Final Report:
Fifth 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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List of Acronyms

ACE	Air, Climate, and Energy (ORD program)
ACM2	Asymmetric Convective Model version 2
AMAD	Atmospheric Modeling and Analysis Division (EPA)
AOD	aerosol optical depth
API	application programming interface
APT	Advanced Plume Treatment (module)
AQ	air quality
AQMEII	Air Quality Model Evaluation International Initiative
BEIS	Biogenic Emissions Inventory System
BELD	Biogenic Emissions Landuse Database
BENMAP	Environmental Benefits Mapping and Analysis Program
CARB	California Air Resources Board
CB	Carbon Bond (chemical mechanism)
CCN	cloud condensation nuclei
CCTM	CMAQ Chemical Transport Model
CMAQ	Community Multi-scale Air Quality (model)
CMAS	Community Modeling and Analysis System
CSD	Chemical Sciences Division (NOAA)
CSS	Chemical Safety for Sustainability (ORD program)
DDM-3D	Decoupled Direct Method 3D
DISCOVER-AQ	Deriving Information on Surface conditions from COlumn and VErtically resolved observations Relevant to Air Quality
DMS	dimethyl sulfide
EFIG	Emission Factor and Inventory Group (EPA)
EPA	Environmental Protection Agency
EPIC	Environmental Policy Integrated Climate (model)
FDDA	four-dimensional data assimilation
FEST-C	Fertilizer Emission Scenario Tool for CMAQ
GCAM	Global Change Assessment Model
GCM	general circulation model
GHRSST	Group for High Resolution Sea Surface Temperature
HEASD	Human Exposure and Atmospheric Sciences Division (EPA)
HTAP	Hemispheric Transport of Air Pollutants
ICARTT	International Consortium for Atmospheric Research on Transport and Transformation
I/O	input/output
IRR	integrated reaction rate
ISORROPIA	not an acronym – meaning is “equilibrium” in Greek
ISAM	Integrated Source Apportionment Method
IVOC	intermediate-volatility organic compounds
KPP	Kinetic PreProcessor
LBC	lateral boundary condition
LSM	land-surface module
MAGIC	Model of Acidification of Groundwater In Catchment model

MARKAL	Market Allocation Model
MCM	Master Chemical Mechanism
MEGAN	Model of Emissions of Gases and Aerosols from Nature
MODIS	Moderate Resolution Imaging Spectroradiometer
MPAS	Model for Prediction Across Scales
MPI	Message Passing Interface
NAAQS	National Ambient Air Quality Standard
NAS	National Academy of Sciences
NASA	National Aeronautics and Space Administration
NEI	National Emissions Inventory
NERL	National Exposure Research Laboratory
NLCD	National Land Cover Dataset
NOAA	National Oceanic and Atmospheric Administration
NRMRL	National Risk Management Research Laboratory
NRT	near real time
OAQPS	Office of Air Quality Planning and Standards
OLAM	Ocean Land Atmosphere Model
ORD	Office of Research and Development
PBL	planetary boundary layer
PM	particulate matter
PMEL	Pacific Marine Environmental Laboratory (NOAA)
P-X	Pleim-Xiu
RACM	Regional Atmospheric Chemistry Mechanism
RFP	Request for Proposal
RWC	residential wood combustion
SAPRC	State-wide Air Pollution Research Center (chemical mechanism)
SHC	Sustainable and Healthy Communities (ORD program))
SHEDS	Stochastic Human Exposure and Dose Simulation model
SIP	State Implementation Plan
SMOKE	Sparse Matrix Operational Kernel Emissions
SNODAS	SNOw Data Assimilation System
SOA	secondary organic aerosol
SREF	short-range ensemble forecast
SST	sea surface temperature
SSWR	Safe and Sustainable Water Resources (ORD program)
STAR	Science To Achieve Results
STE	stratosphere-troposphere exchange
UC	University of California
USGS	U.S. Geological Survey
VBS	volatility basis set
VIC	Variable Infiltration Capacity macroscale hydrologic model
VOC	volatile organic compounds
WRF	Weather Research and Forecasting (model)
WRF-CHEM	WRF model with coupled online CHEMistry
WRF-CMAQ	WRF model with coupled online CMAQ

1. INTRODUCTION

The Fifth CMAQ Model Peer Review Panel conducted a two-and-a-half-day review of the Community Multiscale Air Quality (CMAQ) Modeling Program on June 17-19, 2015. The panel focused on CMAQ model development, evaluations, and applications since the last peer review, which took place in 2011. This report summarizes the Fifth Panel's findings. Note that this report follows the series of reports from four previous peer reviews conducted in 2003, 2005, 2006, and 2011 [see Amar et al., 2004, 2005; Aiyyer et al., 2007; and Brown et al., 2011]. The report is written from the perspectives represented by the seven-member review panel: Marina Astitha, Kelley Barsanti, Nancy Brown, Ajith Kaduwela, Stuart McKeen, Michael Moran, and Ken Pickering. Panel members read a considerable volume of material on CMAQ provided by EPA and attended two days of presentations on CMAQ by EPA staff (see Appendix 1 for the meeting agenda).

The CMAQ model has been developed by the Atmospheric Modeling and Analysis Division (AMAD) of the National Exposure Research Laboratory (NERL), Office of Research and Development (ORD), U.S. Environmental Protection Agency (EPA). AMAD develops comprehensive state-of-the-science air quality models and modeling tools for use in policy, regulatory analysis, and research. This review focused on the work since the last peer review in 2011 that has been conducted by the 16.5 staff scientists (i.e., full-time equivalents) within AMAD who work on CMAQ development and evaluation. This 2015 CMAQ Peer Review emphasized an assessment of the meteorological, physical, and chemical process aspects of the CMAQ Modeling Program, as well as model applications and evaluations of model performance. The review panel focused its attention on the current community version of CMAQv5.0.2, which was released in May 2014, as well as the next community version, CMAQv5.1, which is to be released in October 2015.

The panel was charged with evaluating the overall quality of the applied scientific research in the CMAQ Modeling Program. The panel considered the following five topics within the context of AMAD's mission to develop air quality models for regulatory purposes:

(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 evaluation being conducted as part of the CMAQ Modeling Program to ORD's research program areas;

(4) the integration across different elements of the CMAQ Modeling Program and its usefulness to the EPA, states, and other customer needs, and research community;

(5) the modeling research areas that are relevant to the EPA's regulatory program needs that are not being addressed or given insufficient attention or that could be given less attention or eliminated and the effectiveness of the use made of CMAQ Modeling Program resources.

With respect to the third evaluation topic, ORD research is organized around six national research programs. AMAD's research on CMAQ development, evaluations, and applications primarily falls within four of these programs:

(1) Air, Climate, and Energy (ACE);

(2) Safe and Sustainable Water Resources (SSWR);

(3) Sustainable and Healthy Communities (SHC);

(4) Chemical Safety for Sustainability (CSS).

The core CMAQ development and evaluation work is conducted under the ACE research program. CMAQ applications for ecological studies and applications linking CMAQ to water quality systems are being conducted under the SSWR research program. Use of CMAQ output for both ecological and health assessments falls under the SHC program. AMAD also had a small focused effort on assessing impacts of nano-materials, in particular nanoscale cerium, under the CSS research program, but this effort has come to a close and currently there is no involvement in the CSS program. Currently, AMAD's CMAQ-related research portfolio can broadly be classified as 75% in ACE, 15% in SSWR, and 10% in SHC.

The CMAQ modeling system simulates a wide range of physical, chemical, and biological processes. Some of these processes are well understood, some are reasonably well understood, and some remain poorly understood. This wide range in our level of knowledge about the processes being modeled, and the fact that parameterizations of some of the processes remain areas of active research worldwide, means that some parts of the model code are sufficiently well established as to be considered "good enough" at this time whereas other parts of the code are undergoing continuing development. Because the CMAQ modeling system serves as both a regulatory tool for the evaluation of alternative control strategies and as a research tool, two versions of the model code exist at all times: one version, known as the "community" version, is a reasonably up-to-date and stable version of CMAQ that is used for regulatory and policy simulations while the other is a developmental version of CMAQ that is continually being improved by AMAD's CMAQ development team and by researchers outside the EPA. The CMAQ community of users includes federal, regional, state, local, and non-U.S. agencies involved in either AQ policy and regulation or operational AQ forecasting as well as university and other research groups and consulting companies in the U.S. and elsewhere.

AMAD now follows a development cycle where every three to four years the existing CMAQ community version is replaced by a newer developmental version, thus bringing recent advances in atmospheric science and improvements in computational efficiency to the EPA's regulatory arm and to others in the CMAQ user community. The CMAQ external peer review panel is part of this cycle, and a panel is now convened prior to each major model release. The last such major release was the release of CMAQv5.0 in early 2012, which was preceded by the Fourth External Peer Review in mid 2011. The next major release, CMAQv5.1, is expected in late 2015, thus requiring the current Fifth External Peer Review that is the subject of this report.

For this reason, the Fifth Peer Review Panel focused largely on CMAQv5.1, which will be the new community version, but it also paid attention to how AMAD assesses and transfers new research into its modeling tools and to plans for further CMAQ development. In reviewing the state-of-science in the CMAQ model, the panel recognized that CMAQ is primarily a model for regulatory applications and assessments and hence the panel tried to balance the desire for scientific completeness and rigor in the model with the need for computational efficiency that is required of a regulatory model. However, the community version of CMAQ is also used as a research tool by many groups, so that the research community is another important client of

AMAD (though not its primary client), which introduced another perspective into the panel's deliberations.

The consensus of this panel is that AMAD and the CMAQ team have done an excellent job in responding to the recommendations from the Fourth Peer Review Panel and in improving the CMAQ code over the past four years. CMAQv5.1 appears to represent a significant step forward and the panel sees no reason that it should not be released as planned. In the rest of this report, the panel summarizes major CMAQ developments since the release of CMAQv5.0 (Section 2) and AMAD's responses to the recommendations of the Fourth Peer Review Panel (Section 3), addresses the five charge questions to the panel and makes a number of specific recommendations (Section 4), provides some comments about the review process itself for both the EPA and future panels (Section 5), and concludes with five high-level recommendations related to future CMAQ development for consideration by AMAD (Section 6). With respect to Section 6, the panel considers the need for further model development to be a "given" since it is clear that further advances can be expected in our understanding of air quality science in the coming years, and this new science will need to be incorporated into future model versions.

2. MAJOR DEVELOPMENTS SINCE THE FOURTH EXTERNAL PEER REVIEW

The CMAQ model has continued to evolve since the last (fourth) external peer review in 2011, which preceded the release in February 2012 of CMAQv5.0. This major release was followed by (a) the release in June 2012 of CMAQv5.0.1, a minor release, (b) the release in April 2014 of CMAQv5.0.2, a significant release that included some changes to the science algorithms in the base model and a number of new diagnostic/scientific modules, and (c) the release in April 2015 of a patch for the Decoupled Direct Method (DDM) for CMAQv5.0.2 and the release of CMAQv5.1beta. The final version of CMAQv5.1 is expected to be released in October 2015.

Many improvements and enhancements have been made to the CMAQ code and to the rest of its supporting modeling system over the past four years. These include many science updates, revisions to the code structure and numerics for faster execution, improved physics and data assimilation in WRF (the Weather Research and Forecasting numerical weather prediction model), and improvements to the two-way coupled WRF-CMAQ system. A number of the model improvements address issues related to ozone, sulfate, organic carbon, and $PM_{2.5}$ predictions that were identified by extensive evaluation of CMAQ v5.0 performance (e.g., Appel et al., 2013; Napelenok et al., 2014). Major model areas where there has been significant progress since 2011 include the following:

<u>Emissions</u>

A consistent series of annual U.S. and hemispheric emissions inventories was developed for the 21-year period 1990-2010. The Biogenic Emissions Inventory System (BEIS) model has been updated to version 3.61, which includes a two-layer canopy model and uses BELD4, a new version of the Biogenic Emissions Landuse Database. The treatment of sea-spray PM emissions has been upgraded to enhance fine-mode emissions, add a dependency on sea surface temperature (SST), and reduce coastally-enhanced emissions. Updates were also made to the volatile organic compound (VOC) speciation profile library to support the new CB05e51 chemical mechanism as well as enhancements to the secondary organic aerosol (SOA) module.

Meteorology and Transport

CMAQ has been modified to use WRF version 3.7, which was released in April 2015. This new version of WRF includes improvements to the Pleim-Xiu land surface module (P-X LSM) and Asymmetric Convective Model version 2 (ACM2) options. Among them are better treatment of the evening transition period, convective feedbacks to radiation, updates to the treatment of wetlands and snow albedo, the ability to use any of three land-use data sets (USGS, MODIS, and NLCD), a treatment of impervious urban surfaces, and new high-resolution snowcover and SST data sets. The ACM2 code in CMAQ was also updated to be consistent with the above changes. A new iterative LSM data assimilation scheme has been developed for high-resolution applications.

