February 2005
Volume 2, Issue 2

CMAS Quarterly

The Quarterly Newsletter of the Community Modeling and Analysis System

2005 Models-3 Conference Call for Papers

The CMAS Center and the UNC Carolina Environmental Program are proud to announce that the 4th Annual CMAS Models-3 Users' Conference will be held September 26-28, 2005, at the Friday Center at the University of North Carolina at Chapel Hill. SMOKE and CMAQ training courses will be available before and after the conference.

We are currently accepting abstracts for presentations in the following sessions:

- Model Development
- Emissions Modeling and Analysis
- Air Pollution Management
- Urban/Regional Model Applications and Evaluation
- Regulatory Modeling Studies
- Intercontinental Transport and Climate/Pollution Feedbacks
- Analysis Tools

Attendees may present their work as either platform presentations or posters.

All presenters in the Analysis Tools session will have the opportunity to display their analysis tools at a booth during the poster session to be held on September 27. All presenters in the Model Development session will be invited to submit their papers for consideration for a special edition of the journal *Atmospheric Environment*.

Registrations are now being accepted for presenters and attendees through the CMAS web site. The deadline for submitting presentation abstracts is May 20, 2005. All potential presenters will be notified of their status no later than July 1. Early-bird registration fees are $250 ($150 for full-time students). Fees increase by $50 after August 24.

For more information, please visit the conference web site: http://www.cmascenter.org/html/2005_conference/announcement.html.

Official Summary of the 2004 Conference

The following is the official executive summary of the 2004 Models-3 Users' Conference.

The Third Annual Models-3 Users' Conference was held October 18-20, 2004, at the Friday Center of the University of North Carolina at Chapel Hill. More than 180 scientists participated in the conference, including 25 scientists from South Korea, Spain, Germany, China, Australia, Taiwan, and Canada. The conference included two parallel sessions during its second day (Tuesday, October 19). The sessions conducted over the three days were as follows:

1) Model Evaluations
2) Air Quality Management
3) Fine-Scale Modeling for Exposure/Risk Assessment
4) Model Development
5) Climate/Air Pollution Feedbacks and Multi-scale Applications
6) Computational Issues
7) Air Quality Forecasting

The above sessions were preceded by an introductory session on the current status of the Community Modeling and Analysis System (CMAS), and followed by a session on the future directions of the CMAS. The introductory session and the seven main sessions are summarized below.

Status of the CMAS

The introductory session included presentations on the CMAS Center, the Sparse Matrix Operator Kernel Emissions (SMOKE) modeling system, and the Community Multiscale Air Quality (CMAQ) modeling system.

During 2004, the CMAS Center continued to work with the air quality community and stakeholders to enhance the community's ability to address air quality

Upcoming Training Events:

(All are at UNC-CH unless otherwise indicated)

- SMOKE – March 8-10, 2005 @ NC DENR
- SMOKE – May 2-4, 2005
- CMAQ – May 5-6, 2005
- SMOKE – July 11-13, 2005
- CMAQ – July 14-15, 2005
- SMOKE – September 21-23, 2005
- CMAQ – September 29-30, 2005

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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Conference Summary (cont'd.)

problems. The center held four training sessions on SMOKE, CMAQ, and MIMS; one of these sessions was held off-site in Portland, Oregon. The CMAS also again saw an increase in the number of annual conference attendees, including scientists from foreign countries. Upward trends have also been seen in the number of help desk tickets and model downloads. At the end of 2003, the CMAS organized a peer review of the CMAQ model. The report resulting from this review is posted on the CMAS web site.

Scientists at the CMAS Center have worked on three research topics in 2004 to improve CMAQ: (1) developing an in-line photolysis rate model, (2) including sea salt in particulate matter (PM) simulation, and (3) incorporating the Pleim-Xiu surface model in the Weather Research and Forecast (WRF) model.

