Final Report:
Second Peer Review of the CMAQ Model

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1. INTRODUCTION

The CMAQ Model External Peer Review Panel that conducted its review in May 2005 provides this review report, a follow-on to the report of the first CMAQ Model External Peer Review Panel (Amar et al., 2004). While this review had a mandated focus on particulate matter, mercury and air toxics modeling aspects of the Community Multiscale Air Quality (CMAQ) modeling program, the review panel addressed all aspects of the program in order to assess the current state of the model, to guide its development in the short term, and to assess the appropriateness of resources (institutional support, staffing, and operational funding) in the long term to achieve desired advances. The mission of Environmental Protection Agency's (EPA) program in air quality modeling within the Atmospheric Modeling Division (AMD) of the National Exposure Research Laboratory (NERL) to facilitate transition from research-grade air quality models to operational tools for policy and regulatory analysis was a defining context of the review. The review panel focussed its attention on the current community version of CMAQ, version 4.4, which was released in October 2004.

The report is written from the range of perspectives represented by the seven-member review panel: Praveen Amar, David Chock, Alan Hansen, Michael Moran, Armistead (Ted) Russell, Douw Steyn, and William Stockwell. Panel members read a considerable volume of material on CMAQ provided by EPA, and attended a day and a half of presentations on CMAQ by NOAA/EPA staff (see Appendix for meeting agenda).
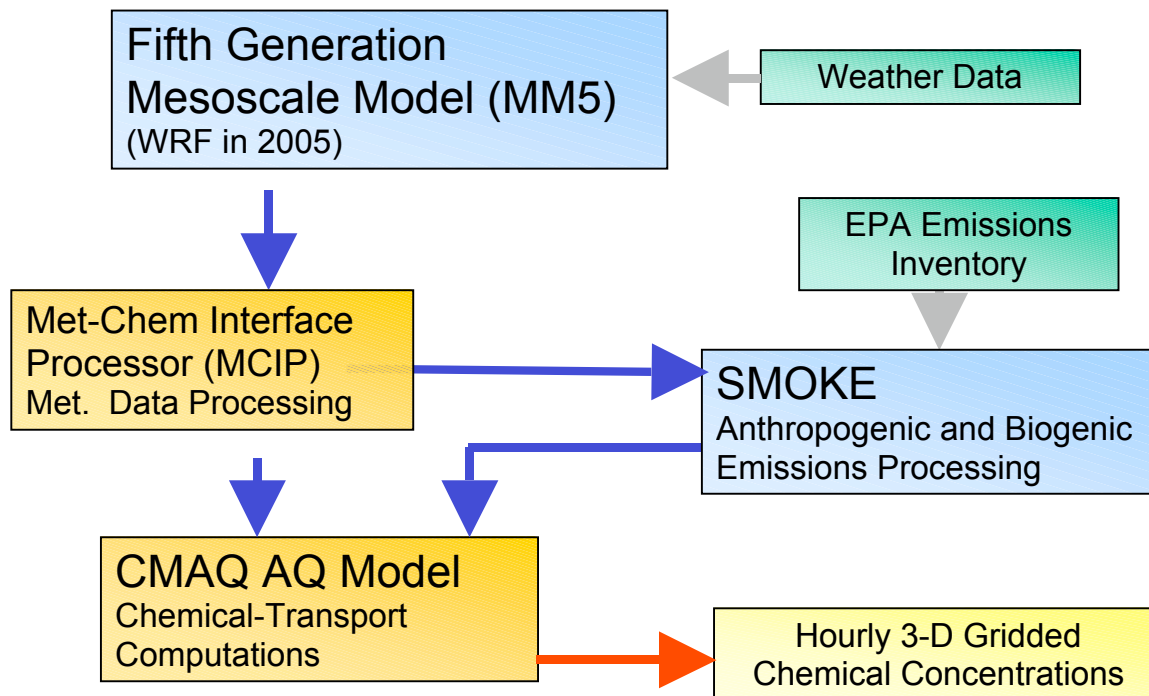
The review panel addressed a set of charges that are described in detail in this report. Among the charges was a request that we assess the effectiveness of resource utilization in relation to the direction and quality of research and model development conducted by the CMAQ modeling program. In the absence of a detailed analysis of available financial resources, this assessment is limited to a consideration of the work done by the complement of 28 staff scientists with AMD, including postdoctoral researchers.

CMAQ is a modeling system that simulates a wide range of physical, chemical and biological processes (see figure below). Some of these processes are well understood, some reasonably well understood, and some only poorly understood. This wide range in the level of knowledge about the processes being modeled, and the fact that uncertainties in characterizing some of the processes correspond to areas of active research worldwide, means that some parts of the model code are sufficiently well established as to be considered fixed, while other parts of the code are under continuing development. Because CMAQ is both a research model and a regulatory tool for the evaluation of alternative control strategies, two versions of the code exist at all times: a currently active, reasonably stable version of CMAQ that is used in an operational and regulatory applications mode, and, in parallel, a developmental version of CMAQ that is continually being improved by the AMD's CMAQ development team and by researchers outside the EPA. From time to time, the developmental version replaces the operational version, thus bringing recent advances in atmospheric science and computational efficiency to the operational realm.

For this reason, the review panel focused largely on the operational version of CMAQ, but also paid attention to how AMD transfers research-grade air quality modeling techniques into operational tools. While we reviewed the state-of-science in the CMAQ model, we did so

recognizing that CMAQ is primarily a model for operational applications and assessments. We have attempted to balance the demand for scientific completeness and rigor in the model with the need for computational efficiency as demanded of an operational model. Nonetheless, we realize that the operational version of CMAQ is also used as a research tool in many contexts. This makes the research community another important, though not the primary customer, necessarily introducing a degree of tension into our considerations.

CMAQ Modeling System

Fifth Generation Mesoscale Model (MM5) (WRF in 2005)	←	Weather Data

| Met-Chem Interface Processor (MCIP) Met. Data Processing | → | SMOKE Anthropogenic and Biogenic Emissions Processing |

EPA Emissions Inventory

| CMAQ AQ Model Chemical-Transport Computations | → | Hourly 3-D Gridded Chemical Concentrations |

(Source: Presentation to Peer Review Panel by Shawn Roselle, May 2005)

2. DEVELOPMENTS SINCE FIRST EXTERNAL PEER REVIEW (DECEMBER 2003)

The review panel is both delighted and highly impressed by the depth and comprehensiveness of AMD's response to recommendations contained in the first peer review report (Amar et al., 2004). It is our sense that CMAQ, as an operational tool, has matured and improved markedly over the past year. A few salient features of the CMAQ modeling team's efforts since the first review include the following:

- The team has managed to strike an appropriate balance between pursuing their main mission in urban/regional modeling and positioning themselves to move into the newly emerging areas of fine-scale and global-scale modeling. The prudence with which they are approaching these developments is applauded. Also admirable is their clear understanding of

the importance that they be well positioned to take advantage of developments in modeling at both finer- and coarser scales.

- AMD is working with NOAA in the area of operational air-quality forecasting, and with NCAR on ongoing research efforts on WRF and WRF-Chem. A major effort by AMD brought the Eta-CMAQ forecast system into the National Weather Service operational realm in September 2004 (for daily ozone forecast guidance in northeast U.S.) We encourage the current work on Eta-CMAQ to expand the forecast domain and to add PM2.5 forecasting capability.

- The modeling team has been very successful in striking an appropriate balance between the competing demands of scientific rigor and operational utility. This balance has been struck while continuing to work on model development on a number of fronts.

- The commitment of AMD to model evaluation is admirable. The development of AMET, and the associated model evaluation toolkit is seen as recognition of the importance of model evaluation, and its planned inclusion in future distributed versions of CMAQ will provide strong guidance to users of these versions. The conduct of annual $PM_{2.5}$ simulations is an important part of overall model evaluation process and should continue to be pursued vigorously.

- We note that AMD has actively worked with PSU and NCAR to ensure that nudging capability exists in WRF, and with NCAR to implement nesting in WRF. We understand that the AMD effort was essential to ensure that these developments are available in WRF.

- We applaud AMD's strategically astute move to build CMAQ along two parallel development tracks: namely, a community version in multiple configurations designed for retrospective modeling for policy and research with annual public releases via CMAS and an air quality forecast version in a single optimized configuration for operational ozone and PM forecasts, integrated with NCEP's weather forecast system. The distinct purposes and configurations of these two versions makes this a powerful strategy.

- We are encouraged by AMD's successful efforts in substantially increasing the computational efficiency of CMAQ, making practical annual simulations of PM2.5 for the continental US. This development alone will encourage the use of CMAQ by the regulatory community to support State Implementation Planning (SIP) and regional haze assessments.

