JANUARY 2012

CMAS Quarterly

The Quarterly Newsletter of the Community Modeling and Analysis System

Upcoming Events

(All are at UNC unless otherwise indicated)

11TH ANNUAL CMAS CONFERENCE:

- Oct. 15–17, 2012

SMOKE Training:

- Apr. 23–25, 2012
- Oct. 10–12, 2012

CMAQ Training:

- Apr. 26–27, 2012
- Oct. 18–19, 2012

BenMAP Training:

- Apr. 30 – May 2, 2012
- Oct. 22–24, 2012

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Can't come to us for training? Have the same courses taught on-site at your location. Visit http://www.cmascenter.org/training/ classes.cfm or e-mail cmas@unc.edu.

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Credits

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www.cmascenter.org

CMAQv5.0, the Latest CMAS Release

The CMAS Center is working with EPA to finalize CMAQ version 5.0 (CMAQv5.0), scheduled for release in January 2012. Jon Pleim of EPA gave a review of this version's new features during the 10th Annual CMAS Conference in October. The model incorporates many scientific advances that reflect the latest research in gas chemistry, aerosol chemistry and thermodynamics, aqueous chemistry, and photolysis, in addition to improved advective and turbulent schemes as well as major structural upgrades that improve flexibility and maintainability. CMAQv5.0 includes the two-way coupled WRF-CMAQ system, a modeling option that is desirable when modeling regional climate / air quality feedback applications. The new version also includes bidirectional surface flux for ammonia and mercury.

A number of optional gas-phase mechanisms in the model have been updated. The SAPR07TB mechanism was fully updated based on current knowledge in atmospheric science on reactive organic compounds and HAPs. Also, additional explicit species that have either high emissions, high toxicity, or high secondary organic aerosol (SOA) formation potential (such as xylene, α-pinene, benzene, and 1,3-butadiene) are now included. The CB05 chemical mechanism was updated to address impacts in urban areas using an updated toluene mechanism. Changes in aqueous chemistry include SO_2 oxidation rate updates.

Another key element of CMAQv5.0 is the improvement in representing photolysis. The in-line photolysis module was revised to read input data from an ASCII file created by a preprocessor, which facilitates updating data or adding new reactions. Also included are spatially and temporally varying surface albedo that varies by wavelength and land use parameters as well, and albedo for snow and sea ice from WRF.

Particulate matter (PM) treatment of NCOM (no-carbon organic mass) was revised to represent source-specific OM/OC ratios in primary emissions and to simulate oxidation of OC to NCOM. PM updates also include the speciation of all PM(other) species under the main $PM_{2.5}$ category. Speciating PM(other) helps in characterizing seasonal bias. Further changes in PM treatment in CMAQv5.0 include (1) updated sea-salt emission speciation, (2) updated aerosol thermodynamic treatment in ISORROPIA v2.1 to include chemistry of additional crustal species, and (3) code optimization to reduce computational time. A new fugitive-dust emissions model based on a wind-blown dust algorithm is also part of CMAQv5.0.

Dry deposition in CMAQv5.0 was improved using a Mosaic approach that quantifies output dry deposition flux for the various land use categories within a grid cell. This feature will be particularly helpful for ecological assessment studies.

The model includes four options for lightning NO_x emissions: a no-NO_x option; reading NO_x emissions from a file calculated outside of CMAQ; an in-line NO_x emissions parameterization based on convective precipitation; or an in-line NO_x emissions parameterization based on convective precipitation and monthly lightning flash count observations.

The transport upgrades include a new scheme for vertical advection that more closely follows mass continuity calculations in WRF with less diffusion in upper model layers and only small deviations from mass conservation. A new scheme for stable boundary layers in WRF and CMAQ is also included. This significantly improves the simulation of nocturnal low-level jets and allows more mixing after the evening transition.

Watch for the release of CMAQv5.0 on www.cmaq-model.org and www.cmascenter.org.

Special Session for 2012 CMAS Conference: Modeling Secondary Impacts from Single Sources or Single-Source Complexes

Part of the CMAS Center's mission is to highlight advances in science that support the air quality community, through conference presentations and training sessions. CMAS received a proposal from Dr. Kirk Baker of EPA to organize a special session at the 11th Annual CMAS Conference next October that focuses on the use of photochemical Eulerian and Lagrangian models for looking at the secondary impacts (ozone, $PM_{2.5}$, mercury, etc.) from single sources or single-source complexes such as fires. His idea was motivated by the increased demand for these types of assessments that is expected in the future, when much of this work is likely to migrate toward the photochemical modeling arena.

Air quality models are increasingly being used to assess secondary impacts from single sources at nearby urban-scale monitors as well as long-range transport to regional-scale locations. Single-source impacts on ozone and secondarily formed $PM_{2.5}$ (e.g., sulfate and nitrate) are important in evaluating how new sources or changes to existing sources impact National Ambient Air Quality Standards (NAAQS) for ozone and $PM_{2.5}$. In addition to near-field impacts, the potential effects from proposed new emission sources on air quality and air-quality-related values (visibility and surface deposition) at Federally protected "Class I" wilderness areas under the Prevention of Significant Deterioration (PSD) program are largely secondary in nature and must be quantified with an air quality model. Other regulatory purposes for assessing the impacts of secondarily formed pollution from a single source include the assessment of prescribed or naturally occurring fires on downwind areas of interest, and the impacts of single sources on mercury deposition.

