Final Report: Fourth Peer Review of the CMAQ Model

Submitted to:

Community Modeling and Analysis System Center

Carolina Environmental Program

The University of North Carolina at Chapel Hill

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1. Introduction

The CMAQ Model External Peer Review Panel conducted a two and a half day review view on June 27, 28, and 29, 2011. This report summarizes its findings, and follows other reviews conducted in 2004, 2005, and 2006 [Amar et al., 2004; 2005 and 2007].

The report is written from the perspectives represented by the seven-member review panel: David Allen, Praveen Amar, Nancy Brown, George Kallos, Richard McNider, Armistead (Ted) Russell, and William Stockwell. Panel members read a considerable volume of material on CMAQ provided by EPA and attended two days of presentations on CMAQ by the EPA staff (see the Appendix for meeting agenda).

The Atmospheric Modeling and Analysis Division (AMAD) of the National Exposure Research Laboratory (NERL) develops operational state-of-the-art air quality models and modeling tools for use in policy and regulatory analyses. This review focused on the work conducted by the group of 21 staff scientists (the CMAQ group) within AMAD. The 2011 Peer Review emphasized an assessment of the meteorological, physical, and chemical process aspects of the Community Multiscale Air Quality (CMAQ) modeling program, as well as applications, refinements, and considerable evaluations of model performance. The review panel focussed its attention on the current community version of CMAQ, version 4.7.1, which was released in January, 2011 as well as the future version, CMAQ 5.0, to be released in October, 2011.

Within the context of the AMAD's mission to develop air quality models for regulatory, research, and operational purposes, the panel was charged with evaluating the overall quality of the applied scientific research in the CMAQ Modeling Program. The panel evaluated: 1) the overall quality of the applied scientific research in the CMAQ Modeling program; 2) the strengths and weaknesses of the science being used within the components of the CMAQ Model development program; 3) the quality and relevance of the model development, applications and evaluations that are conducted as part of the CMAQ Modeling Program to the four Integrated Transdisciplinary Research (ITR) programs; and 4) the integration of different elements of the CMAQ modeling program and its usefulness to the EPA, states, and other customer needs as well as the research community. The panel also evaluated the relevance of the AMAD's modeling program elements in view of the resources available to the CMAQ Modeling Program. The panel was requested to identify relevant modeling research areas that are not being addressed or are given insufficient attention. The panel also identified current research areas that should be given lower priority or eliminated to help advance the four EPA Office of Research and Development (ORD) ITR areas. The four ITR areas are: Air, Climate, and Energy (ACE), Chemical Safety for Sustainability (CSS), Sustainable and Healthy Communities (SHC), and Safe and Sustainable Water Resources (SSWR). The panel was also asked to consider whether the resources made available to the CMAQ Modeling Program are being used effectively in terms of the choice and quality of the applied research being conducted at AMAD in support of the four ITR areas.

CMAQ is the central tool for its user community throughout the US and the world that is being used in regulatory and scientific applications by researchers and the EPA, states, regional, and local agencies in State Implementation Planning (SIP) processes. The community is at ease with using it at its current state of development, even as more difficult policy-oriented demands are being placed on the model (e.g., simulating ozone at lower concentration levels and in the winter).

As noted, even though the CMAQ modeling system is used throughout the US for regulatory purposes, by EPA, states, and regional and local agencies, there are also other models used by many of these entities for SIP activities that are often provided by the air quality consulting community outside the CMAQ framework. There is a need for the nation to have the very best tools for air quality decision making; hence, it would seem appropriate that the CMAQ group should also strive, when feasible, to make subcomponents of CMAQ available to the larger U.S. modeling community. In the past, the CMAQ group has achieved this successfully with biogenic emission modules, and more recently, with the development of model evaluation tools.

The consensus of the panel was that the CMAQ group is doing an exceptional job selecting research topics and conducting their research; hence, we will not comment further on the choice of scientific directions that the group has pursued. The panel was impressed that they have used model error and control strategy sensitivity as a basis for guiding the selection of research directions.

2. Major Developments since the third peer review (December 2006)

CMAQ has evolved significantly since the last review in 2006. The aerosol/particulate matter simulation capabilities have advanced dramatically. The descriptions of the secondary organic aerosol (SOA) formation routes are significantly enhanced, and while still biased on the low side, they capture reasonably the diurnal trends and the scientifically identified routes. Dust emissions are also more realistically treated. Sea salt aerosol emissions from the coastal zone are simulated. Additional species are included in the thermodynamic treatment and reactive gases are now modeled to interact with coarse particles in a dynamically correct fashion. The chemistry has been updated from older to current versions of the CB, SAPRC and RACM chemical mechanisms. In spite of the model becoming more comprehensive and complex, the group is also making strides to make it more user-friendly.