Chemistry

Updates have been made to a regulatory gas-phase chemistry mechanism (CB05) and two research mechanisms (SAPRC07, RACM2) and an improved treatment of organic nitrate has been added to CB05. An optional dynamic aqueous-phase chemistry scheme has been introduced. Two versions of halogen chemistry have been added: as an explicit mechanism and as a parameterized first-order depletion process. In-line photochemistry has been introduced with consistent coupling to PM concentration fields and to WRF meteorological fields such as clouds. Heterogeneous reactions have been restructured and linked to gas-phase chemistry.

Aerosols (Particulate Matter)

Additional sources of SOA have been introduced. Code for a volatility basis set (VBS) treatment for modeling SOA was contributed by the CMAQ community (ENVIRON International Corp.). An improved treatment of ultrafine particles, including revised emissions, size distribution, and nucleation, has been implemented and the gravitational settling of particles is now considered in all model layers, not just the lowest layer.

Deposition and Air-Surface Interactions

A number of refinements were made to the bi-directional flux scheme for NH_3, first introduced in CMAQ version 5.0. These include updates to the Fertilizer Emission Scenario Tool for CMAQ (FEST-C) system to make it more accurate, more user-friendly, and faster. The description of land use has also been made consistent across the WRF, CMAQ, and Environmental Policy Integrated Climate (EPIC) models.

Model Structure and Numerics

A new parallel I/O scheme was implemented to improve I/O performance on large parallel computers, particularly writing data to disk. A more efficient planetary-boundary-layer (PBL) solver was implemented for ACM2 and code for horizontal advection, aerosols, and chemistry was optimized based on profiling (i.e., timing) results. The structure of some mechanisms was also revised to facilitate code changes that are less prone to error.

Two-Way Coupled WRF-CMAQ Model

The coupled WRF-CMAQ model has been updated to WRFv3.7 and CMAQv5.1. Improvements have been made to the calculation of aerosol direct radiative effects, including implementation of an efficient Mie scattering algorithm and a core-shell treatment of black carbon. A research version of aerosol indirect effects and feedback has also been developed. The coupled WRF-CMAQ model was a participating model in Phase 2 of the Air Quality Model Evaluation International Initiative (AQMEII2), whose focus was the evaluation and intercomparison of regional-scale online coupled meteorology/chemistry model simulations [poster, Hogrefe et al.].

Model Evaluation

As one step towards the release of CMAQv5.1, a comprehensive evaluation of the beta version of CMAQv5.1, which was released in April 2015, has been completed for both incremental changes and all changes [presentation, Roselle et al.]; a corresponding evaluation of CMAQv5.1 is underway. Both concentration and deposition predictions have been examined. A concerted effort has been made to explore dynamic evaluation further with a focus on air quality changes associated with the 2002 NOx SIP call and with decadal time trends in 8-hour ozone extremes and annual regional wet deposition [poster, Foley et al.]. As noted above, CMAQ was a participating model in AQMEII2 [poster, Hogrefe et al.]. A developmental version of the WRF-CMAQ system has been running in near real time (NRT) within AMAD since 2013 and model predictions are compared with AIRNOW measurements on an ongoing basis [presentation, Eder et al.].

Instrumented Models

Three different source sensitivity and source apportionment schemes were included with the v5.0.2 release: the Decoupled Direct Method 3D (DDM-3D), the Sulfur Tracking scheme, and the Integrated Source Apportionment Method (ISAM) [poster, Napelenok et al.].

Applications

CMAQ applications since 2011 include a 21-year hemispheric simulation using the coupled WRF-CMAQ system [poster, Xing et al.], WRF-CMAQ ensemble modelling to examine meteorological uncertainty [poster, Gilliam et al.], fine-scale simulations of DISCOVER-AQ field studies on model grids down to 1-km and 2-km horizontal grid spacing [poster, Appel et al.], ecosystem and human-health studies [poster, Garcia et al.], and projections of the impacts of regional climate change on air quality and human health [poster, Nolte and Spero].

3. SPECIFIC RECOMMENDATIONS OF THE FOURTH PEER REVIEW PANEL AND EPA RESPONSES

The 2011 Fourth Peer Review Panel made four high-level recommendations to improve CMAQ performance, usefulness, and relevance, along with a number of more detailed recommendations (Brown et al., 2011). The four recommendations were the following:

(1) Improve the emission inputs to the CMAQ model and allocate more resources to this task;

(2) Work with the Office of Air Quality Planning and Standards (OAQPS) and other groups in the EPA to help them accomplish their goals;

(3) Improve the connections between CMAQ and other AQ-related models, such as global models, local-scale models, and exposure models; and

(4) Develop a comprehensive approach to gas-particle interactions and continue to improve their treatment of secondary inorganic and organic aerosol formation.

AMAD examined and considered all of the recommendations made by the 2011 Panel after that review. At the beginning of the 2015 Fifth Peer Review, Dr. Rohit Mathur of AMAD gave a presentation that summarized AMAD's responses to this earlier set of recommendations. Details of Dr. Mathur's presentation can be found in Appendix 2.

Based on his presentation, which describes the many responses undertaken by AMAD over the past four years, the consensus of this panel was that AMAD and the CMAQ team have done an excellent job in responding to the recommendations from the Fourth Peer Review Panel and in improving the CMAQ code over the past four years.

4. PANEL RESPONSE TO CHARGE QUESTIONS

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

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

Though much of the emissions-related research conducted within the EPA falls within the regulatory realm of OAQPS, those emissions that depend on meteorology, especially emissions from natural sources, are the primary responsibility of AMAD. Work related to emissions by the CMAQ team has been wide-ranging and the scientific quality of the research in this area is very high overall.

Research, development, and evaluation of the bi-directional NH_3 flux scheme in CMAQ and development of the Fertilizer Emission Scenario Tool for CMAQ (FEST-C) are documented examples of AMAD leadership in that particular field (see also the "Deposition and Air-Surface Interactions" section). AMAD also has a well-established role in the field of biogenic emissions through its development, evaluation, and public support of the BEIS biogenic emissions module and its companion Biogenic Emissions Landuse Database (BELD). Recent upgrades to these systems with more recent and comprehensive datasets will ensure that the BEIS/BELD methodology remains a viable and useful platform for determining these important emissions. AMAD should also be recognized and commended for current efforts and future plans to collaborate with the broader ecosystem modeling community related to evaluation and updates of BEIS and BELD.

The CMAQ team's emissions research sometimes overlaps with emissions that are routinely handled by OAQPS, and the CMAQ team contributes to the improvement of the U.S. National

Emissions Inventory (NEI) through CMAQ evaluation and feedback. For example, by combining CMAQ with source apportionment tools (ISAM) and comparisons with southeastern U.S. aerosol composition measurements, including organic tracers, they were able to show a systematic negative bias in residential-wood-combustion (RWC) emissions and possible errors in the RWC temporal profiles within the NEI. On the other hand, case studies of CMAQ wintertime $PM_{2.5}$ overpredictions in the northeastern U.S. pointed to a problem of overallocation of RWC emissions to major urban areas. In a third study, an analysis and evaluation of aerosol composition measurements related to mineral dust and soil provided useful information about uncertainties related to dust emissions in the NEI.

The U.S. emissions trend research for the 1990-2010 period by the CMAQ team is considered unique within the emissions modeling community and is providing an important reference for trend-related AQ research within the U.S. and one of the least uncertain components within global emissions trend research. The CMAQ team augmented and modified an existing 1990-2008 global emissions trend data set (Xing et al., 2015a). The broader, international modeling community in general has a high regard for the quality of the science within EPA's NEI and AMAD's contribution to the NEI. AMAD has been a key contributor to the emissions input files used in two HTAP and three AQMEII model intercomparison study phases.

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

The CMAQ team has been actively experimenting with new techniques to improve the accuracy of the meteorology used to drive the CMAQ model. This activity is important for reducing biases in CMAQ predictions of trace gas and aerosol concentrations, since small errors in PBL height and winds, for example, can lead to large errors in constituent amounts. One goal of the group has been to bring additional observational types into the 4-D data assimilation (FDDA) used with the WRF model, and have less reliance on surface analysis nudging. This is a promising direction for the meteorological modeling. For example, it has been demonstrated that assimilation of wind profiler and Doppler radar-derived winds leads to reduced ozone biases in CMAQ. The importance of determining the uncertainty in the meteorological fields has been recognized by AMAD, and an excellent application of ensemble modeling has led to probabilistic ozone forecasts from the coupled WRF-CMAQ [poster, Gilliam et al.]. The two-way coupling of WRF with CMAQ also has much potential for improving meteorological predictions by including the aerosol feedback effects. Even though this topic needs further investigation, the AMAD CMAQ team is commended for working in this area.

The CMAQ team has also demonstrated the benefits of using new geophysical data sets and of important modifications of the Pleim-Xiu Land Surface Model (PX LSM) and the ACM2 boundary layer scheme in WRFv3.7. New data sets include: (a) impervious surface fraction and canopy fraction data, which affect the surface heat capacity and impact 2-m temperatures; (b) snowcover data from the SNOw Data Assimilation System (SNODAS), which also impact 2-m temperatures; and (c) Group for High Resolution Sea Surface Temperature (GHRSST) data, which is critical for properly simulating coastal circulations. Use of all of these data sets with WRF has demonstrated marked improvement in the meteorological fields used with CMAQ. Improved treatment of wetlands and snow albedo in the PX LSM has also led to reduced bias in 2-m temperatures. The modeling group has recognized that unrealistically weak mixing in the evening and overnight leads to overprediction of surface-emitted species, and they have made appropriate modifications to both the PX-LSM and the ACM2 boundary layer scheme to address this deficiency, thereby improving the quality of science in the model.

Chemistry (quality of science)

The overall quality of the applied scientific research related to chemistry is excellent. The panel is very impressed by both the quality and applicability of various internal scientific investigations conducted by the CMAQ team and their progressive attitude to anticipate (and to be ready for) future challenges related to chemistry.

There are several chemistry research projects in the CMAQ modeling program that deserve special mention here. They are improvements to isoprene chemistry, organic nitrates, heterogeneous chemistry, halogen chemistry, and photolysis rates. Biogenic emissions (mostly isoprene) are important because of their abundance at the global scale and their relative abundance at the regional scale, which will only increase with aggressive emissions control strategies for anthropogenic VOCs. In addition to isoprene's well-known ozone-forming potential, it is now known to be a major precursor for SOA production. Organic nitrates constitute an important class of compounds that are thought to contribute a large (ca. 30%) fraction of total airborne nitrogen and wet-deposited nitrogen (Cape et al., 2011) and that may have implications for emissions control strategies through the hydroxyl radical, NO_x, O_3, and SOA budgets (Mao et al., 2013). In the heterogeneous chemistry of dinitrogen pentoxide (N_2O_5), the inclusion of a second pathway to produce nitryl chloride ($ClNO_2$) is especially important in coastal environments during colder months. This expanded treatment of heterogeneous chemistry has implications for nitrate budgets and emissions control strategies to reduce nitrates. Halogen chemistry is not only important for proper simulation of O_3 production, especially in coastal areas, but it also has implications for deposition of O_3 over oceans. Finally, improvements to in-line calculations of photolysis rates are especially important in environments other than clear-sky conditions. This dynamic calculation can also improve the realism and benefits of coupled models. Thus, the research projects in chemistry undertaken by CMAQ team members are very relevant and we find the quality of them to be excellent.

In addition, CMAQ team members have engaged in several external activities that will lead to further enhancements to the quality of the chemistry research program. First, they have actively participated in organizing/planning of the UC Davis Atmospheric Chemical Mechanisms conference series. This biennial series, started in 2006, has now matured into the premier gathering of international mechanism builders. Second, there is a smaller *ad hoc* group of mechanism builders, convened as a part of this conference series, who meet more often to discuss pressing issues of mechanism updates/development. This group also discusses the development needs for atmospheric chemical mechanisms for future atmospheres resulting from aggressive emissions control strategies and climate change. CMAQ team members are active participants in this group as well. Third, through the aforementioned conferences/*ad hoc* group and through direct contacts, CMAQ team members have engaged with researchers in the United Kingdom (University of Leeds) on the Master Chemical Mechanism (MCM) and its condensed version development. This international collaboration is important to ensure that gas-phase chemistry mechanisms in CMAQ continue to reflect the state of the science.

Recently, the National Academy of Sciences formed an *ad hoc* committee on "The Future of Atmospheric Chemistry Research." This committee is charged with documenting the research needs for the next decade. Although the committee solicited ideas from stakeholders on field, laboratory, and modeling studies, development of chemical mechanisms was not one of the areas highlighted. CMAQ team members, together with the staff from both the California Air Resources Board (CARB) and University of California at Riverside, participated in town-hall meetings organized by this committee and made a strong case for the need to implement results of new basic-science projects in chemical mechanisms. Without that technology transfer, these new findings will not be included in future regulatory applications of models. Highlighting this need was especially important in light of the dwindling funding for mechanism development/updates over the past decade.

