Review of CMAQ Model, December 17-18, 2003

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Introduction:

The external review panel provides this report in order to assess the current state of the CMAQ model, to guide its development in the short term, and to assess the appropriateness of resources (institutional support, staffing and operational funding) in the long term to achieve desired advances. The report is written from the range of perspectives represented by members of the review panel. Panel members read a considerable volume of material on CMAQ provided by EPA, and attended two days of presentations on CMAQ by EPA staff.

Federal, state and local governments as well as regional organizations have used three-dimensional deterministic models such as CMAQ with one fundamental goal in mind: evaluation and the optimum selection of alternative control strategies to attain ambient standards for various criteria pollutants. The main regulatory purpose of such models is to understand how future changes in emissions ("delta E") would result in future changes in concentrations of various pollutants ("delta C"). Ozone (one-hr standard) has been the primary focus so far, and fine particle (those below 2.5 and/or 10 micrometers in diameter) will be the new focus in addition to a continuing focus on ozone (8-hr standard). From the science, policy, and implementation perspectives, Particulate Matter (PM) will be much more challenging than ozone, in that PM has an annual standard (in addition to the 24-hr standard) that requires annual modeling (unlike, ozone which is usually modeled over periods of a few days to a few weeks). Also, our present understanding of PM chemistry and physics is considerably weaker than that of ozone, though that understanding of PM is evolving rapidly. PM modeling has additional problems related to the need for acceptable and quality-assured annual data for emissions, and atmospheric measurements for model evaluation. In addition, the most sophisticated treatments of aerosol chemistry and physics will lead to substantial increases in computational requirements (run time and hardware requirements).

The CMAQ model must take into account the fact that ozone plus PM modeling could involve considerably more than twice the work of ozone modeling alone. In addition to ozone and PM, it is also important for CMAQ to address the issues of air toxics (including mercury) and acid deposition.

These considerations provided a context for our review of CMAQ. Of great interest and concern are efforts to expand the range of scales of applicability of its modeling capability into both the micro- (though "urbanization" of its 1-km scale version) and global-scales. Such scale expansion, while consistent with a growing trend toward "End-to-End" models, presents considerable technical and computational challenges, made more challenging when faced with limited resources.

CMAQ is a massive computer code designed to model a wide range of physical and chemical processes that occur at particular scales in the lower atmosphere. Some of these processes are well understood (for example dispersion of pollutants by mean wind and turbulent fluctuations), some processes reasonably well understood (for example the production of oxidant substances by photochemical reactions between volatile organic substances and oxides of nitrogen), and some processes only poorly understood (for example the production of organic nitrate aerosols by heterogeneous reactions between volatile organic substances and oxides of nitrogen). This range of knowledge about processes being modeled, and the fact that processes subject to uncertainty are the subject of active research worldwide means that parts of the model code are well-established enough to be considered fixed, while other parts of the code are in constant development. The result of this is that there must exist at all times a currently active, reasonably stable version of CMAQ which is used in an operational and regulatory mode. In parallel, there must exist a development version of CMAQ which is continually being improved by the CMAQ development team. From time to time, the development version replaces the operational version, thus bringing recent advances in atmospheric science to the operational realm. The model thus exists in both operational and research realms, a situation not uncommon for computer codes. The existence of two versions (research and operational) considerably complicates the task of this review panel. The panel has concentrated its attention on the operational version of CMAQ, but where appropriate, has referred to characteristics of the development version. Clearly the development version is closer to “state-of-the-science” than the operational version, and the differences will be most marked in areas that are topics of current research.

The main substance of our report is thus a set of recommendations designed to assess the current state of CMAQ, and to guide its development in the short term. These statements are primarily directed at the operational version of CMAQ. Our report is accompanied by appendices consisting of a detailed narrative covering internal panel discussion of the five areas of interest identified in EPA’s charge to the panel, and a set of tables and technical discussion which deal with quite detailed considerations brought forward by individual panel members.

Panel Report

The panel report is presented as a set of recommendations. These are not ranked in order of priority, but are grouped merely for convenience.

Overall

- CMAQ effort should remain focused on its main mission. From the perspective of its major clients, this is urban/regional modeling of PM and ozone for State Implementation Plan (SIP) purposes. The main regulatory purpose of CMAQ and similar models is to provide an understanding of how future changes in emissions would result in future changes in concentrations of various pollutants.

- The core research effort of the CMAQ modeling program should focus on model improvements and urban/regional applications. The research effort in air quality modeling at a fine scale and up to a global scale to study the linkage between air quality-health impacts and global change is important, but should not distract from the main effort of developing CMAQ as an urban- to regional-scale model.

