The Sixth External Peer Review of the Community Multiscale Air Quality (CMAQ) Modeling System

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TABLE OF CONTENTS

I. Introduction

The Sixth CMAQ Model Peer Review Panel conducted a two-and-a-half-day review of the Community Multiscale Air Quality (CMAQ) Modeling Program on May 21-23, 2019. The panel focused on CMAQ model development, evaluations, and applications since the last peer review, which took place in 2015. This report summarizes the Sixth Panel's findings. Note that this report follows the series of reports from five previous peer reviews conducted in 2003, 2005, 2006, 2011, and 2015 [see Amar et al., 2004, 2005; Aiyyer et al., 2007; Brown et al., 2011; and Moran et al., 2015]. The report is written from the perspectives represented by the five-member review panel: Kelley Barsanti, Ken Pickering, Arastoo Pour-Biazar, Rick Saylor, and Craig Stroud. Panel members read a considerable volume of material provided by EPA and attended two days of presentations on CMAQ development, evaluation, and application by EPA staff (see Appendix 1 for the meeting agenda).

The CMAQ model has been developed by the Computational Exposure Division (CED) of the National Exposure Research Laboratory (NERL), Office of Research and Development (ORD), U.S. Environmental Protection Agency (EPA). CED 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 2015 that has been conducted by the 19 staff scientists (i.e., full-time equivalents) within CED who work on CMAQ development, evaluation, and application. This 2019 CMAQ Peer Review emphasized an assessment of the meteorological, physical, and chemical process aspects of the CMAQ Modeling Program, as well as evaluations of model performance and model applications. The review panel focused its attention on the model updates that were implemented in the community version of CMAQ v5.2, released in 2017, and CMAQ v5.3beta3, the final version of which is projected to be released in fall 2019.

The CMAQ Modeling Program Peer Review Panel was charged with addressing the following questions regarding the scientific and computational quality of the CMAQ modeling system for addressing air quality related concerns, bearing in mind that the primary object of the research program is to develop air quality models for use by EPA's program offices and states. The review was conducted to primarily focus on the following four charge questions:

(1) What is the overall quality of the applied scientific research in the CMAQ modeling program? What is the overall quality of the supplemental documentation?

(2) What are the strengths and weaknesses of the science being used within the new components of the CMAQ modeling program?

(3) How responsive are the development-application-evaluation elements of the CMAQ modeling program towards meeting stakeholder needs (EPA, states, and the research community)?

(4) Are there areas relevant to EPA's regulatory program needs that are not being addressed or given insufficient attention? If so, are there areas that could be given lower priority? Are

available resources being used effectively towards the choice and quality of the applied research that is being conducted?

With respect to the third charge question, CED's efforts for CMAQ development, evaluation, and application are aimed at supporting modeling activities within EPA (Office of Air Quality Planning and Standards (OAPS), Office of Transportation and Air Quality (OTAQ), Office of Atmospheric Programs (OAP)) and state and regional air management programs. The work is primarily supported under two of EPA's national programs:

(1) Air and Energy (A & E);

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

The core CMAQ development and evaluation work is conducted under the A & E research program. CMAQ applications for ecological studies and applications linking CMAQ to water quality systems are being conducted under the SSWR research program. Currently, CED's CMAQ-related research portfolio can broadly be classified as ~80% in A & E.

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 most of the time: 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 CED'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.

CED now follows a development cycle where every three or 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 CMAQv5.1 in 2015, which was preceded by the Fifth External Peer Review in mid-2015. An intermediate release, CMAQv5.2, occurred in 2017. The next major release, CMAQv5.3, is expected in late 2019, thus requiring the current Sixth External Peer Review that is the subject of this report.

The Sixth Peer Review Panel focused largely on CMAQv5.2 and CMAQv5.3, which will be the new community version, but it also paid attention to how CED 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 CED (though not its primary client), which introduced another perspective into the panel's deliberations.

The consensus of this panel is that CED and the CMAQ team have done an excellent job in responding to the recommendations from the Fifth Peer Review Panel and in improving the CMAQ code over the past four years. CMAQv5.3 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 CMAQv5.1 (Section II) and CED's responses to the recommendations of the Fifth Peer Review Panel (Section III), addresses the four charge questions to the panel and makes a number of specific recommendations (Section IV), provides seven high-level recommendations related to future CMAQ development for consideration by CED (Section V), and provides some comments about the review process itself for both the EPA and future panels (Section VI). With respect to Section V, 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.

II. Major Developments Since the Fifth External Peer Review

As noted above, the last (Fifth) External Peer review directly preceded the 2015 release of CMAQv5.1. Thus, the current (Sixth) External Peer Review covers the major developments that have followed since the release of CMAQv5.1. A number of model updates, as well as additional features and processes, were included in the June 2017 release of CMAQv.5.2. Patches to a number of CMAQ modules, fixes to default compilation and execution workflow, and a new Developer's Guide were included in the March 2018 release of CMAQv.5.2.1. A beta version of CMAQv5.3 was publicly released in October 2018, and a follow-up version ('Beta3') was released internally in March 2019. The final version of CMAQv5.3 is planned for public release in fall 2019.

Many major developments and model improvements have been made since the release of CMAQv.5.1. The significant changes in CMAQv.5.2 and CMAQv.5.3 are summarized below (see also: Hogrefe and Foley presentations). Relative to CMAQv.5.1, the model updates in CMAQv.5.2 allowed improvements in the modeled mean PM2.5 high bias in winter and low bias in summer. While bias in maximum daily average 8-hr ozone was improved in CMAQv.5.2 for Eastern states, model (negative) bias worsened in Western states. The decrease in modeled ozone between CMAQv.5.1 and CMAQv.5.2 was largely attributed to: WRF updates (meteorology), CB6 updates (chemistry), and lightning NO updates (chemistry). In CMAQv.5.3 relative to CMAQv.5.2.1, maximum daily average ozone bias was improved for a number of locations (including wintertime negative bias and summertime positive bias). However, wintertime negative bias worsened for the Western US during the winter period of evaluation. In CMAQv.5.3 (Beta 3), the model response to changes in aerosols resulted in complex behavior, for which increasing and decreasing biases were observed in roughly equal proportions. Notably, the transition to the H-CMAQ modeling platform allowed better evaluation of individual model changes on spatial and temporal variations in model predictions.

Model Updates/New Features and Processes in CMAQv5.2

Meteorology (emissions, transport):

- Updated sub-grid cloud scheme
- Transition from WRFv3.7 to WRFv3.8
- Assimilation of lightning strike data in WRFv3.8
- Transition from NEI 2011 v2 eh to 2011 v2 ek (updates in MOVES, commercial marine)
- Transition from GEOS-Chem to hemispheric CMAQ (H-CMAQ) for lateral boundary conditions

Land-surface interactions (deposition):

- Multiple updates to O_3 deposition to wetted surfaces resulting in minor net changes
- Added representation of stratospheric-tropospheric exchange for 3-D ozone distributions
- Incorporated a new physics based windblown dust emission model that yields better agreement with observations of fine and coarse PM and constituents

Gas-phase chemistry:

- Incorporated updates to organic nitrate and halogen chemistry
- Implemented the CB6r3 chemical mechanism to incorporate new information on gas-phase kinetics

Aerosol chemistry:

- Modified representation of organic aerosol (OA) volatility to more consistently treat the volatility of secondary OA (SOA) and primary OA (POA)
- Added heterogeneous uptake of glyoxal and methylglyoxal as a new source of SOA
- Added an empirical representation of SOA formation from combustion sources

Model Updates/New Features and Processes in CMAQv5.3

Meteorology (emissions, transport):

- Updated H-CMAQ based boundary conditions
- Update from 2016 ‘alpha fe’ to 2016 ‘beta ff’ emissions platform

Land-surface interactions (deposition):

- Multiple updates to M3Dry deposition scheme (dependence of ozone soil resistance on moisture, gas phase deposition to snow, aerosol deposition)
- Surface Tiled Aerosol and Gaseous Exchange (STAGE) deposition scheme added

Gas-phase chemistry:

- Minor updates to CB6r3 (ClNO3 reaction added; first-order O3 depletion)
- Full halogen chemistry – included in optional detailed mechanism
- Dimethyl sulfide (DMS) chemistry – optional detailed mechanism
- Hazardous Air Pollutants (HAPS)
- CB6r3 mechanism in CMAQ termed CB6-CMAQ

Aerosol chemistry:

- Increased monoterpene SOA
- Added uptake of water onto hydrophilic organic aerosol
- Reorganized anthropogenic SOA

III. Specific Recommendations of the Fifth External Peer Review Panel and EPA Responses

The 2015 Fifth Peer Review Panel made five high-level recommendations to improve CMAQ performance, usefulness, and relevance, along with a number of more detailed recommendations (Moran et al., 2015). The five recommendations were the following:

(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 CED computer facility ends*;

(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;*

(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;*

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

(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).*

CED examined and considered all of the recommendations made by the 2015 Review Panel. At the beginning of the 2019 Sixth Peer Review, Dr. Rohit Mathur of CED gave a presentation that summarized CED'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 CED over the past four years, the consensus of this panel was that CED and the CMAQ team have done an excellent job in responding to the recommendations from the Fifth Peer Review Panel and in improving the CMAQ code over the past four years.

IV. Panel Response to Charge Questions

Question 1. What is the overall quality of the scientific research in the CMAQ modeling program? What is the overall quality of the supplemental documentation?

The quality of the scientific research in the CMAQ modeling program is very high. The continued improved performance of the modeling system with respect to observations over each new release of CMAQ attests to the high quality of the work being performed in improving the scientific content of the model. The scientists involved in the CMAQ modeling group are all high performers and are uniformly well respected in the air quality modeling community. The work described in the materials provided for the review is a comprehensive, accurate presentation of the entire CMAQ modeling program.

Meteorology (emissions, transport):

While the development and maintenance of a meteorological model has not been the primary responsibility of CED and the CMAQ team, and the CMAQ modeling system has always relied on reputable community meteorological models, the continued scientific research by the CMAQ team has led to major contributions to these models that are pertinent to the air quality community. The continued high quality research by the CMAQ team was evident in the material that was presented for review and attested by publications of the team. Participation of the CMAQ team in the weather forecast community has ensured the availability of options that are imperative for retrospective modeling and the practices of regulatory organizations.

The CMAQ team has been able to provide unique physics parameterizations, data assimilation, land surface models, and advanced techniques that improve the realization of emissions, surface deposition, transport and transformation of gases and aerosols in the atmosphere. The scientific contributions of the team are of high quality as demonstrated in their numerous publications.

The panel was pleased by the quality of the material that was presented for review. The posters and presentations were of high quality and illustrated the depth of scientific research performed by the CMAQ team. The presentations on meteorological modeling, the next generation air quality modeling system, as well as the poster describing the surface fluxes and meteorology linkages encapsulated the specific contributions of the team.

