Response to Recommendations from the Sixth External Peer Review of the Community Multiscale Air Quality (CMAQ) Modeling System

Recommendation 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.*

Response: Several efforts are underway to enhance communication of updates in the CMAQ modeling system, for data sharing, and engaging the growing CMAQ user community. The user guide for the CMAQ modeling system has been recently revamped and significantly updated to improve documentation of options available in the CMAQ modeling system and guidance on when they should be invoked. This is now available with the model in the Git repository and as a live document will continue to evolve as the model evolves. We also agree with the suggestion on easier public access to EPA-generated modeling inputs and outputs. We are working with the CMAS Center to explore options for making model input and output data sets available to the external community. Model inputs for annual simulations of 2016 over the Continental U.S. domain are already populated on the CMAS Data Warehouse (https://dataverse.unc.edu/dataverse/cmascenter). We plan to add to this data inventory as new data sets become available, such as for finer resolution domains over specific areas. The CMAS Data Warehouse also offers the ability for CMAQ users and developers outside of EPA to upload their model inputs and outputs to share with the wider air quality modeling community.

Recommendation 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.*

Response: To support the broad set of research and regulatory assessment needs of the CMAQ user community, we incorporate our best understanding of the production of both gas phase pollutant and SOA constituents into reduced-size chemical mechanisms. It is a continuing challenge to find the right balance of detail and condensations so that these mechanisms accurately represent the sensitivity of pollutants to biogenic and anthropogenic precursors yet are also computationally-efficient. Our approach is to supply a suite of mechanisms with different degrees of condensation that are appropriate for different applications. For users that need fast simulations of ozone, for example, we recommend a mechanism that has less detail in SOA but evaluates well for ozone. For applications focused on SOA production, we will recommend a different mechanism with greater detail in SOA precursors and heterogeneous chemistry but might require more computer resources. Going forward, our goal is to make this suite of mechanisms more flexible, easier to update, and more consistent across applications. The recent RFA that we have developed for EPA will provide guidance on innovative ways to accomplish that and tools for creating updated mechanisms with associated evaluation and documentation. Working within this framework, we will continue to expand our representation of toxic air pollutants and feedbacks between biogenic and anthropogenic pollutants. We plan to continue to develop explicit chemical representation of SOA formation when possible (e.g. from autoxidation (Pye et al., 2019) or from organic nitrates (Zare et al., 2019)) and condense them for the most common CMAQ configuration. For some systems (e.g. volatile chemical products), analysis may focus more on uncertainty bounds as mechanistic information is not yet available. We agree with the need for more evaluation and to this end plan to use CMAQ simulations for the past decade to understand how OC is responding to changes in anthropogenic emissions (StRAP planned product). In addition, a submitted manuscript (Kelly et al., 2019) provides OC evaluation as a function of region and time of year, providing more information on current model performance. We will incorporate uncertainty analysis to a greater degree going forward (e.g., Qin et al., in prep).

Recommendation 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.*

Response: We share the view that to adequately assess the model skill over the expanding space and time scales of emerging model applications, model evaluation and analysis must also explore emerging and non-traditional observational data sets. We already use satellite retrievals for assessing the model's ability in representing across space, long-term trends in ambient concentrations, emissions and optical/radiative properties. We are also exploring use of satellite derived information for specification of model input data such as emissions (e.g., GOES geostationary lightning mapper for lightning NO_x, ocean chlorophyll for marine halogen emissions) and sea-surface temperature. Many ongoing applications of the model are focused on assessing unique region-specific air pollution issues – in these cases we are pursuing extensive comparisons with specific fields campaigns (e.g., DISCOVER-AQ, LISTOS). We have also extensively utilized multidecadal ozonesonde measurements to develop a potential vorticity-O_3 relationship to dynamically specify O_3 in the UTLS in CMAQ resulting from stratosphere-troposphere exchange. Since much of the material shared with the panel focused on motivation, updates and testing of the model changes, many of these efforts involving these diverse observational data sets were not necessarily covered. In the past we have evaluated the CMAQ modeling system and in many cases specific process modules with data from field campaigns such as ICARTT, INTEX, SENEX, CARES and expect to continue to expand the model evaluation methods to incorporate data sets from new campaigns as well as emerging platforms (including sensors).