Other areas where there has been significant progress are indicated below:

Model Evaluation

The Air Quality Model Evaluation International Initiative (AQMEII) has played a key role in making the model evaluation more systematic by including operational, diagnostic, dynamic and probabilistic evaluation methods. Probabilistic evaluation is the newest approach and is still under development within the modeling community.

Chemistry

Chemical mechanisms options have been upgraded to include SAPRC07 and CB05. Isoprene chemistry, toluene chemistry, and the kinetics associated with key inorganic reactions $OH + NO_2 \rightarrow HNO_3$ and $HO + SO_2 \rightarrow H_2SO_4 + HO_2$ have been revised. The inline calculation of photolysis rate constants has been improved and implemented for testing. Work is in progress to incorporate a more realistic aqueous-phase chemistry mechanism.

Aerosols (Particulate Matter)

There is an improved treatment of the heterogeneous reaction of N_2O_5 to HNO_3. There has been substantial improvement of the SOA module. There is dynamic mass transfer for coarse aerosols.

Emissions

Improvements have been made in the treatments of estimating biomass burning emissions and anthropogenic fugitive dust. The addition of "lightning NO_x emissions" to CMAQ significantly improves agreement between simulations and measurements.

Transport

Work is in progress to achieve consistency between CMAQ and the Weather Research and Forecasting (WRF) meteorological model. For example, the new mass continuity treatment in CMAQ uses the WRF vertical velocity calculation, which still requires additional attention especially when modeling at finer scales (of a kilometer or less). Since the inherent problem is related to both grid and/or stencil differences, there are likely to be differences in CMAQ and WRF vertical velocities especially relating to the selection of an appropriate top boundary condition.

Air-Surface Interactions

The CMAQ group has adapted a two-layer (vegetation & soil) resistance model for bidirectional exchange for ammonia and mercury. They have continued their excellent work comparing model deposition to field observations.

Two-Way Coupled WRF-CMAQ Model

An efficient and flexible coupled meteorology-chemistry modeling system based on the WRF and CMAQ models has been developed and is being tested. The current one-way and off-line coupling of WRF and CMAQ has the advantage that one only has to run the meteorological model once for multiple control strategy tests. This means that CMAQ and WRF can continue separate internal development tasks. However, ultimately this approach may limit the application of the CMAQ model when small scales (e.g., less than 1 km) are required, where turbulent eddies begin to be resolved by the model. It is difficult to see how the chemistry model can accommodate the segregated effects without using true time-step coupling. Coupling of the chemistry and physics should be required when plume behavior is dominated by the resolvable eddies. The "vertical velocity problem" mentioned previously may also be of concern for applications at the small scales. While the global modeling community has been less concerned about this, the same issues appear to arise when trying to translate the effects of cloud convective transport from the physical model to the chemical model.

3. Specific recommendations of third peer review panel and response to prior review

Recommendations of the Third Peer Review Panel and EPA Response:

The 2006 peer review panel made several key recommendations to improve CMAQ performance and the CMAQ group has made a number of modifications in response. The key "high priority" recommendations included: 1) improvement in the treatment of N_2O_5 chemistry, 2) reduction of the uncertainty in chemical mechanisms for aromatic chemistry, 3) improvement of the representation of SOA production from biogenics and aromatics, and 4) improvement of the evaluation of different mechanisms to quantify their impact on pollutant predictions and responses to precursor reductions.

In response to the above recommendations, the CMAQ group has made substantial efforts to include development of a new parameterization scheme for N_2O_5 chemistry and conducted model comparisons with field measurements. Consistent with the panel's recommendation, a parameterized version of aromatic chemistry (including an updated toluene mechanism in the CB05 version) has been implemented. To improve SOA treatment, new SOA precursors (isoprene, benzene, and sesquiterpenes) have been added, and new pathways have been incorporated (e.g., acid enhancement of isoprene SOA). The panel recommendation relating to responses to precursor reductions is important from a regulatory standpoint and the group's recent work found that both CBM and SAPRC mechanisms exhibited similar responses. The CMAQ group is commended for its work with EPA Office of Air Quality Planning and Standards (OAQPS) in this policy-relevant effort.

In responses to other recommendations of “medium and low priority” a number of actions were also taken. For example, for dry deposition, good progress has been made in the important area of a bidirectional flux treatment for ammonia and mercury that includes comparisons with data from intensive field studies.

4. Panel Response to charge questions

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

Evaluation (quality of science)

The CMAQ group is to be complimented on the extensive efforts they have made to evaluate CMAQ, and to provide the evaluation tools to the user community. Their research in this area is of very high quality and they are the world leader in air quality model evaluation activities. These efforts provide a foundation for the more reliable use of the CMAQ modeling system, not only for traditional applications, but also as the model is used for new and more challenging applications. If the National Ambient Air Quality Standard (NAAQS) for ozone becomes more stringent, new evaluation efforts may be required by the CMAQ group to demonstrate the model’s ability to capture correctly the model response to air pollution control strategies at “mid-high” ozone levels. While the group is arguably the world leader in this area, there are cases where they will need to be even more forward-looking. They need to support the NAAQS review process (e.g., the primary and secondary ozone standards, new primary PM and NOx/SOx standards, and future secondary standards for SOx/NOx) by providing the modeling tools and requisite analyses.