Land-surface interactions (deposition):

In presenting the new CMAQv5.3 system, it is necessary to look backward to previous versions of CMAQ to provide a comparison between the land surface processes and results of the new system versus the old. The provided documentation generally does a good job of this comparison. Some exceptions to the overall positive assessment include: (i) Poster 15: Surface Fluxes and Meteorology Linkages – The poster is a collection of results from changes made in the land-surface modeling of CMAQ, but with very little detail or context for the changes; no reference list was provided; no mention of STAGE and how these two dry deposition options fit within the overall modeling system; (ii) Poster 15: Some papers that are referenced in presentations describing more details of the work were not provided in the Supporting Materials (e.g., "Pleim et al., (2019), in review"); (iii) Poster 6: Modeling Atmospheric Nitrogen Deposition for the Chesapeake Bay Program - another paper in review (Campbell et al., JGR) was not provided, even though it would have provided more detail about the research presented on the poster; (iv) Poster 16: The Surface Tile Aerosol and Gaseous Exchange (STAGE) Model Option in CMAQ v5.3 – it would have been helpful for the review if a more detailed written description of STAGE had been provided in the Supporting Materials.

Gas-phase chemistry:

The overall quality of the scientific research related to gas-phase chemical mechanisms in CMAQ is excellent. EPA scientists are forward thinking in developing chemical mechanisms for current and future application needs. For exposure and health applications, CMAQ has a multi-pollutant approach that addresses both criteria pollutants and hazardous air pollutants (HAPS). CMAQ also supports chemical mechanisms best suited for both regulatory and research applications.

The Carbon Bond (CB) mechanism in CMAQv5.3 has advanced from CB5 (tucl and e51) to CB6 (r3). The main update in moving from CB5 to CB6 is the improved treatment of low NOx chemistry. Longer lived VOCs such as acetone, benzene and propane are now treated explicitly. Three alkyl nitrates are now included with differing formation yields, reactivity and aqueous solubility. Additional updates to CB6-r3 have been made by EPA scientists and implemented in CMAQ, termed CMAQ-CB6. These additional updates/options include expanded SOA precursors, updated photolysis rates, inclusion of HAPS, explicit alpha-pinene SOA formation, formation of sulfate from dimethyl sulfide (DMS) and updated halogen chemistry.

EPA scientists have performed diagnostic evaluations of the CMAQ-CB6 mechanism using vertical profile measurements of odd nitrogen species (NO_2, alkyl nitrates, HNO_3, PANs) from the DISCOVER-AQ study. These detailed evaluations help ensure that ozone is being modeled accurately for the right reasons. Sensitivity analysis considering possible uncertainties in NOx emissions and odd nitrogen rate coefficients were able to improve the predictions of odd nitrogen species. Ozone predictions at the high end of the observed ozone mixing ratio distribution were also improved which should give more confidence to ozone predictions for exceedance periods.

EPA scientists have an impressive publication record over the past 5 years in developing extended halogen (Br, I) and dimethyl sulfide (DMS) chemical mechanisms. These extended mechanisms have been implemented into the hemispheric CMAQ model and result in improved ozone and sulfate predictions over the oceans. The panel is very impressed with the development of the cloud chemistry mechanism (CMAQ-KMT2), particularly the mechanistic approach undertaken, and the development of a flexible numerical solver method based on the community-tool, Kinetic PreProcessor (KPP), developed by Dr. Adrian Sandu. The publication record for the cloud chemistry research is very strong. The updated cloud chemistry mechanism improves predictions for organic acids (oxalic acid, pyruvic acid) compared to aircraft-based observations in the vicinity of clouds and at various ground level locations in the N. Hemisphere. Overall, the atmospheric chemistry projects undertaken by CMAQ scientists are of excellent quality and very relevant for future needs.

The review panel is very pleased to hear that the EPA STAR grant RFA for atmospheric chemical mechanism development has now been announced at a significant funding level. These grants will provide much needed funding to develop the next-generation of chemical mechanisms for air quality models and ensure that the state-of-the-science is maintained for future regulatory applications.

Aerosol chemistry:

The CMAQ development team is publishing high-impact research that addresses current and critical limitations in organic aerosol modeling (one of the largest uncertainties in predicting the spatial and temporal evolution of PM2.5). SOA model development efforts are addressing a wide-range of current topics, e.g., the volatility of POA (Woody et al., 2016), the contribution of intermediate volatility organic compounds (IVOCs) including from new sources such as volatile chemical products (VCPs) (Murphy et al., 2017; P14 Qin et al.), autoxidation (Zhao et al., 2018; Pye et al., 2019), and phase-separation (Pye et al., 2017, 2018). Many of the relevant papers appear in high-impact journals and are highly cited, further indicating their impact and relevance to the broader scientific community.

Many of the developments in the model representation of SOA have led to better agreement with measurements, particularly in the relative contributions of POA and SOA to total organic aerosol. The developments have not all led to better agreement with total PM2.5 measurements, which is likely influenced by: uncertainties and assumptions in implemented model representation of SOA, uncertainties in relevant emissions and meteorology, and spatial/temporal resolution of measurements vs. model output. The modeling group has established itself as a leader in implementing important SOA chemistry in CMAQ, and such comparisons are critical for the continued improvement of modeled PM2.5, particularly the organic fraction.

In addition to the largely gas-phase SOA formation pathways described above, significant progress has been made in the representation of aqueous SOA formation pathways, specifically in-cloud. Since CMAQv.5.1, the cloud chemistry module AQCHEM-KMT (Fahey et al., 2017) has been updated in CMAQv5.3 to KMTBr and KMT2. These model updates and impacts on predicted in-cloud SOA formation and PM constituents (sulfate, oxalate and pyruvate) were presented in Poster 11 by Fahey et al. These model updates represent the state-of-the-science, though model evaluation was limited likely due to lack of relevant observations.

Evaluation:

The scientific underpinning for CMAQ model algorithms has continually been improving with each new version. Considerable evaluation has been conducted for CMAQv5.2, but a more limited amount for CMAQv5.3. The talk presented by Hogrefe et al. is the only one that provided a substantive evaluation of the complete CMAQv5.3 model. Major components of v5.3, such as the CB6 mechanism, the marine (halogen and sulfur) mechanisms, and the aero7 algorithm, have been evaluated independently. The incremental improvements in PM2.5 prediction in CMAQ versions 5.2 and 5.3 are strong evidence of the improvement of the science behind the aerosol scheme, particularly with regard to organic aerosol. Improved meteorology has also had a strong influence on the improvement of CMAQ air quality predictions. One of the most important upgrades in the meteorology was the implementation of lightning data assimilation in WRF, which assists in putting deep convection in the right location and time in the model, and in turn, improves the vertical transport in CMAQ.

Concerning the supplemental documentation, there are no published papers yet on evaluation of CMAQv.5.3. However, there are many papers in the literature that support the development of CMAQ versions 5.2 and 5.3. The most important papers outlining the scientific advancements are as follows:

- *Emissions*: Foroutan et al. (2017) and Foroutan and Pleim (2017) developed an improved windblown dust emission scheme. Kang et al. (2019) developed an improved scheme for specifying lightning flash rates for use in calculating lightning NO_x emissions.

- *Meteorology*: Heath et al. (2016) implemented a lightning data assimilation scheme in WRF, which led to greatly improved transport in CMAQ.

- *Gas-phase chemistry*: Sarwar et al. (2015; 2018) and Gantt et al. (2017) reported on the development of mechanisms for halogen chemistry, an important option in CMAQ 5.3 especially in coastal regions and for use of H-CMAQ. Luecken et al. (2019) implemented the CB6 chemical mechanism in CMAQ. This mechanism greatly improves handling of NO_y chemistry.

- *Aerosols*: Murphy et al. (2017) reported on treatment of semi-volatile POA and parameterized total combustion SOA. Pye et al. (2017) developed improved treatment of liquid water associated with organic aerosol. Xu et al. (2018) and Zhang et al. (2018) reported on the importance of the monoterpene contribution to SOA, as was found in the SOAS experiment in the southeastern US. These model updates greatly improved PM2.5 prediction in CMAQ 5.3, especially over the eastern US.

- *Land surface*: Bash et al. (2018) introduced the STAGE option for dry deposition, and Ran et al. (2018) described the FEST-C agriculture – ecosystem algorithm.

Applications:

Overall, the quality of science used in recent applications is excellent. In these applications, CMAQ scientists have tried different options for key uncertain inputs or processes to assess model sensitivity. Examples include testing different sub-grid scale cloud parameterizations, different land-surface models and applying different spatial resolutions.

For the first time, the base release of CMAQ will include the Integrated Source Apportionment Technology (ISAM) module. This module calculates the contributions to the concentration of a pollutant from all its various emission sources. Gas-phase pollutants, such as ozone, can be assessed, as well as the inorganic aerosol components (sulfate, nitrate, ammonium) and elemental carbon. The ISAM is an excellent innovation that will benefit the regulatory community. A new method, based on Integrated Reactions Rates (IRR) calculations, has resulted in an improved numerical accuracy and computational efficiency. Total species concentration changes and how the reactions contributed to their change are known after each chemistry sub-time step. Source contributions are then estimated using fractions of the reactants in a reaction from each source.

For acid deposition assessments, the aqueous chemistry mechanism in CMAQ has been updated to be more state-of-the-science. An example of a recent acid deposition assessment was the use of CMAQ to calculate atmospheric nitrogen deposition in the Chesapeake Bay region. The assessment was able to demonstrate the improvements in water quality that resulted from reductions in atmospheric nitrogen due to pollutant emission reductions (NOx, SO2) enacted under the US Clean Air Act.

Another example of a recent application of CMAQ was the Kansas City Green Infrastructure study. Green planting can be a cost-effective approach for reducing stormwater runoff and thus improving urban water quality. It was shown that reducing the impervious surface and increasing vegetation can decrease the urban heat island effect and also result in the more efficient dry deposition of pollutants to the increased vegetation surface. However, cooler surface temperatures impact atmospheric stability and mixing which can enhance the surface layer concentrations of primary pollutants. The study demonstrates how coupled land-atmosphere models can assess the feedback between land surface changes and air quality changes.

CMAQ has a multi-pollutant approach, as it can predict both criteria pollutants and hazardous air pollutants for exposure and health applications. CMAQ has been used in areas with complex terrain, along coastlines and for urban areas. In these environments, higher resolution is needed to capture local gradients. One of the inherent problems with chemical transport models is the artificial dilution of emitted pollutants due to the instantaneous mixing into a grid cell. Thus, in regions with point and line emissions, it is best to perform simulations at the highest resolution possible to capture human and ecosystem exposure risk. Examples of recent studies performed at fine resolution (1-km grid spacing) with CMAQ include: DISCOVER-AQ field program simulations, Uinta Basin winter ozone formation, Flint Hills wildland fire impacts, Nooksack-Fraser nitrogen deposition, Long Island Sound tropospheric ozone production and the Colorado Front-Range complex terrain study. Overall, these studies provide valuable information on how to best setup and apply WRF-CMAQ (e.g. cloud parameterization option, land surface data assimilation). It would be helpful for EPA CMAQ scientists to include on github examples of defined high-resolution domains, input files and 'best practice' settings for the user community (recommendation #1).

