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CMAS Quarterly

The Quarterly Newsletter of the Community Modeling and Analysis System

Annual CMAS Conference: Registration Open!

We invite you to join us for the fifth annual CMAS conference to be held October 16-18, 2006, in the Friday Center in Chapel Hill, NC. As always, the conference will address leading edge issues in air quality modeling, analysis, and applications. This year we have added a session on data assimilation, including the many uses of remote sensing data. Other sessions include advances in air quality modeling systems (including the Weather Research and Forecasting Model); emissions inventories, modeling, and analysis; air quality forecasting; regulatory modeling studies; climate/pollution interactions; analysis methods and tools; and fine-scale and urban-scale modeling applications. To register to attend, please visit http://www.cmascenter.org/conference.cfm. Papers on the above topics will be accepted for either oral or poster presentation; the deadline for titles and abstracts is May 24. We look forward to seeing you!

CMAS Center Spearheads Journal Issues

As part of fulfilling its mission, CMAS has helped advance the state of air quality modeling by initiating and participating in the preparation of journal special issues containing peer-reviewed articles on air quality modeling systems such as CMAQ and CAMx. These articles have expanded upon presentations given during specific sessions at the CMAS annual conferences. Ready to hit the streets is a special issue of *Atmospheric Environment* that is based on the "Model Evaluation" session of the 3rd annual CMAS conference (October 2004). Its 25 papers discuss various aspects of evaluating air quality models, including emissions and meteorological processors. The CMAS Director, Adel Hanna, and the CMAS EPA Project Officer, Bill Benjey, are guest editors on the issue. Similarly, papers have been submitted for review to the *Journal of Applied Meteorology* that are based on presentations given during the "Model Development" session of the 4th annual CMAS conference and also at the NOAA/EPA Golden Jubilee Symposium on Air Quality Modeling and Its Applications, both held in September 2005.

CMAS EAC is Key to Success

The CMAS External Advisory Committee (EAC) provides important guidance concerning the CMAS Center's activities. EAC members are selected to represent a broad spectrum of users from industry, consulting groups, federal and state government, academia, and the international arena. The EAC meets with the CMAS Director following the annual CMAS conference. Members receive a Center status report, provide feedback on the conference, and set goals and directions for CMAS activities during the upcoming year. Communications continue throughout the year via e-mail and conference calls. The EAC members volunteer their time and effort; they do not receive compensation from CMAS.

Current EAC members include Praveen Amar, David Chock, Alan Cimorelli, Mark Evangelista, Tyler Fox, Bob Imhoff, Harvey Jeffries, Weimin Jiang, Naresh Kumar, Jeff McQueen, Ralph Morris, Talat Odman, Rich Scheffe, Ken Schere, Christian Seigneur, and Neil Wheeler. In the past, Pete Breitenbach, Daewon Byun, Richard Derwent, Gary Foley, Alan Hansen, Ajith Kaduwela, Mike Koerber, and John Vimont also served as members. CMAS is very grateful to all of these distinguished scientists for their service.

Model Releases

CMAS released CMAQ version 4.5.1 and MCIP version 3.1 on March 31. You can download them from the CMAS web site.

Upcoming Training Events for 2006

(All are at UNC unless otherwise indicated)

SMOKE Training:
- April 24-26
- July 17-19
- October 11-13

CMAQ Training:
- April 27-28
- July 20-21
- October 19-20

Can't come to us for training? Have the same courses taught on-site at your location by the same experienced trainers. Visit http://www.cmascenter.org/cmastraining or contact cmas@unc.edu for more information.

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Please come visit us on the Web!

www.cmascenter.org

CMAS Scientists Develop On-line CMAQ Photolysis Module

To calculate photolysis rates, CMAQ uses the JPROC preprocessor, which applies climatological profiles of ozone and a fixed profile of aerosol extinction to calculate atmospheric opacity. As an alternative, CMAS scientists have created an on-line photolysis module that calculates opacity using the time-dependent O_3 and NO_2 aerosol concentrations developed by CMAQ during a given simulation period. The new module calculates the solar radiative transfer in the same seven wavelength intervals used in Fast-J, a photolysis module used in several global climate models.

The on-line module uses updated absorption cross-sections and quantum yields from the latest available JPL data summary.

The radiative transfer calculations for the irradiances and actinic fluxes are done using an efficient two-stream delta-Eddington approach, with the addition of a pseudo-spherical approximation. In addition to photolysis rates, the module produces aerosol optical depth (AOD) and total surface irradiance at every surface-layer grid cell.

The module's new, efficient aerosol optical code calculates the tropospheric aerosol optical characteristics and subsequent AOD. This code is optimized for the lognormal modal representation of particle size distributions used in CMAQ as well as the range of refractive indices of internally mixed aerosol particles. The real and imaginary parts of the refractive indices for three particle-constituent groups (water soluble, sea salt, and dust-like) are taken from the OPAC software package. All values are taken as constants for all wavelengths within each group. The final refractive index for the internal mixture is a volume-weighted average of the individual constituent-group refractive indices.

New Sea Salt Model Released with CMAQ v4.5 in aero4

Modeling the interaction between sea salt aerosol and other atmospheric species is important for reliable prediction of the atmospheric composition in coastal areas. Sea salt sodium can be associated with sulfate and nitrate, and sea salt in the coarse mode provides an important sink for nitrate via the displacement of sea salt chloride, reducing the fine particulate nitrate concentration. The importance of sea-salt-related halogen atoms (chlorine and bromine) to the chemistry of the troposphere has also been shown in numerous observational and modeling studies. Including sea-salt-derived chlorine in the photochemical reaction mechanism may significantly increase morning ozone predictions. The new sea salt model released in the aero4 module with CMAQ v4.5 is the first phase of enhancing CMAQ's particulate chemistry to simulate the effects of sea salt on aerosol composition. Parallel work is underway at EPA/ORD to enhance the chloride chemistry in the gas-phase chemical mechanism.

In the first phase of development, CMAS collaborated with EPA/ORD to create an algorithm that generates sea salt emissions on the fly. This model uses a parameterization valid for the range of particles with dry radii 0.03-10 µm to estimate sea salt emissions at the ambient meteorological conditions in each grid cell. The emissions for the open ocean are estimated for both sea salt particle number and mass, and include a relative humidity (RH) correction that extends their validity from 80% RH to the entire range of 45% to 99%. The emission algorithm includes a scheme for modal partitioning of the emission fluxes based on truncated lognormals. The model also includes a parameterization for generating sea salt emissions in a 50-m surf zone in coastal grid cells. However, the evaluations performed for this release version have not exercised this capability, due to ongoing work by Computer Sciences Corp. on generating GIS-based gridded input data of surf-zone fractional areas for model applications worldwide. Because surf-zone sea salt concentrations have been shown to be 1-2 orders of magnitude higher than the oceanic background, including the surf zone in the emissions of sea salt should improve the current underprediction in the model-observation comparisons of sodium.

In addition to the new sea salt emissions algorithm, CMAQ v4.5 also has several changes to the aerosol module to include additional species—sodium, chloride, and sea salt sulfate in the Aitken, accumulation, and coarse modes—in the various aerosol processes. A new partitioning scheme has been implemented for mass transfer of volatile species to/from particles from/to the gas phase based on the particulate surface area in each mode. This scheme will be evaluated when coarse-mode chemistry is implemented in CMAQ in the second phase of enhancing the particulate chemistry. The inclusion of the condensable species partitioning to coarse particles is expected to significantly affect the fine-mode nitrate concentration predicted by the model.