

## FUTURE ENHANCEMENTS OF THE CMAQ MODEL

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### 1. INTRODUCTION

The Community Multiscale Air Quality (CMAQ) Model is being applied to an ever increasing variety of issues. These applications require expansion of CMAQ's capabilities to include more chemistry, improved physics, longer simulations, and greater spatial range (intercontinental to urban scales). While the model complexity increases so do the demands for better computational performance for longer retrospective studies (multi-year for regional climate studies) and for air quality forecasting. Thus CMAQ development is proceeding along several parallel tracks both within USEPA/ORD and in the larger CMAQ community.

### 2. CURRENT DEVELOPMENTS

From the beginning of CMAQ development we are continually working to keep abreast of, and occasionally push forward, the state-of-the-science in all key chemical, physical, and meteorological model system components. Examples of this type of development in recent years are the inclusion of a new gas-phase chemical mechanism (SAPRC99; Carter, 2000), updating the aerosol module with state-of-the-science secondary organic aerosol (SOA) yields and adding semivolatile partitioning of SOA (Schell et al., 2001). Developments in components outside of the chemical transport model are also necessary to keep the model system at the cutting edge. Examples include new land surface model development applied to the MM5 (PX-LSM) with its adjunct dry deposition scheme (Xiu and Pleim, 2001, Pleim et al., 2001). Also, an improved and updated Biogenic emissions model has been developed (BEIS3)

(Guenther et al., 2000). Development and testing of the Plume-in-Grid module (PinG) is continuing. Emissions from large point sources are not accurately treated in coarse grid resolution simulations. The PinG option simulates point source plumes by means of a Lagrangian plume model including gas-phase chemistry. Recently, aerosol modeling has been added to the plume model.

### 3. MAINTAINING STATE-OF-THE-SCIENCE

Near future developments that fall into the maintaining state-of-the-science category are planned through collaboration with several scientists at NCAR, including updating the aqueous chemistry and the photolysis modules. These efforts will not only update science but also add new science. For example, the new aqueous chemistry model will update reaction rates and also add new chemical reactions including aqueous photochemistry. A fast online photolysis model will allow for interaction of modeled aerosols with actinic flux calculations. We are also collaborating with University of Alabama in Huntsville to use satellite derived cloud information for improved solar radiation in MM5 and for improved photolysis simulation in CMAQ (McNider et al., 1998).

Another part of our NCAR collaboration will involve contributing to the development of the new Weather Research and Forecast (WRF) model. Specifically, we will add the PX LSM to WRF and work on development of a Newtonian nudging data assimilation system for WRF, as well as developing linkage with CMAQ.

### 4. EXPANDING CAPABILITIES

Ongoing efforts aimed at expanding CMAQ's capabilities are mainly focused on additional pollutants. For example, we are developing expanded versions of CMAQ to simulate mercury, dioxins, and a set of

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additional toxic species. Many of these issues involve multi-phase components such as semi-volatile treatment or aqueous chemistry interactions. Thus, further development of the aerosol module is needed for both toxic pollutants and criteria issues such as fine particulates and visibility. Efforts in this area include development of an improved fugitive dust model, the addition of emission and aerosol modeling of sea salt, and wildfire/prescribed burn emissions.

Research in the formation of SOA is critical for many issues and applications. The 3 main links in the chain leading to SOA formation are emissions (much of which is biogenic), yields of gas-phase reactions forming potential SOA species, and the semi-volatile partitioning of these products. We are actively collaborating with researchers within ORD and the larger scientific community to incorporate results of cutting edge field and laboratory research. In addition to the current tri-modal approach to aerosol size spectra modeling, sectional size resolved models are being added through collaboration with AER, Inc. and University of California at Davis.

## 5. EXPANDING SCALES

Spatial scales of application are expanding at both ends of the spectrum from neighborhood scale to inter-continental. At the small scale (~1 km), we are adding new capabilities to better account for the effects of urban canopies within the MM5/CMAQ system. Urban effects include increased drag and turbulent kinetic energy (TKE), radiation trapping in street canyons, increased surface heat capacity, and anthropogenic heat (Lacser, and Otte, 2002). For large scale and long-term simulations we are improving numerical advection and mass-conservation algorithms. Through collaboration with Harvard University, we are adding one-way nested linkage of CMAQ to the global chemistry model known as GISS-CTM (Mickley et al., 1999).

## 6. AIR QUALITY FORECASTING

We are in the initial stages of developing an air quality forecast system through collaboration with the National Center for Environmental Prediction (NCEP). This effort entails linkage of CMAQ to NCEP forecast models such as Eta and the Non-Hydrostatic Mesoscale Model (NMM; Janjic, 2002). This

project will involve substantial restructuring of the CMAQ system to utilize forecast meteorology fields, create emissions, and run the chemical transport simulation as efficiently as possible on the NCEP operational computer system. We anticipate that analyses of daily operational model forecasts will lead to better understand of model system shortcomings leading to accelerated development. This effort will also lead to computational efficiencies producing a faster running model.

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