EPA scientists also run CMAQ in a near-real time mode to assess the short-term forecast behavior of the model such as whether the model is capturing the observed diurnal pattern of pollutants. The near-real time runs can also identify recurring problematic forecasts and their associated meteorological features. These short-term trends can be missed in a model evaluation that focuses on monthly or annual averages. Examples of recurring problematic forecasts that have been identified include: 1) wintertime ozone over-predictions for cold periods with snow surfaces, 2) windblown dust episodes, 3) summertime ozone over-predictions over water surfaces and 4) cold pool ozone under-predictions in mountain valleys. As the EPA runs a more recent version of WRF-CMAQ than the NOAA air quality forecasting office, a closer collaboration between EPA/CED and NOAA/ARL is recommended to help inform NOAA of which model updates result in the most significant forecast improvements.

The EPA CMAQ team has a strong publication record over the past 5 years on assessing the impact of climate change on predictions of air quality. Since climate change is an important global environmental concern, the panel was pleased to see these applications for human exposure to pollution in U.S. cities (Dionisio et al., 2017), on the economic cost in the U.S. (Fann et al., 2015) and an assessment of effects in year 2030 (Nolte et al., 2018a). EPA scientists were also lead authors on the Impact of Climate Change on Human Health in the United States: Scientific Assessment (Fann et al., 2016) and a chapter on the Impacts, Risks, Adaptation in the US: Fourth National Climate Assessment: Volume II (Nolte, et al, 2018b).

Another important application of CMAQ was an assessment of the effect of aerosol reductions on surface temperature and atmospheric stability (so-called direct radiation effect). EPA scientists co-authored a paper entitled, "Unexpected Benefits of Reducing Aerosol Cooling Effects". They found that reducing aerosol concentrations resulted in less cooling that, in turn, led to more vertical mixing of pollutants in the boundary layer. This had the benefit of reducing human exposure to pollution at the surface (Xing et al., 2016). The panel recommends further studies in the future assessing the feedback of aerosol on meteorology through aerosol-radiation-cloud interactions.

CMAQ scientists have participated actively in several service and outreach activities related to chemistry mechanism development. First, they have been on the organizing committee for the UC Davis Atmospheric Chemistry Mechanism conference. This biennial event is the leading conference for researchers to present their work on chemical mechanism development. Second, CMAQ scientists actively participated in planning the CARB Mobile

Emissions workshop. This event is also biennial and brings together leading researchers in model development and source apportionment techniques.

The panel encourages the efforts that have been made towards modernizing the approach for making CMAQ (model and documentation) available to users, and facilitating interactions within the CMAQ development and user communities, largely through GitHub (CMAQv.5.3 beta). The development team has identified the clear science application and user-oriented development goals, which were presented in the Mathur talk and are listed below. Setting these clear goals facilitates prioritization of resources and allows easy evaluation of strategies and progress. The panel appreciated this goal-driven approach to outreach and communication as presented by Foley in Poster 18.

Science-application goals: improve capabilities for addressing local nonattainment issues; enable examination of US air pollution in context of changing global emissions; quantifying natural contributions vs. anthropogenic enhancements, especially with lower NAAQS threshold; improve cross-media application capability.

User-oriented development goals: greater transparency of emissions source options and scaling; improved diagnostics tools for probing and understanding mode results; increased numerical efficiency with expanded use of modern high performance computing techniques; improved user-oriented design features, such as better-organized output logs with consistent and expanded meta-data.

Question 2. What are the strengths and weaknesses of the science being used within the new components of the CMAQ modeling program?

Meteorology (emissions, transport):

With respect to meteorological needs of air quality community, the CMAQ team has actively engaged the weather forecast community to ensure that the latest science relevant to the air quality community is included in the Weather Research and Forecast (WRF) model and remains as an option for the AQ user community. Furthermore, in light of the ozone standard based on a lower mixing ratio value in the United States, the team has recognized the importance of accurate realization of background air and the need for better representation of long range transport. Thus, developing the next generation of air quality modeling system as a flexible global model with ability of seamless refinement to local scales is a positive response to the needs of the stakeholders and the AQ community. Moreover, selecting the Model for Prediction Across Scales (MPAS) as the meteorological core is in line with the developments in the weather forecast community. This will ensure the continued active engagement of the CMAQ team with the weather community and the availability of air quality relevant options in MPAS for the foreseeable future.

Model errors in cloud prediction remain a concern for air quality simulations as clouds affect emissions, photochemistry, transport, aerosol recycling and heterogeneous chemistry. The implementation of lightning assimilation scheme that limits model deep convection to the areas where lightning is observed, is a promising approach by the CMAQ team. The technique has demonstrated improvements to precipitation as well as reducing ozone bias.

Significant improvements have been made to Pleim-Xiu (P-X) land surface model (LSM). P-X LSM can nudge soil moisture to conform to the observed near surface air temperature. Use of MODIS vegetation fraction to replace the P-X table values has demonstrated improved model performance with respect to boundary layer physics.

P-X LSM is designed to be coupled with ACM2 boundary layer option and performs well when used with surface observations to perform surface moisture nudging. The technique relies on many ancillary data sets, and the system is becoming too complicated with respect to the use of these data (e.g., surface observations, LU/LC, veg. fraction, …). Clear guidelines are needed for the limitations of this technique and its proper use. There are also shortcomings in the current coupled configuration of the model (WRF/CMAQ) with respect to the vertical mixing that is due to the model construct. This shortcoming will be alleviated in the next generation air quality model as it will be a fully integrated online air quality model.

The implementation of P-X LSM, ACM2 boundary layer scheme, multiscale KF convective parameterization, and FDDA in the next generation air quality modeling system (MPAS-AQ) is ensuring that the most relevant physics options for air quality are maintained in MPAS.

The updated Atmospheric Model Evaluation Tool (AMET) is providing a suitable platform with increased functionalities for model evaluation. AMET now is compatible with MPAS and will be a useful tool in the development of the next generation air quality model.

Land-surface interactions (deposition):

The Surface Tiled Aerosol and Gaseous Exchange (STAGE) dry deposition module is a significant advancement in the CMAQ modeling system. Providing the capability to estimate dry deposition onto individual land use types within a grid cell should be useful to both regulatory and research communities and, for many applications, will be the dry deposition option of choice over the legacy M3DRY module. Further, since STAGE has been designed with the potential for bi-directional exchange of all simulated gaseous species, future enhancements to the module may allow for more biologically-driven exchanges of biogenic hydrocarbons between vegetative canopies and the atmosphere. Incremental alterations to the M3DRY module of CMAQ, including changes for deposition to snow and bare soil and reductions in coarse mode aerosol deposition velocity, all appear to be justified and improve certain specific aspects of CMAQ simulation results. It does not seem that these changes to M3DRY are being documented in the peer-reviewed literature, but should be to allow the community to evaluate and provide feedback on the resulting impacts to CMAQ simulations. With the development of STAGE, some thought needs to be given to the future of these two options for dry deposition calculations in CMAQ. It’s not clear whether both of these options will be needed going forward or whether they should be kept for use in different specific applications. Maintaining both of these options in future versions of the modeling system may also strain available limited resources.

The Fertilizer Emission Scenario Tool for CMAQ (FEST-C), version 1.4, including the Environmental Policy Integrated Climate (EPIC) field-scale cropping simulation system, is an important advance in CMAQ's ability to effectively model NH_3 bi-directional exchange. Since volatilization from fertilizers applied to crops is such a key component of total NH_3 emissions, FEST-C/EPIC's ability to more accurately provide these data leads to a remarkable improvement in simulated NH_3 concentrations as compared to data from the Ammonia Monitoring Network (AMoN) and from Cross-track Infrared Sounder (CrIS) satellite retrievals. The WRF-CMAQ-FEST-EPIC integrated modeling system is a powerful tool for a range of applications from crop yield analyses to nitrogen cycling to watershed nutrient loadings. However, as it is currently configured the FEST-C and WRF-CMAQ components are only loosely coupled across multiple-year timescales. Ideally, the FEST-C component should be closely coupled to WRF-CMAQ at an appropriate temporal resolution to provide the highest fidelity interactions between the two systems. At a minimum, the impact of the coarse temporal coupling on the system's simulation results should be quantified.

Total deposition estimates generated in part by CMAQ are an important and useful product for environmental research and regulatory assessments. The applications of these estimates to investigations of deposition to the Chesapeake Bay watershed, the Mississippi River Basin and the Nooksack Fraser Transboundary Nitrogen Study provide extremely valuable information to help protect human health and wellbeing as well as the overall environment. The total deposition maps created in conjunction with the National Atmospheric Deposition Program (NADP) Total Deposition Science Committee serve as a unique guide to the assessment of deposition to sensitive ecosystems across the U. S. However, the dry deposition estimates provided by CMAQ as part of the total measurement-model data fusion are highly uncertain, since dry deposition is notoriously difficult to measure. The uncertainty of modeled dry deposition is not unique to CMAQ but reflects a broader uncertainty within the air quality modeling community, as the algorithms that are used in contemporary models are largely based on data obtained more than 30 years ago. Participation in the Air Quality Modelling International Initiative (AQMEII) Phase 4 model inter-comparison should result in an enhanced understanding of the uncertainties inherent in modeled deposition predictions. However, a renewed emphasis should also be placed on obtaining new measurements, using new technology and approaches, over a variety of land use types to both evaluate current model dry deposition predictions and update the theoretical framework on which dry deposition is estimated. Given the national importance of the deposition-related studies and assessments mentioned above, evaluating and improving the estimates generated by CMAQ for these applications should be a high priority.

The Detailed Emissions Scaling Isolation and Diagnostics (DESID) module is an important and long overdue advance in emissions generation for the CMAQ modeling system. The additional flexibility provided by DESID should be invaluable to the research and regulatory communities for a variety of applications. Because of its potential usefulness to so many in the user community, the new tool should be made as user-friendly as possible. One suggestion to accomplish this is the creation of a graphical interface to DESID that would assist a user in developing the text file input to DESID as well as provide "sanity-checks" on specified emissions adjustments.