Chemistry (quality of science)

The overall quality of the chemistry components is high. It is commendable that the CMAQ group has been developing alternative gas-phase mechanisms to the carbon bond mechanism. These new options will allow CMAQ to be used reliably for a wider range of conditions and applications. Chemical mechanism options have been upgraded to include SAPRC07 and CB05. Appropriate attention is being given to the chemistry of biogenically emitted organic compounds. Photolysis is a major driver of atmospheric chemistry and is very dependent on meteorological conditions; thus the inline calculation of photolysis rate constants in CMAQ is a significant improvement.

Particulate Matter (quality of science)

The overall quality of applied scientific research on particulate matter in the CMAQ modeling program is excellent. The CMAQ group has made significant scientific progress in developing methods for tracking, within CMAQ, sources of primary and secondary aerosol. These advances will enable much more focused efforts to improve CMAQ's under-prediction of Secondary Organic Aerosol (SOA) formation and over-prediction of "other", unspeciated particulate matter (PM) components. The team has also incorporated state of the science descriptions of heterogeneous chemistry into CMAQ gas phase chemistry modeling, particularly for N_2O_5.

While progress has been significant, there is a need for improvement in the following areas:

- Review of the soil dust schemes currently included in limited area models and not those in GCMs (schemes in the GCMs are not refined and less accurate).

- Addition of heterogeneous chemistry processes (e.g., primarily processes associated with SOA formation).

- Treatment of the conversion from concentrations to number density and size distribution, which is especially important if tighter coupling between the met and chemical transport models is required to treat the physics and chemistry of aerosol indirect effects.

<u>Meteorology</u> (quality of science)

The meteorological model (WRF) used in the coupled system is mature and provides the necessary meteorological fields to drive CMAQ using the recently developed coupler. WRF has 2-way nesting capability but CMAQ does not. This imposes some restrictions on how to do coupling. A one-way nesting configuration was applied for most cases where the coupled system is used. The coupler also works in a limited fashion in the reverse way by supplying the necessary information to estimate the direct effects of aerosols on radiation. This is a useful step towards better coupling.

Retrospective studies in which air quality is simulated at locations that exceeded NAAQS in the past are used to evaluate the impact of different emission control strategies. These studies have been a cornerstone of control strategy development for SIPs under the Clean Air Act. The EPA has used such retrospective studies for outlining general population exposures, for designing observation/monitoring networks to observe changes in air quality and to determine what might be possible in terms of atmospheric response as frameworks for new standards are being established. The CMAQ team has made significant contributions in developing techniques for recreating the meteorology and physical atmospheres for these retrospective studies.

In particular they have embraced Four Dimensional Data Assimilation (FDDA) in the MM5 (the model that preceded WRF) framework in the free atmosphere as a way to constrain the model to observations and remove the model drift, which is inherent in a free forecast. Most importantly they have worked with the WRF community to include these FDDA techniques within the WRF framework. Data assimilation in WRF is a useful tool for hindcasting (and forecasting) simulations and this has been clearly demonstrated in their work. Additionally, they have used a new generation of observations including radar profilers and satellite data to improve the fidelity of representing the atmospheric conditions and parameters.

They have led the way by demonstrating, in retrospective studies, that simple models constrained by observations are preferable to more complex models that contain many uncertain and unknown parameter values. Near-surface temperatures are highly dependent on land characteristics of highly uncertain quantities such as soil moisture, soil heat capacity and deep soil temperatures. Their indirect methods of adjusting soil moisture in a simple two-layer surface model based on model error in the morning and similar schemes to adjust the deep soil substrate temperatures at night to improve surface temperatures are two examples of this approach. The corresponding surface flux correction in this indirect assimilation of both sensible heat flux and moisture flux greatly improves the calculation of mixing heights and Planetary Boundary Layer (PBL) turbulent characteristics.

While these are data driven adjustments, they are based upon a thorough understanding of the physics of the lower atmosphere. The CMAQ team has also developed practical methods for including subtle boundary layer characteristics such as asymmetry in convective eddies in boundary schemes and, perhaps most importantly, has worked to include these schemes in the WRF model [Pleim, 2007].

A 12-km resolution was used for continental coverage for most of the cases discussed or referred to in the CMAQ group's publications. The 4 km resolution was only used in a few cases, and it would be useful to perform more testing at the higher resolution. The manner in which the vertical velocity component is used in CMAQ needs to be refined because the current treatment may have important limitations, especially at high-resolution configurations. One area that does not seem to have been explored is the use of a one-dimensional variational assimilation following the approach of O'Brien [1970] for solving the "vertical velocity problem." In this approach the divergence from WRF can be minimally adjusted to meet the same top boundary constraint used in WRF for the CMAQ grid/stencil.