- We applaud the efforts of AMD to build the community of model developers (through maintenance of AMD staff and postdoctoral research fellows, in spite of budgetary pressures) and model testers (in states, RPOs, and the CMAS center).

3. SPECIFIC RECOMMENDATIONS OF FIRST PEER REVIEW PANEL AND AMD RESPONSES

On the first morning of the review meeting, Dr. Ken Schere of AMD presented the following responses to the recommendations of the first External Peer Review Panel (convened in December 2003):

- *Remain focused on main mission ... urban/regional modeling of PM and ozone*
  - Response: This remains the principal focus (especially PM; ozone support is diminishing).

- *Fine-scale and global-scale modeling research should not distract from main mission*
  - Response: These are relatively new emerging areas for AMD research. Support is growing for them, while it is steady or diminishing in traditional areas. Still, they will not obscure the main mission of urban/regional modeling.

- *Air quality forecasting efforts should be coordinated with NOAA and NCAR*
  - Response: This is being done. Major efforts with NOAA on operational forecasting; research efforts on-going with NCAR on WRF and WRF-Chem

- *Enhancing the chemical and dynamical aspects of PM modeling in CMAQ should be a top priority*
  - Response: This is first priority. Need to balance scientific detail with operational utility. We are working on numerous model development and evaluation fronts.

- *Evaluate emissions using inverse modeling*
  - Response: We are making use of inverse, receptor, and source apportionment modeling to help evaluate and improve emissions estimates. We will be adding EC to inverse modeling activities in the near future to supplement our on-going work with NH_3, which started in 2000.

- *Investigate range of scales over which the model (CMAQ) can legitimately be applied.*
  - Response: New investigative areas at fine urban and coarse hemispheric scales will start to explore this. Limits of physical process parameterizations will constrain fine resolution to ~1 km. Larger space and time scales are possible but demand consideration of different or additional processes (e.g., free-tropospheric chemistry and long-lived species, strat/trop exchange mechanisms, inter-hemisphere exchange, oceanic influence, global emissions).

- *Operational evaluation should be expanded into diagnostic/mechanistic/probabilistic evaluations; a guideline for PM evaluation should be published by EPA.*
    - Response: AMD is committed to carrying out both operational evaluations (annual simulations) as well as diagnostic evaluations (focused on field-study periods). Examples from CMAQ model evaluation will be part of the 2005 release package. Operational and diagnostic model evaluation guidance will follow over next two years. A model evaluation "Toolkit" is in development, beginning with meteorological model evaluation (AMET).

- *Should move cautiously down to scale of urban canyons*
    - Response: Agreed; we are exploring this scale with other modeling techniques, including CFD, LES, and Gaussian models. Urban "hot-spot" analyses may include hybrid of CMAQ and local model.

- *EPA should resist pressures to implement nesting in WRF model; EPA should not be responsible for implementing "nudging" FDDA in WRF.*
    - Response: NCAR has implemented nesting into WRF (not EPA). We are supporting and working with Penn State and NCAR to implement nudging into WRF (a "must-have" for air quality applications.

- *EPA, NOAA, and NCAR should work together to develop a real-time version of CMAQ for forecasting.*
    - Response: This is a major on-going activity. A two-year effort culminated in the Eta-CMAQ forecast system becoming fully operational at the National Weather Service in September 2004, for daily ozone forecast guidance in the northeast U.S. Current work is expanding the forecast domain to the continental U.S. and adding $PM_{2.5}$.

- *Ensure sufficient research-level staff to support needed PM modeling efforts.*
    - Response: Retirements of key experienced personnel have been a challenge. We are utilizing EPA post-docs and NOAA-supported contractor positions to help fill gaps. Permanent positions will be filled as resources become available.

- *CMAQ model development team should increase its number of post-doctoral researchers.*
    - Response: Agreed; we currently have 3 EPA post-docs working on CMAQ model development and evaluation, and we will add another next month. We will continue to add post-docs as funding permits.

- *Develop group of beta-testers for research and pre-release versions of CMAQ model code.*
    - Response: We heavily rely on modelers in EPA/OAQPS to test our codes, and are developing beta testers in the community as well (e.g., states,

RPOs, CMAS center). MCIP has a large group of beta testers; we are working to expand the list for CMAQ.

- *Improve acknowledgements for contributions from non-EPA developers and beta testers.*
  - Response: Agree that this area needs improvement. We are working with CMAS center outreach group for more deliberate and public acknowledgements for community contributions.

- *Build collaborative links with non-EPA researchers, e.g., through focused workshops or conferences.*
  - Response: This is a good idea. We are working closely with some of the EPA STAR program grantees that are using CMAQ for development and applications research. Annual CMAS/CMAQ Workshop is helpful also. We need to do more here.

- *Recommend a scientific review of CMAQ be undertaken every two years.*
  - Response: Our goal is to convene a peer-review panel every year, with some years devoted to focused themes, and other years devoted to an overview of the complete system.

- *CMAQ team should work on MM5 (WRF) improvements that do not duplicate efforts of meteorological community.*
  - Response: Agreed. Our efforts focus only on those areas that are most important to air quality, and may not be high priorities of the meteorological community, such as PBL parameterizations, land-use and land-surface effects, and nudging FDDA.

- *CMAS must have sufficient public and private resources to offer training, workshops, etc.*
  - Response: Agreed. CMAS center offers the user community services that a government research organization is not well suited to perform.

4. COMPARISON WITH OTHER U.S. AND INTERNATIONAL PROGRAMS

Based on our national and international experience, the review panel believes that AMD is a world leader in its mission to develop research-grade air quality models and transition them to operational tools for use in policy and regulatory analysis. In making this judgment, we have considered other current regional air-quality modeling efforts in the U.S., Canada, Europe, and Japan, including MAQSIP, PM-CAMx, REMSAD, WRF-Chem, STEM-2K3, AURAMS, the Unified EMEP model, EURAD, and LOTOS. The following characteristics of CMAQ and its development and user communities place CMAQ ahead of comparable models:

- CMAQ is a state-of-the-science air quality model for regulatory applications.

- The CMAQ community has developed research versions that are state-of-the-science as well. Some of these developments are diffusing into the more widely used assessment and regulatory versions of the model.

- CMAQ represents a more balanced mix of science than other comparable models because it does not represent individual research projects, but rather is based on a conscious analysis of what type and level of science and numerical implementation is optimal in an integrated air quality model.

- CMAQ is rather unusual in that it is built in a coordinated national program (Canada has a similar program). By contrast, the EU has a variety of models being developed in and by various countries, and within those countries there are often competing efforts at various institutions, none of which are being conducted in a community approach. Part of this is driven by the unique mission of CMAQ, which is to be a regulatory/policy tool for use by a number of stakeholders, and that regulatory applications in the U.S are based on specific "demonstration of attainment" requirements of the SIP process.

- CMAQ is better documented and more readily used than virtually any other air quality model, including those being developed by other national programs.

- There is an active community helping with the model development, debugging, and wider use. CMAQ benefits from active participation by the user community through the third-party CMAS center.

Operational tools for use in policy and regulatory applications must be comprehensive, realistic, and balanced. That is, they must address all significant atmospheric and surface processes affecting air quality, they must be based on realistic and detailed meteorological and emissions data, and they must balance scientific rigor and completeness with acceptable computational cost. CMAQ meets these characteristics better than other comparable models. Of course, some of these other models also possess features that could be of benefit to future versions of CMAQ.

While air-quality models have traditionally lagged behind weather forecast models in the operational arena, CMAQ can legitimately aspire to join the many operational weather forecast models in terms of reliability, accuracy, comprehensiveness, and utility.

5. PANEL'S RESPONSE TO CHARGE QUESTIONS

Charge Question 1:

What is the overall quality of the applied scientific research in the CMAQ Modeling Program?

The CMAQ modeling system is a comprehensive, state-of-the-science tool for policy applications and it continues to improve with each release. The review panel was asked to review scientific research related to the modeling of fine particulate matter ($PM_{2.5}$), mercury, and

air toxics. The panel was very impressed by the quality of the presentations, which showcased the high competency of the researchers (see Appendix for meeting agenda). The prioritization of the research is also sensible and responsive to the needs at hand.

Presentations at the peer review meeting were made on CMAQ model system physics, including clouds, radiation, planetary boundary layer dynamics, dry deposition, and photolysis. The presentations on the meteorological research component included the future transition to WRF as the meteorological driver for CMAQ, the incorporation of Pleim-Xiu land surface model into WRF, the use of FDDA nudging in WRF, the comparison of MM5 using FDDA with WRF-EM, the status of MCIP, and the development of an automated tool (AMET) for evaluating the performance of a meteorological model.

