SYNERGISMS IN THE DEVELOPMENT OF THE CMAQ AND CAMX PM/OZONE MODELS

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1. INTRODUCTION

Photochemical grid models have been used extensively in the past to aid in the development of emission control strategies to demonstrate compliance with the ozone standard. Until recently, the Urban Airshed Model (UAM) (Morris and Myers, 1990) was the EPA recommended model for addressing regulatory ozone issues. More recently, revised EPA air quality modeling guidance no longer lists the UAM as the preferred model and instead recommends models be approved on a case-by-case basis (Federal Register, 2003). During the development of the UAM during the 1980s, a key test of the model was comparisons to other models. In the 1970s and 1980s, the UAM was compared against the California Institute of Technology (CIT) model. When the California Air Resources Board (ARB) developed the CALGRID model, comparisons of CALGRID and UAM were performed in the late 1980s that helped us better understand photochemical grid modeling of southern California. The early 1990s saw the development of the UAM-V nested-grid photochemical grid model that was used for ozone SIP analysis (Morris, Myers and Yocke, 1992). The comparison of the UAM-V EPA alternative model with the UAM EPA recommended model was required to satisfy EPA's modeling guidelines. During OTAG there were further comparisons of UAM-V with the SAQM and CAMx models.

More recently there have been several model evaluations and intercomparisons of EPA"s Models-3 Community Multiscale Air Quality (CMAQ) modeling system with CAMx for ozone (Morris, Emery and Tai, 2003; Tesche et al., 2001). By running the models side-by-side using the same meteorological and emission inputs, the effects of alternative model formulations and modules can be studied. Such information can be used by the model developers to enhance and improve both modeling systems.

With the movement to "one-atmosphere" models that treat both particulate matter (PM) and ozone issues within the same platform, many additional processes need to be considered by the photochemical grid models. New issues such as aqueous-phase and heterogeneous chemistry, aerosol thermodynamics, deposition of particles and acids, and particle size distributions need to be adequately treated. The development of the CMAQ and CAMx one-atmosphere photochemical grid models has occurred, for the most part, in parallel. However, both models share the same challenges in developing computationally efficient one-atmosphere models for ozone, fine particulate and regional haze planning. There are several emerging issues related to PM modeling that both models are addressing. These include nitrate formation chemistry, wet and dry deposition processes, secondary organic aerosol (SOA) formation, PM size distribution, grid nesting, and computational efficiency. Although the two models have taken similar approaches for addressing many of these issues, they have also taken different approaches to address others. For example, CMAQ has adopted the modal approach to represent PM size distribution, whereas CAMx has adopted a sectional approach. Much can be learned through running the models side-by-side to investigate processes that need improvements.

2.0 PREVIOUS CMAQ AND CAMx MODEL INTERCOMPARIONS

Previously, the CMAQ and CAMx models were intercompared for ozone performance using the same meteorological inputs for 1991 episodes in the Lake Michigan region (Tesche et al., 2001)

Corresponding author address: Ralph E. Morris, ENVIRON, 101 Rowland Way, Novato, CA 94945 and in the Northeast Corridor for the July 1995 NARSTO-Northeast episode (Morris, Emery and Tai, 2003).

2.1 1991 Lake Michigan Intercomparison

Tesche and co-workers (2001) applied the CMAQ and CAMx models for June 26-28, 1991 and July 17-19, 1991 ozone episodes in the Lake Michigan region. The two models were run on a 36/12/4 km grid structure using meteorological data from MM5. CAMx was also run on a 13.5/4.5 km grid structure using RAMS meteorological data. Several sensitivity tests were run with the two models to investigate important processes. In general, no one model or model configuration was performing sufficiently superior to the other to conclude that one model or configuration was better than the other. Both models exhibited similar model performance and similar ozone responses to VOC/NOx controls. In fact, there were more differences between the CAMx ozone estimates using the MM5 and RAMS meteorology than between CAMx and CMAQ using the MM5 meteorology. Some small differences were seen in the ozone estimates using the different CMAQ chemistry solvers with the CMAQ simulation using the QSSA and SMVGEAR chemistry solvers taking approximately, respectively, 5 and 8 times longer to run than CAMx with its CMC fast solver. Since this work, a more efficient Hertel/MEBI chemistry solver has been installed in CMAQ and the latest September 2003 CMAQ release utilizes and even more efficient EBI solver.