Gas-phase chemistry:

The halogen and DMS chemistry implemented is state-of-the-science and supports hemispheric modeling. The halogen and DMS chemistry are supported in the CB6-m mechanism where the 'm' refers to marine. The panel agrees with the mechanistic approach undertaken to SOA formation. The two-stream approach to the current development of the cloud chemistry mechanism is very appropriate and strikes the balance between new mechanism development and computational speed requirements. The on-line coupling of the gas and aqueous species solved simultaneously means that cloud chemistry can feedback and impact gas-phase oxidant levels. The consolidation of the HAPS chemistry into the CB6-CMAQ mechanism will have the benefit that assessments can be made for both criteria pollutants and air toxics in the same simulation. The CB6-CMAQ was published recently in the peer-reviewed literature. The CMAQ team has taken recommendations from the previous 5th Peer Review Assessment and consolidated the CB6 mechanism into two self-consistent versions that can be used for global/hemispheric modeling (CB6-m) and for regional/high resolution modeling (CB6).

There are several weaknesses identified in the chemical mechanisms supported and their current development:

1) The development slowed for some mechanisms (SAPRC07 and RACM2) because of the semi-retirement of their creators. The SAPRC07TIC mechanism remains as a supported mechanism in CMAQ and is largely used for research applications, as it is the most detailed, but also the most computationally intensive (includes toxics, detailed isoprene and chlorine chemistry). The new SAPRC-16 has been evaluated in the peer-reviewed literature, but performance improvements are needed, either in its mechanism or how it is implemented in CMAQ, before it is recommended. RACM2 continues to be supported in the current release of CMAQ and is used internationally for global and regional modeling research applications. Hopefully, the EPA-supported STAR grant RFA will spur continued development of these two mechanisms.

2) The CB mechanism approach is efficient, but it has disadvantages in that multi-generation chemistry is simplified greatly and the evaluation of multi-generation products is not possible unless explicit pathways are included. The review panel was pleased to see the EPA STAR grant call on developing flexible tools and systematic methods to reduce detailed chemical mechanisms. The development and implementation of lumping methods based on reactivity and volatility are needed so that both ozone and SOA formation can be modeled in a coupled manner. This will enable the user community to develop customized mechanisms which can be used for different applications (HAPS, SOA, SO_4, O_3). This will support the higher order recommendation on developing high resolution model configurations for different regions of the U.S. that are experiencing exceedance problems.

3) In conjunction with the flexible mechanism development, there is a need for systematic methods and user-friendly tools to perform the emission mapping between a detailed chemical speciation in the emissions inventories and a generated chemical mechanism.

4) None of the supported mechanisms include the RO_2 isomerization pathway under low NOx to form multi-functional RO_2 radicals (so-called auto-oxidation) which can then combine to form extremely low vapor pressure dimer species. These highly oxygenated dimer species are important in particle nucleation mechanisms.

5) There is a need to evaluate the CB-CMAQ mechanism for the toxic compounds predicted. This will provide an assessment of the uncertainties in their prediction. There are also other North American data sets that can be used to extend the available toxic measurements (e.g. NAPS).

Overall, the review panel was very impressed with the scientific rigor and scope of the research performed by the EPA CMAQ group. Continued efforts will be needed to ensure that the state of the science is transferred into CMAQ so that new research will be included in future regulatory applications.

Aerosol chemistry:

The strengths of the science represented in CMAQv.5.2 and v.5.3, with regard to aerosol chemistry, include: improved representation of the volatility of POA and SOA formation from known precursors (e.g., monoterpenes); new NO_x-mediated SOA formation pathways (particulate organic nitrate, autoxidation); and an increasingly mechanistic approach. The weaknesses/limitations include: limited characterization of uncertainty and modeled sensitivity to changes to the aerosol modules (individually and in total); and the combined use of engineering and mechanistic approaches, which creates significant potential for double counting.

CMAQv.5.3 includes four options for treatment of aerosols: aero6/6i/7/7i. The “i” denotes explicit isoprene SOA treatment and requires the use of SAPRC07tic as the gas-phase chemical mechanism. This mechanism is largely intended for research applications. Regarding inorganic aerosols, the use of the thermodynamic model ISORROPIA II for inorganic constituents (in all aerosol modules) was tested against more comprehensive thermodynamic models (e.g., AIOMFAC, Pye et al., 2018) and measurements. ISORROPIA performed reasonably well, and measurement-model comparisons highlighted the potential for errors in Aerosol Mass Spectrometer (AMS) and Chemical Speciation Network (CSN) measurements. This effort illustrates the importance and utility of using models also for evaluation of measurements. Regarding coarse mode aerosols, CMAQv.5.2 and v.5.3 have a physics-based windblown dust option available. The models with this option performed well for most scenarios, but overestimated emissions in some cases. The composition of coarse aerosol was also updated to reflect current measurements. Strengths and weaknesses of specific updates for organic aerosols in CMAQv.5.2 and v.5.3 (following presentation of Pye and Murphy) are provided below.

In CMAQv.5.2, the properties of models species were revised to more accurately represent measurements. Properties include molecular weight, OM/OC ratio, and enthalpy of vaporization (v.5.3), which affect predicted hygroscopicity and volatility. In prior versions of CMAQ, the properties of the model surrogates were derived from older chamber studies, and thus may not be representative of ambient OA characterized by more recent instrumentation. Given that predicted hygroscopicity and volatility will be sensitive to the properties of the surrogates, this is an important model update. Even with more recent chamber studies, the measured SOA is typically sufficiently less oxidized than what is measured in the atmosphere. The panel encourages the development team to consider this limitation in using chamber data (even recent chamber data) to derive the properties of the model surrogates.

Also in CMAQv.5.2, the new aerosol modules allow treatment of POA as non-volatile or semi-volatile as a function of source category. It is now well established that primary PM emission factors are likely too high, and due to sampling conditions, represent the partitioning of gas-phase compounds to the condensed-phase under non-dilute conditions. When such measurements are used *and* POA is considered non-volatile, SOA is underpredicted in urban areas and errors are likely in the ratio of POA:SOA and the spatial/temporal distribution of SOA. Therefore, as long as such measurements are used, treatment of POA as semi-volatile is likely to yield better results. However, this assumes that a reasonable volatility distribution of the POA exists. If volatility distributions are highly uncertain or absent, it may be better to assume non-volatile POA. It is likely that this is the reason that the model development team has enabled the option of semi-volatile POA by source category. Sufficient documentation of modeled sensitivity (i.e., errors associated with assuming non-volatile POA vs. uncertain/unconstrained volatility assumptions) and user guidelines (e.g., under which scenarios/model configurations should non-volatile vs. semi-volatile POA be assumed) are greatly needed.

Treating POA as semi-volatile allows consideration of SOA formation from “non-traditional” precursors, including semi-volatile and intermediate-volatility compounds (SVOCs, IVOCs respectively) largely of anthropogenic origin. Another approach for representing such pathways, is accomplished through the inclusion of the potential combustion SOA (pcSOA) pathway in CMAQv.5.2 and v.5.3. The pcSOA formation pathway accounts for SOA formation from: IVOCs that are not captured in emissions inventories (but notably maybe double counted when treating POA as semi-volatile), multi-generation oxidation of S/IVOCs that may not captured in chamber-based parameterizations of SOA formation, and SOA formation from IVOCs lost to chamber walls and therefore also not captured in chamber-based parameterizations. Given the uncertainties of each of the contributing pathways, this simplified representation of a range of processes is an appropriate way to add relevant chemistry with general observational constraints (i.e., an engineering vs. mechanistic approach). However, the panel has some concerns with the use of this parameterization in addition to other parameterizations to represent similar and even same processes, these include SOA formation from anthropogenic precursors as updated in aero7 and the treatment of POA as non-volatile (with subsequent aging to form SOA).

Similarly to the mechanistic development of isoprene SOA chemistry in CMAQv.5.1, the model development team has expanded the mechanistic representation of monoterpene SOA chemistry in CMAQv.5.2 and v.5.3, specifically including particulate organic nitrates (aero7/7i) and autoxidation products. The continued efforts to build mechanistic representations of SOA formation are considered a strength, as they better capture the dependencies of SOA formation on NO_x and SO_x, and allow more accurate estimates of the properties of particle-phase species. As these mechanistic approaches are evaluated, the panel recommends evaluation of the multi-generation, gas-phase products (in addition to particle-phase products/properties) using the latest measurement technology (e.g., tof-PTR-MS, 2D-GC/MS, CIMS). This has been done to some extent with the consideration of alpha-pinene autoxidation products (P12 Pye et al.).

There is the potential for double-counting when the mechanistically-based SOA formation pathways are added to (or layered on) existing empirically-based SOA parameterizations. When the mechanistically-derived parameterizations have been sufficiently evaluated and documented, the panel strongly recommends replacing the empirically-derived parameterizations (or deriving new reduced-form parameterizations based on the mechanistic approach). One note regarding the monoterpene parameterizations, while the parameters have been updated in CMAQv.5.3 using more recent laboratory data, further improvement is needed, as the parameters are derived from alpha-pinene experiments only and do not differentiate between ozone- and OH-initiated chemistries.

In summary, as complexity is built into the aerosol modules, it is important to characterize sensitivity and uncertainty, and implications for regulatory modeling. This is a difficult but important challenge, particularly with regard to modeling SOA. Further, while there is a desire to maintain flexibility given the diversity of CMAQ users, research and regulatory versions should be structured to limit unconstrained predictions and sufficient documentation of modeled sensitivity and user guidelines ("best practices") should be provided.

Evaluation:

Overall, CED has a very strong program of model evaluation, which includes four different types of evaluation: operational evaluation, dynamic evaluation, diagnostic evaluation, and probabilistic evaluation. The operational evaluation includes basic statistics such as monthly mean bias for PM2.5 and monthly mean bias for daily maximum 8-hour averages, primarily based on AQS data. However, a more rigorous evaluation would result from use of evaluation statistics closely related to those used in air quality regulatory affairs (e.g., fourth highest daily maximum 8-hour average ozone over the ozone season; maximum 24-hr PM2.5). Examination of model performance at the high end of the distributions of pollutant concentrations would strengthen the group's evaluation of the model. In addition, evaluation of the low end of the distributions would allow evaluation of the background values of pollutants in the model.

It is obvious that CED has devoted a tremendous amount of work to evaluation of the model changes going from v5.1 to v5.2, but evaluation of v5.3 is still in progress. A long-term v5.3

simulation (2002 - 2018) is planned for later this year. This work is definitely to be encouraged.

Improved meteorology has made a large impact on improved air quality predictions. A variety of changes to the POA and SOA schemes in the model have been made, including the uptake of water on OA. As a result, OA treatment in CMAQv5.3 is reaching state-of-the science, and significant reductions in PM2.5 biases are noted. CB6r3 updates have significantly improved predictions of NO_y species. Implementation of halogen and DMS chemistry options will be a major benefit for H-CMAQ simulations. Decreased ozone deposition to snow surface appears to have substantially improved prediction of wintertime ozone at northern latitudes. Increased ozone deposition to soil may likely had a role in reducing ozone high biases (particularly in summer), which occurred going from CMAQv5.1 to v5.3. However, the ozone bias increased in v5.3 relative to v5.2.1 for the months of March through June. This is now a low bias, the reason for which has not been assessed. Possible reasons include excessive ozone deposition to soil and the change in lateral boundary conditions.