Emissions (quality of science)

The overall quality of the emissions component of CMAQ is satisfactory. The emissions component includes three major categories (anthropogenic, biogenic, and natural). The main improvements since the 2006 review include improvements in the characterization of existing emission sources (including new species, optimization and streamlining of emissions processing, and adding new emission sources (lightning-NOx and windblown dust in CMAQ v 5.0). The Panel believes that CMAQ must have an emissions component of high quality for it to have success in its regulatory applications. Evaluation of the effectiveness of alternative emission control strategies and accurate representations of emissions (as well as changes in emissions) are very important; however, historically, sufficient attention has not been devoted to this because of the difficulty associated with it and the large labor requirements for doing this task correctly.

The new CMAQ effort on improving emission estimates from three categories of 1) windblown dust emissions for PM2.5 and PM10, 2) biogenic emissions (BEIS, MEGAN, and BELD3 vegetation database), and 3) emission speciation including the SPECIATE data base (v. 4) will be of great use to future CMAQ applications. Additionally, there has been reasonable progress in emissions related to biomass burning, though it has not taken into account the potential heterogeneous reaction on the particles produced in the fire [see Buscu et al., 2006].

Land-surface Interactions (quality of science)

The land surface team has continued to perform quality research in actively comparing models to field observations of deposition. They have also begun to embrace crop models as a path to further improve plant uptake parameterizations. When possible, the CMAQ team should use existing crop models rather than developing new models.

Coupled WRF-CMAQ (quality of science)

The ability to run WRF and CMAQ inline and offline is highly desirable for climate research and air quality forecasting applications. The system is somewhat outside of the CMAQ group's current mission because it is used less for these applications than for efforts concerned with the development of control strategies where CMAQ is used to simulate many scenarios. The coupled WRF-CMAQ model could be used to develop the base case meteorology for multiple off-line simulations.

The WRF-CMAQ coupling is obtained through direct writing to the allocated memory of each system. Both models have been programmed for Shared Memory and Distributed Memory Platform computers that allow fast execution and utilization of relatively inexpensive computer infrastructures. The WRF-CMAQ coupler is efficiently designed. There are questions related to its use in other computer cluster configurations.

The coupler is designed to work primarily on a one grid configuration of CMAQ, and this imposes some restrictions on the optimal use of the WRF capabilities (2-way nesting). This affects accuracy (e.g., in the calculation of the vertical wind component). While we recognize that achieving two-way nesting for the coupled system is difficult to achieve, we encourage the CMAQ group to continue to work to improve the coupler to achieve greater flexibility.

The coupled system has been tested by using boundary conditions (BC) from global modeling systems. This is a good step for climate-type simulations. The CMAQ Group's hemispheric configuration of the coupled system is promising and can be used for the preparation of better lateral BCs and to perform higher resolution simulations. These useful features could be enhanced further if a fully coupled two-way nesting system for WRF-CMAQ were to be developed.

4.2 Charge Question 2: What are the strengths and weaknesses of the science being used within the components of the CMAQ Model development program?

Evaluation - strengths and weaknesses:

Model evaluation is a tremendous strength of the CMAQ Group, and their work in this area is of extremely high quality. The CMAQ group is the world leader both in terms of the level and range of model evaluation activities. In addition to constantly evaluating CMAQ in its various revisions using traditional and diagnostic model evaluation approaches, they have pioneered dynamic, operational and probabilistic air quality model evaluation approaches. More importantly, they have used their evaluation activities to spur model improvements in innovative and practical ways. They have also made the model evaluation tools available to the user community.

A potential weakness is that they need to examine their model evaluation efforts in a meta (overall or global) fashion, that is, they need to identify and synthesize what they have really learned from all their evaluation activities. One of their emerging activities, probabilistic evaluation, will require more development and applications to realize its full potential.

Recently the NAAQS process required characterizing the uncertainties in CMAQ's simulations of nitrogen and sulfur oxides deposition. This uncertainty characterization was not readily available to OAQPS as part of one of the more important EPA functions, establishing and revising secondary NAAQS.

Chemistry - strengths and weaknesses

The caliber of expertise and research on the CMAQ atmospheric chemistry components is high. Substantial uncertainties in gas-phase and aqueous-phase mechanisms remain including key inorganic reactions, aromatic and biogenic reactions and aqueous-phase chemistry. We encourage the group to devote more attention to the field validation of the calculated photolysis rate constants (actual actinic flux comparisons, for example). The work to incorporate more realistic aqueous-phase chemistry mechanisms is very good and efforts are needed to elevate the standards of the aqueous-phase chemistry mechanisms to those of the gas-phase mechanisms. Future directions might include incorporation of stratospheric chemistry as the CMAQ spatial domain increases and climate applications are considered.