Recommendation 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.*

Response: The need to accurately model air pollutant concentrations ranging from background to extreme values has further emphasized the need to accurately represent processes regulating concentrations in the low-moderate range. As a persistent sink of air pollutants at the surface, the role of dry deposition parameterizations in regulating concentrations especially at the low to moderate range has received renewed attention. Recent CMAQ versions in particular have incorporated improvements in dry deposition of: (1) gas-phase species to snow, (2) ozone to bare ground and cuticle, (3) organic nitrogen species, and (4) accumulation and coarse model aerosols. We have also improved the parameterizations of vegetation characteristics (LAI, vegetation coverage) in the PX LSM used in WRFv4.0 and later, which are passed through to CMAQ, with both a revised land-use category look-up table and a new option to directly use MODIS satellite products. We agree with the reviewers that characterization of uncertainty in model estimates of both ambient concentrations and deposition amounts, associated with uncertainties in the dry deposition parameterization schemes will help objectively convey and interpret model results. The incorporation of an alternate dry deposition scheme, i.e., STAGE, in CMAQ in fact was motivated by the need to also characterize the diversity in dry deposition parameterization (and assumptions) and their impact on model results. We are also closely working with colleagues both within the Agency and externally to facilitate and use measurements of dry deposition fluxes for various species. Additionally, to better characterize the performance and variability of dry and wet deposition fields simulated by multiple state-of-science air quality models for both grid-based and sub-grid land-use specific values, we are co-leading and actively participating in phase 4 of the Air Quality Model Evaluation International Initiative (AQMEII). We expect that these evolving research activities will provide insights on key drivers of differences and parameters that must be improved to reduce the uncertainty in dry deposition parameterizations used in the models.

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

Response: The near real-time (NRT) WRF-CMAQ test-bed has played a key role in identifying systematic errors in the modeling system (e.g., excessive wind-blown dust, boundary-layer heights over Great Lakes, temporal allocation of residential wood combustion emissions, vertical allocation of wildfire emissions) and served as a useful environment to test alternate process representations and enhancements. In fact the motivation for undertaking NRT simulations as a means for continuous CMAQ testing and evaluation stemmed from prior involvement in the development and deployment of the NOAA NAQFC. We recently met with colleagues from NOAA-ARL to explore potential collaborations in areas of mutual interest and have also been in discussions with NOAA NWS and OAR on possible re-establishment of a NOAA-EPA MOA on collaboration in air quality modeling.

Recommendation 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).*

Response: Significant progress has been accomplished in linking components of the CMAQ modeling system with MPAS. This integration is providing a basis for the initial prototyping and testing of the next generation global-to-local scale coupled meteorology-chemistry modeling system. To support a broad user community with a wide array of applications, the design of the next generation model should be able to be configured both as an online and off-line system as well as support "stand alone" regional simulations. To minimize code maintenance across multiple systems, we are exploring design options wherein CMAQ based chemistry and aerosol modules can link in with different dynamical models both in online and off-line paradigms. In the online configuration, transport calculations should clearly be conducted consistently using the dynamical model physics and numerical algorithms, which on surface suggests coupling could be accomplished with a 0-D version of the chemistry-aerosol modules. However, representation of the atmospheric chemical system is also intricately linked with emissions, air-surface exchange, cloud processes (aqueous chemistry, scavenging) and for some processes vertically (e.g., coarse-mode settling). Consequently, it is not readily apparent whether a 0-D or 1-D version of CMAQ would provide the most efficient and maintainable approach. We thus are exploring different approaches that provide flexibility to couple CMAQ with different atmospheric dynamics models to support broad air quality applications from local to global scales across for both research and policy assessment applications.

Recommendation 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).*

Response: We echo the panel's acknowledgement on the need for additional resources (computing and labor) to robustly support the increasing application demands. While the demands of expanding CMAQ to hemispheric scales, addressing finer resolutions for urban applications and running simulations spanning multi-decadal periods are currently accommodated on EPA's HPC resources, for emerging air pollution problems, model application complexity is expected to increase significantly (e.g. additional diagnostic simulations with DDM and ISAM, operational global to local simulations with mesh refinement) and will require enhanced computational resources. We thank the reviewers for recognizing the need to maintain adequate resources (computational and labor) to support the development, evaluation, and application of the CMAQ modeling system.