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A CMAQ and WRF/Chem Model Intercomparison for August 2006

Jerold A. Herwehe and Tanya L. Otte
Atmospheric Modeling and Analysis Division
U.S. EPA/Office of Research and Development/National Exposure Research Laboratory
Research Triangle Park, North Carolina

Introduction

Traditional air quality (AQ) modeling systems compute the meteorology separately from the chemistry and then drive the chemical transport using saved meteorological variable fields. One example is the released version (v4.7) of the Community Multiscale Air Quality modeling system (CMAQ; Byun and Schere, 2006), an offline chemical transport model driven by stored meteorological dynamics from weather prediction models such as the Weather Research and Forecasting model (WRF; Skamarock et al., 2008). But offline chemistry does not allow aerosol feedbacks to affect the radiation budget and cloud microphysics of the meteorology. One solution is to use an online coupled chemistry and dynamics model, such as the WRF with Chemistry model (WRF/Chem; Grell et al., 2005). The online-coupled WRF/Chem provides a framework to study two-way interactions between the chemistry, aerosols, radiation, cloud microphysics, and meteorology.

Objective

The purpose of this study is to conduct a model intercomparison between CMAQ and a modified version of WRF/Chem, focusing on ground-level AQ predictions and statistical analyses. Reported here is the work in progress.

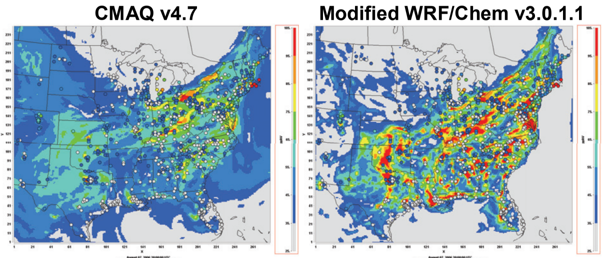
Approach

- Conducted a one-month simulation (August 2006) using a modified WRF/Chem to compare with an existing CMAQ v4.7 simulation.
- A more compatible model intercomparison required several steps:
  – implemented the CB05 chemical mechanism (Yarwood et al., 2005), the same as employed by CMAQ (Sarwar et al., 2008), into WRF/Chem v3.0.1.1 and coupled the gas phase chemistry to the existing WRF/Chem MADE/SORGAM modal aerosol scheme;
  – converted and used the same emissions for both the WRF/Chem and CMAQ simulations;
  – wrote the `cmaq2wrfchem` program and used it to convert CMAQ initial and boundary condition (IC/BC) data for use by WRF/Chem, complete with the necessary aerosol units conversions;
  – and specified many of the same physics options in WRF/Chem as were specified for the WRF meteorology used to drive CMAQ, such as RRTM long-wave radiation, Pleim-Xiu surface layer and land surface model, ACM2 boundary layer, IC/BC data, and FDDA.
- Conducted statistical analyses of the month-long WRF/Chem and WRF-driven CMAQ simulations using the Atmospheric Model Evaluation Tool (AMET; Gilliam et al., 2005; Appel and Gilliam, 2008). Additional steps were required to prepare WRF/Chem chemistry output for use by the CMAQ-centric AMET package:
  – extracted layer 1 of all gas and aerosol species fields;
  – concatenated hourly extractions into daily files containing 25 times;
  – renamed species to match those used by CMAQ;
  – converted these netCDF files into I/O API format using `dpp` tool;
  – and generated METCRO3D files needed for AMET AQ module by running MCIP v3.4.1.1 on WRF/Chem meteorological output.

Quick Surface Ozone Comparison to AQS

Instantaneous Mixing Ratios at 20 UTC on 7 August 2006

CMAQ v4.7 | **Modified WRF/Chem v3.0.1.1**



NOTE: Filled circles indicate observed ozone (O_3) values from EPA's Air Quality System (AQS).