2.2 July 1995 NARSTO-Northeast Intercomparison

The NARSTO-Northeast CMAQ and CAMx intercomparison modeling study also could not make any definitive conclusions regarding whether one model is superior to another. The differences in model performance between the CAMx/MM5 (net underprediction) and CAMx/RAMS (net overprediction) simulations emphasize the fact that the photochemical ozone modeling results are highly dependent on their inputs. Thus, it is difficult to separate the effect of model formulation from model inputs. However, this does point out that preparing high quality and representative meteorological and emissions inputs is probably the most important activity for a successful photochemical grid model application and such applications cannot be performed in a “cookbook” fashion.

Model performance of the different models is mixed. CMAQ/MM5 and CAMx/RAMS simulate late afternoon and nighttime ozone concentrations much better than CAMx/MM5, but CAMx/MM5 estimates the afternoon ozone levels better. Some of the key findings were:

- The BEIS2 biogenic VOC emissions are overstated in some regions.
- The Quasi-Steady-State-Assumption (QSSA) chemistry solver is slow and can be inaccurate.
- In most cases (see next point), the more four-dimensional data assimilation (FDDA) that is used with the MM5 meteorological model the more representative the meteorological fields are.
- Care should be taken using observation nudging FDDA or using overly strong nudging as it may introduce artifacts that destroy good meteorological features.
- The Smolarkiewicz advection solver is overly diffusive and should not be used.
- The SAPRC97 chemistry is more reactive producing higher ozone than the CB-IV chemistry.
- The CMAQ horizontal diffusion coefficient parameterization that is inversely proportional to grid size may mask some of the benefits of using higher resolution grids.
- The use of the higher-resolution grid increases the local NOx disbenefits of NOx control in the major urban areas.
- Meteorological modeling of convective activity is a particularly challenging task and more research to interface meteorological model output with air quality models is needed.
- There are more differences between the CAMx model simulations using the MM5 and RAMS meteorology than between CMAQ and CAMx using the MM5 meteorology.

3.0 EMERGING MODEL DEVELOPMENT ISSUES

The CMAQ and CAMx model developers have been independently addressing many of the same emerging PM modeling issues. These issues include nitrate, secondary organic aerosols (SOA), deposition, primary PM performance and computationally efficiently. The latest version of CAMx (Version 4) was released April 2003, whereas CMAQ Version 4.3 was released September 12, 2003. Examples of how the two models have addressed emerging PM modeling issues are as follows.

3.1 Aqueous-Phase Chemistry

The PMCAMx model adopted the multi-section Variable Size Resolution (VRSM) CMU aqueous-phase chemistry module. However, the computational requirements of the VRSM module were quite extensive so that the model's use for annual modeling would be very limited. Thus, like CMAQ, the RADM aqueous-phase chemistry module was implemented in CAMx Version 4 to make it more computationally efficient.

3.2 PM Size Distribution

CAMx has adopted a section representation of PM size distribution where PM size is represented with, say, 10 size sections. CMAQ uses a modal approach whereby PM size distribution is represented by 3 lognormal distributions. A two-section version of CAMx was developed where all secondary PM was assumed to be in the fine mode, an assumption shared by CMAQ. However, tests between the 2 and 10 section versions of CAMx suggested there could be significant differences in the model estimates. Figures 1 and 2 display examples of 24-hour $PM_{2.5}$ nitrate concentrations on October 18, 1995 in Southern California using the 2 (Mechanism 4, M4) and the 10 section approach.

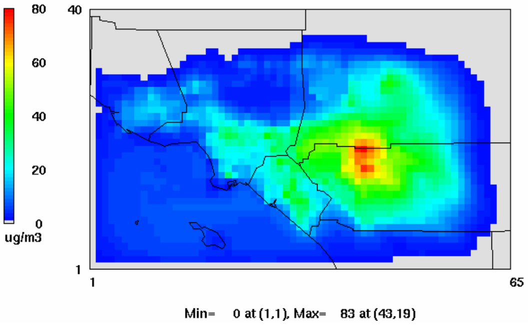

Figure 1 24-hour average $PM_{2.5}$ nitrate estimates using 2 size sections.

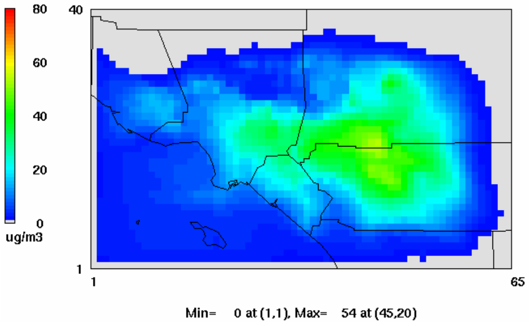

Figure 2 24-hour average $PM_{2.5}$ nitrate estimates using 10 size sections.