In addition to the types of evaluation already being performed, it would benefit the regulatory community if more emphasis was placed on evaluation oriented toward the particular issues that air regulators face (e.g., long-range transport of pollutants from Asia; regional transport and chemistry (e.g., Ohio Valley to East Coast); local transport at coastlines and complex terrain (e.g., sea breeze, up/down slope)). To address these issues more use of alternative data sets will be needed (CASTNET, IMPROVE, ozonesondes, aircraft profiles, lidar, satellite, etc.) in the evaluation process. In particular, more evaluation of the model vertical profiles of trace gases and aerosols is needed, as a large portion of regional and long-range transport occurs above the boundary layer. Further evaluation of the lightning NOx schemes in CMAQ should be conducted using aircraft data from the Deep Convective Clouds and Chemistry (DC3) experiment conducted over the US in 2012.

Applications:

The CMAQ modeling system has been used in a variety of applications since the last review, mostly to provide guidance and support for EPA Programs and Regions, states and multi-jurisdictional planning organizations (MJOs). These applications include the Chesapeake Bay deposition study, the Uinta Basin Winter Ozone study, The Flint Hills Wildland Fire Study, the Nooksak-Fraser Transboundary nitrogen deposition study, the Kansas City Green-Infrastructure project and integrated hydrology and water quality modeling for the Mississippi River Basin. In most of these applications, CMAQ provides the atmospheric component of complex, integrated modeling studies. The strong science content that has been and continues to be implemented in CMAQ provides a sound basis for confidence in the model's input to these projects. The CMAQ group seems to be responding to stakeholder needs and requests with the inherent variety of these applications, both geographically and programmatically. In most cases, results from the studies are being (or planned to be) published in the open peer-reviewed literature. One concern related to these applications is whether the model's predictions can be fully evaluated. Species-specific total deposition estimates are critical components of many of these applications, but, as noted elsewhere, these model outputs have large uncertainties and need to be better quantified. Another concern is whether, with limited resources, the group is able to effectively balance the addition of new science to the model with application requests from stakeholders. Applications consume substantial resources and time, but represent a prime reason for the model's existence.

Next-Generation CMAQ:

The next-generation, global version of CMAQ is currently being developed by a small, select team within the modeling group. With the air quality improvements that have occurred in the U.S. over the past 20-30 years, it is recognized that the resulting lower concentrations of regulated pollutants are being impacted increasingly by sources outside our national boundaries. With this recognition, it is clear that a long-range pollutant transport model is needed to provide accurate model representations of these external sources. The hemispheric-CMAQ (H-CMAQ) is providing a transitional system to meet this need, but a longer-term, more robust solution is required. A truly global, CMAQ-quality modeling system will provide valuable flexibility for air quality modeling issues important to the U.S. over the next 20-30 years or longer. Moreover, the legacy CMAQ code is probably overdue for extensive redesign and code refactoring, and development of the Next-Gen CMAQ provides an excellent opportunity for this kind of model refreshening. However, the development of a global chemical modeling system is an enormous project, one which numerous modeling groups around the world have been undertaking for many years. With the current level of resources devoted to this effort, it is unclear how long it will take before a useful global modeling system can be operational. One of the key resources that will be required to make the Next-Gen system possible is sufficient computational power. Group leadership is aware of this challenge and is exploring possible solutions, including cloud computing, but at this time there is a great deal of uncertainty how this challenge will be met. In an environment of limited resources, leadership will need to carefully balance the competing resource demands of regional- and global-model development along with stakeholder applications.

Question 3. How responsive are the development-application-evaluation elements of the CMAQ modeling program towards meeting stakeholder needs (EPA, states, and the research community)?

EPA CED has focused the development and modification of CMAQ toward reduction of model biases for surface ozone and PM2.5. They have been responsive to stakeholders in this regard, but the evaluation process needs to be aimed more rigorously toward the ozone and PM2.5 statistics with which the states must demonstrate compliance for attainment of the NAAQS. In addition, the evaluation has not been sufficiently aimed at the needs of the states and regions with regard to particular air quality transport and chemistry regulatory issues (see the discussion under Charge Questions #2 and #4).

Based on the survey of CMAQ user community and in response to the recommendations from the previous CMAQ peer review panel, CED scientists have been considering alternatives to the current IOAPI in CMAQ. A new centralized I/O system (CIO) is under development and the preliminary testing of the system is promising. CIO adds to the computational efficiency of the model by eliminating the need for successive recurring interpolation for the same variable in different modules. Additionally, CIO is more appropriate for MPAS-AQ and the future needs of the air quality community as it will include the recent advances in multiprocessing. Stakeholders will certainly welcome the move away from the current IOAPI and associated separate I/O and interpolations within each science module. The Centralized I/O approach will definitely decrease memory requirements and improve run time for the model.

CMAQv5.3 is an advanced model and includes the latest science. It offers options and enough flexibility so that it can be configured to address the needs of diverse users. Thus, overall it is responsive to the needs of the stakeholders. The inclusion of physics options developed by the CMAQ team in the weather forecast model and continued scientific research and updates to these techniques in order to embrace the latest scientific advances and reduce the uncertainties in air quality simulations is in response to the needs of the air quality community.

EPA scientists are forward thinking in developing CMAQ for current and future application needs.

- For exposure and health applications, CMAQ has a multi-pollutant approach that addresses both criteria pollutants and toxics. EPA has made a good effort at balancing between all the client needs (e.g. CARB uses SAPRC, global modeling community uses RACM), improving SOA chemistry in ALL mechanisms, consolidating toxics chemistry into the CB6 regulatory mechanism, and removing outdated mechanisms.

- For acid deposition assessments, CMAQ has updated the aqueous chemistry mechanism to be more state-of-the-science. EPA scientists could consider a surface analysis product for acid deposition, combining model and network observations for critical load assessment.

- Often the air sheds in non-attainment of standards have unique emissions and/or atmospheric conditions leading to pollutant episodes. It is recommended that EPA consider supporting higher spatial resolution nested model domains over these non-attainment areas to better address the unique conditions for an air shed, both in terms of emission development, improved land surface properties/fluxes, resolved met features (convection, lake breezes) and more customized chemical mechanisms.

- Additional methods/tools for evaluation should also be considered, such as, evaluating both meteorology and chemistry together, especially in surface layer. Typical met evaluations focus on mid-troposphere conditions (using sondes) for development of weather systems, but for air quality the surface layer is the most critical.

- A clustering method for network sites could be developed and then statistics calculated on the clustered sites. This can provide an evaluation on an air shed basis, so that redundant sites do not bias the evaluation.

This is a difficult (if not impossible) question to fully answer without direct input from the stakeholders (see the comments of the review panel concerning the review process in Section 5). The presented applications seem to provide significant value for the particular localities involved (Chesapeake Bay, Kansas City, Nooksak, WA, Long Island Sound, etc.). However, we have no way to know if other localities or other parts of EPA have needs that are not being met. One stakeholder, the NOAA National Weather Service's National Air Quality Forecasting Capability (NAQFC), which uses CMAQ, is not even mentioned in the question. For the research community, the high-quality science produced by the CMAQ group is very useful, especially for active users of CMAQ.

Question 4. Are there areas relevant to EPA's regulatory program needs that are not being addressed or given insufficient attention? If so, are there areas that could be given lower priority? Are available resources being used effectively towards the choice and quality of the applied research that is being conducted?

There are a number of air quality chemistry and transport issues that are faced by the regulatory community. The evaluation of CMAQ has not been sufficiently focused on these issues. We would suggest that the operational and diagnostic evaluation processes be enhanced to include "Issue-driven Evaluation" as described below:

Issue #1: Impact of long-range transport of pollutants from Asia on US air quality. H-CMAQ should be evaluated at remote sites on the West Coast and in the interior of the western US.

Issue #2: Regional transport of pollutants (e.g., impact of Ohio Valley sources on East Coast ozone). This will require inclusion of detailed evaluation in rural areas using CASTNET sites.

Issue #3: Local transport (e.g., impact of sea or bay breezes on air quality at coastal locations, which often have the largest ozone mixing ratios on the East Coast). We recommend greater use of data (aircraft, ozonesondes, remote sensing) from DISCOVER-AQ, LMOS, LISTOS, and OWLETS campaigns.

Issue #4: Vertical distributions of gases and aerosols (important for evaluation of regional and long-range transport and for evaluation of magnitude of downward mixing of pollutants from residual layer following morning inversion breakup). Additional evaluation using aircraft profiles from DISCOVER-AQ is needed.

Issue #5: Extremes of the ozone distribution (NAAQS exceedances for ozone are based on maximum daily 8-hr average > 70 ppbv). Evaluations need to be performed using model data from specific days with observed MD8A > 70 ppbv. This approach will better evaluate the model in a regulatory sense.

The distribution of labor resources among the various focus areas appears to be appropriate. Additional personnel may be needed in moving the Next Generation modeling system toward completion. Following recommendations from the last panel, it was good to learn that computer resources have been improved. However, further increases in computing capacity will likely be needed to accommodate greater use of the MPAS-CMAQ system, as well as more fine-resolution WRF-CMAQ simulations. EPA may embark on use of a cloud computing platform in the future. However, if this approach is not taken, in-house computing resources will again likely need to be enhanced.

There is a realization in the scientific community that air quality should be viewed globally. With respect to U.S. regulations, the background air and natural variability of ozone is becoming more important for decision makers. Thus, long-range (intercontinental) transport and natural emissions are becoming more important. Due to these concerns, the development of the next generation air quality modeling system, a modeling system that can realize global chemical transport as well as fine scale regional/local air quality, has a higher priority. This also requires engaging the larger air quality community, researchers and end users, to ensure that such a modeling system will be responsive to the needs of the user community. This next generation model should be a community model in order to enjoy the success that CMAQ has enjoyed.

It appears that the majority of effort within the CMAQ modeling program is geared towards improving model performance for regulatory purposes and that available resources are being used effectively in this endeavor. In particular, performance of the model in simulating ground-level O_3 and $PM_{2.5}$ concentrations have been a primary focus of many of the model improvements made over the span of many years. And, the continual improvement of model biases for these species over this span attests to the success of the effort and is largely due to improvements in incorporating the latest scientific understanding into the system and recognition of the importance of accurate boundary conditions for sub-hemispheric applications. Although deposition of particular species is not currently regulated, the creation of the NADP Total Deposition maps, using CMAQ in part, has sparked the use of these data for assessment purposes. Since these deposition estimates are now being more widely used, more attention should be paid to quantifying the uncertainties inherent in their creation. In particular, establishing how uncertainties in dry deposition modeling affect the overall total deposition estimates and in what areas of the U. S. these uncertainties may be more important than in other areas.

