NEW DEVELOPMENTS IN THE COMMUNITY MULTISCALE AIR QUALITY (CMAQ) MODEL

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1. INTRODUCTION

CMAQ model research and development is currently following two tracks at the Atmospheric Modeling Division of the USEPA. Public releases of the community model system for research and policy analysis are continuing on an annual interval with the latest release in September 2004. The publicly released system includes the latest advancements in scientific modeling research and improvements for model efficiency and is intended for research and policy development. The other CMAQ track is for the National Air Quality Forecast (AQF) system, which is a joint NOAA/USEPA project to provide nationwide operational model forecasts of ozone and aerosols. The AQF system includes an optimized version of CMAQ coupled to NOAA/NCEP's North American Mesoscale forecast model, which is currently the Eta model. The version of CMAQ used in the AQF system has been specifically tailored to the forecast application and NCEP's operational computing environment.

2. TWO TRACKS OF DEVELOPMENT

While CMAQ development has diverged between the version for community release and the Air Quality Forecast version, there is a continuous exchange of learning, testing, and new developments between the two systems.

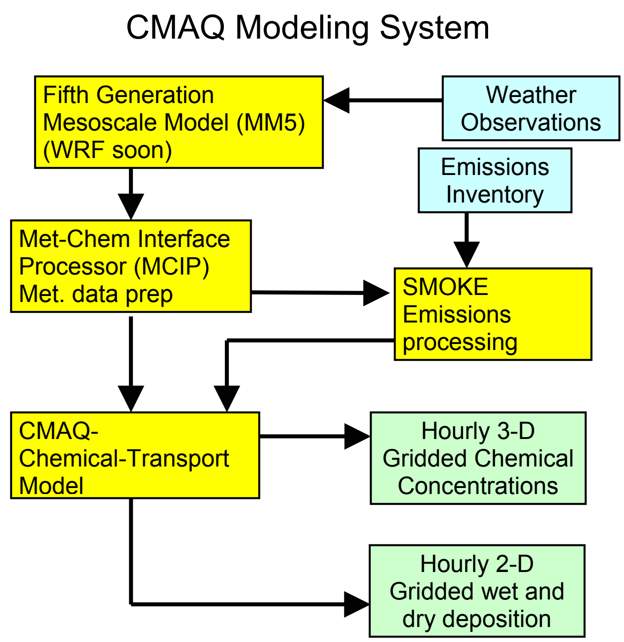

Figure 1. Schematic of the community release version of the CMAQ system

The CMAQ code itself has only minor differences whereas the overall systems are quite different. Figure 1 shows a schematic of a typical system configuration for running the community release CMAQ in retrospective mode for research or policy. Note that, while MM5 is not a required part of the system and other mesoscale meteorology models such as RAMS and MC2 have been used with CMAQ, MM5 with four dimensional data assimilation (FDDA) has been most commonly used. However, since the MM5 is soon to be replaced with the Weather Research and Forecast (WRF) model we are working on a version of MCIP that will read WRF output.

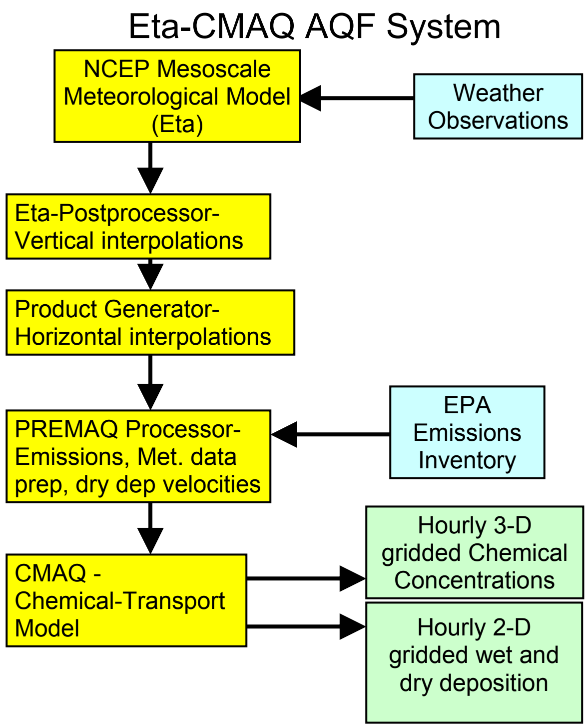

Figure 2. Schematic of the Air Quality Forecast system

The Air Quality Forecast System is shown schematically in Figure 2. The most important difference is that the meteorological data are provided by NCEP's Eta forecast model, which is run four times daily at 12 km grid resolution over North America. Downstream, a series of processors interpolate and regrid the meteorological data vertically (Eta-Post) and horizontally (Product Generator). PREMAQ replaces MCIP and performs the final adjustments to provide meteorological parameters on CMAQ's grid. PREMAQ includes a dry deposition model customized to Eta parameters. PREMAQ also computes meteorologically-dependent emissions, thus replacing part of the function of SMOKE. Other SMOKE functions are pre-computed off-line because SMOKE is too slow to be included in an operational forecast system. See Mathur et al. (2004) for an overview of the AQF system and Otte et al. (2004) for a detailed description of PREMAQ.