The proposed topics for this special session will include (but are not limited to) the following, where "single source" can include source complexes and fires:

- Application and evaluation of a photochemical model with subgrid treatment of single-source impacts on ozone and on secondarily formed $PM_{2.5}$ and/or toxics (e.g., mercury).
- Application/evaluation of single-source Lagrangian models that include the chemical and physical processes needed to estimate ozone and secondarily formed $PM_{2.5}$ and/or toxics.
- Application of single-source modeling systems to assess nitrogen and sulfur deposition impacts.
- Evaluation of near-field and long-range transport of pollutants in a single-source Lagrangian model and/or photochemical model.

The Community Remembers Dr. Daewon Byun

During the 10th Annual CMAS Conference last October, a special session titled "Air Quality Modeling Applications" was dedicated to the memory of Dr. Daewon Byun, who passed away in January 2011. Daewon made distinguished contributions to the air quality modeling community in all phases of his career, which culminated in working as an academic professor at the University of Houston and NOAA at the time of his death.

Mrs. Chin Byun was invited by the CMAS Center to attend a special ceremony held in honor of her husband. Session chairs Rick Saylor and Pius Lee gave presentations on Daewon's life and his professional contributions. Jon Pleim, on behalf of former colleagues of Daewon from EPA, presented Mrs. Byun with a signed copy of the CMAQ science documents on which Dr. Byun was the chief editor and co-author during the late 1990s. CMAS Director Adel Hanna gave Mrs. Byun a plaque in recognition and appreciation of her husband's many contributions to the air quality modeling community. In addition, speakers and presenters during that session spoke about Daewon's scientific contributions to their particular topics of research.

Collaborative Studies of Fine Grid Scale and Urban Model Research Using the WRF Model

Typical sub-grid-scale PBL parameterization closure schemes may no longer be adequate or appropriate when applied at grid sizes on the order of 1 km, which is the so-called terra incognita regime (Wyngaard, JAS, 2004); thus, mesoscale models will not be able to accurately simulate flow details at such scales. Observational analyses indicate the presence of 2-D horizontal roll vortices or 3-D quasi-stationary persistent mesoscale structures on the order of 1-10 km, but these are not resolvable at that corresponding grid size. Simulations using MM5 and WRF that employ grid sizes of ~1 km or less do capture the essence of these features, but at the expense of introducing stochastic or "model" noise.

This fundamental issue poses a serious and important challenge to the mesoscale meteorological and air quality modeling communities interested in fine-scale model applications. Given the rapid rate of growth of these user communities (e.g., it has been noted that the number of WRF and CMAQ downloads is growing at a rapid rate) and the continually improving computational speed and memory capabilities of modern computing systems, fine-scale modeling will become increasingly more possible and popular to perform. Thus, it is critically important at this juncture to address this model scale issue; without further resolution or advancements on this issue, model-generated uncertainties (and errors) will inadvertently and increasingly propagate into all fine-scale modeling results. Dr. Jason Ching of UNC's Institute for the Environment joins a group of scientists from NCAR, El Centro de Investigaciones Energéticas, Medioambientales y Tecnológicas (CIEMAT, in Spain), and San Jose State and New York Universities that is pursuing several avenues of investigation designed to address this important issue. He will provide project facilitation on site at NCAR later this year.

Please contact Jason (jching@unc.edu) if you are interested in these activities.

CMAS Web Portal and Links

The CMAS web site, http://www.cmascenter.org, is the main web portal to the Center. This central site has links to multiple other sites that provide access to various components of the supported modeling systems, data acquisition and analysis tools, and user support. The CMAS Center also hosts e-mail listservs (e-mail forums) to facilitate communication between community members; a listserv is an electronic mailing list that uses one address to distribute e-mail to all members of a specified group. These are the web sites and listservs hosted by the CMAS Center:

- http://www.cmascenter.org: Central web portal to the CMAS Center
- http://www.cmaq-model.org: Air quality modeling
- http://www.smoke-model.org: Emissions processing
- http://www.benmap-model.org: Economic and health impact modeling
- http://www.verdi-tool.org: Visualization and graphics
- http://bugz.unc.edu: E-mail–based technical support
- http://www.cmascenter.org/irods: Model output data distribution
- http://cmas.wikidot.com: Model development wiki
- m3user@listserv.unc.edu: E-mail forum for technical support
- m3list@listserv.unc.edu: E-mail forum for announcements
- m3dev@listserv.unc.edu: E-mail forum for software development discussion
- emregional@listserv.unc.edu: E-mail forum for emissions-related announcements and discussion
- benmap-user@listserv.unc.edu: E-mail forum for BenMAP-related announcements and discussion

The CMAS web sites are regularly updated with new information, including model releases, documentation, conference announcements, and training schedules.

EPA Recognizes Efforts of Fellow Scientists

Following the 10th Annual CMAS Conference in October, Dr. S.T. Rao, Director of the EPA/NERL Atmospheric Modeling and Analysis Division, presented EPA Certificates of Appreciation to Dr. Adel Hanna, CMAS Director, in recognition of his outreach and training on CMAQ to scientists around the world; Dr. William Benjey, for effectively managing the CMAS contract over the past decade; Dr. Bernard Fisher, for promoting the use of CMAQ in the United Kingdom for scientific and regulatory applications; and Dr. Stefano Galmarini, for his contributions toward advancing the objectives of the Air Quality Model Evaluation International Initiative (AQMEII) throughout Europe and North America.

In accepting his certificate, Dr. Hanna presented it to all of his colleagues at the CMAS Center for their dedication in supporting the community for over 10 years.