The presentations on the CMAQ particulate matter research included discussions on increasing the computational efficiency of treating coagulation and secondary organic aerosols, the addition of sea salt, eliminating one source of numerical instability in ISORROPIA thermodynamics, addition of tracking tools for sulfate and carbon and adding the contribution of wildfires. Future plans were presented, including further reducing numerical instabilities in ISORROPIA, comparing it with Clegg's AIM treating thermodynamics at low relative humidities, implementing a ternary nucleation module, adding coarse-mode chemistry, adding a tool for apportioning coarse "other" to sources, adding a sectional approach to particle dynamics, and adding a capability for representing an external mixture of size modes based on different sources. An additional presentation described sectional approaches in CMAQ developed by others, including CMAQ-MADRID and CMAQ-UCD. Several presentations were made on evaluating various aspects of PM representation in CMAQ, including the diagnostic evaluation of carbonaceous aerosol and inorganic aerosol representations. An inverse application of CMAQ for assessing ammonia emissions was also described.

Presentations also discussed the treatment of mercury in CMAQ, including added Hg-specific chemistry and physics and the results of evaluations. Modifications of CMAQ to treat a number of air toxics in CMAQ were presented. One example was the combining of results from local-scale dispersion models with regional-scale CMAQ results to estimate ambient exposures at the census-tract level; another was the use of embedded fine-grid results within coarse grids to estimate probability density functions for ambient exposures.

We are very impressed by the overall quality of the applied scientific research in the CMAQ modeling program, in terms of the breadth of coverage and the quality of the scientific staff. The current (and expanded) use of post-doctoral positions is having a very positive impact on the CMAQ program, and its continuation should be encouraged. This has significantly improved the level of science in CMAQ and its applications.

The program is quite broad, from atmospheric physics to homogeneous and heterogeneous chemistry, from ozone to PM, air toxics, and mercury, from local to regional spatial scales, and from hourly to annual temporal scales. AMD staff maintain awareness of current developments elsewhere in their fields of specialization and this contributes to their own high-quality research. In many instances the researchers have established formal or informal collaborations with outside scientists and engineers that help to leverage their own resources and to broaden their

perspectives by exposing them to diverse ideas, approaches, and applications.

AMD staff understand their clients' needs, and are trying to respond in a timely and scientifically sound fashion. They should expand their view of their clients to include the states, and interact more directly with the state and RPO modelers. AMD needs to find other parallel and direct channels to sophisticated parts of the regulatory community (California, Texas, New York, Northeast, LADCO and other RPOs, etc.). One specific recommendation is for them to participate in meetings of the regulatory modeling community (e.g., RPOs' modeling meetings) to get first-hand knowledge of how models are being applied and evaluated by these groups. This would actually serve OAQPS as well. One gets the feeling that AMD staff interact solely with OAQPS and look to OAQPS to interact with the states. This could delay response to states' needs and dilutes the information that is transmitted from them.

Increased interaction between AMD staff and clients at all levels could be facilitated by CMAS. CMAS has proven to be an integral aspect of the evolution of CMAQ and it has been instrumental in improving the utility of CMAQ to the regulatory and scientific community. The Models-3 list server is a tremendous benefit to the community. The annual CMAS conference has been very successful for widening the use of CMAQ and for discussions of its capabilities and limitations.

Charge Question 2:

What are the strengths and weaknesses of the science being used within the components of the CMAQ Model development program?

CMAQ, as part of the Models-3 system, represents the state-of-the-science of widely used models, particularly those used in a regulatory context. This is not to say that each scientific component reflects the most recent research in that particular area, nor should it, as there should be a thoughtful delay to allow the scientific community to reach a level of consensus on how to best simulate processes. Further, the user community has specific operational modeling needs that may not be met by a model having the most complete science. As a particular example, the user community, including OAQPS, the states, and many research teams, cannot tolerate the significantly increased computational costs that would result from having a large number of aerosol sections or from using source-oriented, external-mixture representations of aerosols. Further, our understanding of SOA (Secondary Organic Aerosol) formation is still evolving relatively rapidly, and numerical description and treatment of SOA formation should probably evolve at a measured pace to avoid following many false leads. AMD staff should continue to assess what has been done and is being done in this area, and make a scientific judgment as to how to proceed. They have been making significant headway in terms of improving computational efficiency, which the community needs.

Specific strengths of the science in CMAQ include, but are not limited to, the following:
- A relatively convenient coupling to a widely-used meteorological model (MM5), allowing more direct use of the physical details from the meteorological model;
- A one-atmosphere modeling approach that already treats ozone, PM, and acid deposition in significant detail, and the next (Sept. 2005) release of CMAQ will add a number of air toxics, including mercury, to this unified modeling framework;

- Comprehensiveness: almost all significant processes affecting ozone, PM, acid deposition, and many air toxics are represented;
- Computational efficiency: CMAQ is fast enough to permit longer simulation and evaluation periods;
- Flexibility: a number of processes (e.g., gas-phase chemistry, advection) have more than one parameterization available;
- Ability to treat a variety of scales and being relatively easy to allow use of nested grids;
- Inclusion of a plume-in-grid capability; and
- Extensive use and testing of the model's various science modules.

Specific weaknesses of the science in CMAQ that should be addressed include:
- Heterogeneous chemistry of N_2O_5;
- Limited description of the aerosol size distribution using a modal approach with only three modes;
- No physical or chemical interaction between gases and the coarse mode;
- Lack of treatment of the effects of meteorology on fugitive dust emissions (similar to how CMAQ deals with sea salt);
- Re-emissions of volatile and semi-volatile compounds such as mercury and some other air toxics are not yet addressed;
- Source apportionment tools (particularly for non-linear, secondary PM production);
- SOA chemistry;
- Subgrid-scale (SGS) vertical transport in deep convection (current treatment is simplistic and inconsistent with treatment of deep convection in MM5);
- Inconsistency between treatment of vegetation phenology in dry deposition module and BEIS3;
- Weak measurement base for evaluation of the CMAQ-Hg, especially air concentrations and dry deposition of Hg; and
- Weak and inconsistent coupling with global chemical transport models.

Little was presented in terms of how the PinG capabilities are evolving, and it appears as though this option is not being used as often as might be expected. Such a capability might become important when doing more detailed studies of mercury (e.g., assessing mercury chemistry in a concentrated plume), and it would be valuable to gain more experience now rather than waiting. The PinG PM capabilities should be assessed, and consideration should be given to how to make this an attractive component for wider use.

The Panel recognizes that for a number of the areas identified as weaknesses, a strong scientific foundation may still be lacking. In these cases the science should be allowed to mature before changes are made in CMAQ.

While not part of the "science in CMAQ", there are some related issues dealing with emissions that should be addressed. One is that the characterization of chemical composition and size distribution of primary PM emissions is weak (possibly the pending release of SPECIATE3.4 may help). A second is the need to better treat criteria, air toxic, and mercury emissions from wildfires. A third is that SMOKE is probably the weakest link in the Models-3 suite. It is the most cumbersome to use, and the documentation is less detailed than that for CMAQ. One of us

(AGR) has also experienced some strange results in that removing a source has led to increases in predicted concentrations of some species. A fourth issue is the need for a better temporal treatment of emissions and increased ease with using non-default activity patterns. It is felt that many of the current weaknesses in using CMAQ (and air quality models in general) are due to weaknesses in the emission inputs.

Charge Question 3:

What is the quality and relevance of the model applications and evaluations being conducted as part of the CMAQ Modeling Program?

AMD staff are very aware of the need to conduct both routine as well as diagnostic model evaluations and have been taking this aspect of model development seriously. Significant resources have been assigned by AMD to the evaluation of CMAQ performance, and we find the model applications and evaluations being conducted to be relevant and of high quality. In many ways, they are now limited by the lack of sufficient observational data rather than by their ingenuity.

Given the requirements for long-term model runs related to the annual $PM_{2.5}$ standard and the planned thrust towards all-year PM operational forecasting, the operational evaluation of CMAQ for all seasons is an important step forward, and the different results for different PM chemical components provide insight into some model strengths and weaknesses. CMAQ participation in various model intercomparisons is very valuable: these include the summer 2004 ICARTT real-time model intercomparison organized by NOAA-Boulder, the MSC-E series of Hg-model intercomparisons in Europe, and the ongoing Hg-model intercomparison for North America. The various diagnostic studies undertaken to date are very relevant, including those for inorganic PM species, for carbonaceous PM component, and for seasonal variations in ammonia emissions. Noteworthy was the use of the unusually comprehensive SEARCH data for diagnostic evaluations involving the comparison of simulated and observed "gas ratios." The immediate day-by-day feedback offered by the NOAA/EPA operational AQ forecasting program for ground-level ozone via comparison with AIRNOW network measurements provides an additional window on CMAQ performance. The air toxics modeling work with CMAQ is innovative and highly relevant to population exposure evaluations, but it is limited by availability of evaluation data, both on the national scale and on the local and community scale. Investigation of additional evaluation data sources, including the remote sensing of atmospheric trace constituents by satellites, is relevant and worth continuing.