It is thus very encouraging to learn that the EPA is working through their STAR program on a future RFP on atmospheric chemical mechanisms for the next-generation air quality models. This is important on three fronts. First, it will provide much needed funding to develop the next generation of chemical mechanisms for air quality modeling. Second, it will allow the air quality modeling community to attract and train the next generation of mechanism builders: the current generation has aged without a new generation following them. Third, it will allow the community to migrate towards a true, community-based mechanism-building paradigm. Currently, mechanisms are built by individuals with very little communication/collaboration among them. The UC Davis Atmospheric Chemical Mechanism Conference series mentioned above can help to provide a foundation for this community-based effort. Thus, the funding and the leadership provided by the proposed STAR grant will be vital to the future viability of atmospheric chemical mechanism building.

Aerosols (Particulate Matter) (quality of science)

CMAQv5.1 contains significant advances in the science being used to model PM. The PM modeling is scientifically rigorous and recent publications by the CMAQ model development team, particularly as related to organic and nitrogen-containing compounds, are highly cited within the scientific community. For example, the paper by Pye et al. (2013) on the role of acid-catalyzed isoprene SOA formation has already been cited 30 times. The CMAQ model development team has been leading the scientific community in improving model representation of SOA formation from isoprene; in CMAQv5.1, SOA formation by reaction with nitrate radical, and oligomer formation via epoxide channels have been added [poster, Pye et al.].

Scientific advances in the representation of SOA also include additional formation mechanisms, as well as an option to use the Volatility Basis Set (VBS) partitioning model (a community contribution to CMAQv5.02 by ENVIRON International Corp.). In CMAQv5.1, a treatment of SOA formation from PAHs and longer-chain alkanes (> 6 carbons) has also been added (Pye and Pouliot, 2012). Interest in these higher-molecular-weight intermediate-volatility organic compounds (IVOCs) has been spurred by research at Carnegie Mellon University led by Robinson et al. (2007). Other investigators have demonstrated the importance of longer-chain alkanes/alkenes in SOA formation (e.g., Lim et al., 2009). These external publications highlight the importance of including such pathways in the CMAQ model.

These developments in the SOA mechanism have produced good agreement with field measurements of “isoprene SOA” from 2011 and 2013 [presentation, Pye et al.]. In addition, a reduction in summertime monthly average $PM_{2.5}$ bias was demonstrated for the eastern U.S. with the updated SOA mechanism [poster, Pye et al.; presentation, Roselle et al.]; more PM sulfate and organic carbon are predicted, largely in the south and southeastern U.S. Identifying and removing sources of sulfate bias was one of the recommendations put forth by the Fourth Review Panel.

Since publication of the Fourth CMAQ Peer Review in 2011, the CMAQ model development team within AMAD has made considerable progress in application of the CMAQ model for predictions of particulate matter (PM) and subsequent air quality and climate effects. Those applications address the recommendations of the Fourth Review Panel to improve connections between CMAQ and other (/local-/global-scale) models. From the human health perspective (relevant to the ORD Sustainable and Healthy Communities program), CMAQ model output has been used to provide approximations of $PM_{2.5}$ concentrations at higher spatial resolution than provided by existing monitoring stations, thus facilitating improved exposure estimates [poster, Bash et al., 2015].

From the AQ–climate perspective (relevant to the ORD Air, Climate, and Energy program), a 21-year hemispheric run has been completed using the coupled WRF-CMAQ model, which allows for treatment of aerosol-radiation feedbacks. Predictions from this run, which was a monumental achievement, are being used to investigate the magnitude and direction of the aerosol radiative effect in specific locations around the globe [poster by Xing et al. and references therein]. On the regional scale, application of the coupled WRF-CMAQ model improved performance, including predictions of $PM_{2.5}$ concentrations and surface shortwave radiation, in California during a period of intense wildfires [presentation, Mathur]. These applications demonstrate the ability of the CMAQ model to account for climate-air quality feedbacks, which will be increasingly important in coming years (e.g., Fiore et al., 2015). More generally, such efforts strongly support the mandate of the CMAQ development team for applied research relevant to ORD's research programs.

While the multi-decadal hemispheric run is a laudable achievement, given the limited resources available to the model development team, the team is encouraged to proceed in this direction with caution (both in spatial and temporal scales). It is recommended that the team continue to evaluate external collaborative opportunities, pursuing these applications internally only as deemed necessary to support AMAD's mission.

Deposition and Air-Surface Interactions (quality of science)

The CMAQ team has been a world leader in their work to develop a coupled meteorology-agriculture-AQ modeling system. The Environmental Policy Integrated Climate (EPIC) agroecosystem model is used to simulate the daily, gridded, plant-demand-driven amount of fertilizer that is applied to U.S. commercial cropland. These detailed estimates of fertilizer application are then fed to the bi-directional ammonia flux scheme in CMAQ to estimate time-step- and grid-cell-specific NH_3 fluxes. EPIC is a semi-empirical biogeochemical process model that was developed by the U.S. Department of Agriculture and that is sufficiently detailed to allow consideration of scenarios in which land use, agricultural practices, or climate are changed. This WRF-EPIC-CMAQ system is an excellent example of a response to recent recommendations for more integrated and transdisciplinary multimedia modeling approach to link agriculture, hydrology, and meteorology/climate models in a "One Biosphere" framework (e.g., Cooter et al., 2012). Land-use data is needed by the bi-directional scheme and the CMAQ team has also worked to make the land-use description used by WRF, EPIC, and CMAQ more consistent and more flexible.

The CMAQ team has also developed an innovative approach to combine CMAQ dry deposition fields with ambient-air and wet-deposition network measurements to estimate annual sulfur and nitrogen total deposition fields. These deposition fields can then be used with critical load and other ecological analyses to inform the development of new secondary standards. Concerns over the contribution of organic nitrates to nitrogen deposition also provided motivation for the improved representation of organic nitrate chemistry described in the "Chemistry" section. And since the last peer review in 2011 the CMAQ team has also made more use of wet deposition measurements for model evaluation to complement ambient measurements.

Model Structure and Numerics (quality of science)

With CMAQ applications in general requiring more and more computer resources, the CMAQ team is acutely aware of the need to improve computational performance: they have had some success in improving model efficiency with the new CMAQv5.1 release. Input/output (I/O) was shown to consume about 24–35% of model run time (Wong et al., 2015). To address this bottleneck, several new parallel I/O schemes based on the pnetCDF software package were implemented in CMAQ and tested in order to speed up writing data to disk on large parallel computers. A more efficient PBL solver was implemented for ACM2 and the in-line photolysis code introduced in CMAQv4.7 was restructured and made more efficient. The CMAQv5.1 beta code was also profiled and the model code for horizontal advection, aerosols, and chemistry was then optimized, resulting in some significant speed-ups: e.g., time in chemistry was reduced by ~60% and overall run time was about 15% faster than v5.0.2 despite the use of a larger chemical mechanism.

Other changes to numerics for CMAQ v5.1 included making the solution of heterogeneous chemical reactions simultaneous with the solution of the gas-phase reactions and implementing the aqueous-phase chemistry mechanism in the Kinetic PreProcessor (KPP) for improved extensibility and access to multiple solvers. One area where further efficiencies might still be achieved on some computer architectures is by implementing hybrid MPI/OpenMP parallelization in order to benefit from both coarse- and fine-granularity parallelization.

Two-Way Coupled WRF-CMAQ (quality of science)

The coupling of the two modeling systems has been designed efficiently and effectively. Even though it is not an online integrated coupling, where the two modeling systems would share the same structure and code as well as the scientific benefits of such a structure, the continued development and improvement of the WRF-CMAQ coupling scheme has shown that it is an effective tool based on a well-thought-out methodology. The coupled WRF-CMAQ model has been effectively ported to various cluster configurations in the U.S. and abroad (U.K., Greece, China), alleviating the concerns raised for the portability of the code during the last panel review (Brown et al., 2011). The same portability is anticipated for the new version release (CMAQv5.1). The 2-way nesting capability for the coupled WRF-CMAQ model has not been pursued by the CMAQ team, mainly because of the mass conservation issues that were identified in previous research work by CMAQ team scientists. Nevertheless, the CMAQ team recognizes the need and benefits from multiscale modeling for atmospheric processes and is exploring alternative approaches for grid refinement that will address the mass conservation of chemical constituents more appropriately [presentation, Pleim et al.]. This effort is commended by the panel. Collaboration with research groups worldwide on integrated meteorology-chemistry modeling is thought to be very important for future research directions that the CMAQ team is considering with regards to the coupled model.

The diverse applications of the coupled WRF-CMAQ system (multi-decadal hemispheric, regional and local scale) are a good example of the importance of the coupling to account for realistic feedback processes (i.e., direct and indirect aerosol effects). The online treatment of direct and indirect aerosol effects are vitally important for the improvement of particulate matter prediction and the investigation of climate-air quality effects (see "Aerosol" section above). Because of the uncertainties in the treatment of such processes, it is crucial that the EPA continues to lead and advance our knowledge and understanding of those interactions through ongoing use and development of the coupled model. The panel agreed that the quality of the science is high and the coupling of the two models is very positive and necessary for leading the science of air pollution modeling forward for both research and regulatory applications.

<u>Model Evaluation</u> (quality of science)

AMAD is a leader in model performance evaluation both nationally and internationally. They are also very collaborative both externally and internally. They have pioneered a number of innovative approaches to characterizing model performance. In particular, AMAD proposed and has continued to develop a Model Evaluation Framework that includes four different model evaluation approaches, each of which is suited to answer specific questions regarding model performance. These are:

- Operational Evaluation: compares model output to routine observations to characterize the fidelity of the predictions (i.e., "is the model getting the right answer?").
- Diagnostic Evaluation: focuses on the use of non-routine analysis tools and data sets to discern whether the model "is getting the right answers for the right reasons".
- Dynamic Evaluation: focuses on changes to model inputs like emissions and meteorology to determine whether the model is able to predict observed changes in air quality.
- Probabilistic Evaluation: relatively new and often very computationally intensive, used to quantify uncertainties (and hence confidence) in model predictions.

The CMAQ team has routinely used results from different CMAQ evaluations to guide the current and future development of the CMAQ model. Their most recent major evaluations include (1) their involvement in and leadership of Phase 2 of the Air Quality Model Evaluation International Initiative (AQMEII2), an international collaboration to evaluate and intercompare online coupled meteorology-AQ models, and (2) multiple evaluations of the performance of different prototypes of the newest model version, CMAQv5.1, against observations and previous versions.

AQMEII2 included a range of operational, diagnostic, and dynamic evaluations to examine climate-chemistry-aerosol–cloud interactions (e.g., Im et al., 2015; Hogrefe et al., 2015; Campbell et al., 2015). It involved 16 research groups from North America and Europe, eight different online coupled models, two simulation years (2006 and 2010), North American and European modeling domains, and online and offline simulations. Four groups applied three coupled models, including WRF-CMAQ, on the North American domain. The AQMEII2 community has in effect conducted a meta-analysis through the publication of over 20 evaluation papers that focus on model outputs of selected gases (O_3 and precursors) and particle composition ($PM_{2.5}$ and PM_{10}), radiation budgets, aerosol optical depths, top-of-the-atmosphere radiative fluxes, and variables important in cloud microphysics. While radiation budgets and major column gases are predicted reasonably, the various physical parameters that are important in describing cloud physics are not, and the latter are identified as targets for further research. It was also concluded that more research is required to characterize the aerosol indirect effect, and that the use of online modeling is crucial to this effort. The various analyses and evaluations conducted in AQMEII2 continue to drive the development of online coupled models across scales from local to hemispheric and have most certainly confirmed the importance of online modeling for treating climate-air quality interactions.

The CMAQ team also completed a number of CMAQ-specific performance evaluations as part of the CMAQv5.1 development process. The performance of various CMAQ v5.0.x developmental versions run in near-real-time by the CMAQ team between 2013 and 2015 underwent a variety of objective and subjective analyses [presentation, Eder et al.]. The CMAQv5.1beta model version underwent operational, diagnostic, and dynamic evaluations [presentation, Roselle et al.]. A fine-scale version of CMAQv5.0 was applied for two DISCOVER-AQ field campaigns, the 2011 Baltimore–Washington, D.C. campaign and the 2013 San Joaquin Valley campaign [poster, Appel et al.]. Dynamic evaluations were performed on two multi-year time series, one for maximum daily 8-hour ozone concentration for the 1990-2010 period (CMAQv5.0) and another for annual regional wet deposition for the 2002-2011 period (CMAQv5.0.1) [poster, Foley et al.]. “Cross” simulations were also performed with CMAQv5.0.1 to separate the combined impacts of emissions changes and meteorological differences in dynamic-evaluation studies of the impact of the NOx SIP call between 2002 and 2006 (Foley et al., 2015). Lastly, a holistic evaluation has been performed to examine the impact of multiple model changes on the representation of the isoprene system [poster, Pye et al.].

Overall, the CMAQ team has successfully used ground-based observations and satellite retrievals in their operation and dynamic evaluations. They have investigated the roles of changes in emissions, chemistry, boundary conditions and meteorology in affecting the air quality changes between 2006 and 2010, and in so doing they have uncovered important issues that impact control strategy design.