2.1 Synergistic Development

There has been a synergistic exchange of new developments between the community system and the AQF system right from the inception of the AQF project. The initial development of the AQF system required new additions to the community model such as a faster chemical solver (Euler Backward Iterative or EBI) and a more robust scheme for mass conservation. The EBI solver has since been added to the community system. In the other direction, continuing developments in the community model, such as advances in aerosol modeling and efficiency improvements are being added to the AQF version. The last two years of pre-operational testing and evaluation of the AQF system have produced many new insights into the strengths and weaknesses of model components. These insights, in turn, lead to modifications of several algorithms that are currently being tested. Examples include modification of the minimum eddy diffusivity (K_z), modification of the cloud cover algorithm used for photolysis, and modification of the subgrid convective cloud scheme. The change in the minimum K_z, in particular, has proven to result in better ozone forecasts at night. The minimum K_z was changed from 1.0 m^2/s to values ranging from 0.1 to 2.0 m^2/s depending on the fraction of urban land use. This change produced more titration in non-urban areas resulting in lower ozone concentrations overnight while preventing precursor concentrations from building to unrealistically high levels in urban areas. This change is now in the operational AQF system and will be added to the community version soon (at least by the FY05 release).

3. NEW FEATURES OF THE 2004 RELEASE

The 2004 release of CMAQ, designated as version 4.4 (CMAQv4.4), includes advances in science, several bug fixes and corrections, and many modifications for improved efficiency.

3.1 Aerosols

The most extensive and important changes for the 2004 release of CMAQ were in the aerosol module. These changes are described in detail by Bhave et al (2004) and are summarized here. Two modifications were made that greatly improve computational efficiency without significant change in results. The coagulation calculation, which previously consumed about half of the computation time of the aerosol module, has been replaced with a look-up table approach that takes almost no computation time at all. Also, the calculation of the gas to particle partitioning of secondary organic aerosols was made more efficient by improving the initial guess of the iterative solver. Together, these modifications halved the computation time of the aerosol module. Several other improvements and corrections were made including corrections for instability in the ISORROPIA thermodynamic module, corrections to the sulfate condensation rate, and improved treatment of the geometric standard deviation of the modal size distributions.

3.2 Gas Chemistry

Most of the changes in gas phase chemistry are related to the numerical solvers. We now have two highly accurate generalized solvers: SMVGEAR and ROS3. ROS3, a Rosenbrock-type solver developed by Sandu et al. (1997) was added for this year's release and has replaced our QSSA since it is both faster and more accurate than QSSA. In addition to the generalized solvers we have the mechanism-specific Euler Backward Iterative solver (EBI). EBI for the SAPRC99 mechanism has been added for CMAQv4.4. Since EBI is now available for CB4 and SAPRC99 the Modified EBI (MEBI) which has similar accuracy but slower performance has been discontinued for these mechanisms.

3.3 Corrections and other updates

Two significant bugs in the advection and vertical diffusion modules were found and corrected for the new release. The Piecewise Parabolic Method (PPM) advection scheme had a coding error which mis-computed the flux divergence for non-uniform grid spacing. The effect was to not conserve mass in vertical advection since the vertical grid spacing expands with height above ground. This bug caused errors of about 10% in ground-level concentrations.

In the vertical diffusion module the dry deposition velocity was erroneously specified in flux form (velocity x air density). The correction, removing the density so that the dry deposition velocity is in velocity units, typically reduces dry deposition flux by about 10%. There were also minor corrections to the eddy diffusion coefficients that have insignificant effects.

Another important advancement in CMAQV4.4 is the upgrading of the Plume-in-Grid (PinG) module to include aerosols. Godowitch (2004) describes the PinG module in detail and shows selected test simulation results.

In addition to the efficiency improvements obtained though modifications of numerical algorithms in aerosol and gas phase solvers there were also significant improvements in computational efficiency gained through code optimization. Scalar and parallel operations were optimized in collaboration with DOE's

Sandia National Laboratories. The most significant outcome of this effort was a dramatic improvement in parallel scalability through revision of the parallel I/O system.

4. FUTURE DEVELOPMENT

CMAQ development will continue along two tracks with synergistic exchange between them. The most important developments planned for the next release (FY05) include:

- Extension of the aerosol module to include sea salt with heterogeneous interactions with gas-phase species
- Updates to the CB4 gas-phase chemical mechanisms
- Linkage to the WRF meteorology model
- A new hybrid local and nonlocal closure PBL model
- Upgrades to cloud-photolysis interactions
- Modifications to the subgrid convective module

Other developments that will probably follow the FY05 release include:

- A generalized solver for aqueous chemistry
- On-line photolysis calculations with aerosol interaction
- Updates to other gas phase chemistry mechanisms (e.g. SAPRC99, RACM2)

5. REFERENCES

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