Evaluation of the air toxics and mercury aspects of CMAQ is somewhat behind ozone and PM. In part this is because these are newer issues, but another aspect is the lack of appropriate measurement data. AMD should get involved in targeted air toxics studies such as MATES III for multiple reasons. First, MATES III will provide a good data set for model evaluation. Second, this will enable more direct model comparison (albeit to a rather old model). Third, it can lead to wider adoption of CMAQ, further facilitating OAQPS's future activities in support of regional, state and local governmental agencies.

Seasonal and annual operational evaluations of model performance should include greater use of wet deposition measurements, given the good continental coverage of existing networks, the

sizable number of species sampled (including base cations), and the importance of wet removal to atmospheric mass budgets. Characterization of model performance should be extended to consider daily (e.g., daily PM chemical components) and even hourly measurements (e.g.,TEOMs for $PM_{2.5}$ mass) in order to examine and characterize model performance for shorter averaging periods as well as for the longer averaging periods now being considered (monthly, seasonal). The ammonia inverse modeling performed for 2001 should be expanded to another annual period such as 2002.

Given that the CMAQ domains typically being modeled include much of southern Canada, where possible, use should be made of available Canadian measurement data to augment the U.S.-based measurements. This is already being done for the operational forecasting version of CMAQ through use of AIRNOW data. For example, the Canadian NAPS network includes ambient measurements of $PM_{2.5}$ chemical components, including inorganic species and heavy metals, and some gaseous air toxics such as benzene and 1,3-butadiene. More recent Canadian toxics emission inventories than the 1995 inventory are available, and the 2002 Canadian toxics inventory will include emissions from mobile and area sources as well as point sources.

Finally the CMAQ evaluation team needs to continue to advocate for the addition of new measurements to existing networks, such as ambient air concentrations of NH_3, Hg, and selected air toxics.

Charge Question 4:

What are your perceptions of the integration across different elements of the CMAQ Modeling Program (links between model development, applications, evaluation)? What is your perception of the usefulness of the CMAQ Modeling Program to the EPA, states, other customer needs and research community?

The three key components of the CMAQ modeling program — model development, model application, and model evaluation — need to interact with each other and function smoothly for the overall CMAQ modeling program to succeed. The links within various branches of AMD between model development and model evaluation appear to be strong and well integrated. This perception is based, in part, on how well the presentations prepared by AMD staff for the peer review were prepared and organized to show how the various elements fit together to make CMAQ both scientifically up-to-date and computationally efficient.

Historically, CMAQ model development and part of the evaluation has taken place primarily within AMD with substantial help from the outside research community in the academic and private sectors, and the linkage between the CMAQ developers in AMD and the external research community is quite strong and should continue. Some improvements to CMAQ (for example, CMAQ-MADRID) have come from outside the AMD core development team. However, if such outside contributions are to be of most benefit to the user community, they should be incorporated into the core model version rather than having to be reinserted into every new release.

Model application and associated evaluation for appraisal of control strategies to demonstrate attainment of NAAQS for pollutants such as $PM_{2.5}$ and ozone, for assessment of federal rules

such as CAIR (for SO_2 and NOx) and CAMR (for mercury) or for examination of the human-exposure impact of toxic pollutants, however, is conducted by groups outside the AMD. These groups include other offices of EPA (OAQPS, OAR, and CAMD) and many regional, state, and local governments. The intra-EPA linkage appears to be adequate. However, the linkage between AMD and regional, state, and local governments is rather weak and we make recommendations below to improve it.

Practical CMAQ model applications are generally performed by client divisions of EPA (OAQPS, CAMD, and OAR) and by various local and state governments and the RPOs. The major applications within EPA are undertaken to provide technical support for national rulemakings. The two recent applications are the Clean Air Interstate Rule (CAIR) and the Clean Air Mercury Rule (CAMR). CMAQ modeling for the CAIR application evaluated the impact of future major reductions in emissions of SO_2 and NOx from large electric generating units (EGUs) in the 28 eastern states and District of Columbia on progress towards achieving 8-hr ozone and $PM_{2.5}$ standards. The planned application of CMAQ to simulate a complete year for a number of years instead of just one year is very useful for a more robust evaluation of CMAQ.

The CAMR application, on the other hand, is not as robust mainly because of knowledge gaps in atmospheric science of mercury and also because of lack of sufficient measurements of ambient concentrations and dry deposition of mercury. However, the AMD efforts underway with OAQPS to evaluate the impact of CAMR for years 2010 and 2020, and multi-model intercomparisons with outside groups including EPRI and Environment Canada (with the same input emission inventory and meteorology) for the 2001 test year as well as the same control scenarios are very useful and must continue so that advances are made in the science and modeling skills in this emerging area. Here, we especially commend AMD's choice of an outside third party (New York Department of Environmental Conservation) for independent model results analysis.

The other, and perhaps more important, applications of CMAQ are by the local, state, and regional governmental bodies (for SIP applications for 8-hr ozone and $PM_{2.5}$ and regional haze assessments). Here CMAQ has been "adopted" at a slower rate than what is needed for technology transfer to result in rapid improvement in modeling skill. Part of the problem can be explained by the comfort level state and locals have with existing modeling technology (CAMx and REMSAD) and the usual inertia that thwarts the adoption of new tools. However, a major reason appears to be that ORD considers EPA's other divisions (OAP, OAR, OAQPS) as its major, if not only, client. OAQPS, in turn, has traditionally considered regional entities and state and local governments as its clients in the model application field.

What is needed is a more direct involvement of the CMAQ development and evaluation team with RPO, state, and local users in the field. This could be done either independently or in cooperation with OAQPS. The goal should be for the researchers to get first-hand knowledge of challenges being faced by the model application and evaluation community outside of the EPA. We recommend that appropriate members of AMD model development and evaluation teams participate in various modeling conferences sponsored by the RPOs and OAQPS to provide feedback to future model development paths. Additionally, RPOs, state and locals would

become more aware of CMAQ's current and anticipated capabilities. AMD should identify six to eight key "client" states and RPOs for direct and mutually beneficial involvement. This recommendation would supplement the excellent coordination already being done by CMAS, especially its increasingly well attended annual workshops.

Finally, AMD is to be commended for the recent progress in dramatically increasing in computational efficiency (run time of about one week for one year of $PM_{2.5}$ modeling for the eastern domain). This improvement in overall computational efficiency, more than any other factor, is expected to expedite the acceptance and technology transfer of CMAQ to RPOs and state and local governments. If there are additional avenues to increase efficiency even further (for example, in the aerosol module), they should be pursued.

Charge Question: 5

> *Are there modeling research areas that are not being addressed or are given insufficient attention within the CMAQ Modeling Program? Are there current areas of research emphasis that might be given lower priority or eliminated? For the resources available to the CMAQ Modeling Program, are they being used in an effective manner in terms of the choice and quality of research being conducted?*

Given the resources available, AMD has done a tremendous job in improving the scientific content of CMAQ. In addition to its own research effort, AMD also relies in large part on fundamental research conducted elsewhere. Part of its job is to synthesize and integrate research results from others into the modeling system so that it represents our current understanding of emissions and their transformations, transport and fate in the atmosphere. Applications and evaluations then determine how well the inputs and processes in the model simulate reality. In this sense, AMD is doing an excellent job of following relevant emissions and atmospheric research results and incorporating them into the modeling system. Even though the internal research within AMD is impressive, AMD can also use its powers of persuasion to encourage other parts of EPA (or even other research agencies) to focus on neglected or under-funded areas of research that could lead to modeling improvements.

Some of the areas of research that can benefit from greater attention are listed below:

- The current practice of model performance evaluation has emphasized the comparison of model predictions and observation. However, because the model contains many parameters, good agreements in absolute concentrations do not guarantee good model performance. A more stringent performance criterion ought to be based on comparing predicted changes with observed concentration changes due to changes in emissions. An obvious area to look into initially is the weekday/weekend emission differences and their predicted outcome. This means that an emission inventory needs to be developed for the weekend conditions for model comparison with observation.