Particulate Matter - strengths and weaknesses:

One of the principal strengths of the CMAQ group's work on particulate matter is its relevance to the Agency. Recent analyses of the costs and benefits of the Clean Air Act (http://www.epa.gov/cleanairactbenefits) indicate that the cumulative benefits of the Clean Air Act will exceed $2 trillion by 2020, far exceeding its cost. Most of the benefits are attributed to the reduced mortality and morbidity associated with reductions in fine particulate matter. Yet significant scientific uncertainty remains regarding the relative strengths of the sources of major components of fine PM, especially organic carbon and metals/dust. The CMAQ model improvements developed by the CMAQ group, which allow for tracking of molecular and atomic tracers of aerosol sources, will enable a much more integrated approach to addressing this uncertainty in PM sources. The scientific community has recognized this contribution, and the. journal publication describing this advance is one of the most frequently cited papers published in Atmospheric Environment over the past 5 years (Kleindienst, et al., Atmospheric Environment, 41, 8288-8300, 2007; cited 62 times as of 6/28/2011).

Model predictions of sulfate formation now exhibit significant bias. Recent changes to gas phase chemical mechanisms and cloud processing have improved certain aspects of model performance, but have led to increased bias in predictions of sulfate formation. Identifying and removing these sources of bias should be a high priority for the Division.

There is increasing evidence that multiple heterogeneous processes will have significant impacts on predictions of criteria pollutant concentrations. These include cycling of oxides of nitrogen, aerosol chloride/reactive chlorine gas cycling, gas and particle phase reactions of semi-volatile organics, and other processes. While the Division is commended for developing methods for approaching problems individually, there is a need to examine the problem in a more comprehensive and integrated manner. As an example of a solution to one problem making solutions to others more difficult, using techniques such as volatility basis sets for characterizing physical partitioning of organic semivolatiles may make treating the reactivity of those same semi-volatile species more difficult.

As the largest group dedicated to regional air quality model development, the Division should continue to play a leadership role in defining comprehensive modeling approaches to gas-particle interactions.

Meteorology - strengths and weaknesses

As previously mentioned, embracing simple models constrained by observations is a clear strength of the program. This has led to increased efficiency in having models simulate the atmospheric processes rather than the approach of using endless tuning of a large number of parameters. The allegiance of the CMAQ team to the fundamentals like mass conservation as expressed in the governing equations is noteworthy. While such attention to detail might not make much difference in short-term simulations, the longer-term simulations inherent in the proposed hemispheric work would require mass to be conserved.

Their recent work on including the effects of aerosols in the photolysis rates is also important. However, given the errors in aerosol prediction and uncertainty in emissions and fire characteristics, the CMAQ team should consider using observations such as satellite-derived Aerosol Optical Depths (AOD) or even reflectance to constrain results id their uncertainties are not too large. They demonstrated that better specification of albedo determined from land use dependent albedo derived from satellite retrievals improves photolysis rates.

As previously indicated, data assimilation in WRF is a useful tool for hindcasting (and forecasting) simulations and this has been clearly demonstrated in their work.

<u>Coupled WRF-CMAQ</u> - strengths and weaknesses

The effort concerned with creating an on-line coupling code for the WRF-CMAQ system is viewed positively and is well thought out. While some reviewers are persuaded that having the coupling as it is currently designed is sufficient and allowing CMAQ and WRF to advance independently, other panel members believe that a closer coupling between the meteorological and air quality models is desirable. The CMAQ group should continue to weigh the advantages and disadvantages of the coupling design. One direction to consider is to have a workshop of experts in the field who have considered various coupling issues. OAQPS and other clients should be participants in the coupling design decision-making process.

4.3 What is the quality and relevance of the model development, application, and evaluation being conducted as part of the CMAQ Modeling program to the four ITR Programs?

The approach this group has taken to develop CMAQ and to foster and support its use should be taken as a model of success within EPA. This program has been, is, and will continue to be, very relevant to the needs of EPA and state regulatory agencies in their policy and regulatory applications as well as to the scientific community. The model enjoys a remarkably wide and growing user community because it is viewed as being of scientifically high quality, relatively easy to use and well supported by EPA, CMAS, and the community. Furthermore, it has continued to evolve successfully to become a state-of-the-science model. The range of applications (e.g., assessment of emission change impacts, identification of source impacts, support of potential regulatory direction changes, evaluation of impacts of climate change on surface level air quality, design of monitoring and observation networks, and providing spatial pollutant fields for health and exposure assessments) are all extremely relevant to the needs of

EPA and state and local governments. The efforts of the group are central to the role that the Air, Climate and Energy and the Sustainable and Healthy Communities components of ITR will play in ORD and EPA. The CMAQ group will also play important roles in the Chemical Safety for Sustainability (e.g., by the development of a version to evaluate toxic air contaminants) and the Safe and Sustainable Water Resources (e.g., by providing depositional loadings of acidifying and eutrophying species). EPA ORD researchers in all of the four ITRs should be made aware of CMAQ and its capabilities.