Work continued on the development of SMOKE, which has been used extensively for regulatory and research activities. SMOKE processes emission inventories for input into air quality models; it handles criteria, particulate, and toxic pollutants. Its basic functions include gridding, speciation, temporal allocation, and plume rise. SMOKE version 2.0 was released in the fall of 2003, with updates to toxics support for all source categories. In September 2004, the CMAS released SMOKE version 2.1. Version 2.1 uses MOBILE6.03, the latest version of MOBILE6. The new version of SMOKE can extract humidity and barometric pressure data from gridded meteorology files, and it has better temporal modeling of on-road emissions processes. SMOKE version 2.1 also includes an updated BEIS3 model (it can use BEIS3.09 or BEIS3.12). In addition, it supports the polar stereographic map projection. Work in progress on SMOKE includes updates for variable-grid processing, a new method for handling aircraft emissions, and a new QA tool (EmisView).

Also presented during the introductory session were highlights of the newly released CMAQ version 4.4. This version includes new modules and improvements to CMAQ, especially in aerosols, chemistry, and cloud treatment. For example, for aerosols, a computationally efficient coagulation routine and an improved secondary organic aerosol (SOA) solver have been added. For chemistry, two chemical solvers have been added: the EPI_SAPRC99 and Rosenbrock solvers. For clouds, CMAQ version 4.4 includes the capability to account for "graupel" in the resolved cloud model.

Model Evaluations

The main theme of the conference this year was "Model Evaluations." Journal articles based on papers and posters presented under this session are being considered for journal publication. A special issue of *Atmospheric Environment* will be published on this topic during 2005. About 30 papers are expected. They will undergo the normal peer review process for *AE* publications. The CMAS Director, Adel Hanna, and the CMAS Project Officer, Bill Benjey, are the guest editors for the special issue.

Air Quality Management

The air quality management session included eight oral presentations. The Emission Data Management System (EDMS) was introduced as an emission inventory tool that can be used to analyze emissions data, perform emissions comparisons, and perform trend analysis. EDMS, from the Western Regional Air Partnership (WRAP), is an emission inventory data warehouse and web-based application that provides a consistent approach to regional emissions tracking to meet the requirements for State Implementation Plan (SIP) and Tribal Implementation Plan (TIP) development and periodic review and updates. The system includes GIS data query/

CMAQ GUI in Development

The CMAS Center is developing a CMAQ Graphical User Interface (CMAQ-GUI). The CMAQ-GUI is an installer that steps a user through installing the code and libraries on a client computer and installs a GUI interface for compiling and running the model. The CMAQ-GUI will be easy to install, easy to use, and well-documented; it will provide flexible options for compiling and executing CMAQ, and will be easily extensible to support new code versions. It will allow users to run CMAQ through the GUI interface instead of from scripts.

In addition, the CMAQ-GUI will have an integrated on-line help system. The help system will give users information about the GUI and the available options, plus provide links to other documentation and facilitate the submission of queries to Bugzilla and M3list. The documentation provided by the GUI will be in the form of HTML files that could be referenced from within the GUI or outside of it.

For more information or to make suggestions on the CMAQ-GUI project, please e-mail us at cmas@unc.edu.

New Login Procedures for CMAS Web Site

The CMAS web site continually undergoes updates and modifications to better serve the modeling community. We have recently completed the integration of a login system to the web site that will allow users to provide their contact information only once and have access to all of the model downloads, training and conference registration, and help desk information.

To create a user name, please access http://cf.unc.edu/cep/empd/cmas/html/register.cfm. You will be asked to provide your basic contact information, including a valid e-mail address, and to select your own user name and password. This user name will allow us to keep track of the models and data that you are downloading, as well as the trainings and conferences that you are attending, and will allow us to better meet the needs of the modeling community. This information will not be sold or distributed to anyone.

If you have any problems with this new registration process, please contact us at cmas@unc.edu.

Conference Summary (cont'd.)

view of data, data import and export, and report preparation.

Sensitivity analyses using air quality models are important tools to support environmental decision making. The CMAQ-HDDM is an extension of the DDM (the decoupled direct method) for three-dimensional air quality modeling applications. HDDM was presented as a powerful modeling tool for policy applications of air quality models, especially when examining numerous source contributions or control measures, and the interactions between the pairs.