- In model performance evaluation, there is always a problem of mismatch in spatial resolution between point measurements and model grid cells. This problem is well known, but it is also often ignored. Obviously, secondary pollutants are more forgiving in general, but there is no guarantee (consider ozone). Ammonia would most likely be a

serious challenge because of its short-range "footprint" due to its high removal rates and rapid interaction with sulfuric and nitric acids. AMD is using fine-scale modeling for air toxics, which are often primary pollutants. In this connection, the fine-scale dynamics, including plume rise from vehicle exhausts, may need to be considered. But when chemistry is involved, the scale mismatch issue is quite often ignored. Even though temporal averaging would help relax the constraints of the spatial resolution, some investigations need to be done with the emissions and observation teams to gain understanding of the level of acceptable tolerance in the resolution mismatch between model predictions and observation. In this connection, one or more mobile monitoring laboratories may be a cost-effective way of investigating the issues more thoroughly.

- Predicting clouds and precipitation is a difficult issue in meteorology. AMD may consider use of satellite data to infer precipitation fields for assimilation into the modeling system to improve precipitation simulation accuracy. AMD may want to incorporate the most up-to-date cloud parameterization scheme in CMAQ to improve the accuracy of cloud chemistry. Also, AMD may want to investigate whether a subgrid convective parameterization should be used for finer grids (on the order of 4 km). Here the work from the Pennsylvania State University may be helpful (Deng and Stauffer, 2004).

- An emerging issue that AMD may want to pay attention to is the interaction of air quality and climate change. This interaction may require two-way coupling of the air quality and meteorological models. It is hoped that more effort will be put into this area as it is bound to loom large in the not too distant future.

For the most part, the CMAQ team is very aware of the needs and their own capabilities. This has made them identify what is most important to them and their clients. There is very little superfluous project work underway, if any, and it has been virtually impossible to identify any aspects of the model development/application/evaluation that should be eliminated. There are areas (listed below), however, that might be given a somewhat lower priority if priority ranking becomes necessary due to resource constraints.

- The CMAQ team should proceed cautiously in terms of adding another chemical mechanism to those currently supported by ORD (CB4, SAPRC and RADM2). Updates to these mechanisms may be appropriate depending upon community needs. Let the community add other mechanisms and identify advantages that might argue for their adoption and support by CMAS. Recognize that the user community is interested in speed and chemical accuracy and that $PM_{2.5}$ is the likely driving force for change.

- Caution is also warranted in trying to make CMAQ applicable to a wider spatial range than it is now, i.e., going to very small or global scales . Their current approach, melding the Gaussian Plume model results with CMAQ results in a sensible fashion, is providing the type of information that can be used effectively by exposure modelers (though other alternatives, e.g., empirical analyses of the spatial and temporal variability, exist that might better capture the range of exposures across a range of scales and should be used to evaluate model results).

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- Immediate incorporation of WRF as a replacement of MM5 may be premature because WRF is still largely in the early application and model evaluation stage. No four-dimensional data assimilation effort has been initiated, which is an important component for CMAQ applications other than air quality forecasting. Accordingly, incorporation of WRF into the developmental CMAQ system should not take a high priority, although the work undertaken already to modify MCIP to add an ingest capability for WRF output files strikes a reasonable balance by letting the CMAQ community test WRF.

- Large-eddy simulations, while helpful in gaining insights on interactions across different scales and in providing better model simulations, are computationally intensive. In addition, many parameters need to be specified with little or no experimental or observational support. Unless there are justifications for specific applications, their use may not be a high-priority item.

We believe that the CMAQ Modeling Program has made very effective use of its resources, especially in the creation and use of a unified modeling platform (cf. CMAQ, CMAQ-AT, CMAQ-Hg), in fostering of collaborations and partnerships, and in developing flexible, multi-purpose tools (e.g., AMET).

6. PM MODEL DEVELOPMENT AND EVALUATION – DETAILED QUESTIONS AND PANEL'S RESPONSE

1. Which aspects of the aerosol modeling components warrant the most attention in order to improve the reliability of CMAQ for regulatory applications? Please rank the following in order of priority and provide specific recommendations wherever applicable.

In response to these questions, the Review Panel has developed consensus rankings and recommendations, with commentary as to why a particular ranking has been given. While some of the topics are of great scientific interest, if they were perceived as being of less concern to improving the reliability of CMAQ for regulatory application, the ranking is not high. An example is nucleation, which is a scientific "hot topic" but for which the current description within CMAQ is sufficient as this process is not viewed as impacting the results significantly and a generally accepted scientific description is not available. The rankings given to the specific topics are High (H), Medium (M), and Low (L).

Primary PM emissions (list specific source categories)   Priority: H
The Panel views this as one of the most important issues to be addressed by the CMAQ development team, though it is not apparent where their piece of this pie begins in relationship to other groups at EPA in charge of understanding and quantifying emissions. Particular areas where the group should focus are emissions of/from: vegetative detritus; biomass burning; road and wind-blown dust; heating oil; and sea salt. In terms of fugitive dust emissions, it is suggested that CMAQ and/or SMOKE include a capability to describe how meteorology impacts emissions, similar to how they are now treating sea-salt emissions. For most of these sources, information is needed in terms of chemical profiles and size distributions. Again, given the

limited resources, AMD must identify what they can and should do within SMOKE and CMAQ, and those issues that need to be addressed by other groups at EPA.

Emissions/chemistry of secondary inorganic aerosol precursors   Priority: M, except for ammonia, which is H
The panel views this with a medium priority as most of the relevant sources appear to be relatively well characterized, except where mercury is concerned. The work on inverse modeling of ammonia is applauded, though there is now a need to make sure that the loop is closed on this issue; that is, that other groups now use this information to improve their inventories (as has been done), the improved inventories are retested, and iteration is conducted until a satisfactory level of model performance is reached.

Emissions/chemistry of secondary organic aerosol precursors   Priority: H
This is another of the truly top issues. They must keep up with the various modeling approaches to SOA formation and be judicious in how to proceed. They should consider doing inverse modeling for identifying SOA precursors, similar to how they are addressing ammonia emissions.

Aqueous-phase chemistry   Priority: L
The current scientific treatment in CMAQ, for PM formation, is viewed as adequate at this point although the numerical algorithm in the model could be improved.

Heterogeneous chemistry   Priority: M
Here, the perceived need is in better understanding N_2O_5 hydrolysis and HNO_3 reaction with sea salt.

Inorganic aerosol thermodynamics (NH_4/SO_4/NO_3/H_2O system, sea salt, dust)   Priority: M-H
Here, the topics of concern are the treatments of the coarse mode, nitrate replacement, and comparison to AIM II.

Secondary organic aerosol formation pathways   Priority: H
The panel felt strongly that this is a high priority. If there is a scientific basis for doing so, updates should be made. They should look towards bounding their results given the uncertainties and assess where advances might be most profitable, e.g. understanding acid catalysis impact.

Interactions between organic and inorganic aerosol components (via hygroscopicity or activity)   Priority: (L)
This is not perceived as being fundamental to providing a scientifically well-founded model for regulatory application. Although it is an area where the evolving scientific understanding does not warrant significant effort on the part of the CMAQ-ORD modeling team, they should still keep a close eye on continuing developments.

Hygroscopic aerosol state (metastable vs stable)   Priority: L-M
This is not perceived as being fundamental to providing a scientifically well-founded model for regulatory application, plus it is an area where the scientific understanding does not warrant significant effort on the part of the CMAQ-ORD modeling team.

Nucleation   Priority: L
This is not perceived as being fundamental to providing a scientifically well-founded model for regulatory application, plus it is an area where the scientific understanding does not warrant significant effort on the part of the CMAQ-ORD modeling team.

Coagulation   Priority: L
The current approach is adequate.

Gas/particle mass transfer with fine particles   Priority: M
As noted above, there is a need to address nitric acid interaction with sea salt, and fine particle SOA formation.

Gas/particle mass transfer with coarse particles   Priority: M
As noted above, there is a need to address nitric acid interaction with sea salt.

Deposition, wet and dry   Priority: H
At a minimum, they should assess how improved descriptions might impact results. There appears to be some need to look at wet deposition results and the underlying description.

Aerosol size representation (e.g., modal vs. sectional)   Priority: M
They are working in this area, and should continue to do so. Their planned work appears appropriate.

Aerosol mixing characteristics (e.g., internal vs. external mixtures)   Priority: L
Again, scientifically interesting, but the computational burden likely does not make this attractive to most users. Allow the research community to make headway in this area, for possible adoption in about five (5) years.

Visibility calculations   Priority: M
They should consider adding capabilities directly to CMAQ to provide visibility fields that account for aerosol loadings that vary in space, and possibly spend a little time to make it a direct output with source attribution.