Air, Climate and Energy (ACE) (quality and relevance)

Though this team is new to the climate arena, we believe they have selected an important topic: changes in the observed diurnal temperature range. This is one of the biggest signals in the observed surface global temperature records, and it has not been simulated well by the GCMs. While there have been many hypotheses for this change (e.g., from increasing clouds, to airplane contrails, to land use change or dynamics of the stable boundary layer), the role of anthropogenic aerosols in relation to this change deserves attention. The role that dimming of insolation by aerosols has in decreasing day time temperatures and the enhanced Long Wave forcing at the surface at night that leads to warming is reasonable and has been proposed by others. However, the CMAQ team has the type of complete model that can add specificity of to the quantification of this process; however, here, the team must be careful. They have found several areas where running the models for the longer hemispheric time periods leads to large scale balance and drift problems (in both the chemistry and physics). Global models have always had drift or flux corrections built in. Working with other global modelers may be useful here and they may have a niche if they can concentrate on shorter-term simulations using the constrained meteorology through FDDA.

Because of EPA's extensive past efforts on the climate change-air quality interface, including the work under the STAR program, the panel believes that CMAQ group is well positioned to participate in the ORD's refocused research program on ACE as one component of the new organizing paradigm of ITR. Past efforts have focused on the effects of climate change on surface-level ozone ("climate change penalty"). The Panel strongly suggests that CMAQ group extend this work to consider the effect of climate change on PM2.5 and on the effects of projected emissions (for the American Continent) of ozone and PM2.5 precursors (say, to the years 2050 or to 2100) on ground-level air quality. For the energy component of the ACE research program area, CMAQ group should work with the EPA's National Risk Management Research Laboratory to develop realistic future energy (production and consumption) scenarios that can be used with the CMAQ modeling efforts.

Chemical Safety for Sustainability (CSS) (quality and relevance)

The CMAQ team needs to carefully define its mission within this area. Is the CSS application long-term regulatory planning, emergency response, or something else? CMAQ is a potentially useful tool for chemical safety applications, but it may be “overkill” for many of them. Dispersion modeling without atmospheric chemistry is normally used for planning the emergency response to chemical accidents, and a tool such as the NOAA Ready system is currently more suitable for this purpose. Another limitation to using CMAQ is that the chemical mechanisms included in the model are not particularly relevant to the broad range of chemicals that may need to be modeled.

Sustainable and Healthy Communities (SHC) (quality and relevance)

CMAQ has the potential to be used widely for health studies if it can overcome some barriers, including limits on its application scale and resource requirements. EPA has explored some of these possibilities, and the results are inconclusive. Potential benefits could be achieved if the SHEDS (a multi-media exposure model) efforts were more closely linked to CMAQ and if the two groups identified how the two models could work together best.

Safe and Sustainable Water Resources (SSWR) (quality and relevance)

CMAQ is relevant to water resource modeling. It includes modules to simulate the deposition of acids and other chemicals to dry and aqueous surfaces. It simulates the aqueous phase chemistry that affects precipitation composition. There has been less research on deposition and aqueous phase chemistry recently due to reduced concerns about acid deposition. New process based research may be required to develop the data base that the CMAQ team will need before further development of the SSWR model.

4.4 What are your perceptions of the integration across different elements of the CMAQ modeling program (links among 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?

With respect to the usefulness of the CMAQ modeling program to the EPA, there are areas where the CMAQ group needs to be especially vigilant. A primary user of CMAQ type tools is OAQPS EPA. While the effort should not be viewed negatively, OAQPS is using a competing model, because CMAQ does not have all the capabilities they desire (tools to provide source impacts on ozone and particulate matter). If this capability is important and scientifically appropriate, the group should consider adding it. If there are scientific reasons why the approaches taken by OAQPS are scientifically less well founded, this concern should be clearly communicated to them.

The CMAQ group can provide other very important function to EPA. In the recent NOx/SOx secondary NAAQS review, the CASAC panel was critical of the level of evaluation provided for the CMAQ simulations. CASAC was critical of the approach, specifically in reference to the use of CMAQ results in the development of parameters for the Atmospheric Acidification Index (AAI). Since that time, the EPA Administrator decided that the uncertainties in determining the factors as part of the AAI were too large to go forward using the approach for determining AAI. As a step toward reducing the uncertainties and preparing for the next NAAQS review, the Administrator has proposed a five-year pilot field study. The CMAQ team should be very actively involved in the design and analysis of the pilot field study. Further, the CMAQ team should use this as a platform for a very detailed evaluation of the modeling system's ability to provide the needed information, including providing well-assessed, quantitative uncertainties, and quantitatively identify the sources of the uncertainties.

