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.

Response: We thank the reviewers for recognizing the need to maintain adequate computer resources to support the development, evaluation, and application of the CMAQ modeling system. The CMAQ modeling team relies primarily on computer resources provided by EPA's Office of Environmental Information at its High Performance Computing Center (HPCC). Since 2009, computational power at the HPCC has increased by a factor of 9, although its funding has decreased by a factor of 2. Meanwhile, the nine-fold increase in power has been outpaced by the demands of expanding CMAQ to hemispheric-global scales, addressing finer resolutions for urban applications, and running simulations for multi-scale decadal periods. AMAD is attempting to increase its access to additional computer resources by serving on ORD's Informational Management Governance Board, which provides guidance to ORD for allocating Working Capital Funds for HPCC resources. In addition, AMAD staff have been working closely with HPCC staff to explore options in the "cloud", by performing pilot tests over the past three years on NOAA and NASA supercomputing centers. While the tests have been encouraging, a much greater bandwidth will be necessary for the "cloud" option to be feasible for CMAQ development and application. We plan to continue to be proactive with our EPA and external government partners to secure access to adequate computer resources.

Recommendation #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.

Response: We wholeheartedly agree with the reviewers that new ways of approaching the development of chemical reaction schemes should be a focus of future research in atmospheric chemistry modeling. It is becoming clear that the current chemical mechanisms and the minimal connections between gas, aerosol and aqueous chemistry are insufficient to meet the challenges of EPA's future needs for the regulatory and research models, especially under changing atmospheric conditions. It is difficult to incorporate new chemical information into the current chemical reaction schemes, and we are pushing them beyond their capabilities. This has been a topic of much discussion within the CMAQ chemistry workgroup. Our resources are limited to in-house expertise because we have no funding from the National Program, and this in-house work has largely been exploring how and where to incorporate feedback between phases, and which framework might provide the most flexibility for extension. CMAQ v5.1 is the first demonstration, albeit on a small scale, of a better way to represent multiphase chemistry, because it provides a simultaneous integration of gas and heterogeneous chemistry, and allows feedback between gas and organic aerosols, for the first time. Adding the KPP option for the aqueous chemistry now gives us the flexibility to expand the aqueous chemistry and incorporate organic feedback between the gas and aqueous phases. CMAQ v5.1 also includes a more deliberate consideration of the aspects of remote and marine chemistry that are necessary as we expand the domain for climate studies, long-range transport and background ozone, as well as a refined calculation of photolysis rates – important as the atmosphere changes and more accuracy in radiative impacts becomes critical. Each of these fields of chemistry is huge and our team is small, so we highly leverage professional connections with the scientific community.

With CMAQ v5.1, we have learned a lot about where we need to go with an updated mechanism, but the next step (making it truly flexible, efficient, responsive to new research, and something that the entire modeling community could use) requires a substantially larger investment. We think this would make an excellent opportunity to harness the best ideas of the atmospheric chemistry community, and an ideal EPA STAR grant! To this end, we have been pursuing discussions with the STAR grant program in EPA/ORD/NCER for over 2 years. Although competition is fierce within EPA for development of STAR grant RFAs, we believe this is a critical component of a next-generation AQM and plan to continue pushing for EPA to choose this as one focus area for a STAR grant.

Recommendation #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.

Response: The panel's recommendation is very much in sync with our current thinking and planning for the development of the next-generation air quality model. We will proceed on a parallel 2-track approach noting that much of the model process development is independent of the spatial structure of the model's domain and therefore applicable to both continued development of CMAQ including hemispheric applications and the new Next Generation Air Quality Model (NGAQM). Due to the fractional time-step approach used in air quality models, processes such as gas-phase, aqueous phase, and heterogeneous chemistry as well as aerosol microphysics and chemistry are integrated in independent boxes. Furthermore, surface processes such as biogenic emissions, dry deposition and bidirectional surface flux, dust emissions, point source plume rise, gravitational settling, and boundary layer turbulent transport can all be modeled in a 1-dimensional (vertical) model configuration. These components could thus structurally be isolated from the dynamical components that inherently are reliant on the underlying grid system. Therefore, while process research and development continues, with a particular emphasis on globally relevant processes, we will develop a new 1-D AQ model, which will first be tested as a prototype by coupling to WRF so that we can compare to our current WRF CMAQ system. As recommended, we will work on adding some of our AQ application related features that we have developed for WRF over the years to global models such as MPAS. Also, as recommended, we will investigate and test various ways of coupling the 1-D AQ component to various dynamic models, with particular emphasis on mass-consistency. In terms of coupling strategies, in addition to the current method used in WRF-CMAQ (in-memory buffer files that are accessed like I/O), we are looking into the CIME modeling infrastructure which was developed at NCAR and is used for coupling various components of the CESM.

Recommendation #4: Consider investing additional resources in emissions processing and emissions modeling.

Response: We agree that additional resources (in personnel and extramural funding) could improve the characterization of emissions for the CMAQ modeling system. The CMAQ team seeks to leverage its expertise and avoid duplication of emission-related work performed by other EPA offices. For example,

we work very closely with the Office of Air Quality Planning and Standards' Emission Inventory and Analysis Group (EIAG) to ensure that the most up-to-date and accurate emission estimates are available for CMAQ modeling. Indeed, George Pouliot from the CMAQ team participates in weekly EIAG workgroup meeting to identify needed emission improvements and to exchange information. Our collaboration with EIAG ensures that our emission inputs for CMAQ development, evaluation and testing are consistent with the emission inputs used for regulatory modeling. Elsewhere, several CMAQ scientists are collaborating with the National Risk Management Research Laboratory who is performing flux measurements of reactive nitrogen. The goal of our participation with NRMRL is transfer the analysis of field data into improved algorithms for ammonia fluxes (including emissions, especially over heavily-fertilized agricultural fields). In addition, the Division is able to sustain a modest in-house effort to improve emission characterization and surface-exchange with compounds such as biogenic VOCs, soil NO, lightning NO, wind-blown dust, and sea salt. As improvements are realized, algorithms and databases will continue to be transferred to the CMAQ modeling community. Recognizing that emissions are a huge uncertainty with air quality models like CMAQ, we will seek opportunities to bring on additional post-doctoral support and the hiring of a permanent federal scientist, as resources permit.

Recommendation #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).

Response: Over the years of CMAQ development, as the problem size significantly expanded, we have continued to explore methodologies to keep the computational efficiency and run time under control. We strongly agree that this aspect of AQ modelling is of paramount importance. We have done model run profiling varying from developing in-house tools to using third-party applications such as Intel's Vtune. These tools have helped to find "hot spots" that we have been able to address (as in CMAQv5.1), with solutions ranging from code modifications, e.g. eschewing Fortran character string comparisons, to addressing the ubiquitous I/O bottleneck, especially in the large number of writes-to-disk for a typical model run. For the latter in particular, we have been developing a true parallel disk access using pNetCdf. We are looking at other coding structures throughout the model for computational efficiency opportunities and have found a number, but with more to go. Using MPI as the primary basis for parallelization can also be supplemented with multithreading in some parts of the code. Exploring this approach is still in its infancy but is in serious consideration. We also acknowledge that the overall model IO and data flow will need to be considered as we explore alternate structuring of the model components discussed in response to recommendation #3.