- We believe that air quality forecasting is an important and worthwhile goal that could be accomplished with CMAQ, supplemented with other less intensive tools such as Auto regression Integrated Moving Average (ARIMA) or Artificial Neural Net (ANN) statistical models. Since long-term air quality forecasting (> 1 month) may provide potentially important information for SIPs, EPA should coordinate their efforts and resources effectively with the lead organizations, such as National Oceanographic and Atmospheric Administration (NOAA) and National Center for Atmospheric Research (NCAR), charged with achieving this capability.

Core model capability and applicability

- We recommend that enhancing the chemical and dynamic aspects of PM modeling in CMAQ become a top priority. We note that the primary objective of AMD's CMAQ model research program is to develop **operational air quality models** for use by EPA and the states in making emission management decisions. A continuing focus of scientific improvement should be on CMAQ's aerosol treatments. Much effort has gone into improving these treatments over the past several years, but there remains room for improvement. It is also important to note that while CMAQ is a leader in this area among other operational air quality models, all such models lag noticeably behind worldwide research efforts.

- We recommend that EPA maintain its position in the forefront of model evaluation for the types of applications for which CMAQ is used. Operational evaluation should be expanded into more insightful diagnostic/mechanistic/probabilistic evaluation. A guideline/protocol for PM evaluation should be published by EPA.

- We recommend that the CMAQ team perform an in-house evaluation of emissions modeling by use of techniques such as "inverse modeling".

Fine-scale and global scale model applicability

- We recommend that EPA and others undertake an investigation of the range of scales (temporal and spatial) over which the model can legitimately be applied. Results of this investigation should be publicized to all users.

- Recognizing pressure from users and regulators to provide a nested modeling capability down to the scale of urban canyons, we recommend EPA move cautiously in this logical next step, given the significant challenges on the meteorological side of developing a linkage of Pennsylvania State University/NCAR mesoscale model (version 5) (MM5) to Computational fluid Dynamics (CFD) and/or Large Eddy Simulation (LES) codes.

Air quality forecasting

- We recommend that EPA resist pressures to implement nesting within the Weather Research and Forecasting model (WRF), as we believe that this task should be undertaken by NCAR. We note also that WRF will have to incorporate nudging capability for it to be an appropriate driver for CMAQ, but such data assimilation capabilities are also demanded by weather forecasters. Thus, EPA should also not be responsible for implementing nudging, but should work to ensure that this capability is included into WRF in a manner well-suited to both weather forecasters and air quality modelers.

- We recommend that EPA coordinate efforts and resources effectively with other organizations (e.g., NOAA, NCAR) to develop a version of CMAQ for real-time operational forecasting that leads to development of a nation-wide air quality forecasting program.

CMAQ User and Developer communities

- Recent key staff retirements in the CMAQ group raise concern about continuation of the PM modeling effort. Given the importance of PM modeling to EPA's mandate in the PM-2.5/10 areas and given the complexity of aerosol physics and chemistry, we recommend that the modeling group work actively to ensure they have sufficient research level staff to support needed PM modeling efforts.

- We recommend that the CMAQ model development team increase its number of postdoctoral researchers, as these personnel will be most likely to introduce continuing improvements into CMAQ.

- We recommend that EPA, or others, develop a group of beta testers who will test research and operational (pre-released) versions of CMAQ, while the current released version is in active use.

- We recommend that EPA widely, and publicly acknowledge the contributions of non-EPA developers and beta testers of CMAQ. This should include those providing code extensions, modifications, corrections and bug fixes. An established mechanism to implement bug fixes discovered in this way should be established.

- We recommend that EPA staff be given time and resources to build collaborative links to non-EPA researchers, so as to ensure that CMAQ reflects state-of-the-science in all its aspects. This could be achieved through focused workshops or conferences on topics central to the development of CMAQ.

- We recommend the creation of a mechanism for the periodic review of CMAQ to ensure that it remains state-of-the-science. We strongly recommend that the scientific review of CMAQ be made an ongoing activity and be undertaken about every two years.

- We recommend that the CMAQ team consider carefully efforts underway to improve MM5, so as to avoid working in problem areas that parallel the efforts of the meteorological community. This will free staff to work on problem areas that are "CMAQ-specific".

- We support EPA's current and quite successful efforts in its outreach to scientific and regulatory communities through CMAS. It is extremely important that CMAS have sufficient public and private resources to offer focused training classes and workshops relating to various components of CMAQ.