The CMAQ group has done a fine job in developing CMAQ as a stand-alone model and continues to enhance its strengths. In the future, regional models will not be stand-alone and will require more integration with other models. There will also be pressure to expand the domains where CMAQ is used. Yet, in a time of diminishing resources, the group will need to be very careful about setting priorities and should focus on doing a limited number of things very well, as opposed to doing many. We recommend that the CMAQ group should continue to develop and enhance the strengths of CMAQ.

Of particular concern is that future model development will require close collaboration with experts who develop other modeling systems. The CMAQ group will need to be careful to choose problems that they contribute their expertise to. The Division's role in this expanding community has not yet been articulated and needs to be defined. The user community should be an active participant in helping the CMAQ group define its future directions.

The CMAQ group has been especially successful in their efforts to continually advance the science to address new problems, increase user confidence, and make the model usable both inside and outside the agency. They need to continue to advance the scientific and application capabilities and articulate the importance of these activities to the broader community both inside and outside the agency. If CMAQ were to fall behind, other key activities of EPA would become more vulnerable to outside attack.

The CMAQ group is one of the very few groups worldwide that has the expertise and size to develop, maintain, and evolve such a model. This is a unique capability that needs to be maintained. This recognition re-enforces the need to stay focused and not to go beyond their core mission and competencies.

The CMAQ group needs to define and communicate their priority setting process better. This is particularly important and timely because they will soon be searching for a new director. They have done well by using their very extensive efforts in model evaluation to identify model development needs. They have also been cognizant of their impacts on control strategies. They should extend their model evaluation culture to other groups at EPA. They should also maintain their international collaborations.

4.5 Are there any modeling research areas that are relevant to the EPA's regulatory program needs not being addressed or given insufficient attention within the CMAQ Modeling Program? Are there any current areas of research emphasis that could be given a lower priority or eliminated to help advance the above four ITR areas? Are the resources made available to the CMAQ Modeling Program being used effectively in terms of the choice and quality of the applied research being conducted at AMAD in support of the four ITR areas?

The CMAQ group should review their efforts over the past decade to identify their successes, discern the reasons for them, and use this information to help guide their future research. The CMAQ group also needs to be cognizant of the costs associated with maintaining the increasing complexity of the models and the data used. This should be actively considered in their priority setting process.

There are many groups involved in global modeling efforts concerned with projecting future climates based on hypothesized feedback and process assumptions as well as assumed emission scenarios. However, there are few that are investigating process sensitivities or emission sensitivities in detailed retrospective runs. Given the CMAQ team's successes in recreating the past atmospheres in retrospective studies, this could be a niche that they could play in the global climate arena.

Throughout the review there were many examples that indicated 1 to 3 ppb changes in ozone concentrations occurred as a result of improvements the CMAQ team made to the surface albedo, chemical mechanisms, land surface characteristics, deposition and temperatures. There was not much attention given to cloud errors (misplacement in time and space) in impacting ozone prediction. In past studies with university partners, there were examples [Pour-Biazar et al., 2007] that showed that replacing model transmittance with satellite derived transmittance made differences of 50 ppb or more dwarfing the impact of the other changes. While the university partners may have developed the core techniques, they may not be in a position or have the skills to bring this research into an operational framework as well as the core CMAQ team. This may be low hanging fruit that can make a big impact on ozone prediction that could be facilitated with assistance from the CMAQ team.

5.0 Comments on the Review Process

Copies of the power point files for the talks and the posters should be provided to the Committee prior to the review. Assignments should be given to the reviewers ahead of time, e.g., the specific areas that they will be expected to lead should be identified. The review should begin with more direct interactions with the group leaders (two to four of the high level leaders) and the Committee. The expectations for the review should be discussed and the type of information that would be most useful should be identified. After that, there should be a 30-minute planning meeting of the Review Committee to organize their effort.

6.0 Panel Recommendations

The panel made four recommendations that they would like the CMAQ group to implement over the next few years, provided that they have resources to accomplish this. They are:

1. Improve the emission inputs to the CMAQ model, and allocate more resources to the overall task concerned with improving emission inputs to the CMAQ model even if they are taken from another activity. They should enhance collaborations with the developers of emissions data, OAQPS and OTAG.
2. Work with OAQPS and other groups in EPA to help them accomplish their goals. The relationship with OAQPS is strong, but the CMAQ group needs to be more proactive in anticipating and responding to the needs of OAQPS, the Office of Atmospheric Programs, the Office of Air and Radiation, and other user needs.
3. Improve the connections between CMAQ and other models, and as they move forward, they should consider the relationship(s) between CMAQ and other models as (e.g., global chemical models, local scale models, and personal exposure models), and determine how to best mesh with such a diverse set of platforms.
4. Develop a comprehensive approach to gas-particle interactions, and continue to improve their treatment of secondary aerosol (inorganic and organic) formation.