Instrumented Models (quality of science)

The “instrumentation” of CMAQ has been an area of ongoing improvement. One updated source-sensitivity tool and one new source-apportionment tool were included with the CMAQv5.0.2 release in 2014: high-order sensitivity analysis for particulate matter was implemented in the Decoupled Direct Method 3D (DDM-3D), which was first released in CMAQv4.7.1; and the Integrated Source Apportionment Method (ISAM) was introduced. These schemes supplement other instrumented-model schemes in CMAQ such as process analysis, Integrated Reaction Rate (IRR) Analysis, the Sulfur Tracking scheme, and the Primary Carbon Apportionment Model. Work has also been underway on a CMAQ adjoint for several years and a working gas-phase version is now available.

Applications (quality of science)

AMAD has been conducting applications of CMAQ and the coupled WRF-CMAQ system for a variety of topics, including investigation of air quality and health effects in future climates, atmospheric deposition and its effects on watersheds, fine-resolution simulations for periods of airborne field experiments, hemispheric simulations to examine trends in air quality and aerosol direct radiative forcing, and a comprehensive assessment of a new chemistry scheme for $ClNO_2$ added to the model. All of these applications are very worthy of the expenditure of time by AMAD staff, and each of them has been conducted in a rigorous manner.

The CMAQ team has worked in a careful and systematic manner for some years on a dynamical downscaling methodology: they have now been able to run CMAQ to estimate the future health effects from a changing climate using downscaled meteorological fields from 2030 scenarios run by two different global climate models. The hemispheric coupled WRF-CMAQ is a relatively new tool, but it has been put to excellent use in the two-decade-long simulation used for estimating trends. The application of the hemispheric model output as boundary conditions for a regional simulation yielded a fine result, which was better than that obtained from using the global GEOS-Chem model to supply chemical boundary conditions. The fine-resolution coupled simulations have yielded excellent simulation results for the NASA DISCOVER-AQ experimental periods of July 2011 in Maryland and January-February 2013 in the San Joaquin Valley of California after some model improvements were implemented for land-surface description and for meteorological data assimilation (described above in the “Meteorology and Transport” section).

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?

Emissions (strengths and weaknesses)

In terms of emissions one obvious strength is the CMAQ team’s commitment to provide information covering a broad and diverse set of atmospheric components and emission sectors for both regulatory and research applications. As such, the emissions component is closely integrated with other aspects of CMAQ model development. Specific examples of improvements and evaluations that have been published, presented, or incorporated into the NEI include emissions of NH_3, dust, sea-salt, biogenic species, RWC, ultrafine PM, and crop and peat burning. In this sense, the CMAQ team has been responsive to one of the 2011 panel’s primary recommendations: “Improve the emission inputs to the CMAQ model and allocate more resources to this task”.

Another strength is the CMAQ team’s ability to test model sensitivity related to emissions uncertainty. The Jathar et al. (2014) reference provides a good example, by showing the impact on SOA and $PM_{2.5}$ of plausible volatility assignments of the unspeciated VOC fraction within the NEI. Additional material related to emission sensitivity is inherently imbedded within the “model evaluation” work presented to the panel.

Although the CMAQ team strives to use the best available science for the emission processes modeled within CMAQ, the panel noted that one area needing improvement is the evaluation of emission components. For example, very limited comparisons were made to coastal or open-ocean observations in the evaluation of the updated sea-salt emissions algorithm or to PM size-distribution measurement data for the evaluation of emissions specified for the treatment of ultrafine PM within CMAQ even though extensive, high-quality observational data sets (e.g., NOAA/PMEL and NOAA/CSD) are available for comprehensive evaluations. Obtaining and utilizing such relevant data, especially from other federal agencies, could be a higher priority within the CMAQ emissions evaluation protocol.

One new area of emissions research is the top-down estimation of emissions from network observations and intensive field studies that is increasingly appearing in the scientific literature. These estimates can be based on direct mass-balance measurements, adjoints of comprehensive models, or Bayesian-based inversions using modeled and observed meteorology. They have the potential to provide very useful information for EPA inventory evaluation and to provide constraints on emissions from certain sectors. AMAD could further improve the scientific basis of their models by including more accurate emissions estimates, either by adopting top-down capabilities themselves or by judiciously using available observation-based emission estimates. Similarly, emission estimates and constraints for specific species (e.g., NO_x) from increasingly accurate and reliable satellite determinations could be used effectively in emissions evaluations.

The panel also noted that certain species/constituents are missing from AMAD emissions processing and evaluation. With increases in oil/gas production throughout North America and associated public concern, methane, ethane, a host of toxics, and additional SOA precursors may need to be considered within scientific assessments, source apportionment, and public exposure studies. Methane also plays an important role in background chemistry and provides a link between air quality and climate change.

<u>Meteorology and Transport</u> (strengths and weaknesses)

The major strength of the improved FDDA efforts has been the demonstration that wind profiler and radar-derived wind data improve the prediction of transport above the PBL, which is important for improving the accuracy of regional ozone prediction. The movement toward ensemble modeling by the AMAD group is to be commended. Use of the Short-Range Ensemble Forecast (SREF) ensemble output from NOAA for initial conditions and for nudging in the coupled WRF-CMAQ is an excellent idea. All of the additional data sets that AMAD recommends using with WRF simulations have led to error reduction in 2-m temperatures. In addition, recent modifications to the P-X LSM and ACM2 code in WRFv3.7 have reduced errors in temperature, water vapor and wind speed predictions, which in turn has reduced biases in ozone and $PM_{2.5}$ predictions.

The improvements implemented with the FDDA procedure and use of additional data did not lead, however, to improved boundary-layer wind predictions, indicating that more work is needed in this area. The ensemble runs of WRF-CMAQ using SREF data appear very promising. Therefore, AMAD should do more to promote the use of such a technique as a means of determining meteorological uncertainty in air quality predictions. This would include promoting the ensemble approach within the research community as well as within the regulatory community. The only perceived weakness among the additional data sets recommended for use with WRFv3.7 is the lack of a method to incorporate diurnal variation of SST, which can be important for shallow water bays and lakes.

It is well known that the stratosphere is an important source of tropospheric ozone both climatologically and episodically. For example, Tarasick et al. (2005) showed that both the trends and the interannual variability of tropospheric ozone levels over Canada are highly correlated with ozone amounts in the lower stratosphere. Lin et al. (2015) recently presented evidence that deep stratospheric intrusions can impact ozone levels in the western U.S. in the springtime, directly impacting human health but also complicating non-attainment determinations. In past years the CMAQ team has investigated different approaches to representing stratosphere-troposphere exchanges of ozone, but it appears that a satisfactory treatment has been elusive. However, representation of this process is important for hemispheric modeling, AQ-climate modeling, and regulatory modeling and the CMAQ team should continue to work to address this gap.

<u>Chemistry</u> (strengths and weaknesses)

The chemistry represented in the CMAQv5.1 is compatible with the current state-of-the science. CMAQv5.1 will feature three gas-phase chemical mechanisms that are already being used by the modeling community. The first is the Carbon Bond V (CB05) mechanism, which was developed in 2005 (Yarwood et al., 2005). CB05 is less detailed than the other two mechanisms but is heavily used by the modeling community mainly due to its computational efficiency. There are two versions of CB05 in CMAQv5.1 with two different levels of improvements: CB05tucl (Whitten et al., 2010), which was introduced in CMAQv5.0, and CB05e5, which has 14 additional species and updates to NOy, SOA, and photolysis.

The second is the second version of the Regional Atmospheric Chemistry Mechanism (RACM2) (Gollif et al., 2013). This mechanism is more detailed than CB05 and has more reactions and model species, but there is only one version of this mechanism in CMAQv5.1. This is the first time that a RACM mechanism has been made available in CMAQ so usage statistics for regulatory/research applications with this mechanism are not yet available.

The third is the SAPRC07 mechanism (Carter, 2010) which is the latest peer-reviewed version of the SAPRC series. (As an aside, note that SAPRC used to be an acronym for the "State-wide Air Pollution Research Center" at the University of California at Riverside, but that center is no longer in existence. Therefore, SAPRC is now simply a name for this series of mechanisms.) CMAQv5.1 contains two versions of SAPRC07: a regulatory version (SAPRC07TB) and a research version (SAPRC07TIC). SAPRC has the largest number of reactions and model species and thus is the most computationally demanding. Of the three chemical mechanisms available in CMAQv5.1, SAPRC is the mechanism that has been most thoroughly peer-reviewed. CARB conducted an external peer-review of the SAPRC07 mechanism that is implemented in latest versions of CMAQ. A SAPRC14 mechanism is now being developed and it is expected to be peer-reviewed with the same vigor in the 2015-16 timeframe. Despite its robustness, however, outside of California the SAPRC mechanism is not used routinely for regulatory applications.

Detailed descriptions of all three base chemistry mechanisms have been published in the peer-reviewed literature and represented the state-of-the-science for individual mechanisms at the time of publication. Since then CMAQ team members have improved each mechanism as described in Section 4.1.

The panel is concerned that the inclusion (and updating) of three chemical mechanisms in CMAQ may be a burden that diverts resources from maintaining one mechanism comprehensively and well. We understand that there are various reasons to maintain multiple mechanisms, but it may be best if the U.S. EPA selected one mechanism to focus on and designated other mechanisms as "user contributions." There is already a precedent for community contributions to CMAQ in the VBS method for calculating secondary organic aerosols. Two versions of the chosen mechanism could be offered in future CMAQ releases. One version would be highly condensed for computational efficiency while the other could be more detailed and targeted for research applications.

Aerosols (Particulate Matter) (strengths and weaknesses)

In addition to the improved representation of SOA in CMAQv.5.1, there have also been new developments in the CMAQ model of the representation of heterogeneous processes and of the PM size distribution. Isoprene SOA formation via the epoxide route also represents an advance in the representation of heterogeneous SOA formation (aqueous aerosol); the mechanism was developed from a holistic perspective, in which the gas- and aqueous-phase reactions were developed to facilitate tracking of the compounds between the phases. The need for this "coupling" of phases was raised by the Fourth Review Panel, and it continues to be a need and a challenge with the gas/organic aerosol formation mechanisms as well.

In CMAQ v5.1, the binary nucleation scheme was updated to that presented by Vehkamäki et al. (2002), which can result in significantly higher nucleation rates. In addition, an Aitken mode was added such that 10% of primary $PM_{2.5}$ mass emissions are emitted to this "nucleation" mode [poster, Fahey et al.]. Accurate representation of the formation and growth of these small particles are critical for predictions of cloud condensation nuclei (CCN), and thus for predictions of the aerosol indirect effect and aerosol-climate feedbacks. Several modeling studies have demonstrated that uncertainties in predictions of CCN are linked to uncertainties in the nucleation mechanism (e.g., Pierce and Adams 2009; Zhang et al., 2010). More recently, Carslaw et al. (2013) have highlighted the potentially greater importance of primary emissions for modeling CCN. The CMAQ team has demonstrated that the addition of primary emissions to the Aitken mode significantly increased particle number concentrations (3-500 nm) and improved measurement-model agreement at the Pittsburgh Air Quality Site [poster, Fahey et al.]. The updated nucleation scheme and/or Aitken-mode emissions also improved the measurement-model agreement for the number size distributions, specifically for particles < 1 μm (although the panel had some concerns about the representativeness of the assumed primary PM size distribution that was used: see "Emissions" section).

The implementation of the online desert dust emission scheme in the CMAQ model permits an important contribution to the total aerosol burden to be modeled and, consequently, aerosol feedback effects on climate to be investigated. Desert dust particles dominate the aerosol mass over some continental regions and play a major role in the aerosol-cloud-radiation cycle (Boucher et al., 2013). In addition, the long-range transport of desert dust particles is of considerable importance for assessing the aerosol burden in downwind areas, including the eastern and western U.S. The hemispheric simulations with WRF/CMAQ have indicated the transport pathways of desert dust particles towards the North American continent, and the CMAQ team has continued to refine and test the dust emission scheme first included in

CMAQv5.0 [presentation, Mathur]. The panel recommends that the CMAQ team continue to develop and evaluate the desert dust mechanism so as to achieve a reliable prediction of the desert dust cycle that will be important to research topics related to air quality, PM exceedances, and aerosol effects on climate.

The CMAQ model development team has made excellent progress in developing isoprene SOA mechanisms that are particularly relevant to the southeastern U.S. (and other isoprene-rich environments). While improving the traditional "two-product" approach, the CMAQ team also has allowed for representation of SOA formation using the more recent VBS approach. Echoing the concerns raised by the Fourth Review Panel about the pros and the cons of the VBS approach, the panel is supportive of advancing and maintaining both approaches at this point. The panel encourages the team to evaluate more closely model bias in other U.S. locations (perhaps using external data sets), and to apply the same level of scientifically-rigorous model development in those regions to improve model representation of $PM_{2.5}$ (and individual components).

While the use of the Vehkamäki binary nucleation mechanism represents an update to the CMAQ model and improves model performance, there have been a large number of experimental and modeling studies that suggest the additional role of bases (e.g., ammonia and/or amines) and/or organic compounds in nucleation (e.g., Berndt et al., 2014; Jen et al., 2014). Furthermore, it has been shown that not only nucleation, but also the subsequent growth of these small particles to climate-relevant sizes, is important for predicting CCN (e.g., Kuang et al., 2010; Riipinen et al., 2012). The panel recommends that the CMAQ modeling team evaluate available parameterizations and consider including these additional processes in a future CMAQ model release.