CMAQ has been used to examine the impacts of PM on health. The analysis shows that the model is best used when addressing regional health issues related to SO_4 and $PM_{2.5}$.

A decision support system has been developed for the Beijing, China, area. The objectives of the system are to produce next-day air quality forecasts, provide source apportionment tools, simulate control decisions, and help users understand the parameters that contribute to poor air quality in the Beijing area. The system uses the MIMS framework and has the modeling components CMAQ, SMOKE, AERMOD, Chemical Mass Balance (CMB), and a cost-effectiveness tool. The architecture also includes visualization tools such as PAVE and GIS mapping capabilities.

CMAQ has been used to examine the impact of three sets of future vehicle emissions standards on ambient PM concentrations in the lower Fraser Valley, Canada. The study shows that the emission standards will be effective in controlling on-road mobile-source contributions to ambient $PM_{2.5}$ levels. The average impact will vary noticeably with location and time. CMAQ has also been used to determine the impacts of aircraft emissions on regional air quality for $PM_{2.5}$ and ozone. Preliminary analysis of the results shows that the Hartsfield-Jackson airport in Atlanta, Georgia, contributes to elevated levels of elemental carbon (and organic carbon in southern metropolitan-area counties.

Fine-Scale Modeling for Exposure/Risk Assessment

The presentations in this session targeted modeling applications for urban scales relevant to the assessment of health risks due to exposures of the population. The CB4TX chemical mechanism has been expanded to handle 20 gas-phase air toxics from the NATA list of 33, including those produced from nontoxic VOC emissions. Primary and secondary emissions were separated from secondary production. The application targeted the Philadelphia area using 4-km CMAQ simulations. Modeled toxics concentrations were compared with measured concentrations at various sites. The annual CMAQ concentrations were linked to the Hazardous Air Pollutant Exposure Model (HAPEM5). A software statistical package, CDFware, was developed to produce probability density functions (pdfs) based on the CMAQ outputs. This will account for the stochastic description of the subscale pollutant variability of CMAQ. The results of the study show the applicability of CMAQ for air toxics modeling. Research in progress investigates the integration of CMAQ into the ISCST3 and AERMOD Gaussian models and into the Stochastic Human Exposure to Dose model (SHEDS). Also planned is the application of CMAQ at a finer resolution (1 km).

Model Development

The inclusion of mercury processing in CMAQ was the subject of a number of presentations. New mercury chemistry and reaction kinetics are implemented in CMAQ. Modules to generate sea-salt aerosols and reactive halogen species are important for mercury transport and deposition. More experimental data are needed to better describe Hg(II) sorption in the aqueous phase. Mercury modeling using

Conference Summary (cont'd.)

CMAQ indicates that identifying the correct boundary conditions for mercury is very important. Natural emissions of mercury are a critical input for accurate prediction. The mercury concentration is strongly influenced by global, regional, and local sources.

CMAQ applications worldwide included the development of an emissions model to provide emission inventories to CMAQ for the complex configuration of the northeastern Iberian Peninsula (Catalina, Spain).

CMAQ also has been used to predict air pollutants resulting from wildfires. An emission processor, Daysmoke, was developed to inject smoke into CMAQ. Daysmoke is composed of four modeling components that account for the plume changes during the course of the burn, how high emissions go, and the distribution (how much and when) of smoke emissions among vertical levels.

A vertical wind adjustment method is recommended for use in CMAQ to ensure mass conservation. Mass conservation errors result from using different wind discretizations in the meteorology and air quality models. In the case of the MM5 and CMAQ, MM5 outputs are stored less frequently than the CMAQ advection time step.

Plume simulations within CMAQ are configured with a new version, CMAQ-APT. The impact of plume-in-grid (PinG) treatment on CMAQ simulation of ozone and HNO_3 shows a spatial distribution with increases or decreases compared to a control case. The effect of PinG treatment on HNO_3 is important for PM nitrate and regional haze modeling.