In terms of meeting EPA regulatory needs:

- The use of CMAQ-adjoint modeling would be useful. Adjoint sensitivity analysis can assess the impact of proposed emission reduction strategies for specific non-attainment locations. It is recommended that EPA develop some in-house expertise to implement and maintain the adjoint code into the latest CMAQ versions. Now that the forward sensitivity model (ISAM) has been developed and implemented with great success, efforts could move to the adjoint model.
- The use of measurement-derived emissions (e.g. satellite, aircraft box flights) can also help to improve base case emissions in CMAQ simulations, particularly for sectors

where reported emissions are uncertain or not reported. Improving forest fire emissions is a priority given the increased frequency of fires and their large emissions close to populated areas.

- The panel was pleased that a new proposal calls for an EPA STAR grant for chemical mechanism development was announced. This will help foster new researchers in this field and hopefully a more systematic approach to mechanism development and condensation.
- Maintaining CMAQ code flexible and consistent with meteorological model (WRF) developments is a challenge. It is recommended that a researcher focused on WRF development tailored for air quality applications be considered. This can reduce the workload on all the other EPA scientists so that they can focus on their CMAQ area of specialty. This researcher can also focus on the direct and indirect effect of aerosol on meteorology, particularly assessing the impact of the great research being done on organic aerosol modeling.

V. Panel Recommendations

The panel would like to make the following seven overarching recommendations for the CED CMAQ modeling team to consider and, if judged to be helpful and achievable, to implement as resources permit:

1. Due to the increased complexity of CMAQ and the diverse user community, EPA/CED should prepare guidance on recommended model inputs and configurations for different types of applications, and provide inputs and high resolution domains for different non-attainment regions that have unique emissions, chemistry and meteorology.

Rationale: Local non-attainment presents unique modeling challenges due to a combination of unique emission sources, meteorological conditions and geographical features. The regional scale CMAQ model is developed with a holistic approach of trying to improve overall scores from the national ambient data networks. However, there are clear differences in model performance for east vs. west and north vs. south U.S. For example, air sheds along the lee side of the Rocky Mountains experience impacts from complex terrain and stratospheric intrusions. Urban areas along the shores of water bodies experience systematic land-water breezes that impact vertical mixing and can recirculate emissions. Certain regions are impacted by oil and natural gas extractions while other regions are impacted by highly reactive VOC emissions from oil refining. Agricultural areas that are impacted by aged urban emissions often have poor air quality which reaches standard exceedance levels for both ozone and $PM_{2.5}$.

Clearly, due to the number of diverse regions, it would be beneficial to engage the user community in tackling these problems. However, the user community does not always have the knowledge on how to set up CMAQ most appropriately for a particular region. It is recommended that EPA/CED prepare model inputs and guidance documents based on their experience in understanding the most appropriate chemical mechanisms, surface models and meteorological processes for a particular region. The pollutant emissions could also be provided for a recommended chemical mechanism and gridded to a prepared high resolution domain. This would save the user community much time in learning how to best configure all of these inputs and most importantly make sure that parameterizations are not selected that are not compatible with each other and produce unrealistic results.

2. To encourage continued development of multiphase chemical mechanisms and SOA modules, as well as the adoption of these model updates, we recommend development of reduced form mechanisms and SOA modules that represent the state of the science and meet the needs of the broadest user community.

Rationale: The CMAQ aerosol model development team is recognized for their leading excellence in the implementation of mechanistic and parameterized representations of SOA formation in CMAQ. The study of SOA formation is relatively new, and advances in instrumentation are leading to rapid advances in understanding of relevant chemistries. That said, observations are not necessarily sufficient for constraining and evaluating model representation. Therefore, the panel recommends the development and evaluation of reduced form mechanisms and SOA modules that include representations of known chemistries, while maintaining computational efficiency. Distributions of PM2.5 predictions (and other relevant metrics, such as OC), as a function of uncertainties in the reduced form modules (e.g., autoxidation yields), should be well documented. With appropriate evaluation and documentation, the use of such reduced form modules in regulatory applications is preferable to using older CMAQ model versions, since such models will allow more accurate assessments of the sensitivity of criteria pollutants (specifically PM2.5) to changes in emissions and other air quality mitigation strategies.

3. Given the increasing complexity of chemical processes and continuous refinement of meteorological processes and grid meshes, we recommend diversifying the datasets that are used for model evaluation. These include: vertical profile data (aircraft, lidar, sondes), remote/rural data, and satellite data (e.g., OMI, TROPOMI, MODIS, TEMPO). We also recommend the use of satellite data for constraining emissions.

Rationale: Increasingly, stakeholders are required to use CMAQ in addressing air quality issues involving long-range and regional transport and in complex meteorological conditions. Most of the evaluation seen in this peer review is based on AQS data (biased toward urban and suburban sites), with a very occasional use of rural data such as CASTNET or vertical profile data such as that from DISCOVER-AQ. The panel calls for much greater use of these types of data sets from rural/remote areas and from the many intensive air quality field programs that have been conducted in the US over the past decade or more. The panel saw no use of satellite data in the presentations and posters, whereas the literature from the atmospheric community as a whole contains much use of satellite retrievals of NO_2, SO_2, HCHO, and AOD for evaluation of other models and in constraining emissions (the top-down approach).

4. Uncertainty estimates for CMAQ-generated dry deposition, and ultimately total deposition, should be developed, preferably based on measurements resulting from leveraging activities of groups within and external to EPA, and supplemented by results from Phase 4 of AQMEII.

Rationale: Dry deposition estimates from air quality models, including CMAQ, are highly uncertain because of a lack of high-quality measurements that can be used to evaluate the modeled deposition rates. Total deposition estimates generated wholly or in part by CMAQ are now being used both within EPA and externally to perform environmental assessments and planning. Uncertainty estimates for these modeled deposition rates would provide needed clarity in their use for these activities.

5. Renew coordination with NOAA NAQFC through comparative evaluations of NRT simulation results against NAQFC forecasts and pursue other collaborative research efforts.

Rationale: Most regulatory applications of CMAQ consider retrospective simulations, and model evaluations concentrate on longer term statistics. Near real-time CMAQ simulations (CMAQ-NRT), however, allow the CMAQ team to evaluate the model performance continuously at finer temporal and spatial scales and to identify systematic errors that would otherwise be obscured in longer retrospective evaluations.

EPA's CED began CMAQ-NRT simulations in 2014 when EPA was directly involved with NOAA's National Air Quality Forecast Capability (NAQFC). This has been a valuable activity as it has identified several model deficiencies and provided feedback to the CMAQ development team to prioritize model update activities. However, such information is also valuable to the NOAA NAQFC as they provide real-time forecasts. Thus, better coordination between the CMAQ-NRT activity and the NOAA NAQFC will be beneficial for both groups. While CMAQ-NRT might be using the latest advances in CMAQ and there will be differences in model science and configuration, sharing the evaluation tools and comparative evaluation of CMAQ-NRT against NAQFC forecasts should be constructive for both groups.

6. The panel is encouraged by the ongoing efforts to design CMAQ to support smooth integration with next-generation coupled met/chem models. We recommend the consideration of a 0-D version of CMAQ (rather than 1-D), which supports coupled chemical and meteorological predictions (e.g., aerosol-radiation-cloud interactions).

Rationale: As the influence of background air and natural variability of ozone is becoming ever more important in designing an effective local emissions reduction strategy, attempts to construct a global-to-regional-to-local next generation air quality modeling system are in line with the needs of regulators as well as the scientific community. The CMAQ team has demonstrated notable competence in defining a vision for such a model and in creating a working prototype that preserves the critical components of CMAQ modeling system. The team also recognizes the need for a complete redesign of CMAQ for seamless integration within a global meteorological model.

In transitioning to the next generation MPAS-AQ and redesigning CMAQ, it is imperative to take note of the reasons for CMAQ success as a community model and to address some of the deficiencies of the current model construct. The success of the CMAQ as a community model is attested by the growing number of users worldwide and the growing number of publications using CMAQ. This has been possible due to model flexibility to integrate the latest scientific knowledge as well as its flexibility to be used for different applications. Therefore, for the new MPAS-AQ to enjoy the success of CMAQ, it should maintain this flexibility.

Furthermore, the original CMAQ was designed as an offline model with a meteorology-to-chemistry interface processor (MCIP) to provide the meteorological input to the chemical transport model (CTM). This was done to allow the CTM to be independent of the meteorological model and have the flexibility of being used with different meteorological inputs. However, in doing so, many of the atmospheric processes were recreated in CTM. This construct led to inconsistencies between the meteorological model and the CTM for some of the processes. Even, the current coupled version of CMAQ suffers from this deficiency. To address this issue for the next generation model, the redesigned CMAQ should avoid replicating physical processes and remain only as a chemistry processor. In doing so, the chemical processes for each grid volume will be represented by the 0-D CMAQ while the transport will be treated by the meteorological model. Such a construct will enhance the flexibility of CMAQ and will address the current model deficiencies.

7. Given the importance of additional fine-resolution simulations and the next generation modeling system for CMAQ users and stakeholders, we highlight the need for additional resources (computing and labor FTEs).

Rationale: The peer review revealed that the CMAQ team intends to undertake a greater amount of fine-resolution (1 km horizontal resolution) simulations for limited domains and time intervals, as well as greater use of the hemispheric version of CMAQ to evaluate intercontinental transport and to provide lateral boundary conditions for CONUS CMAQ simulations. In addition, there is the ongoing program to develop the next general modeling system, which will be based on the MPAS meteorological model with EPA-developed physics parameterizations. CMAQ chemistry is being added to this model. All of these activities will lead to the need for increased labor and computing resources. The panel is encouraged that in the four years since the Fifth Review, CED has managed to increase the CMAQ team from 16.5 to 19 FTE, and significantly increase its computing capacity. However, with the planned activities for the coming years, we foresee an increasing need for both labor and computing resources well into the future that will need to be addressed.

VI. Comments on the Review Process

The overall peer review process was greatly improved for the 2019 Sixth Review compared with the 2015 Fifth Review. This outcome was due to several of the specific recommendations made in the final report from the Fifth Review Panel: 1) advance communication of relevant information (topics, agenda, schedule, logistics) to the panel before the meeting; 2) panel members identifying and agreeing to individual topic assignments; 3) receipt of copies of talks and posters prior to the meeting; 4) having a closed-door meeting of the panel at the beginning of the first day for organizational purposes; and 5) having two panel members assigned to each poster.

The relative distribution of time between presentations, posters, and closed-door sessions was appropriate, and allowed for sufficient time for the panel to interact with CED personnel and with each other. The time scheduled for follow up questions with CED on the third morning was not needed; it is recommended that this time be allocated to the panel for closed-door report and recommendation writing.

It is recommended that the panel be given two weeks from the last day of review to prepare and submit the first draft of the summary report.