<u>Deposition and Air-Surface Interactions</u> (strengths and weaknesses)

The CMAQ team's successful efforts to couple an agroecosystem model (EPIC) with CMAQ has expanded the range of applications that CMAQ can address, including the impacts of future climate change on ecosystems and agriculture and the estimation of N_2O emissions. CMAQ has also been linked with the Variable Infiltration Capacity (VIC) macroscale hydrologic model and the Model of Acidification of Groundwater In Catchment (MAGIC) surface water chemistry model to estimate groundwater acidification. Such linked-model systems already allow more complex environmental problems to be tackled by modeling various relationships and interactions across multiple source types, pathways, and scenarios. They also provide a platform for further development, including coupling nitrogen and carbon biogeochemical cycling.

At the same time, the CMAQ team has noted that the CMAQ bi-directional NH_3 flux scheme has many uncertainties and that to this point it has only been compared with a limited number of land-cover types. Evaluation of the scheme for a greater variety of managed and natural land-cover types will likely lead to improvements and also to the possibility of harmonization of the representations of some surface properties such as cuticular resistance with those used in related CMAQ parameterizations such as those for dry deposition and biogenic emissions.

Some improvements may also be possible for the EPIC model. These include the addition of missing soil processes and the acquisition of compatible soil data and agricultural-management information for Canada and Mexico (especially important for simulations focusing on border states). There may also be merit in examining the possibility of developing a reduced-form version of EPIC model output (e.g., county-specific temporal profiles and spatial surrogates) that could be used for CMAQ climate-scenario simulations or by other AQ models via emissions processing.

Model Structure and Numerics (strengths and weaknesses)

As noted in Section 4.1, the CMAQ team is very aware of the need for improved computational efficiency, and they have been successful with CMAQv5.1 in speeding up a number of model components. However, the age of the CMAQ model computer code itself has become a weakness. Work on CMAQ began in the 1990s (e.g., Dennis et al., 1996; Byun et al., 1998) and the overall model design and structure and much of the model code dates from this period. In the intervening years the model code has undergone a succession of revisions made by many developers, which open the door to inconsistencies across the model and to convoluted code. The nature of various model applications and hence CMAQ requirements have also evolved over this period, including new needs for greater spatial and temporal range and for earth system and climate linkages. Computer science in general has also made great strides in the last two decades, including advances in computer languages, hardware, algorithms, data structures, and numerical methods.

The CMAQ team is developing plans for a next-generation air quality model that include a thorough model redesign and code revamp. Envisioned features include a single, flexible global mesh, an integrated and consistent formulation of chemistry, dynamics, and physics, mass conservation, state-of-the-science numerical schemes, strong modularity and interoperability of model code, and an emphasis on code efficiency, flexibility, and extensibility. This is a challenging vision, but if successful it would provide an improved modeling platform that could be applied to many different applications while undergoing further development to keep pace with advances in air quality science over the next two decades. The panel supports the need for a next-generation air quality model but recognizes the realities of finite resources and the need to minimize duplication and leverage the accomplishments of other modeling groups. It has thus made some suggestions about one possible strategy for pursuing this major development effort (see Section 6). The panel notes that there may be some further computational improvements that can be made in the short term to future CMAQ model versions that also could be carried forward to a next-generation model in an "encapsulated" CMAQ air quality module.

Two-Way Coupled WRF-CMAQ (strengths and weaknesses)

The two-way coupled WRF-CMAQ model and its applications are viewed very positively. The coupled-model approach is essential for the success of other model parameterizations, and this is considered to be a significant strength of the system. The coupled system and natural aerosol processes are inter-related: for example, improved estimates of desert-dust and sea-salt emissions and transport improve the treatment of direct and indirect aerosol feedback effects.

Comparison of the coupled WRF-CMAQ system with the offline WRF-CMAQ and with WRF-Chem or other fully integrated modeling systems is important to determine the relative advantages and disadvantages of coupled models and different coupling strategies. A lot of work has been done in this respect by the CMAQ team. However, additional comparisons will be required to determine the overall performance of the coupling methodology and collaborations with research groups that work on related areas will be essential. One question that can be posed related to the findings in other activities of the CMAQ team is the following: "Does the coupled WRF-CMAQ model, in its current state, improve the biases in the air quality prediction that are related to meteorological inputs?" As one example, the biases in SO_4^{2-} predictions associated with uncertainties in the precipitation and cloudiness might be expected to benefit from the use of the two-way coupled model, but do they? Participation by the CMAQ team in AQMEII2 and other activities have provided insights on this question and are commended by the panel.

Continued work is also needed on the parameterization of the indirect aerosol effects that is undergoing development and testing because the science itself is evolving rapidly in this area. Such work is planned according to AMAD.

Recent work by the CMAQ team showing a positive feedback of anthropogenic emissions on PM surface concentrations (through reduced PBL mixing) further highlights the impact of two-way coupling and the importance of continued research. For example, the relative importance of this effect compared to other factors, such as the urban heat island and land-use changes, remains an open question. Likewise, the impact of model resolution on the feedback effect, as well as on other semi-direct effects, has yet to be characterized.

One potential weakness identified by the panel concerns the differences in the advection scheme between WRF and CMAQ. The impact of these difference should be investigated through comparisons with fully integrated modeling systems.

Model Evaluation (strengths and weaknesses)

Model evaluation is a tremendous strength of the CMAQ team. The CMAQ team devotes considerable resources to this activity and they are leaders both in terms of the level and range of model evaluation activities. In addition to evaluating various version of CMAQ on an ongoing basis using traditional operational model evaluations, they have pioneered diagnostic, dynamic, and probabilistic air quality model evaluation techniques, including adding new model instrumentation. Most importantly, they have used their evaluation activities to spur model improvements in innovative and practical ways. They have also made many of their model evaluation tools available to the user community.

AMAD's development of the probabilistic evaluation approach offers a more robust quantitative approach to estimating model uncertainties and establishing confidence limits with which to guide efforts to achieve compliance with current and more stringent standards. One weakness at this point is that they have only performed this analysis for a few cases. However, conducting probabilistic evaluations of modeled ozone and PM is extremely computationally intensive. While AMAD scientists have developed computer strategies and architectures that optimize their use of computer resources, increased computer resources will be required to make progress in this area. The panel's concern about the computer resources available to AMAD is reiterated in Section 6.

If the NAAQS for ozone (both primary and secondary) are made more stringent, there will likely be a need for further model improvements to reduce the bias associated with high and mid-levels of ozone. Some evaluations looking at lower and mid-range O_3 levels have already been performed but this topic is likely to be a focus going forward. It is likely that the CMAQ team will also need to improve the treatment of background ozone and other lateral boundary conditions and their ability to predict NOx, NOy, and SOx for primary and secondary O_3 standards and for $PM_{2.5}$ standards.

<u>Instrumented Models</u> (strengths and weaknesses)

The CMAQ team has also worked closely with OAQPS to develop and implement source apportionment modules for O_3 and PM in CMAQ to complement existing sensitivity analysis tools. Source apportionment is also of great interest to the states, tribes and local air districts. Adding a CMAQ adjoint would provide another powerful tool and a receptor-based perspective to the instrumentation suite.

<u>Applications</u> (strengths and weaknesses)

The different CMAQ applications performed since 2011 by the CMAQ team display a number of strengths. Many of the additional data sets (e.g., high-resolution SST, SNODAS, impervious surface fraction, etc.) recommended for use with CMAQv5.1 were used in the fine-resolution simulations with the coupled WRF-CMAQ model for two DISCOVER-AQ campaign periods, which likely aided in generating reasonable simulations. Use of the iterative data-assimilation approach to WRF simulations also contributed to the high quality of the DISCOVER-AQ simulation results. With regard to the hemispheric simulations, a major strength is that the Aerosol Optical Depth (AOD) and radiation fields generated by the coupled WRF-CMAQ are compared with satellite observations for a decade-long period. A major advancement was the addition of heterogeneous $ClNO_2$ chemistry to CMAQ, which was used in a hemispheric simulation and evaluated using hemispheric surface ozone measurements. The ecosystem applications of CMAQ are enhanced by the linkage of CMAQ with surface runoff and ground-water acidification models. The climate downscaling applications of WRF and CMAQ benefit from the use of output from multiple GCMs, which gives some indication of the uncertainty associated with future climate and air quality prediction.

The panel believes that some of these applications can be further refined. The air quality portion of the coupled WRF-CMAQ simulations for the DISCOVER-AQ periods was evaluated primarily by use of surface air quality data. They can be further evaluated using the aircraft profile data and remote-sensing data (e.g., column amounts of trace gases and AOD) to yield a more comprehensive (3-D) view of the quality of the simulations. The uncertainties in the emissions data used in the two-decade hemispheric simulations should be more rigorously evaluated. This need is brought to the forefront because of some deficiencies evident in the simulations (e.g., inability to simulate the nitrate trend over the U.S. and the SO_2 and NO_2 trends over China properly; underestimates of AOD over deserts). The hemispheric model simulations would be more state-of-the-science if they could be run at higher spatial resolution: by contrast, global GCMs with online chemistry are now being run by other agencies with resolution as fine as 12 km. The future climate and air quality downscaling should also be done at higher spatial resolution than 36 km. Such results would improve accuracy of the ozone predictions, as well, as the accuracy of the health effects, especially in urban areas. The relatively coarse resolutions used in these studies are likely due to the limited computing environment within which AMAD is working. See Section 6 concerning our recommendation with regard to computing resources.

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 ORD's research program areas?

The quality of the model development, evaluation, and application being conducted by the CMAQ group is very high. As evidence of this, many recent peer-reviewed journal articles authored or co-authored by members of the CMAQ group were provided to the Panel as part of this review. The CMAQ modeling system is also used by a remarkably wide and growing domestic and international user community outside of the EPA because it is viewed as being of scientifically high quality, relatively easy to use, and well supported by EPA, CMAS, and the community. The range of applications (e.g., assessment of emission change impacts, identification of source contributions, support for potential regulatory policy changes, evaluation of impacts of climate change on surface air quality, design of monitoring networks, and provision of spatial pollutant fields for health and exposure assessments) supported by CMAQ are all extremely relevant to the needs of the EPA and state and local governments. As a consequence, the CMAQ modeling 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.

With respect to ORD's research program areas, the model development, evaluation, and application carried out by the CMAQ group are well aligned with some of the goals of ORD's Air, Climate and Energy program as well as its Safe and Sustainable Water Resources program (e.g., by providing estimates of depositional loadings of acidifying and eutrophying species to ecosystems and water quality systems) and Sustainable and Healthy Communities program (e.g., CMAQ output is used for both ecological and health assessments).

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?

The level of integration and coordination between the subgroups with AMAD working on model development, evaluation, and applications appears to be very high. For example, the regular meetings of each subgroup are attended by members of the other subgroups. Moreover, the development subgroup work plan is influenced by model performance results from the evaluation subgroup and by needs and findings communicated by the applications subgroup. Members of the CMAQ team also participate in regular meetings with the EPA's policy arm (i.e., OAQPS) and its emissions inventory group (i.e., EFIG). Feedback from the CMAQ user community is also provided to the CMAQ team at the annual CMAS conferences, by the CMAS 'm3user' forum, and through collaborations with individual agencies and research groups.

The CMAQ Modeling Program has been very successful in its efforts to advance the science to address new problems and increase user confidence and to make the model more usable both inside and outside the EPA. As noted in Section 4.3, the many capabilities and possible applications of the CMAQ modeling system make it very useful to the EPA, states, and local agencies and to the research community. Going forward AMAD will need to continue these efforts and to articulate the importance of these activities to the broader community both inside and outside the Agency.

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 ORD's research program 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?

As noted in one of the CMAQ group's responses to the Fourth Peer Review Panel (see Section 3, p. 15), although the primary focus of CMAQ applicability within the Agency is on the continental U.S. scale, current and emerging AQ issues require consistent treatment of air pollution from urban to hemispheric scales. Given the reality of resource constraints and the growing number of application needs (e.g., secondary NAAQS, human and ecosystem exposure), the CMAQ group has adopted a "problem-oriented" approach to ongoing CMAQ development and applications while keeping in mind future extensibility and overall system maintenance. This pragmatic approach seems to be a very suitable response to current realities and limited resources.

Much of the prioritization of modeling research topics to pursue is guided by the CMAQ team's examination of model evaluation results and the research literature. The CMAQ team also participates in regular meetings with OAQPS, so that internal feedback about any regulatory program needs that are not being addressed is ongoing. However, as noted in Section 6, emissions processing and emissions modeling is one area that may warrant additional resources. In addition, one challenge facing AMAD as they go forward in an era of shrinking resources will be how to fill gaps in their research capabilities that have been opened up by the departure of subject specialists due to retirement or other reasons.