Others (please specify)   Priority: H
Boundary conditions (e.g., trans-Pacific transport)

Other issues beyond PM (across pollutants)
    A. Subgrid-scale deep vertical transport (beyond ACM)
    B. Precipitation impacts on pollutant concentrations (Here, the scientific foundation to make significant improvements might be lacking. Need to understand and assess how this uncertainty impacts your mission.)

2. Which aerosol diagnostic tools would be most helpful to EPA and the states for devising air quality control strategies for PM2.5 and regional haze?

Aerosol Diagnostic Tool	Priority
Sulfate apportionment by formation process (i.e., sulfate tracking model)	**M**
Primary PM source apportionment (suggest DDM be considered)	**H**
Integrated process rate analysis for PM	**L**
Direct decoupled sensitivity method for PM	**H**
Secondary PM source apportionment (suggest DDM with tagged S)	**H**
Others (please specify) – None	

We gave a low priority to IPRA because the large memory and postprocessing requirements have discouraged its widespread use. If approaches could be found for reducing the intensity of these requirements, the priority would be raised because of the deep insights this type of analysis provides.

3. What types of diagnostic evaluations would be most promising in terms of improving model performance for PM and its components? Please indicate specific data sets for evaluation if those are known.

For the most part, EPA has shown that they are aware of the most promising datasets. Two possible data sources that might warrant further examination for their model evaluation potential are the Chemical Speciation Trends Network (STN) data set and the growing body of single particle mass spectrometer data. The latter, in particular, could give valuable insights into how realistic are the PM size distribution and mixing state (external or internal) assumptions in the PM processing parameterizations. ESP 01/02 should be utilized, studied, etc., extensively. Also look into weekday-weekend comparisons, MANE-VU: RAIN, SEARCH continuous data.

4. In what ways should CMAQ be refined to better assess impacts on particulate matter from potential automobile emissions control strategies, considering effects from both direct emissions and secondary formation from gaseous emissions?

Even though emissions from mobile sources are fairly well characterized, there are still issues related to the reliability of Federal Test Procedure-based MOBILE6 inventory. EPA is developing a physically-based model called MOtor Vehicle Emission Simulator (MOVES). This should eventually be the model used for CMAQ. An area requiring more attention is the emissions from high emitters. They are responsible for most mobile source emissions yet they are not well characterized. For primary pollutants like organic carbon aerosol and black carbon, fine-scale modeling taking into account the plume rise of the exhaust is clearly needed. On the chemistry side, our understanding of organic nitrogen-containing compounds (nitrates, amines, amides) remains deficient. The need to better understand ammonia emissions from all sources near an urban area is also needed. Also, the involvement of semivolatile organic compounds from diesel vehicles in secondary organic aerosol formation needs to be incorporated in the chemistry.

5. Is the CMAQ model development team effectively incorporating scientific contributions from the aerosol research community? How could this process be made more efficient? Among the new scientific advancements implemented in research-grade models but not yet in CMAQ, which do you consider the most important (i.e., highest priority) to incorporate into the CMAQ modeling system?

The AMD team has effectively identified most justifiable scientific improvements by the scientific community to be incorporated. They may wish to consider making improvements to the characterization of emissions, including chemical and size distributions, and the incorporation of tracers for primary aerosol emissions and/or DDM for both primary and secondary aerosol. The CMAQ model development team ought to consider the sectional approach more diligently because of the generality, flexibility and scientific correctness of the approach. In this connection, the work done by ENVIRON on the incorporation of the PM modules developed by Carnegie Mellon University (CMU) needs to be considered for potential incorporation into CMAQ. There has been a concern about the diffusive nature of the solution to the condensation/evaporation equations. However, the Trajectory-Grid approach, which is highly accurate and fast, especially for the present application, has been incorporated into the CMU module. The model development team may want to pay attention to that development if it has not already done so. This research can be made more efficient by expanding the postdoctoral program to about six post docs, at least half of whom are dedicated to PM model development, application and evaluation.

6. Is the PM model evaluation program incorporating the right kind of components to build a comprehensive evaluation study? What major components do you consider missing, if any?

When a global chemical transport model is used to provide the background concentrations for all necessary pollutant concentrations, the reliability of the global chemical transport model is assumed. This is a big leap of faith that has to be investigated. Comparison of the model with IMPROVE or other rural database needs to be carried out. It would be valuable if EPA could secure one or more mobile labs to collect ambient data as needed to assist model evaluation. Clearly, a very big void in concentration measurement and model evaluation is in the vertical dimension. No models can be considered fully reliable without some kind of comparison with observations in the vertical dimension.

7. Is the model evaluation program targeting the right process-level or input-level issues for diagnostic evaluation and other specific analyses, given the areas of model and input uncertainty and data availability? What other aspects of the PM model performance should be included as a high(er) priority that are not yet being addressed?

The team should get involved with studies such as MATES III. Also weekday/weekend comparison would be a high priority activity that needs to be considered for model evaluation. Of course, this activity entails the development of a separate set of weekday and weekend anthropogenic emission profiles.

Although there appears to be interaction between the team responsible for the CMAQ-ETA operational runs and the developmental CMAQ team, there may be additional value that could be extracted from that interaction. The operational forecast runs constitute a tremendous resource that could potentially find greater use in diagnosing input and process representation weaknesses. Perhaps more creative thought should be devoted to how to better exploit this resource.

8. Are there model evaluation activities from which you would recommend divesting to replace with higher priorities?

The currently planned model evaluations appear to be focused on appropriate areas based on known or inferred areas of weakness in the modeling system. Consequently, we have not identified any evaluation activities that we would recommend divesting.

9. The overview presentation on PM model evaluation included several emerging areas for the program (e.g., remote sensing, extensions for inverse modeling, instrumented models). Are there other emerging areas that are of equal or greater importance that the evaluation program should consider?

The emerging areas for PM model evaluation that were presented all appear to be worthy of investigation, and it was not obvious to the panel that any important emerging areas had been overlooked. What might be considered is the application of these approaches in new ways or to new data sets. For example, special data sets from field experiments such as the Pittsburgh supersite and SEARCH have already been used for diagnostic evaluations of CMAQ, but other field experiments should also be considered. One candidate is the 2004 ICARTT field experiment, which included a considerable number of flights by instrumented aircraft plus marine boundary-layer sampling by an instrumented ship (NOAA's ***Ronald H. Brown***) in the northeastern U.S. Similarly, some diagnostic insights have been obtained from the sulfate tracking version of CMAQ, but an 'instrumented' version of CMAQ using the direct decoupled sensitivity method also has much potential. Inter-model comparisons also offer the possibility of new insights. These could include comparisons of the performance of the policy and AQ forecasting versions of CMAQ for the same case studies.

7. MERCURY MODEL DEVELOPMENT AND EVALUATION – DETAILED QUESTIONS AND PANEL'S RESPONSE

1. Which aspects of the mercury modeling components warrant the most attention in order to improve the reliability of CMAQ for regulatory applications? Please rank the following in order of priority and provide specific recommendations wherever applicable.

We see many gaps in our understanding of mercury dynamics in the environment. One problem is that the modeling group is now primarily limited by the fundamental scientific foundation of what level of science might go in to CMAQ. They do not have a good data set for evaluation, though measurements are becoming more widespread, and they should (and appear to be planning to) use this evolving data set. As noted in the responses below to needs in particular

areas, we view almost all of them as high priority, but also not falling fully within the CMAQ model development and application team's area.

Anthropogenic mercury emissions (list specific source categories)   Priority: H
The priority here is to influence others to address this problem. The CMAQ team should work with the inventory experts to identify areas of need, noted discrepancies, etc. Here, categories such as steel mills and foundries, industrial boilers burning fuel oil (both activity factors and emission factors), and refineries should be high priority. For modeling purposes, the new data on recently controlled municipal waste combustors is also very important (approximately 90 to 95 percent reduction).

Natural mercury emissions (list specific source categories)   Priority: H
Again, one priority here is to influence others, but also they should work with others to understand how to model these emissions. The CMAQ team should work with the inventory experts to identify areas of need, noted discrepancies, etc.

Re-emission of previously deposited anthropogenic mercury   Priority: H
Again, one priority here is to influence others, but also they should work with others to understand how to model these emissions. When a supportable approach becomes clear, the CMAQ team should include this in CMAQ.

Gas-phase chemistry   Priority: H
Again, one priority here is to influence others, but also they should work with others to understand how to model these transformations. They currently understand that some of their reactions may be wrong.

Aqueous-phase chemistry   Priority: H
Again, the priority here is to both influence others and work with them to improve our state of knowledge.

Sorption/desorption of aqueous mercury to suspended particles   Priority: M
Again, the priority here is to both influence others and work with them to improve our state of knowledge.