7.0 References

Buzcu, B., Z. W. Yue, M. P. Fraser, V. Nopmongcol and D. T. Allen "Secondary particle formation and evidence of heterogeneous chemistry during a wood smoke episode in Texas," *Journal of Geophysical Research*, II, DIOS13, doi: 10.1029/2005JD 006143, 2006)

O'Brien J.J., 1970: Alternative solutions to the classical vertical velocity problem. J. Appl. Meteor., 9, 197-203.

Pleim, J.E., 2007: A combined local and non-local closure model for the atmospheric boundary layer. Part 1: Model description and testing. J. Appl. Meteor. Climatol., 46, pp 1383-95.

Pour-Biazar, Arastoo, et al. (2007), Correcting photolysis rates on the basis of satellite observed clouds, *J. Geophys. Res*, 112, D10302)

CMAQ PEER REVIEW MEETING

June 27-29, 2011

Agenda

<u>June 27</u> (***Room C112***)

8:30am	Refreshments
9:00am	ORD Research Directions: Integrated Trans-disciplinary Research (Bob Dyer; Director, NERL)
9:15 am	Purpose and Charge to Panel (ST Rao)
9:30 am	Summary of 2006 Review Recommendations and AMAD Response/Progress (Rohit Mathur)
10:30 am	BREAK
11:00 am	Using evaluation to shape improvements and provide guidance for model development (v4.6 to v4.7 to v5.0) (Tom Pierce)
12:00	LUNCH
1:00-4:00pm	POSTER SESSION and Interaction with AMAD Scientists (***Building B Atrium***)

Diagnostic Evaluation (multiple topics)

1. Diagnostic analysis of carbonaceous aerosol predictions by CMAQ (Prakash Bhave)
2. Improving meteorology and climate simulations using Four Dimensional Data Assimilation (Rob Gilliam)

Operational Evaluation

3. Incremental testing and evaluation of CMAQv4.7 (Shawn Roselle)
4. Application of the CMAQ model for the Air Quality Model Evaluation International Initiative (AQMEII) (Wyatt Appel)

Enhancements

5. DDM implementation, development, and application (Sergey Napelenok)

Dynamic Evaluation

6. Recent Dynamic Evaluation Studies of the CMAQ Model (Jim Godowitch)

Probabilistic Evaluation

7. Probabilistic Evaluation of AQ Models: Motivation, Concepts, and Applications (Kristen Foley)

Emerging Application Needs

8. Model applications motivate CMAQ model development and evaluation (Ken Schere)

4:00pm Overview of CMAQv5.0 (Rohit Mathur)

June 28 (***Room C111B***)

8:30am Recap of Day 1 and Questions from Panel

9:00am-Noon: CMAQv5.0: Updates to process modules (20 min talk +10min discussion)

9:00am Atmospheric Chemistry Mechanisms in CMAQ (Deborah Luecken)

9:30am Treatment of Aerosol Processes (Golam Sarwar)

10:00am Characterization and Modeling of Emissions (George Pouliot)

10:30am BREAK

11:00am Representation of Transport Processes (Jon Pleim)

11:30am Advancements in the science and applications of CMAQ air-surface exchange (Jesse Bash)

12:00 LUNCH

1:00pm WRF-CMAQ 2-way model: Overview (Jon Pleim/Rohit Mathur)

2:00-5:00pm POSTER SESSION and Interaction with CMAQ GROUP Scientists (***Building B Atrium***)

Chemistry

1. Major changes of gas phase chemistry in CMAQv5.0 (Bill Hutzell)
2. Improving the treatment of oxidized nitrogen (Rob Pinder)
3. Understanding the impact of isoprene nitrates and OH reformation on regional air quality using recent advances in isoprene photo-oxidation (Ying Xie)

Aerosol updates

4. Speciation of PM_{other} in CMAQ (Heather Simon)

Emissions

5. Improvements in characterization of emissions for air quality modeling (Tom Pierce)

Deposition

6. Enhanced Land Surface and Land Management Treatments for CMAQ Air Surface Exchange (Ellen Cooter/Donna Schwede/Robin Dennis)

Computational and Structural Aspects

7. Making CMAQ more user friendly (Jeff Young)
8. Numerical models on high performance computing (HPC) systems (David Wong)

Hemispheric Extensions

9. Hemispheric Extensions of CMAQ: Motivation, Challenges, and Progress (Rohit Mathur)

June 29 ***(Room C112)***

8:30am *Recap of Day 2 and Questions from Panel*

9:00am *Panel work time*

11:30am *Debriefing to AMAD Management and PIs*

12:00noon *END OF PEER REVIEW MEETING*