The CMAQ Modeling Program is making very effective use of the resources provided in terms of the choice and quality of the applied research being conducted at AMAD. Evidence for this can be seen in the summary of recent major developments to CMAQ provided in Section 2. In addition, the CMAQ group has also actively sought opportunities to leverage additional resources through collaborations with internal partners, university research groups, and other agencies, participation in external research activities (e.g., AQMEII, EuMETCHEM), and access to Agency funding programs for post-doctoral fellows and university research. They should continue to pursue such opportunities.

A large impact was shown for North Carolina ammonia concentrations predicted by CMAQ when simple temporal emission profiles were replaced with the bi-directional flux calculations.

Although further evaluations were recommended (see "Deposition and Air-Surface Interactions" section), it is not clear how the coupled bi-directional NH_3/EPIC-database research will propagate into the broader EPA emissions program. For example, EPA gives detailed recommendations, from a regulatory perspective, on how to treat dust emissions within a modeling framework (http://www.epa.gov/ttn/chief/emch/dustfractions/). Should bi-directional NH_3 emissions/EPIC likewise be publicly recommended, or required, within certain regulatory applications?

The importance of lateral boundary conditions, either directly specified or supplied from the hemispheric model, were shown to have a significant impact on CMAQ O_3 predictions [presentation, Pleim et al.]. In terms of EPA's regulatory program it is unclear how boundary conditions from a hemispheric model would be generated, archived, and supplied to the general CMAQ community. Likewise, the impact of stratospheric O_3 on surface O_3 exceedances has been documented in the western U.S. The CMAQ team first needs to develop the modeling capability to quantify stratospheric influence adequately. Once it does this, should AMAD be responsible for making the boundary conditions for these discrete episodic events available to the CMAQ community? These issues and questions will become more critical if the NAAQS for O_3 becomes more stringent.

5.0 COMMENTS ON THE REVIEW PROCESS

The panel felt that the review process worked quite well overall. It is clear that this Fifth Review Panel benefited from the experiences of and lessons learned by the first four review panels. Nonetheless, it may be helpful to the EPA, CMAS, and future panels to provide some specific comments about the review process.

The panel recommends that CMAS and the EPA should hold a call with the chair of the next external peer review panel in advance of the face-to-face review meeting to discuss expectations for the review, high-priority topics, agenda, schedule, and logistics. The panel chair should then communicate relevant information to the other panel members before the review meeting. The panel members should also try to identify and agree to individual topic assignments, i.e., the specific areas that they will be expected to lead, before the start of the meeting. Copies of the PowerPoint files for the talks and the posters for the review meeting should be provided to all panel members prior to the meeting. The agenda for the first day of the review meeting should begin with a closed-door meeting of the panel for organizational purposes, since in some cases the panel members may not have met each other previously and there will not have been a previous opportunity for any face-to-face discussion. The poster sessions are an excellent mechanism for the panel to interact with more members of the CMAQ team, and breaking the panel into smaller groups (e.g., pairs) to circulate between the posters should be considered. In addition, given the limited time available for panel members to meet with each poster presenter, if it would be possible to provide a separate opportunity after each poster session for individual panel members to meet with selected presenters, that would be beneficial.

6.0 PANEL RECOMMENDATIONS

The panel would like to make the following five recommendations for the CMAQ Modeling Program to consider and, if judged to be helpful and achievable, to implement as resources permit:

(1) *Work with ORD and Agency management over the next year to secure access to enhanced computer resources and enhanced data transfer capabilities before the lease on the current AMAD computer facility ends*.

<u>Rationale</u>: Going forward the CMAQ team plans to pursue higher spatial resolutions on domains ranging from the urban to the hemispheric scale, to simulate more multi-year periods, to adopt more general and more sophisticated physical and chemical process representations, and to explore greater use of the ensemble technique for both air quality studies and air-quality/climate-change studies. All of these new directions will require access to increased computational resources. In addition, improved data transfer capabilities are needed to support the exchange of CMAQ output data sets and other data sets (e.g., satellite data) with external agencies and partners and to allow access, if required, to off-site computer centers, including cloud computing. This request for access to expanded computer resources might be made jointly with major internal CMAQ clients and users such as OAQPS.

(2) *Work to develop a more integrated, extensible, maintainable, flexible, and efficient comprehensive chemistry package for use by CMAQ. This package would likely include further upgrades to the treatment of organic aerosol, background chemistry, marine chemistry, and possibly stratospheric chemistry. Consideration should also be given to developing a single package with different forms to be used in different parts of the domain.*

<u>Rationale</u>: In developing CMAQv5.1, the CMAQ team has succeeded in producing a more tightly linked and consistent multiphase, multipollutant chemistry package. However, continued development of and updates to this package will be required to incorporate ongoing advances in our understanding of atmospheric chemistry. The current application of CMAQ to the hemispheric scale and planned application to the global scale will require chemistry mechanism extensions to address chemical regimes other than the moderately polluted continental troposphere for which CMAQ was originally designed, such as those found over oceans and remote continental regions and in the stratosphere. Making updates and extensions to multiple gas-phase chemical mechanisms results, on an ongoing basis, in a dilution of resources that could be put to other uses. Being able to use different forms of a singular chemical mechanism/package over different regions or vertical layers also might result in computational savings.

(3) *Take a two-track approach to the development of a next-generation air quality model. In the near-term the CMAQ team should continue to develop and apply the online hemispheric version of CMAQ in order to build a version of CMAQ with an expanded set of chemical and physical process representations and parameterizations that are better suited to application at the hemispheric- (and global-) scale. Work can proceed in parallel on other aspects of the next-generation model. Multiple coupling strategies should be considered. Prototyping with a column version of CMAQ should be done within several global dynamics models to ensure flexibility.*

Rationale: The CMAQ team plans to continue the development and application of the hemispheric version of CMAQ and also to begin work on a global, multiscale, online version of CMAQ. One consideration is that there likely are further developments to CMAQ process representations that could improve its applicability and performance on the hemispheric scale. These code modifications could be useful right away for hemispheric applications but they would also prepare the model for future global applications. A second consideration is the fact that there already are a number of existing global dynamics models that could serve as a "host" model for adding CMAQ as an "encapsulated" air quality module. Given uncertainties around the future development of some of these global dynamics models, it may not be appropriate to focus on only one of these models in the near term, which in turn suggests the need to emphasize flexibility and portability in the development of the CMAQ column model for global chemistry. However, it would still be reasonable to make use of one or two global dynamics models as a testbed(s) for prototyping. A third consideration is that the CMAQ team has had to work with the WRF development community over the past decade to introduce changes to WRF for compatibility with process treatments in CMAQ. It is very possible that analogous changes would also be required in any global dynamics model that hosts CMAQ. Lastly, the coupling of meteorology and chemistry in a single integrated modeling system is still a new technology, and the coupling approach to be used in the next-generation system should be revisited and reconsidered. Note that development of the next-generation version of CMAQ is also seen by AMAD as an opportunity for a "root-and-branch" overhaul of the CMAQ model computer code, which has undergone extensive serial modification over the past several decades.

(4) *Consider investing additional resources in emissions processing and emissions modeling*.

Rationale: Gridded emissions fields are a key input to CMAQ. New or evolving CMAQ capabilities and applications will pose new requirements for input emissions on an ongoing basis. For example, hemispheric modeling requires the provision of anthropogenic emissions for other continents as well as emissions from numerous natural sources, including biogenic emissions, wildfires, wind-blown dust, sea salt and other oceanic emissions, volcanoes, and lightning. New chemical process representations and the consideration of additional emitted species (e.g., IVOCs, trace metals, base cations, methane and ethane, ultrafine particles, …) will likely require changes to emissions processing and/or emissions modeling. And CMAQ applications on finer-scale grids may require the development of new spatial surrogate fields for the spatial allocation to these higher-resolution grids of emissions reported in the inventories by political jurisdiction.

(5) *Improve the numerical methods used in CMAQ. This could begin with a thorough profiling of the code to identify bottlenecks. The CPU-intensive portions of the code could be re-written to improve the efficiency on parallel architectures that are now routinely used to run CMAQ. This could also involve careful re-evaluation of MPI calls made in the code. Judging from the comments made by the users on the CMAS "m3user" forum, it appears that the CMAQ I/O API implementation is causing difficulties. We encourage the CMAQ team to consider other alternatives in future CMAQ versions that are also compatible with pNetCDF implementations (which seems to improve I/O considerably).*

Rationale: CMAQ is now being applied in large modeling domains in relatively high resolution (e.g., California state domain with 4 km^2 grid size) and for longer time frames (e.g., decadal simulations for climate change studies). Thus, the computational efficiency of the model is an important aspect that needs further consideration.

7.0 REFERENCES

Aiyyer, A., D. Cohan, A. Russell, W. Stockwell, S. Tanrikulu, W. Vizuete, and J. Wilczak, 2007:*Final Report: Third Peer Review of the CMAQ Model*. Report submitted to Community Modeling and Analysis System Center, University of North Carolina at Chapel Hill, Feb., 23 pp.

Allen, D., D. Burns, D. Chock, N. Kumar, B. Lamb, and M. Moran, 2009: *Report on the Peer Review of the Atmospheric Modeling and Analysis Division, National Exposure Research Laboratory, Office of Research and Development, U.S. Environmental Protection Agency*. Report submitted to the National Exposure Research Laboratory, U.S. Environmental Protection Agency, Feb., 46 pp.

Amar, P., R. Bornstein, H. Feldman, H. Jeffries, D. Steyn, R. Yamartino, and Y. Zhang, 2004: *Final Report Summary: December 2003 Peer Review of the CMAQ Model*. Report submitted to Community Modeling and Analysis System Center, University of North Carolina at Chapel Hill, July, 7 pp.

Amar, P., D. Chock, A. Hansen, M. Moran, A. Russell, D. Steyn, and W. Stockwell, 2005:*Final Report: Second Peer Review of the CMAQ Model*. Report submitted to CommunityModeling and Analysis System Center, University of North Carolina at Chapel Hill, July, 31 pp.

Appel, K.W., G.A. Pouliot, H. Simon, G. Sarwar, H.O.T. Pye, S.L. Napelenok, F. Akhtar, and S.J. Roselle, 2013: Evaluation of dust and trace metal estimates from the Community Multiscale Air Quality (CMAQ) model version 5.0. *Geosci. Model Dev.*, **6**, 883-899.

Berndt, T., M. Sipilä, F. Stratmann, T. Petäjä, J. Vanhanen, J. Mikkilä, J. Patokoski, R. Taipale, R.L. Mauldin III, and M. Kulmala, 2014: Enhancement of atmospheric H2SO4/H2O nucleation: organic oxidation products versus amines. *Atmos. Chem. Phys.*, **14**, 751-764.

Boucher, O., D. Randall, P. Artaxo, C. Bretherton, G. Feingold, P. Forster, V.-M. Kerminen, Y. Kondo, H. Liao, U. Lohmann, P. Rasch, S.K. Satheesh, S. Sherwood, B. Stevens and X.Y. Zhang, 2013: Clouds and Aerosols. In: Climate Change 2013: The Physical Science Basis. Contribution of Working Group I to the Fifth Assessment Report of the Intergovernmental Panel on Climate Change [Stocker, T.F., D. Qin, G.-K. Plattner, M. Tignor, S.K. Allen, J. Boschung, A. Nauels, Y. Xia, V. Bex and P.M. Midgley (eds.)]. Cambridge University Press, Cambridge, United Kingdom and New York, NY, USA.

Brown, N.J., D.T. Allen, P. Amar, G. Kallos, R. McNider, A.G. Russell, and W.R. Stockwell, 2011: *Final Report: Fourth Peer Review of the CMAQ Model*. Report submitted to Community Modeling and Analysis System Center, University of North Carolina at Chapel Hill, Sept., 22 pp.

Byun, D.W., J.K.S. Ching, J. Novak, and J. Young 1998: Development and implementation of the EPA's Models-3 initial operating version: Community Multi-scale Air Quality (CMAQ) model. In: *Air Pollution Modeling and Its Application*, S.E. Gryning and N. Chaumerliac, Eds., Vol. 12, Plenum, 357–368.

Campbell, P., Y. Zhang, K. Yahya, K. Wang, K., C. Hogrefe, G. Pouliot, C. Knote, A. Hodzic, R. San Jose, J.L. Perez, P. Jimenez Guerrero, R. Baro, and P. Makar, 2015: A multi-model assessment for the 2006 and 2010 simulations under the Air Quality Model Evaluation International Initiative (AQMEII) phase 2 over North America: Part I. Indicators of the sensitivity of O3 and PM2.5 formation regimes. *Atmos. Environ.*, doi:10.1016/j.atmosenv.2014.12.026, **115**, 569-586.

Cape, J.N., S.E. Cornell, T.D. Jickells, and E. Nemitz, 2011: Organic nitrogen in the atmosphere – Where does it come from? A review of sources and methods. *Atmos. Res*., **102**, 30–48.

Carslaw, K.S., L.A. Lee, C.L. Reddington, G.W. Mann, and K.J. Pringle, 2013: The magnitude and sources of uncertainty in global aerosol. *Faraday Discuss.*, **165**, 495-512.

Carter, W.P.L., 2010: Development of the SAPRC-07 chemical mechanism. *Atmos. Environ*., **44**, 5324–5335.