Wet deposition   Priority: H
Again, the priority here is to both influence others and work with them to improve our state of knowledge.

Dry deposition of reactive gaseous mercury   Priority: H
Again, the priority here is to both influence others and work with them to improve our state of knowledge.

Dry deposition of elemental mercury (or two-way exchange)   Priority: H
Again, the priority here is to both influence others and work with them to improve our state of knowledge. The surface exchange of Hg^0 is going to be updated, but it is not apparent how to

further improve this area given the lack of knowledge. This is one of the weakest links in current Hg models and needs serious effort to improve.

Additional atmospheric constituents that react with mercury   ***Priority: M***
Again, the priority here is to both influence others and work with them to improve our state of knowledge. It is not apparent which constituents might be important. It would be imprudent to introduce reactions that are suspected but not verified.

Others (please specify)   ***Priority: H***
They should encourage studies of Hg^{2+} reactions in simulated power plant plumes to better understand results emerging from field studies, begin incorporating mercury chemistry in to their PinG, and assess possible impacts of Hg^{2+} reduction in plumes.

2. Is there value at this point in adding a mercury emissions tagging capability to CMAQ so that the fate of mercury from specific sources can be followed? On the other hand, can the current science offer such differentiated assessments of mercury fate?

There is a strong value at this point to include tagging capability in CMAQ-Hg similar to CMAQ and, given that this is relatively straightforward, it should be done. The results should always be treated with caution and communicated with caveats as to the scientific limitations in the understanding of the chemistry of various components of Hg.

3. What types of diagnostic evaluations would be most promising in terms of improving model performance for mercury and its components? Please indicate specific data sets for evaluation if those are known.

An in-depth diagnostic evaluation of CMAQ performance in simulating the fate of mercury is limited by the lack of data. Others need to improve the technology for measuring mercury and its compounds. Current datasets are limited to measurements of elemental mercury, gaseous mercury compounds and particulate mercury (compounds adsorbed onto aerosol particles). At this time there are no practical analytical techniques for the measurement of specific gaseous or particulate mercury compounds. Considerable development in analytical techniques for mercury and its compounds will be necessary before adequate datasets may be generated. Given the lack of analytical instrumentation, dry deposition studies of mercury and its compounds are not yet possible.

There may be greater hope for a diagnostic evaluation of CMAQ performance in simulating wet deposition of mercury because of the availability of data from the Mercury Deposition Network. However, the time resolution is low because data are available on a weekly basis only. Simulated and measured wet mercury deposition may be compared. The modeling system's performance in simulating precipitation is an important diagnostic. Precipitation amounts strongly affect measured and modeled mercury concentrations. One possibility for future field studies is the analysis of event-based precipitation samples and samples of actual cloud water.

4. In what ways should the mercury model components be enhanced to improve the usefulness of CMAQ, specifically in relation to the Clean Air Mercury Rule?

Ensure that mercury chemistry is included in the PinG and that the CMAQ-PinG is used for any emissions management assessments involving mercury emissions from power plants. The chemical environment in power plant plumes varies from plume to plume and is quite different from that in the surrounding air such that dominant chemical reactions influencing the oxidation state of plume mercury may differ from plume to plume and from those of mercury in the surrounding air. This is important because the oxidation state (chemical form) of the mercury determines, in part, its dry deposition, scavenging, and transport behavior. From the results presented at the peer review meeting, there appears to be a continuing tendency for CMAQ to over-predict mercury concentrations in precipitation. This may be an indication that CMAQ has a bias toward too high a ratio of Hg (II) to Hg(0). If this is so, it would behoove the CMAQ developers to ensure that the mercury chemistry in the operational version of CMAQ is updated as soon as possible after new reactions and/or rates are published in the peer-reviewed literature, to ensure that mercury emissions management decisions are based on the best possible science and will achieve the results expected. It is worth noting that the mercury modeling PI in the AMD carefully monitors the literature and is broadly networked with other researchers in the field, so that this recommendation would probably be implemented in the developmental version of CMAQ whether or not it appeared here.

5. Is the CMAQ model development team effectively incorporating scientific contributions from the mercury research community? How could this process be made more efficient? Are there any new scientific advancements implemented in research-grade models, but not yet in CMAQ? Which do you consider the most important (i.e., highest priority) to incorporate into the CMAQ modeling system?

While other models do have different representations of the physical and chemical dynamics of mercury, the one contained in CMAQ is appropriate for now. The CMAQ team has identified areas of scientific uncertainty which must be studied for possible change. They recognize that the current treatment of deposition is simplistic and may need to be improved, but they also recognize that uncertainty will remain here as well. For now, having a significant amount of the research being conducted by others, and in some cases being incorporated in CMAQ elsewhere, is proving to be very efficient.

Given that a major anthropogenic contributor to US mercury emissions is the utility sector, and, as discussed above, that there may be significant chemistry in power plant plumes, it is appropriate that the CMAQ team get ahead of this issue and develop mercury capabilities in their PinG such that they can incorporate scientific advances rapidly, and in the mean time, study what the implications might be.

8. AIR TOXICS MODELING – DETAILED QUESTIONS AND PANEL'S RESPONSE

1. Are there other inhalation hazardous air pollutants, beyond the NATA list of 33, that are of higher interest/importance to the scientific community for examining with regional/urban scale air quality models? Should we be focusing on nitro-PAHs, specific compounds rather than "diesel PM", or other carbonyls, for example?

Consistent with the approach that the CMAQ team has already followed, the choice of additional inhalation hazardous air pollutants should be guided by (a) the potential impact of the pollutant based on an assessment of its activity and ubiquity and (b) the availability of good emissions data and ambient measurement data for the pollutant. Based upon these selection criteria, diesel PM would appear to be a priority candidate, since it will likely have the most widespread impact given its association with mobile diesel sources, its targeting by some health studies, and its association with PM number concentration and EC mass component. A few heavy metals, such as Cr(VI), may also be potential candidates: heavy-metal levels are quantified in a number of PM emission speciation profiles and are measured in the elemental analyses performed for PM speciation networks such as IMPROVE. Finally, a number of current and legacy pesticides and herbicides are a concern from the viewpoints of bioaccumulation and water quality. Emission inventories have been constructed for some pesticides (e.g., Li et al., 2003), and ambient concentrations and/or wet deposition of some pesticides are measured by networks such as the Great Lakes' Integrated Atmospheric Deposition Network (Buehler and Hites, 2002) and the new Canadian Atmospheric Network for Currently Used Pesticides (CANCUP). Given that CMAQ has already been applied to modeling the atmospheric transport of the herbicide atrazine (Cooter and Hutzell, 2002; Cooter et al., 2002), pesticide modeling with CMAQ would appear to be a natural extension if these compounds are of interest to the Agency.

2. Given the limited availability (spatial and temporal) of ambient HAP measurements, what is the best approach and criteria to use for evaluating model predictions of toxic air pollutants?

The alternative to ambient measurements of HAPS is to use copollutants that could serve as surrogates. CO is the obvious one for volatile HAPs that are primarily associated with gasoline exhaust such as BTEX and 1,3 butadiene. Less desirable would be 24-hour averages of elemental carbon from the Speciation Trends Network (STN). Because these pollutants are directly emitted, it is very important to carefully characterize the site before the ambient measurements are used for evaluating model predictions. The site should be representative of neighborhood-scale exposures and should be free of the influence of nearby traffic. There should be an expectation that the measurements from this site would be roughly comparable to the average concentration within the modeling grid in which the site is located. These concentrations are obviously much lower than exposures in certain microenvironments such as in commuter traffic. The regional and urban models need to be supplemented with some estimates of the gradients in exposures from source areas (e.g., major roadways) to the central monitoring site. One way to obtain this information is to supplement the existing air monitoring network with regular mobile monitoring along roadways with contrasting mix of diesel and gasoline vehicles. This monitoring should be repeated at least every other year on the same prescribed route.

9. COMMENTS ON THE PEER REVIEW PROCESS

We applaud AMD for its foresight in establishing a regular external peer review process for CMAQ. We recognize that the review addresses the model itself, the work of scientific and support teams that produce the model, and CMAS that disseminates the model. Because we believe the peer review process to be an important part of the development of CMAQ, we would like to offer some thoughts and suggestions on the review process itself.