The difference in the fine nitrate peaks using 2 (83 :g/m^3) and 10 (54 :g/m^3) sections is quite pronounced. An analysis of the reasons for these differences reveals that in the 10 section simulation, nitrate is allowed to grow to the coarse mode where it more efficiently dry deposits than in the fine mode, as assumed in M4. As both CAMx M4 and CMAQ assume all nitrate is in the fine mode, this is an important finding that pertains to both models.

3.3 Computational Efficiency

To address the new fine particulate standard as well as regional haze issues, annual PM modeling will likely be needed. Thus, both CMAQ and CAMx are trying to make the models more computationally efficient without sacrificing technical rigor. In the April 2003 release of CAMx, the integration time step for horizontal advection in different vertical layers was calculated independently so that larger time steps could be taken in the lower layers where wind speeds are lower and shorter time steps can be taken in the upper-layers. Recognizing the strong coupling of layers below the Planetary Boundary Layer (PBL), a single time step is calculated for all layers below the PBL. The September 12, 2003 release of CMAQ Version 4.3 has implemented a similar approach that improves computationally efficiently. These similar approaches to increase the computationally efficiency of CAMx and CMAQ were likely arrived at independently in a convergence of ideas, but they illustrate how synergistic model development for the two models can be.

As noted above, the CAMx M4 and CMAQ assumption that all secondary PM is fine may result in overestimations of secondary PM if they have a tendency to grow into larger particles, like nitrate does. However, the computational requirements of a 10-section PM model may be too great for routine annual modeling. Thus, analysis of how many size sections are needed to correctly depict particle size distribution without a severe computational penalty has been investigated. A 4-section simulation was performed and the results compared against the 10 section simulation. Figure 3 displays an example comparison of the 4 and 10 section simulation. Although the 4 section simulation did not capture all of the details of the 10-section simulation, it did agree with the 10 section run fairly well and did not exhibit the overestimation bias of the 2 section approach that assumes all secondary PM are in the fine mode. The increase in run times from the 2 to 4 section model is approximately 20%, this compares to almost a factor of 3 increases in run time going from the 2 section to 10 section model.

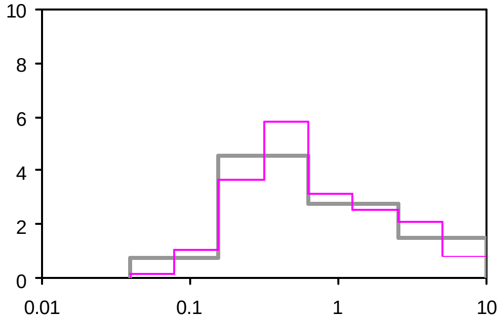

Figure 3 Comparison of sulfate particle size distribution for a CAMx 10 section (purple) and 4 section (black) size section distribution.

3.4 Particulate Nitrate

The simulation of particulate nitrate is particularly challenging due to uncertainties in the nighttime nitrate formation rate, partitioning among particulate nitrate and gaseous nitric acid and dry deposition rates of the nitrate components. In the September 12, 2003 release of CMAQ the reaction rate for the gas-phase conversion of N2O5 to HNO3 has been set to zero and a heterogeneous reaction has been added. These updates have been done in part to help eliminate a nitrate overestimation bias that has been seen in previous versions of CMAQ. CAMx also exhibits a nitrate overestimation bias and the innovative approach in the latest version of CMAQ is intriguing. However, it appears that the nitrate overprediction bias may be due in part to insufficient dry deposition due to assuming that the entire nitrate is in the fine mode that deposits out much more slowly than nitrate in the coarse mode. Thus, more investigations looking at nitrate dry deposition is warranted. Combinations of revised fine/coarse dry deposition and heterogeneous reactions will likely be used in the future for modeling nitrate.

4.0 CONCLUSIONS

The CMAQ and CAMx photochemical grid models represent two distinct one-atmosphere modeling platforms to address ozone, PM, visibility and other air quality issues. Through testing of alternative module formulations in these two platforms, more reliable and definitive findings on the appropriateness of alternative algorithms can be achieved. In particular, the likelihood of introducing compensatory errors in the modeling systems is reduced when two platforms are tested with new modules.

5.0 REFERENCES

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