Cooter, E.J., J.O. Bash, V. Benson, and L. Ran, 2012: Linking agricultural crop management and air quality models for regional to national-scale nitrogen assessments, *Biogeosciences*, **9**, 4023-4035.

Dennis, R.L., D.W. Byun, J.H. Novak, K.J. Galluppi, C.J. Coats, and M.A. Vouk, 1996. The next generation of integrated air quality modeling: EPA's Models-3. *Atmos. Environ*., **30**, 1925-1938.

Elleman, R.A. and D.S. Covert, 2010: Aerosol size distribution modeling with the Community Multiscale Air Quality modeling system in the Pacific Northwest: Part 3. Size distribution of particles emitted into a mesoscale model. *J. Geophys. Res.*, **115**, D03204, doi:10.1029/2009JD012401, 14 pp.

Fiore, A.M., V. Naik, and E.M. Leibensperger, 2015: Air quality and climate connections. *J. Air Waste Management Assoc.*, **65**, 645-685.

Foley, K.M., C. Hogrefe, G. Pouliot, N. Possiel, S.J. Roselle, H. Simon, and B. Timin, 2015: Dynamic evaluation of CMAQ part I: Separating the effects of changing emissions and changing meteorology on ozone levels between 2002 and 2005 in the eastern US. *Atmos. Environ*, doi:10.1016/j.atmosenv.2014.12.038, **103**, 247-255.

Goliff, W.S., W.R. Stockwell, and C.V. Lawson, 2013: The regional atmospheric chemistry mechanism, version 2. *Atmos. Environ*., **68**, 174-185.

Hogrefe, C., G. Pouliot, D. Wong, A. Torian, S. Roselle, J. Pleim, and R. Mathur, 2015: Annual application and evaluation of the online coupled WRF-CMAQ system over North America under AQMEII phase 2. *Atmos. Environ.*, **115**, 683-694.

Im, U., R. Bianconi, E. Solazzo, I. Kioutsioukis, A. Badia, A. Balzarini, R. Baro, R. Bellasio, D. Brunner, C. Chemel, G. Curci, J. Flemming, R. Forkel, L. Giordano, P. Jimenez-Guerrero, M. Hirtl, A. Hodzic, L. Honzak, O. Jorba, C. Knote, J.J.P. Kuenen, P.A. Makar, A. Manders-Groot, L. Neal, J.L. Perez, G. Pirovano, G. Pouliot, R. San Jose, N. Savage, W. Schroder, R.S. Sokhi, D.

Syrakov, A. Torian, P. Tuccella, K. Werhahn, R. Wolke, K. Yahya, R. Zabkar, Y. Zhang, J. Zhang, C. Hogrefe, and S. Galmarini, 2015: Evaluation of operational online-coupled regional air quality models over Europe and North America in the context of AQMEII phase 2. Part I: Ozone. *Atmos. Environ*., doi:10.1016/j.atmosenv.2014.09.042, **115**, 404-420.

Jathar, S.H., T.D. Gordona, C.J. Hennigan, H.O.T. Pye, G. Pouliot, P.J. Adams, N.M. Donahue, and A.L. Robinson, 2014: Unspeciated organic emissions from combustion sources and their influence on the secondary organic aerosol budget in the United States. *Proc. Nat. Acad. Sci*., **111**, 10473-10478.

Jen, C.N., P.H. McMurry, and D.R. Hanson, 2014: Stabilization of sulfuric acid dimers by ammonia, methylamine, dimethylamine, and trimethylamine. *J. Geophys. Res.*, **119**, 7502-751.

Kuang, C., I. Riipinen, S.L. Sihto, M. Kulmala, A.V. McCormick, and P.H. McMurry, 2010: An improved criterion for new particle formation in diverse atmospheric environments. *Atmos. Chem. Phys*, **10**, 8469-8480.

Lim, Y.B. and P.J. Ziemann, 2009: Chemistry of secondary organic aerosol formation from OH radical-initiated reactions of linear, branched, and cyclic alkanes in the presence of NOx. *Aerosol Sci. Technol*., **43**, 604-619.

Lin, M., A.M. Fiore, L.W. Horowitz, A.O. Langford, S.J. Oltmans, D. Tarasick, D., and H.E. Rieder, 2015: Climate variability modulates western US ozone air quality in spring via deep stratospheric intrusions. *Nature Commun*., **6**, art. no. 7105, DOI:10.1038/ncomms8105, 11 pp.

Mao, J., F. Paulot, D.J. Jacob, R.C. Cohen, J.D. Crounse, P.O. Wennberg, C.A. Keller, R.C. Hudman, M.P. Barkley, and L.W. Horowitz, 2013: Ozone and organic nitrates over the eastern United States: Sensitivity to isoprene chemistry. *J. Geophys. Res.*, **118**, 11,256–11,268, doi:10.1002/jgrd.50817.

Napelenok, S.L., H. Simon, P.V. Bhave, H.O.T. Pye, G.A. Pouliot, R.J. Sheesley, and J.J. Schauer, 2014: Diagnostic air quality model evaluation of source-specific primary and secondary fine particulate carbon. *Environ. Sci. Technol*., **48**, 464-473.

Pierce, J.R. and P.J. Adams, 2009: Uncertainty in global CCN concentrations from uncertain aerosol nucleation and primary emission rates. *Atmos. Chem. Phys*., **9**, 1339-1356.

Pye, H.O.T. and G.A. Pouliot, 2012: Modeling the role of alkanes, polycyclic aromatic hydrocarbons, and their oligomers in secondary organic aerosol formation. *Environ. Sci. Technol*., **46**, 6041-6047.

Pye, H.O.T., R.W. Pinder, I.R. Piletic, Y. Xie, S.L. Capps, Y.H. Lin, J.D. Surratt, Z.F. Zhang, A. Gold, D.J. Luecken, W.T. Hutzell, M. Jaoui, J.H. Offenberg, T.E. Kleindienst, M. Lewandowski, and E.O. Edney 2013: Epoxide pathways improve model predictions of isoprene markers and reveal key role of acidity in aerosol formation. *Environ. Sci. Technol.*, **47**, 11056-11064.

Riipinen, I., T. Yli-Juuti, J. Pierce, T. Petäjä, D.R. Worsnop, M. Kulmala, and N.M. Donahue, 2012: The contribution of organics to atmospheric nanoparticle growth. *Nat. Geosci*., **5**, 453-458.

Robinson, A.L., N.M. Donahue, M.K. Shrivastava, E.A., Weitkamp, A.M. Sage, A.P. Greishop, T.E. Lane, J.R. Pierce, and S.N. Pandis 2007: Rethinking organic aerosols: Semivolatile emissions and photochemical aging. *Science*, **315**, 1259-1262.

Tarasick, D.W., V.E. Fioletov, D.I. Wardle, J.B. Kerr, and J. Davies, 2005: Changes in the vertical distribution of ozone over Canada from ozonesondes: 1980-2001. *J. Geophys. Res*., **110**, 1-19.

Vehkamäki, H., M. Kulmala, I. Napari, K.E.J. Lehtinen, C. Timmreck, M. Noppel, and A. Laaksonen, 2002: An improved parameterization for sulfuric acid-water nucleation rates for tropospheric and stratospheric conditions. *J. Geophys. Res.*, **107**, doi:10.1029/2002JD002184.

Whitten, G.Z., G. Heo, Y. Kimura, E. McDonald-Buller, D.T. Allen, W.P.L. Carter, and G. Yarwood, 2010: A new condensed toluene mechanism for Carbon Bond: CB05-TU. *Atmos. Environ.*, **44**, 5346–5355.

Wong, D.C., C.E. Yang, J.S. Fu, K. Wong, and Y. Gao, 2015: An approach to enhance pnetCDF performance in environmental modeling applications. *Geosci. Model Dev*., **8**, 1033–1046, doi:10.5194/gmd-8-1033-2015.

Xing, J., R. Mathur, J. Pleim, C. Hogrefe, C.-M. Gan, D.C. Wong, C. Wei, R. Gilliam, and G. Pouliot, 2015a: Observations and modeling of air quality trends over 1990–2010 across the Northern Hemisphere: China, the United States and Europe. *Atmos. Chem. Phys*., **15**, 2723-2747.

Xing, J., R. Mathur, J. Pleim, C. Hogrefe, C.-M. Gan, D.C. Wong, and C. Wei, 2015b: Can a coupled meteorology-chemistry model reproduce the historical trend in aerosol direct radiative effects over the northern hemisphere? *Atmos. Chem. Phys. Discuss.*, **15**, 14027-14073.

Yarwood, G., S. Rao, M. Yocke, and G.Z. Whitten, 2005: Updates to the Carbon Bond Mechanism: CB05. Final Report to the U.S. EPA. Available at: http://www.camx.com/publ/pdfs/CB05_Final_Report_120805.pdf

Zhang, Y., P.H. McMurry, F. Yu, and M.Z. Jacobson, 2010: A comparative study of nucleation parameterizations: 1. Examination and evaluation of the formulations. *J. Geophys. Res*., **115**, 148-227.

APPENDIX 1. FIFTH CMAQ PEER REVIEW MEETING AGENDA

Agenda

Peer review panel: Mike Moran, Chair (Environment Canada); Marina Astitha (University of Connecticut); Kelley Barsanti (Portland State University); Nancy Brown (Lawrence Berkeley National Laboratory); Ajith Kaduwela (CARB & University of California, Davis); Stu McKeen (NOAA/ESRL); Ken Pickering (NASA Goddard Space Flight Center)

June 17 ***(C-114)***

8:30am	Review panel kick-off meeting (private discussion)
9:10am	Welcome from NERL (Tim Watkins, NERL Deputy Director)
9:20am	Summary of 2011 Review and AMAD response; Purpose and Charge to Panel (Rohit Mathur)
10:30am	BREAK
11:00am	Model evaluation/applications overview (v5.0 to v5.1) (Shawn Roselle)
11:30am	Near-real-time application and evaluation of CMAQ (Brian Eder)
12:00	LUNCH
1:00-4:00pm	POSTER SESSION and Interaction with AMAD Scientists (***Building B Atrium***)

Evaluation

1. Ensemble air quality modeling using coupled WRF-CMAQ (Rob Gilliam)
2. Application of the CMAQ model for Phase 2 and Phase 3 of the Air Quality Model Evaluation International Initiative (AQMEII) (Christian Hogrefe)
3. Assessment of the interactions among tropospheric aerosol loading, radiative balance and clouds through examination of their multi-decadal trends (Jia Xing/Chuen-Meei Gan)
4. Fine-scale applications of the coupled WRF-CMAQ system (Wyat Appel)
5. Dynamic evaluation of CMAQv5.0 (Kristen Foley)
6. Integrated Source Apportionment Method (ISAM) (Sergey Napelenok)

Applications of CMAQ for Ecosystem, Health Effects, and Climate-Air Quality Impacts

7. CMAQ applications for ecosystem and human health (Val Garcia)
8. Using CMAQ to project the impacts of future climate change on air quality (Tanya Spero)

4:00pm	Overview of CMAQv5.1 (Jon Pleim)
4:45pm	ADJOURN

<u>June 18</u> ***(C-114)***

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

9:00am - Noon: CMAQv5.1: Updates to process modules (20 min talk +10 min discussion)

9:00am Atmospheric chemistry mechanisms in CMAQ (Deborah Luecken)

9:30am Treatment of aerosol processes (Havala Pye)

10:00am Heterogeneous and aqueous chemistry (Golam Sarwar/Kathleen Fahey)

10:30am BREAK

11:00am Advances in meteorology and transport processes (Rob Gilliam)

11:30am Emissions and air-surface exchange (George Pouliot/Jesse Bash)

12:00noon LUNCH

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

1:30pm Next Generation model (Jon Pleim)

2:00-5:00pm POSTER SESSION and interaction with AMAD Scientists (***Building B Atrium***)

Chemistry

1. Updates to in-line calculation of photolysis rates (Bill Hutzell)
2. Enhanced ozone deposition and halogen chemistry (Golam Sarwar)
3. Understanding biogenic and anthropogenic influences in the isoprene system through improvements in multiple CMAQ components (Havala Pye/Jesse Bash/Deborah Luecken)

Emissions

4. Development of emission inputs for the CMAQ modeling system (George Pouliot)
5. Updating sea spray aerosol emissions in CMAQ version 5.0.2 (Brett Gantt)

Air-Surface Exchange

6. Air-surface exchange of trace gases and aerosols (Jesse Bash)

Computational and Structural Aspects

7. Enhanced parallel I/O with application level data aggregation (David Wong)

<u>June 19</u> ***(E-201)***

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

APPENDIX 2. DETAILED EPA RESPONSE TO RECOMMENDATIONS OF THE FOURTH PEER REVIEW PANEL

This appendix gives a condensed version of the summary presentation made by Dr. Rohit Mathur of AMAD on 17 June 2015 to describe AMAD's responses to both high-level and specific recommendations made by the Fourth CMAQ Model External Peer Review Panel. His presentation was organized by topic: recommendations made by the Fourth Panel are shown below in italics with a detailed reference and EPA responses follow each recommendation in a blue regular font.