Review Frequency
We believe that the highest reasonable frequency for reviews should be once every 18 months or, preferably, two years. At this frequency it would be appropriate to alternate between broadly based and focused reviews. The lower frequency takes into account that changes in AMD staff and their activities and in CMAQ itself accumulate to a stage worthy of review on a time period generally longer than a year. A higher frequency would be likely to result in "reviewer saturation". CMAS should consider conducting an electronic survey of a selected set of users and targeted non-users prior to the on-site reviews. This survey would involve about 20 users from the various communities (others in EPA, state modelers, researchers, consultants) to identify specific needs and suggested directions. If done before the annual CMAS conference, an on-site discussion session, possibly involving the CMAS Board, could help tie up some loose ends, and the CMAQ program peer review would "close the loop." If a two-year frequency is chosen, the survey could be conducted yearly, along with the CMAS session. As was evidenced by this review, the EPA team understands its mission and direction, and is responsive to past review comments, so a more frequent on-site review is not necessary.

Panel Continuity
We recommend that review panels consist of six or seven members, and that every panel contain two, or preferably three members from the previous panel. This will ensure a continuity of panel deliberations and coherence between reports.

Review Materials
The review panel appreciated having a package of relevant publications to review, and especially having an electronic copy of all review presentations for reference.

CMAS Involvement
We suggest AMD consider using the CMAS workshop to provide direct input to the review process (see above). This will give EPA and the review panel an opportunity to consider opinions of users and potential users of CMAQ. Possibly, a one-hour session at the workshop could be devoted to learning the primary needs of the community.

Review Schedule
The second review worked within a schedule that allowed ample opportunity for panel members to interact with AMD staff, while also allowing them opportunities to plan their review (see Appendix for schedule). The schedule was near optimal, and we recommend that future reviews employ a similar schedule.

10. CONCLUSIONS

This external CMAQ Model Peer Review Panel conducted its review in May 2005 on the basis of a day and a half of presentations by AMD staff and documents provided by them. This assessment was limited to an evaluation of work performed by 28 staff scientists, including postdoctoral researchers. The charge of the review was to focus on the modeling of particulate matter, mercury and air toxics. However it was necessary for the panel to consider all aspects of the program. CMAQ is a modeling system that captures a wide range of physical, chemical and biological processes with applications ranging from ozone to PM, air toxics, and mercury, from local to regional space scales, and from hourly to annual time scales. CMAQ is both a research model and a regulatory/operational tool. Although the panel reviewed the quality of the science, it focused equally on its fitness for use in operational applications and assessments.

The presentations were of very high quality and were given by very competent researchers. The review panel was both delighted and highly impressed by the improvements in CMAQ over the past year. The review panel believes that AMD is a world leader in its mission to facilitate transition of research-grade air quality models to operational tools for use in policy and regulatory applications and that CMAQ represents the state-of-the-science in air quality models applied within a regulatory context.

The scientific content and performance of the CMAQ modeling system continues to improve with each release due to the excellent efforts of AMD staff. CMAQ, as part of the Models-3 system, represents the state-of-the-science of widely used models, particularly models that are used in a regulatory context. Not every scientific component reflects the most recent research in a given area. However, this is not necessarily a criticism since there should be such a thoughtful delay before incorporating new research results into a regulatory model so as to allow the scientific community to reach a level of consensus. AMD has made significant progress in improving computational efficiency, which more than any other factor is expected to expedite the acceptability and technology transfer of CMAQ to RPOs and to state and local governments for regulatory applications.

Part of AMD's job is to synthesize and integrate research results from others into the modeling system so that it represents current understanding of emissions and their transformations, transport and fate in the atmosphere. It has done an outstanding job of incorporating fundamental research conducted elsewhere into CMAQ. AMD staff members are to be commended for maintaining awareness of current developments elsewhere in their fields of specialization that are necessary for leveraging their own resources. AMD staff priorities for research are sensible and they are responsive to client needs. The modeling team has been very successful in striking an appropriate balance between the competing demands of scientific detail and operational utility. AMD is well positioned to assume major new efforts in operational air quality forecasting (for nationwide daily ozone and $PM_{2.5}$ forecast guidance), and in fine-scale and global-scale modeling. The panel applauds the thoughtful approach with which they are approaching these developments.

The panel commends AMD for its commitment to model evaluation. They are very aware of the need to conduct model evaluation at both routine and diagnostic levels. They have been taking this aspect of model development very seriously. Significant resources have been assigned by AMD to the evaluation of CMAQ performance, and the model applications and evaluations being conducted are relevant and are of high quality. The development of AMET, and the associated model evaluation toolkit is seen as recognition of the importance of model evaluation, and its planned inclusion in future distributed versions of CMAQ will provide users with strong evidence of its importance. In many ways, model evaluation is now limited by lack of sufficient observational data. The CMAQ evaluation team needs to continue to advocate for the addition of new measurements to existing networks, such as ambient air concentrations of NH_3, Hg, and selected air toxics.

The CMAQ team is very aware of its mission and client needs. They have prioritized their work well and there is no work that is obviously superfluous. The panel found it difficult to identify any aspect of CMAQ model development/application/evaluation that should be eliminated. The practical application of the CMAQ model generally occurs within client divisions of EPA (OAQPS, CAMD, and OAR) and by various local and state governments and the RPOs. The major applications within EPA are undertaken to provide technical support for national rulemakings. AMD staff should expand their view of their clients to include the states and RPOs, and interact more directly with the state and RPO modelers. AMD needs to find other parallel and direct channels to communicate with sophisticated modelers in regulatory community. AMD should identify six to eight key "client" states and RPOs for direct and mutually beneficial involvement. This would actually complement the mission of OAQPS as well. This recommendation would supplement excellent coordination being done by CMAS, especially its increasingly well attended annual workshops.

Finally we congratulate AMD for its foresight in establishing a regular external peer review process for CMAQ and encourage them to continue with the on-site schedule and format that was used for this second review panel. We believe that the highest reasonable frequency for reviews should be once every 18 months or, preferably, two years. The number of panel members appears to be near optimal and we recommend every panel contain two, or preferably three members from the previous panel to ensure a continuity of panel deliberations and coherence between reports.

11.   REFERENCES

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12. APPENDIX. AGENDA FOR SECOND CMAQ PEER REVIEW MEETING

CMAQ PEER REVIEW MEETING
May 17-19, 2005
U.S. EPA – Research Triangle Park, NC
C114 (May 17, 18); E249 (May 19)

<u>Agenda</u>

May 17, 2005

8:30am	Introductions / Background / Charge to Reviewers	S.T. Rao
8:45am	Summary of December 2003 Peer Review Findings and EPA Response	K. Schere
9:15am	Overview of 2005 CMAQ Model System Release	S. Roselle
9:45am	BREAK	
10:00am	CMAQ Model System Physics (Clouds, Radiation, PBL, Dry dep, Photolysis, etc)	J. Pleim
11:00am	Meteorological Modeling (transition to WRF, PX in WRF, nudging in WRF, eval, MCIP, etc.)	T. Otte
11:45am	WORKING LUNCH	
1:15pm	CMAQ – Particulate Matter (sea salt, ISORROPIA/thermodynamics, organics/diagnostics, emissions issues: fires, biogenic precursors, organics, source apportionment)	P. Bhave/ G. Pouliot
2:15pm	PM- Sectional Methods for CMAQ (CMAQ-UCD, CMAQ-MADRID)	C. Nolte
3:00pm	BREAK	
3:15pm	PM Evaluation – Overview (Summary of operational and diagnostic evaluation research, related meteorological and emission activities, introduction of remote sensing)	A. Gilliland
4:00pm	Diagnostic Evaluation of Carbonaceous Aerosols	P. Bhave
4:30pm	Diagnostic Evaluation of Inorganic Aerosols: Gas Ratio	R. Dennis
5:00pm	Ammonia Emissions – Inverse Application	A. Gilliland
5:30pm	END OF FIRST DAY	

May 18, 2005

8:30am	CMAQ – Mercury	R. Bullock
	(Model science overview, 2005 public release, 2001 Evaluation, North American model intercomparison, collaborations, etc)	
9:30am	CMAQ – Toxics	D. Luecken
	(Overview, 2005 public release, NATA application/evaluation, work with OAQPS, emissions issues)	
10:30am	BREAK	
10:45am	CMAQ – Toxics – Urban scale	V. Isakov
	(Philadelphia application, link to human exposure, hybrid approach for hotspots)	
11:30am	WORKING LUNCH	
1:00pm	CMAQ – Toxics – Houston application	J. Ching
1:30pm	Wrap-up Comments	K. Schere
1:45pm	Small group or one-on-one discussions between Peer Reviewers and CMAQ scientists	
4:00pm	Panel deliberations and work time	
5:30pm	END OF SECOND DAY	
6:30pm	GROUP DINNER	

May 19, 2005

8:30am	Panel deliberations and work time
11:00am	Debriefing to AMD Management and PIs
12:00pm	END OF PEER REVIEW MEETING