Climate/Air Pollution Feedbacks and Multi-scale Applications

The intercontinental transport of pollutants across the Pacific has been simulated for the year 2001. The modeling platforms include CMAQ, the global chemistry model GEOS-CHEM, MM5, and SMOKE. Initial and boundary conditions of the trans-Pacific CMAQ simulation were provided by GEOS-CHEM. The modeling of ozone, PM, and mercury demonstrates strong transport during certain episodes. Some of the elevated PM values on inland locations in the United States were related to origins in Southeast Asia.

Using the IPCC A2 and B2 future greenhouse gas scenarios, CMAQ predicts an increase in average and extreme ozone concentrations for future decades as a result of climate change. Projected land-use change can also have an important impact on air quality. In addition, a number of sensitivity studies were conducted to examine the effects of climate change identified by changes in temperature on air pollutant concentrations. CMAQ results were derived based on meteorological patterns related to temperature changes only ("direct effect") and based on changes in temperature and the resulting induced emissions ("emission-induced"). The results showed that moderate to significant changes in SO_4 and ozone occur in both the direct effect and emission-induced cases. They also showed that the current emission controls are still robust and applicable for the future.

Computational Issues

Significant efforts have been devoted to increasing the computational efficiency of CMAQ. As an example, EPA is collaborating with Sandia National Laboratories to examine the software architecture of the CMAQ modeling systems; they have been examining the computational performance of various modules within the architecture. One finding, for instance, has been that placing the I/O processor at the end of the allocated processor group enhances the performance of the computational model. The performance improvements target applications on the commonly used Linux platforms.

Air Quality Forecasting

Initial results of the NOAA/EPA initiative to develop an air quality prediction system were presented. The prediction system includes CMAQ, the Eta model, and the preprocessor PREMAQ. PREMAQ is a newly developed program that combines the functionality of the Meteorology-Chemistry Interface Processor (MCIP) and parts of SMOKE in a single real-time processor. PREMAQ was specifically designed to link NCEP's Eta model with CMAQ, and it uses meteorological fields that are specific to the Eta model outputs. A forecast domain for the northeast United States was successfully defined using NCEP's software, and a sample data set has been processed on that grid in GRIdded Binary (GRIB) format. The initial applications are for ozone and precursors.

Again, thank you to all those who attended the 2004 Conference. Be sure to check out the updated information on the 2005 Models-3 Users' Conference to be held September 26-28, 2005.

Spotlight on CMAS Research: Adding Sea-Salt Emissions

CMAS has three research projects currently underway. In this issue of the *CMAS Quarterly*, we spotlight the progress made on incorporating sea-salt emissions into the models.

After some discussions within EPA's Office of Research and Development (ORD), it was decided that SMOKE would not be used to provide the sea-salt emission rates to CMAQ, due to the prohibitive disk requirements for speciated hourly emission rates for each sea-salt component in each mode for an annual simulation. Instead, the sea-salt emission rates will be calculated in CMAQ. Testing of the new sea-salt flux integration scheme is underway in SMOKE; once it is completed, the scheme will be ported to CMAQ for these online calculations. We will perform intercomparisons between MAQSIP and CMAQ for the 1996 June 19-29 episode using this enhanced SMOKE version to generate the MAQSIP emissions inputs.

The sea-salt fluxes for the open ocean are based upon an extension by Gong (2003) of the Monahan et al. (1986) flux parameterization at 80% relative humidity (RH). The extended model allows the simulation of sea-salt particles in the range of 0.03-20 μm dry radius. Enhancements by Zhang et al. (2005) to the Gong formulation extend its applicability to ambient RH. Zhang's method to calculate emission rates involves integration of the sea-salt fluxes over the relevant particle size range at ambient RH using a rectangular rule applied to 50 size bins. As an alternative, in this quarter we completed the development of an analytical integration scheme assuming the flux function to be a bimodal lognormal distribution, spanning the accumulation and coarse particle size ranges. Dr. Bhave of ORD did the fitting using MATLAB and provided parameters of the best-fit bimodal distribution in a lookup table as a function of RH. The integration scheme uses these parameters to calculate the number and mass emission rates in each mode as a difference of two error functions evaluated using the maximum and minimum diameters at the ambient RH, corresponding to the maximum and minimum dry radii. We also generated the polygons to calculate the fractional areas in coastal grid cells that can be treated as surf zone, using the MIMS spatial allocation tool linked to a GIS database. Initially a 100-m width was assumed for the surf zone, but based on observations from the Tampa Bay area that showed an overestimate of the sea-salt emissions, we have reduced the width to 50 m, generated a netCDF file of gridded data for the surf zone fractions, and given the file to ORD for future use in continental simulations. The surf zone flux integration cannot be done analytically, as the source function is an exponential function; this integration is therefore performed numerically, and the emissions for the surf zone are added to the coarse mode, assuming that the mean diameter for the emissions is the same as for the open ocean source. The SMOKE implementation of the scheme is ongoing.