Since two of the charge questions (3. and 4.) were related to how responsive the CMAQ program is to its stakeholders, some thought should be given to ways that stakeholder input could be provided to the review committee prior to the review. This could potentially be accomplished either by mounting a stakeholder survey prior to the in-person review or having key stakeholders attend the review for private onsite meetings with the panel. Without this direct input from stakeholders, the panel has to rely solely on its knowledge (or assumptions) about stakeholder needs and experiences to provide useful input on these types of charge questions.

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Appendix 1.

Sixth CMAQ External Peer Review Meeting Agenda

AGENDA
6th CMAQ PEER REVIEW MEETING
May 21-23, 2019

<u>May 21, 2019</u> *(Room C114)*

8:15am	Pre-meeting Reviewer Discussion (Reviewers only)
8:50am	Welcome from Versar (Laura Williams)
9:00am	Welcome from NERL/CED (Tim Watkins/Tom Pierce) Purpose and Charge to Panel (Tom Pierce)
9:15am	Summary of 5th CMAQ Review and CMAQ-Team response (Rohit Mathur)

10:00am - Noon: What drives CMAQ evolution?

10:00am	Model evaluation overview: lessons from CMAQv5.1 to CMAQv5.3 (Christian Hogrefe)
10:30am	BREAK
11:00am	Model evaluation to support application and development of CMAQ (Kristen Foley)
11:30am	Atmosphere-land connection applications (Donna Schwede)
12:00noon	LUNCH

1:00-4:00pm POSTER SESSION & Interaction with CED Scientists (*Building E Atrium*) (1:00-2:30pm)

CMAQ Evaluation

P1 Modeling Regional Air Pollution in the Context of a Changing Global Atmosphere (Christian Hogrefe)

P2 Continuous, Near Real-Time Application and Evaluation of WRF-CMAQ (Brian Eder)

P3 Improving Emissions for Local to Global Air Quality Modeling (George Pouliot)

P4 Fine-scale Applications of the WRF-CMAQ Modeling system (Wyat Appel, Rob Gilliam)

P5 Integrated Source Apportionment Method (ISAM) (Sergey Napelenok)

(2:45-4:00pm)

CMAQ Applications

P6 Modeling Atmospheric Nitrogen Deposition for the Chesapeake Bay Program (Jesse Bash)

P7 FEST-C v1.4: An integrated Agriculture, Atmosphere, and Hydrology Modeling System for Ecosystem Assessments (Limei Ran)

P8 Green Infrastructure Scenario Analysis using the WRF-CMAQ Modeling System: Kansas City Case Study (Shawn Roselle)

P9 Climate Change Applications of CMAQ (Chris Nolte/Tanya Spero)

P15 Surface Fluxes and Meteorology Linkages (Limei Ran) (*Moved from Day2*)

4:00pm	Overview of CMAQv5.3 (Rohit Mathur)
4:45pm	ADJOURN

<u>May 22, 2019</u> ***(Room C114)***

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

9:00am - Noon: CMAQv5.3: Updates to process modules

9:00am Multi-phase chemistry updates in CMAQv5.3: gas and aqueous phase chemistry (Deborah Luecken/Kathleen Fahey)

9:30am Treatment of aerosol processes in CMAQ v5.2-5.3(Havala Pye/Ben Murphy)

10:00am Advances in retrospective meteorology modeling from global to local scales (Rob Gilliam)

10:30am BREAK

11:00am Status and plans for the Next Generation Air Quality Modeling System (O. Russell Bullock)

12:00noon LUNCH

1:00-5:00pm POSTER SESSION & Interaction with CED Scientists (*Building E Atrium*)
(1:00-2:30pm)

Chemistry

P10 Improving Atmospheric Chemistry over Marine Environment (Golam Sarwar)

P11 Enabling Examination of Cloud Chemistry Pathways for PM formation: AQCHEM-KMT (Kathleen Fahey)

Aerosols

P12 Anthropogenic Enhancements to Production of Highly Oxygenated Molecules from Autoxidation (Havala Pye)

P13 Improvements in Representing Aerosol Emissions (Ben Murphy)

P14 Secondary Organic Aerosols (SOA) Formation from Volatile Chemical Products (VCPs)

(Momei Qin)

(2:45-4:00pm)

Air-Surface Exchange

P15 *Moved to Day 1*

P16 The Surface Tiled Aerosol and Gaseous Exchange (STAGE) Model Option in CMAQv5.3 (Jesse Bash)

CMAQ Structure and Outreach Activities

P17 Centralizing the Input/Output Functions (CIO) in CMAQ (David Wong)

P18 Engaging a Growing CMAQ Community: Communication & Outreach (Kristen Foley)

5:00 pm ADJOURN

May 23, 2019 ***(Room E249)***

8:30am	Recap of Day 2 and questions from Panel
9:00am	Panel work time
11:30am	Panel Debrief to CED
12:00noon	END OF PEER REVIEW MEETING
12:00noon	LUNCH and continued panel work time

Appendix 2.

Detailed EPA Response to Recommendations of the Fifth Peer Review Panel

Below are the five high level recommendations from the Fifth Peer Review Panel and the responses from CED as presented by Dr. Rohit Mathur on the first day of the Sixth Review. In addition, CED responses to specific items of concern from the Fifth Panel as presented by Dr. Mathur are summarized.

Panel Recommendation #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

- T. Pierce serves on ORD's Information Management Governance Board which provides guidance on HPC resource allocations
- EPA's National Computer Center acquired a new Dell cluster in 2017; compared to earlier system:
  - 2.5x number of cores
  - 8x the compute capacity (Gflops/s)
- Demands of expanding CMAQ to hemispheric scales, addressing finer resolutions for urban applications and running simulations spanning multi-decadal periods are currently accommodated, though application complexity is expected to increase (e.g. additional diagnostic simulations with DDM and ISAM)
- The CMAQ Team has been working with CMAS Center and a cross-agency workgroup to create a cloud-based modeling platform (Poster by K. Foley)

Panel Recommendation #2
Work to develop a more integrated, extensible, maintainable, flexible, and efficient comprehensive chemistry package for use by CMAQ. Consideration should also be given to developing a single package with different forms to be used in different parts of the domain

- Agree that current mechanisms and connections between gas, aerosol, and aqueous chemistry in CMAQ (and other models) are insufficient to meet emerging challenges
- Current efforts to integrate/extend/maintain multi-phase chemistry
  - Codes to create the EBI code for mechanisms
  - Simultaneous integration of gas-and heterogeneous-chemistry starting in CMAQv5.1
  - *Posters on further development of the AQCHEM-KMT (K. Fahey), SOA pathways (H. Pye), marine chemistry (G. Sarwar)*
- To augment our limited resources & harness expertise in scientific community, we worked with the A&E NPD and the EPA STAR grant program to develop an RFA "Chemical Mechanisms to Address New Challenges in Air Quality" (open till June 24)

Panel Recommendation #3
Take a two-track approach to the development of the next-generation air quality model -(1) near-term: develop (process representations) & apply HCMAQ; (2) in parallel explore column-version of CMAQ, multiple coupling strategies, coupling with several global dynamics models to ensure flexibility

- The panel's recommendation was very much in sync with our next-generation model development plans
- CMAQv5.3 can be configured for urban to hemispheric scale applications

- Extensive applications with HCMAQ have been conducted and analyzed
  - Multi-decadal (1990-2010); NRT; AQMEII (posters by C. Hogrefe & G. Sarwar)
- Fractional step approach allows integration of gas-phase, aqueous phase, and heterogeneous chemistry as well as aerosol microphysics and chemistry in independent boxes
- Surface processes (biogenic emissions, dry deposition, bi-directional exchange, dust emissions), plume-rise, gravitational settling, boundary layer turbulent transport can be modeled in a 1-d (vertical) configuration
- MPAS-CMAQ prototype has been created by integrating a column version CMAQ with MPAS (*presentation by J. Pleim*)
  - CMAQ column code shared with NOAA-ESRL for linkage with FV3
  - Centralized IO and additional restructuring are exploring flexibility in coupling strategies to different dynamical models

Panel Recommendation #4

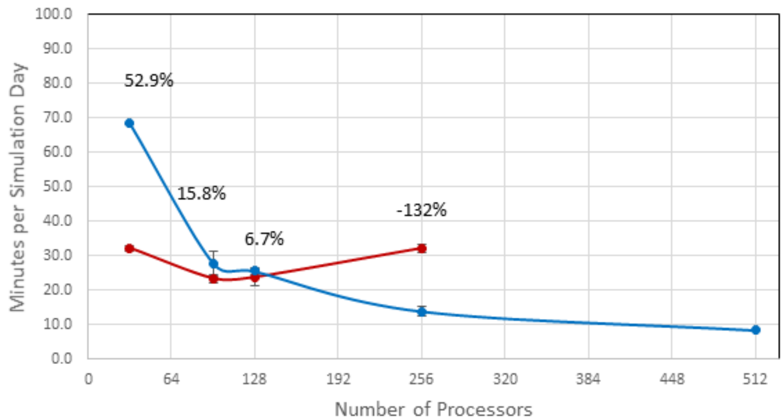
Consider investing additional resources in emissions processing & modeling

- We recognize that new and evolving CMAQ capabilities will continue to pose new requirements for input emissions
  - Recruited a post-doc to research wildfire emission specification (e.g., vertical allocation)
  - Recruited a post-doc to reconcile estimates of volatile chemical product emissions
  - Work closely with OAQPS Emission Inventory and Analysis Group (EAIG)
  - Work with National Risk Management research Laboratory on NH3flux measurements
  - Sector specific emphasis (e.g., agricultural NH3; poster by L. Ran)
  - Working with OAQPS on emission specification for Northern hemisphere
- Standardized and expanded the capabilities in CMAQv5.3 to directly modify emissions inputs and avoid reprocessing of emissions for typical use-cases
  - Improves transparency & flexibility in model use
- *Posters by G. Pouliot and B. Murphy*

Panel Recommendation #5

Improve numerical methods in CMAQ. Conduct profiling to identify bottlenecks and guide rewrite/restructuring.

- To provide a point of comparison, CMAQ profiling results compared to that of CAMx
  - Similar relative proportions (but CMAQ has many additional species)
  - Reduced the number of PM constituents to enhance model speed
  - Conducted extensive tests to identify optimal compiler options
  - CMAQ-scalability:



CMAQ: 8.4 min/simulation-day; ~ 2.2 days for an annual run with 512 processors

Judging from CMAS "m3user" comments, encourage CMAQ team to consider alternatives to IOAPI

- A new IO system for CMAQ is under development and testing that will replace the current IOAPI in an upcoming (interim) model release (Poster by D. Wong).