Model Evaluation

While the group is arguably the world leader in this area, there are cases where they will need to be even more forward looking (Support of NAAQS review process: primary & secondary standards; new primary PM.) [Brown et al., 2011, p. 7]

- Secondary NAAQS
  - Evaluation of modeled sulfur and N (reduced and oxidized) deposition (wet & dry); accounting for biases in modeled precipitation using 2002-2012 model simulations.
- Primary PM
  - Evaluation of crustal PM constituents
  - Evaluation of single-source modeling approaches (DDM-3D, ISAM, APT, Brute-force)
  - Evaluation of fine-scale WRF-CMAQ applications with field intensives

A potential weakness is that they need to examine model evaluation efforts in a meta (overall or global) fashion and need to identify and synthesize what they have learned from all evaluation activities [Brown et al., 2011, p. 11]

- Participation in AQMEII
  - Common evaluation approach for all models – looking at diversity across models
  - Results synthesized and disseminated through journal special issues
- Evaluation results are guiding development of linked models across scales (local to hemispheric), media (air-water-land), and issues (AQ-climate)

One of their emerging activities, probabilistic evaluation will require more development and application to realize its full potential [Brown et al., 2011, p. 11]

- We agree that the area of probabilistic evaluation is important for both regulatory and forecast applications. Examples of our continued efforts:
  - Intrinsic uncertainty in models (see poster on "Ensemble air quality modeling using coupled WRF-CMAQ")
  - Ensemble model analyses in AQMEII phase 1 & 2

Chemistry

Commended and encouraged the continued development of alternate approaches for chemical mechanisms [Brown et al., 2011, p. 7]

- We have tested and included the RACM2 gas-phase chemical mechanism which will be available in CMAQv5.1.
- Numerous updates to the CB05 and SAPRC mechanisms to extend their use for emerging applications (e.g., treatment of organic nitrates, linkage with SOA and heterogeneous chemistry)
- Active participant in chemical mechanism development community:
  - Organizing/planning the UC Davis Atmospheric Chemical Mechanisms conference
  - Engaged with the researchers in the UK on MCM and condensed version development
  - Participated in the recent meetings of NAS Committee on The Future of Atmospheric Chemistry Research
  - Working with the EPA STAR program on an future RFP on atmospheric chemical mechanisms for the next generation models

Encourage group to devote more attention to field validation of calculated photolysis rates [Brown et al., 2011, p. 11]

- Modeled photolysis rates have been compared with aircraft measurements during field campaigns (ICARTT, DISCOVER-AQ). Clear-sky rates appear to be in reasonable agreement. Challenges are more in assessment of representation of attenuation by clouds (placement and cloudiness) and aerosols (lack of measurements when loading is high).
- CMAQv5.1 includes revisions to the treatment of cloud effects on photolysis

Future directions might include incorporation of stratospheric chemistry [Brown et al., 2011, p. 11]

- We agree that representation of the stratosphere could be important for emerging applications (e.g., background O_3) and have explored, but not actively pursued incorporation of explicit stratospheric chemistry because (1) current model extent only includes the lower stratosphere, and (2) simulation durations are not long enough to sufficiently represent the key reactions.
- Investigated the use of a potential vorticity scaling for representing impacts of STE on tropospheric O_3 – developing a seasonal and spatially varying scaling.

Particulate Matter

While progress has been significant, need for improvement in:

(1) review of soil dust schemes (in limited area models and not GCMs) [Brown et al., 2011, p. 8]

- Refinement and testing of the wind-blown dust scheme included in CMAQv5.0, both for continental U.S. and hemispheric applications is an area of continued work. Efforts have also been devoted to improving seasonal estimates of anthropogenic dust in the inventories.

(2a) addition of heterogeneous chemistry processes [Brown et al., 2011, p. 9]

- Current model: Uptake of N_2O_5on aerosols

  $N_2O_5(g) + H_2O\ (aq) \rightarrow 2\ HNO_3(g)$

- When particle contain Cl, uptake of N_2O_5 can also produce $ClNO_2$

  $N_2O_5(g) + H_2O\ (aq) + yCl\ (aq) \rightarrow y(\ HNO_3(g) + ClNO_2(g)\ ) + 2(1\text{-}y)\ HNO_3(g)$
- Alters partitioning of reactive nitrogen, impacts oxidant chemistry, and thus impacts production of secondary pollutants

(2b) addition of heterogeneous chemistry processes [Brown et al., 2011, p. 9]

- CMAQv5.1 will also include heterogeneous SOA additions:
  - Uptake of IEPOX based on water, sulfate, & acidity in the particle (CB and SAPRC)
  - Uptake of MAE (in SAPRC)

(3) Treatment of number density and size distribution (important for met-AQ coupling and aerosol indirect effects) [Brown et al., 2011, p. 8]

- CMAQv5.1 incorporates:
  - corrections to the current binary nucleation scheme (Vehkamäki et al., 2002), and
  - updates to PM emissions modal mass fractions and size distribution based on modern measurements (Elleman and Covert, 2010)

Identifying and removing sources of bias in sulfate predictions should be a high priority for the Division [Brown et al., 2011, p. 12]

- We agree that amongst all PM constituents, predictions of SO_4^{2-} should (and do) have the highest confidence, since SO_2 emissions are well quantified and gas and aqueous formation pathways are well understood.
- Bias in SO_4^{2-} predictions stem from a combination of effects: (1) ability of mechanisms to predict OH and H_2O_2 and thus the relative importance of gas vs aqueous pathways; (2) representation of non-precipitating clouds; (3) bias in precip amounts regulating the removal from the atmosphere.
- We have examined other plausible pathways for SO_4^{2-} formation to account for the small summertime deficit (e.g., through stabilized Criegee intermediates), but the kinetics of this pathway are still quite uncertain.
- Multi-decadal (1990-2010) trends for SO_2 and SO_4^{2-} simulated by the model match well with observations providing confidence in the ability to represent changes in response to changes in emissions and atmospheric dynamics, and thus model inferences drawn on a relative sense.
- Expansion of CMAQ to hemispheric scales is now enabling more consistent representation of space and time varying SO_4^{2-} LBCs. DMS chemistry is also being included to complete the tropospheric SO_4^{2-} budget.

Continued emphasis on the need to examine problems in a more integrated manner [Brown et al., 2011, p. 12]

- We agree that gas-aqueous-aerosol phase connections need to be examined in an integrated manner and have continued to evolve the CMAQ system along those lines
- Example: see poster on "Understanding biogenic and anthropogenic influences in the Isoprene system through improvements in multiple CMAQ components"

Meteorological Modeling

It would be useful to perform more testing at higher resolutions [Brown et al., 2011, p. 9]

- Significant effort has been devoted towards improving the representation of meteorology and coupling with the CTM for finer resolution simulations. Model development and evaluation at these fine resolutions (1-4 km) have focused on the DISCOVER-AQ field campaigns.

Coupled WRF-CMAQ

The WRF-CMAQ coupler is efficiently designed. There are questions related to its use in other computer cluster configurations [Brown et al., 2011, p. 10]

- The coupled WRF-CMAQ system has been exercised by AMAD on two different clusters at EPA. We have also ported the model to two different DOE machines. We have collaborated with groups in the UK, Greece, and China on WRF-CMAQ applications on different machines. We have not received any specific feedback from the user community on issues related to WRF-CMAQ deployment on different cluster configurations.

The coupler is designed to work primarily with one grid configuration and this imposes some restrictions on optimal use of WRF capabilities (2-way nesting)… The hemispheric configuration of the coupled model 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. [Brown et al., 2011, p. 10-11]

- Multiple grids can still be configured for one-way nesting. Our previous work suggests that 2-way nesting poses many fundamental issues related to mass conservation in non-linear chemical flow problems. We thus have not pursued 2-way nesting for non-linear chemistry problems. Nevertheless we acknowledge the need for multiscale modeling for atmospheric problems and instead are exploring alternate approaches for grid refinement that circumvent the issues of discrete boundaries of 2-way nesting (e.g., prototype development of OLAM-Chem; testing of tracer-transport in MPAS).

Weigh advantages/disadvantages of coupling design and have workshop of experts in the field [Brown et al., 2011, p. 13]

- Hosted a workshop on integrated meteorology-chemistry modeling
- Participated in the EuMETCHEM project
- AQMEII phase 2 focused on coupled models

Quality and Relevance of CMAQ Modeling Program to ORD's Research Programs

Assess climate change impacts on $PM_{2.5}$ [Brown et al., 2011, p. 14]

- We have examined the impact of climate change (based on 2030 projections) on distribution and levels of $PM_{2.5}$. Large uncertainties however exist in projections of natural emissions (wildfires and fugitive dust) in response to climate change and these can influence future regional predictions of $PM_{2.5}$.

Collaborate with NRMRL on development of realistic future energy scenarios [Brown et al., 2011, p. 14]

- Active collaborations with NRMRL researchers are underway on using MARKAL (and GCAM in future) to estimate emissions associated with future energy scenarios.

Benefits could be achieved if SHEDS efforts were more closely linked with CMAQ and the two models could work together [Brown et al., 2011, p. 15]

- Linkages of CMAQ output with the SHEDS exposure model are being discussed with scientists in HEASD. In particular, as starting point, linkage of the 12/4/1-km CMAQ predictions for the Baltimore region with the SHEDS model to estimate (and contrast) various exposure metrics (and their sensitivity to spatial resolution) is being explored.

<u>Usefulness of the CMAQ Modeling Program to EPA, States, and Research Community</u>

While the effort should not be viewed negatively, OAQPS is using a competing model because CMAQ does not have all capabilities they desire (tools to provide source impacts). If the capability is important and scientifically appropriate, the group should consider adding it. If there are reasons the current approaches are scientifically less well founded, the concern should be clearly communicated. [Brown et al., 2011, p. 15]

- “Backward” attribution and apportionment of non-linearly evolving concentration fields to specific sources (or sectors) pose many numerical and mass conservation challenges. We have worked closely with OAQPS scientists in developing and implementing in CMAQ, source apportionment techniques for PM and O_3. The formulation, assumptions, and applicability of the tools were documented in two peer-reviewed articles. The tools were made available in an interim CMAQ release (v5.0.2) to the broader community.
- See poster on “Integrated Source Apportionment Method (ISAM)”

In a time of diminishing resources, we recommend that the CMAQ group should continue to develop and enhance the strengths of CMAQ.
Stay focused and not go beyond core mission and competencies [Brown et al., 2011, p. 16]

- Though the primary focus of CMAQ applicability within the Agency is on the continental US scale, current and emerging AQ issues require consistent treatment of air pollution from urban to hemispheric scales. Recognizing resource constraints and the growing application needs (e.g., secondary NAAQS and human & ecosystem exposure), we have adopted a “problem-oriented” approach to CMAQ expansions keeping in mind future extensibility and maintenance of the over system.

Develop close collaboration with experts who develop other (media) models [Brown et al., 2011, p. 16]

- Extensions of CMAQ to the “One-environment” concept is based on close collaboration with experts of other models that are being connected (e.g., Hydrology, Agriculture, Water Quality). However, some understanding of these systems (space/time scales, first principles vs. calibration) is needed to determine how to link them. Additional details may be found in poster on “CMAQ Applications for Ecosystem and Human Health”.

Should continue to maintain international collaborations [Brown et al., 2011, p. 17]

- We continue to foster and extend international collaborations:
  - Air Quality Model Evaluation International Initiative (AQMEII)
  - European framework for online integrated air quality and meteorology modelling (EuMETCHEM)
  - US-UK collaboration on air quality modeling and chemical mechanisms
  - Collaboration with Tsinghua University on WRF-CMAQ applications in China
  - Collaboration with IIT-Mumbai on WRF-CMAQ applications in India
  - Participation on scientific and organizing committees for many international conferences/workshops
  - CMAQ applications across the globe provide many opportunities to collaborate and evolve the model for diverse set of conditions

<u>Additional Recommendations</u>

Given the CMAQ team's successes in recreating past atmospheres in retrospective studies, this could be a niche that they could play in the global climate arena. [Brown et al., 2011, p. 17]

- We agree that our experience puts us in a unique position for examining past atmospheres.
- The development of the downscaling methods have used retrospective time periods to verify the fidelity of the techniques.
- Multi-decadal simulations for 1990-2010 have been conducted to examine the impacts of aerosol radiative effects on atmospheric dynamics and air quality.
- Additional details are provided in posters on (1) "Using CMAQ to Project Impacts of Future Climate Change on Air Quality" and (2) "Assessment of interactions among tropospheric aerosol, radiative balance, and clouds through examination of their multi-decadal trends"

Improve emission inputs to CMAQ model [Brown et al., 2011, p. 18]

- Biogenic emissions (see poster on "Development of emission inputs for the CMAQ modeling system")
- Residential wood combustion
- Marine environments: Sea-salt, Halogens (see posters on "Updating sea spray aerosol emissions in CMAQ version 5.0.2 " and "Enhanced ozone deposition and halogen chemistry")
- Emission trends (see poster on "Assessment of the interactions among tropospheric aerosol loading, radiative balance and clouds through examination of their multi-decadal trends")