We completed modifications to CMAQ for the addition of sea-salt species in the two fine-aerosol modes in all the relevant include files and aerosol subroutines, including the mass transfer algorithm originally formulated for MAQSIP. The adaptation of this algorithm to CMAQ currently contains no chemical interaction of the coarse-mode sea-salt particles with the other inorganic aerosol species. Further, the modifications to the aqueous chemistry and cloud mixing for the presence of sea-salt species are pending. In the next stage, we will include these modifications, as well as a scheme for mass partitioning to the coarse mode, and a modified hybrid approach for the thermodynamics of the fine and coarse particles. We submitted the new source code and documentation to ORD for review, and based upon recommendations from that review, have further revised the code prior to testing.

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What Types of Analysis Tools Do You Use?

From the Help Desk: CMAQ Tip

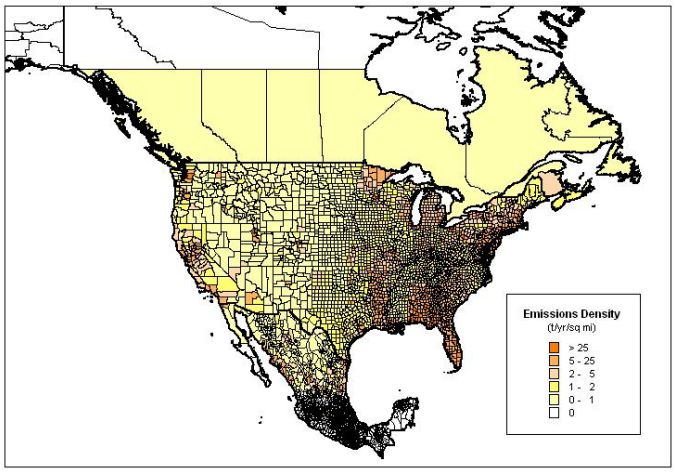
To access past releases of CMAQ, download the unified archive. The CMAQ unified archive contains source code and build scripts for all past release versions of CMAQ, including CMAQ-MADRID. The unified archive allows users to compile all of the CMAQ programs and libraries from a single script interface for Linux systems with either the Portland Group or the Intel compilers.

Visit Us on the Web!

www.cmascenter.org

The CMAS Center is currently trying to create a catalogue of freely available analysis tools commonly used by the modeling community. We are particularly interested in finding out (1) what kinds of analyses are being performed and (2) what tools are being used to create these analyses. What are some of the key statistics used to examine the model performance and model results? What types of graphics are used to display differences? Do you have a stand-alone package to perform your analyses or do you rely on multiple methods?

To add a link to your tools to the list of analysis tools, please send an email to cmas@unc.edu that includes your contact information and a brief description of the tools you use and how you use them in your modeling analyses.



Example analysis plot from a GIS to calculate emission densities.

Demonstrate your Analysis Tools at the 2005 Models-3 Users' Conference

There will be a special session at the 4th Annual CMAS Models-3 Users' Conference devoted entirely to analysis tools. In addition to 10 minutes to present his or her suite of tools, each presenter in the Analysis Tools session will be able to display and demonstrate the tools at a booth during the poster session at the conference. We hope that this will allow all attendees to get a better understanding of the modeling analysis tools available throughout the community.

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CB # 6116
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Printed on recycled paper.
No state funds were used to produce this publication.