (in addition to the climate change – air pollutant effects work) through which CMAQ could prove to be a useful scientific tool. This direction is encouraged if available future funds allow.
- Continued development of the CMAQ mercury model is encouraged. Since mercury science is at a fairly early stage of development, new reactions and rates are likely to appear often, and this new knowledge and information should be incorporated into the mercury model on a regular basis. The recent rejection of CAMR by the court further highlights the need to support the CMAQ mercury model by continued updating in anticipation of likely future mercury policy explorations within EPA.
- An increasing body of scientific information suggests strong links between mercury and sulfur deposition in predicting levels of methyl mercury in fish. Future explorations of the mutual roles of mercury and sulfur deposition in mercury bioaccumulation within ecosystems is encouraged. Development of combined sulfur and mercury deposition modeling scenarios using CMAQ would allow researchers a means to test hypotheses about how strongly sulfur deposition affects mercury bioaccumulation.

- Continued mercury model intercomparisons with CMAQ and other leading models are encouraged with an aim of further refining the temporal and spatial scales from emissions to deposition. Such comparisons will help to better bound the geographic range of sources of mercury deposition to ecosystems within the US.

# Acronyms

| | |
|---|---|
| ACM2 | Asymmetric Convective Model version 2 |
| AMS | American Meteorological Society |
| AMAD | Atmospheric Modeling and Analysis Division |
| AMET | Atmospheric Model Evaluation Tool |
| AQ | Air Quality |
| AQAD | Air Quality Assessment Division |
| AQFM | Air Quality Forecast Model |
| AQME | Air Quality Model Evaluation |
| BEIS | Biogenic Emissions Inventory System |
| BENMAP | Environmental Benefits Mapping and Analysis Program |
| BRACE | Bay Regional Air Chemistry Experiment |
| CAIR | Clean Air Interstate Rule |
| CAMR | Clean Air Mercury Rule |
| CB | Carbon Bond (chemical mechanism) |
| CCTM | CMAQ Chemical Transport Model |
| CIRAQ | Climate Impact on Regional Air Quality |
| CLAD | Critical Loads Ad-Hoc Subcommittee of the National Atmospheric Deposition Program |
| CMAQ | Community Multi-scale Air Quality (model) |
| CMAQ-CA | CMAQ-Carbon Apportionment |
| CMAQ-ST | CMAQ-Sulfur Tracking |
| CMAS | Community Modeling and Analysis System |
| DDM | Decoupled Direct Method |
| DMS | Dimethyl sulfide |
| EPA | Environmental Protection Agency |
| FDDA | Four dimensional data assimilation |
| FHWA | Federal Highway Administration |
| GEOS | Goddard Earth Observing System |
| GHG | Greenhouse Gas |
| GISS | Goddard Institute for Space Studies |
| ICARTT | International Consortium for Atmospheric Research on Transport and Transformation |
| IPCC | Intergovernmental Panel on Climate Change |
| ISORROPIA | not an acronym – meaning is “equilibrium” in Greek |
| MEGAN | Model of Emissions of Gases and Aerosols from Nature |
| MM5 | Mesoscale Meteorological Model (version 5) |
| NAAQS | National Ambient Air Quality Standard |
| NAQFS | Nationwide Air Quality Forecast System |
| NASA | National Aeronautics and Space Administration |
| NCLD | National Land Cover Dataset |
| NEAQS | Northeast Air Quality Study |
| NEOPS | Northeast Oxidant and Particle Study |
| NERL | National Exposure Research Laboratory |

| | |
|---|---|
| NOAA | National Oceanic and Atmospheric Administration |
| NMM | NCEP Meteorological Model |
| OAQPS | Office of Air Quality Planning and Standards |
| ORD | Office of Research and Development |
| PinG | Plume in Grid |
| PM | Particulate Matter |
| PRISM | Parameter-elevation Regressions on Independent Slopes Model |
| PBL | Planetary Boundary Layer |
| RADM | Regional Acid Deposition Model |
| RPO | Regional Planning Organization |
| SAPRC | State-wide Air Pollution Research Center (chemical mechanism) |
| SEARCH | Southeastern Aerosol Research and Characterization Study |
| SMOKE | Sparse Matrix Operational Kernel Emissions |
| SOA | Secondary Organic Aerosol |
| TexAQS | Texas Air Quality Study |
| TMDL | Total Maximum Daily Load |
| VOC | Volatile Organic Compounds |
| WDT | Watershed Deposition Tool |
| WRF | Weather Research and Forecasting |
| WRF-CHEM | Weather Research and Forecast model coupled with Chemistry |
| WRF-CMAQ | Weather Research and Forecast model with coupled online CMAQ |