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THE MODELS-3/CMAQ MODEL: 2002 RELEASE – NEW FEATURES

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1. INTRODUCTION

The Models-3/Community Multiscale Air Quality (CMAQ) Modeling System has been revised, with the latest version available since June 2002. Since 1998, the CMAQ model has been used at EPA for regional through urban air quality research and policy applications. The latest version of the modeling system has extensive changes/additions made in the gas-phase chemistry and aerosol processes, as well as changes in the meteorological and emissions drivers. The modeling system is available for downloading at ftp://ftp.epa.gov/amd/stand_alone_models3/cmaq/. The scripts for this release have been tested on Linux (specifically, Redhat Linux 2.1 with the Portland Group F90 compiler, pgf90 version 3.2).

2.0 NEW CMAQ MODEL FEATURES

In the latest model release we have added a third gas-phase chemical mechanism to CMAQ, the SAPRC-99 (Carter, 2000). This mechanism joins the existing CB4 and RADM2 mechanisms as user choices. (The SMOKE emissions model also supports the generation of primary emissions according to the species categories of these chemical mechanisms.) Also, the Modified Euler Backward Iterative (MEBI) chemical solver (Huang and Chang, 2001) has now been extended for all variants of CB4, SAPRC-99, and RADM2 mechanisms. This new solver has proven to be very fast and nearly as accurate as the slower comprehensive Gear numerical solver. The MEBI solver is not as flexible or general as the other CMAQ chemical solvers, but its efficiency more than compensates for any loss of generality.

Also added to this latest version of the CMAQ model is a new aerosols module, aero3, which includes improved treatment for secondary organic aerosol formation (Schell *et al.*, 2001) by including semivolatile compounds that partition between gas and aerosol phases. The process for sulfate nucleation has been updated and the heterogeneous conversion of N2O5 to nitric acid is now added. Also, the earlier aerosol thermodynamics model has been replaced with the ISORROPIA model (Nenes *et al.*, 1998). Emissions injection of aerosols has been moved from the aerosol module of CMAQ to the vertical diffusion process, where all other source emissions are included in the chemical simulation. Aerosols will be added to the Plume-in-Grid option of CMAQ later this year. A change in the order of the time splitting for science processes was made in the latest version of CMAQ to provide a better linkage between gas-phase chemistry and aerosols. The sequence change is from chemistry -> clouds -> aerosols to clouds -> chemistry -> aerosols.

A second vertical diffusion scheme, the Asymmetric Convective Model, ACM (Pleim and Chang, 1992), was added to CMAQ to supplement the existing standard eddy diffusivity approach. The ACM provides an efficient non-local vertical turbulence calculation under convective conditions.

A change was made in CMAQ to dynamically allocate the horizontal grid for the chemistry model and the initial and boundary concentration pre-processors (ICON and BCON), thus allowing one executable to run any horizontal domain that CMAQ supports. In conjunction with this dynamic allocation, the CMAQ model now can window from meteorology and emissions datasets, so that runs on many subdomains can be executed using one dataset that encompasses all those subdomains. Finally, an output option was added for hour-averaging for any CMAQ chemical species. Previously only instantaneous values for each hour of simulation were output.

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3.0 NEW METEOROLOGICAL FEATURES

The Meteorology-Chemistry Interface Processor (MCIP2) has been completely recoded and streamlined. It prepares data from the meteorological model (usually MM5) for input to the SMOKE emissions and CMAQ chemical transport models. MCIP2 is compatible with the most current versions of the MM5 model (version 3) and allows for a "pass through" option of meteorological data to CMAQ. Earlier versions of MM5 did not output all parameters needed by CMAQ, such as boundary layer height. Thus these parameter values were derived in MCIP from state variables. MCIP2 passes through boundary layer height and other parameters directly from MM5 to CMAQ. Also, MCIP2 contains options to use the more detailed surface data coming from the Pleim-Xiu (PX) land surface model in MM5 (Xiu and Pleim, 2001) to drive a new optional dry deposition scheme, M3dry (Pleim *et al*., 2001). This dry deposition scheme makes use of the soil moisture, surface wetness, and high resolution land cover data that are part of the PX scheme to derive more accurate deposition velocities of trace gases and particles for CMAQ.

4.0 NEW EMISSIONS FEATURES

Several changes to CMAQ's emissions processing were effected in the testing of the June 2002 version. First, BEIS3 (Guenther *et al*., 2000) replaced BEIS2 as the biogenic emissions model within the SMOKE emissions processing system. BEIS3 contains updated yields of biogenic emissions from vegetation and a more resolved vegetated land use inventory. Also, for emissions of fine particles, the new 1996 National Emissions Inventory contains a chemically speciated breakdown (sulfates, nitrates, organic and elemental carbon, and unspeciated mass) of the PM2.5 primary mass by source type. This is an improvement over earlier inventories containing no chemical species resolution of the particle mass.

Early testing of the new version of CMAQ revealed several problems in the plume rise algorithms within the SMOKE emissions model. Corrections were made to the stable plume rise method which greatly reduces low level emissions. The neutral and unstable plume algorithms were also updated. The initial vertical plume spread generally produces a more narrow plume then earlier versions. These changes to the plume rise algorithms are being more fully tested, and may be available in a future release of the SMOKE model.

5.0 REFERENCES

Carter, W.P.L., 2000: Documentation of the SAPRC-99 Chemical Mechanism for VOC Reactivity Assessment. Final Report to California Air Resources Board, Contract 92-329 and 95-308, SAPRC, University of California, Riverside, CA.

Guenther, A., C. Geron, T. Pierce, B. Lamb, P. Harley, and R. Fall, 2000: Natural emissions of non-methane volatile organic compounds, carbon monoxide, and oxides of nitrogen from North America. *Atmos. Environ*., **34**, 2205-2230.

Huang, H-C. and J.S. Chang, 2001: On the performance of numerical solvers for a chemistry submodel in three-dimensional air quality models. I. Box model simulations. *J. Geophys. Res*., **106**, 20175-20188.

Nenes, A., S.N. Pandis, and C. Pilinis, 1998: ISORROPIA: a new thermodynamic equilibrium model for multiphase multicomponent inorganic aerosols. *Aquatic Geochemistry*, **4**, 123-152.

Pleim, J.E. and J.S. Chang, 1992: A non-local closure model for vertical mixing in the convective boundary layer. *Atmos. Environ.*, **26A**, 965-981.

Pleim, J.E., A. Xiu, P.L. Finkelstein, and T. Otte, 2001: A coupled land-surface and dry deposition model and comparison to field measurements of surface heat, moisture, and ozone fluxes. *Water, Air, and Soil Pollution: Focus*, **1**, 243-252.

Schell, B., I.J. Ackermann, H. Hass, F. Binkowski, and A. Abel, 2001: Modeling the formation of secondary organic aerosol within a comprehensive air quality model system. *J. Geophys. Res*., **106**, 28275-28293.

Xiu, A. and J.E. Pleim, 2001: Development of a land surface model. Part I: Application in a mesoscale meteorology model. *J. Appl. Meteor.*, **40**, 192-209.