<u>Emissions</u>:

The panel noted that one area needing improvement is the evaluation of emission components Could further improve scientific basis of their models either by adopting top-down capabilities or by judiciously using observation-based estimates

- Collaborating with colleagues in OAQPS/OTAQ on assessing the suggested bias in mobile NOx emissions (*Presentation by K. Foley; Poster by G. Pouliot*)
- Analyzing trends relative to measurements

With increase in oil/gas production, methane, ethane, a host of toxics, and additional SOA precursors may need to be considered

- CMAQ modeling analysis for Uinta Basin, Utah:
  - Increase VOCs by a factor of 5 to match measurements, methane by a factor of 3

<u>Meteorology and Transport</u>:

WRF-CMAQ ensemble results are encouraging; CED should promote the use of such techniques in both research and regulatory community

- We agree that use of ensembles is a good approach for characterizing uncertainty in AQ predictions. Current resource constraints however limit routine ensemble modeling. We however continue to pursue such investigations through initiatives such as AQMEII

Perceived weakness: lack of method to include diurnal variations in SST, which could be important for shallow water bays and lakes

- We are using high resolution (1km) GHRSST
- Combining GHRSST with other data sets to prescribe a diurnal variation requires further investigation
  - Initial application of a diurnal temperature range on a base SST in the Galveston Bay (shallow Bay) did not appear to impact the predicted meteorology (e.g., sea breeze strength and positioning) in an appreciable manner
- Additional testing is being conducted as part of modeling for LISTOS

A satisfactory stratosphere-troposphere exchange treatment has been elusive. Representation of this process is important for hemispheric modeling, AQ-climate modeling and regulatory modeling –CMAQ team should continue to work to address this gap.

- We have developed a seasonally and spatially varying PV-scaling methodology using 21-years of modeled PV fields and ozonesonde measurements at 50mb (Northern hemisphere)
- We are exploring "nudging" of O_3 above the tropopause to GFS 6-hr, 0.25° analysis (global coverage; *Presentation by J. Pleim*)

Chemistry:

Expressed concern on effort devoted towards maintaining 3 chemical mechanisms and suggested: (1) EPA choose one mechanism to focus on and designate the other as "user contributions"; (2) Offer two versions of the chosen mechanism- highly condensed for computational efficiency and another for research applications

- We agree, and in v5.3 have tried to balance between satisfying client needs, continuously improving chemistry, and reducing maintenance burden, given that:
  - Diverse regulatory applications need slightly different mechanisms formally released
  - Don't want to lose community users (i.e., CARB) when CMAQ code is updated
- In CMAQv5.3, we have implemented new tools (i.e., git and CMAQ preprocessor improvements) so that maintenance of multiple mechanisms is easier

- We hope that the upcoming STAR RFA on "Chemical Mechanisms to Address New Challenges in Air Quality" will help
  - spur community contributions
  - develop approaches to consistently condense mechanisms tailored for application needs

Aerosols (Particulate Matter):

Continued emphasis on the need to couple chemistry across phases

- Improvements to the coupling between gas-, aerosol-, and aqueous phase chemistry have continued to be implemented in the CMAQ modeling system; additional details in
  - Talks by D. Luecken ad H. Pye
  - Posters: K. Fahey, H. Pye

Panel recommends that CMAQ team continue to develop and evaluate the desert dust mechanism to achieve reliable predictions of desert dust cycle –important for air quality, PM exceedances & aerosol effects on climate

- A new windblown dust emission parameterization was included as a science option in CMAQv5.2; the physic-based scheme considers wind speed, soil texture, soil moisture, and surface roughness (Foroutan et al. 2017)
- Similar to other schemes, we have noted variable performance especially in estimation of source strength
- We continue to apply and assess the performance of the scheme in both NRT and retrospective cases

The panel encourages the team to evaluate more closely model bias in other U.S. locations and to apply the same level of scientifically-rigorous model development in these regions to *improve PM2.5 and constituents*

- Extensive evaluation with CARES, SENEX and (ongoing) WINTER measurements

The panel recommends that CMAQ team evaluate available nucleation parameterizations and consider including these additional processes (roles of bases/amines; organic compounds in nucleation) in future CMAQ releases

- Significant effort underway to improve ultrafine particle formation & distribution (Ben Murphy)

Air-Surface Interactions:

Evaluation of bi-directional NH_3 flux scheme for greater variety of land-cover types will likely lead to improvements as well as harmonization of surface properties representation (e.g., cuticular resistance) in CMAQ parameterization for dry deposition and biogenic emissions

- Evaluation of ambient NH_3 predictions have been conducted against measurements from the AMoN network as well as retrievals from the Cross-track Infrared Sounder (CrIS) (posters by J. Bash and J. Pleim)
- Harmonization of land-use data sets and surface properties continues to be a goal in CMAQ evolution design of the next generation system

Possible EPIC improvements: soil and agricultural-management data for Canada/Mexico. There may be merit in examining possibility of a reduced-form version of EPIC

- Information on crop land use, soil, and management practices is needed. We did compile crop information for 2011, but progress on other data is hampered by resources and contacts (and urgency in application needs)
- Poster by L. Ran reviews progress in use of EPIC. Due to process inter-dependencies, “reduced-forms” versions would likely be application specific –an approach we have not explored.

Two-way Coupled WRF-CMAQ:

Continued work is needed on the parameterization of the indirect aerosol effects

- WRF-CMAQ includes an option to represent aerosol indirect effects on grid-scale clouds. Though the scheme has been tested for regional (Yu et al., ACP, 2014) and limited hemispheric applications, more extensive testing needs to be conducted.
- Development efforts have been on the back-burner due to (1) large uncertainties in representation of convective cloud and extensions of the schemes for sub-grid clouds; (2) lack of observational data sets to robustly evaluate such schemes, and (3) de-emphasis on climate related research in the EPA portfolio.
- We, however, would welcome external contributions in improving model representation of this important process

A potential weakness identified by the panel concerns differences in advection scheme in WRF and CMAQ

- We recognize that differences in transport schemes between WRF (hydrometeors) and CMAQ (aerosol constituents) could lead to potential inconsistencies
- The design was however motivated by:
    - Being able to retain identical configurations for both online and offline calculations (other than radiative feedbacks)
    - To ensure strict mass-consistent tracer advection for air pollution simulations
- MPAS-CMAQ design however enables consistent advection for tracers and met variables

Model Evaluation:

CED's probabilistic evaluation approach offers a more robust quantitative estimation of model uncertainty and establishing confidence limits with which to guide compliance assessments – a weakness is that analysis performed only for few cases

- Ensemble approaches are limited by computational resources. Resource availability for end-users is also a consideration – cloud computing and data sharing may help address some issues!
  - Participation in AQMEII has also enabled assessment of approaches to develop "optimal AQ ensembles"
- We have continued to explore alternate approaches to characterize "intrinsic variability" in measurements (and model ability to represent these)
  - Analyzed variability in synoptic and baseline components from spectral decomposition of 1981-2014 DM8O3time-series.
  - Combining the projected change in the ozone baseline level with adjusted synoptic forcing in historical ozone observations could also provide probabilistic assessments of emission projections. Early results from Luo et al., AE, 2019.

Panel comments emphasized (with more stringent NAAQS) continued efforts to characterize and reduce bias across the spectrum of O_3 mixing range. CMAQ team will also need to improve treatment of background O_3 and LBC contributions for NOx , NOy , SOx.

- Efforts have focused on improving representation of dry deposition – a persistent sink that modulates low-mid range O_3
  - Presentation by D. Schwede; Posters by J. Bash and J Pleim
- H-CMAQ development and evaluation has continued to provide improved (and consistent) LBCs for regional calculation
  - Posters by C. Hogrefe & G. Sarwar; C. Hogrefe presentation

Instrumented Models:

Source apportionment is also of great interest to the states, tribes, and local air districts

- The ISAM source apportionment technique is being released with the base CMAQv5.3 Model
- Several improvements in ISAM (algorithmic and computational efficiency) have been implemented – poster by S. Napelenok

Adding a CMAQ adjoint would provide another powerful tool and a receptor-based perspective to the instrumentation suite

- We agree that a CMAQ-adjoint would provide a powerful diagnostic tool
- We are leveraging diverse expertise in the external (academic) community that has spearheaded the development and scientific evolution of the CMAQ-adjoint system
- Ongoing collaborations with this group are exploring:
  - Applications of the adjoint model
  - Approaches to enable (ease in) updates to the adjoint system to keep up with newer CMAQ versions
  - Availability of the latest version of the CMAQ-Adjoint code via GitHub repository

Model Applications:

Uncertainties in emission used in hemispheric simulations should be more rigorously evaluated

- While we agree with the recommendation, we have largely been reliant on country specific information publicly available or incorporated in global inventories
- Where possible we are using large scale satellite retrievals to identify inconsistencies (e.g., N. Africa)
- AQMEII-HTAP collaboration enabled updates to global inventories with country specific information (NEI, East Asia projections)
- Collaboration with the OAQPS emission group is also facilitating updates to specific sector emissions

DISCOVER-AQ applications can be further evaluated using aircraft profile data

- Continued evaluation of the DISCOVER-AQ applications, LNOxparametreizations, chemical mechanism assessments have utilized the aircraft measurements

Hemispheric simulations would be more state-of-science if run at higher spatial resolution. Climate downscaling assessments should also be done at higher resolution; Panel acknowledged the computational resource limitation

- Resolution choice driven by application needs and resource constraints. For HCMAQ applications, we have focused resources on diverse applications (additional time periods) and process enhancements to better characterize large-scale air pollution distributions
- Climate-AQ impacts focused on maximizing # of GCMs, longer time periods & greater number of climate scenarios
- RCM (and associated AQM) applications at 12km resolution are underway for a 23-year historical period as well as projections for 2025-2100

Resource Utilization, Relevance & Priorities:

CMAQ Program is making very effective use of resources provided and leveraging through collaborations – they should continue to pursue such opportunities

- We continue to foster and extend national & international collaborations
    - Health Scientists –Use of CMAQ for AQ-Health Impact assessments
    - NADP –deposition fields in TDEP
    - NOAA –on use of CMAQ in the NAQFC
    - Facilitating international collaboration on understanding & quantifying aerosol acidity
    - Air Quality Model Evaluation International Initiative (AQMEII)
    - UK-US collaboration on AQ modeling
    - Collaboration with Tsinghua University & Zhejiang University on application of coupled WRF-CMAQ
    - Hong Kong University –urban CMAQ development & applications

How will EPIC and NH_3 bi-directional approach propagate to the broader community

- FEST-C facilitates linkage between EPIC-WRF-CMAQ-SWAT & is publicly available
- EPIC/bi-di system is used to guide fertilizer NH3emissions in the NEI

It is unclear how LBCs from HCMAQ will be generated, archived, distributed to general community for regulatory applications

- On a request basis, we have extracted LBCs from existing HCMAQ applications
- The BCON utility can now extract LBCs for a user specified domain from existing hemispheric runs
- CMAS data warehouse will be used host HCMAQ output
  - 2016 CONUS (12km) LBCs from HCMAQ
  - Seasonally averaged HCMAQ output
  - Long term: additional years as need/resources allow