Evaluation of CMAQ and WRF/Chem Results

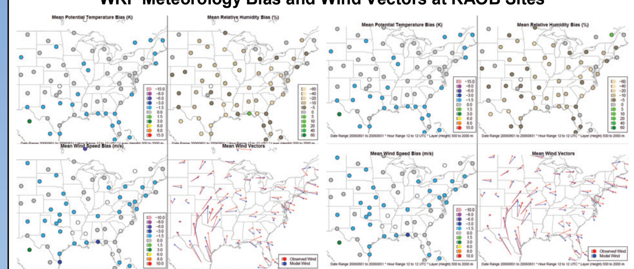
Though both model simulations were configured with like options and conditions on the same domain (E. US 12 km grid with 34 layers), the previous figure shows a significant problem of overprediction of afternoon O_3 values by the modified WRF/Chem v3.0.1.1 model.

To help diagnose this problem, analyses of these model results were then conducted using the AMET package, as shown below.

AMET Evaluation, 1-31 August 2006

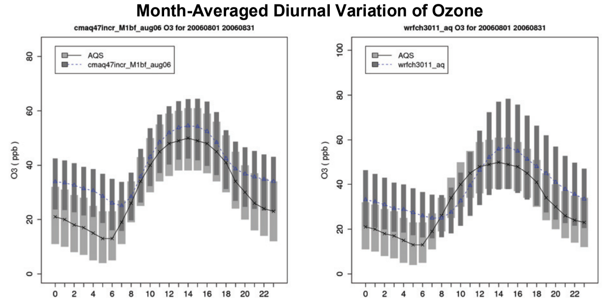
CMAQ v4.7 (left figures) | **Modified WRF/Chem v3.0.1.1 (right figures)**

Month-Averaged 500-2000 m AGL Layer-Averaged WRF Meteorology Bias and Wind Vectors at RAOB Sites

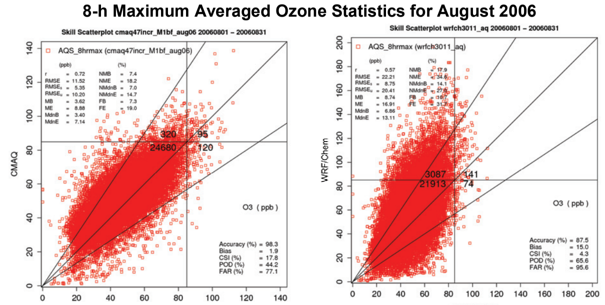


Slight differences in humidity at a few sites, but otherwise similar boundary layer meteorology for the two model simulations.

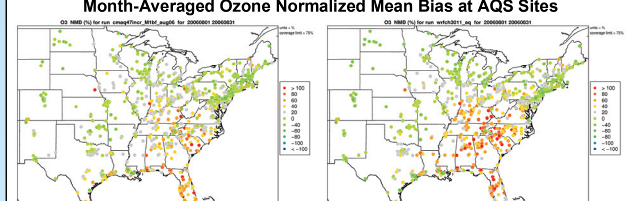
Month-Averaged Diurnal Variation of Ozone



8-h Maximum Averaged Ozone Statistics for August 2006



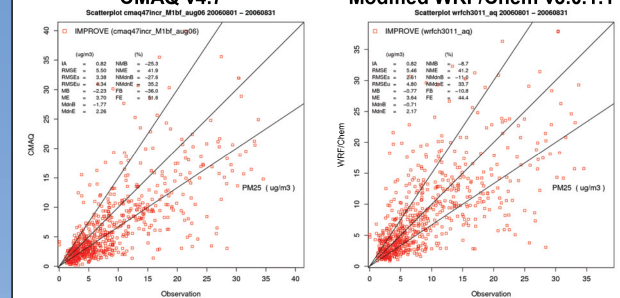
Month-Averaged Ozone Normalized Mean Bias at AQS Sites



O_3 statistics from the WRF/Chem v3.0.1.1 simulation show a 1-h diurnal phase lag, positive bias, and exaggerated extreme values for afternoons of August 2006, mainly in the southeastern U.S.

AMET $PM_{2.5}$ Evaluation, 1-31 August 2006

CMAQ v4.7 | **Modified WRF/Chem v3.0.1.1**



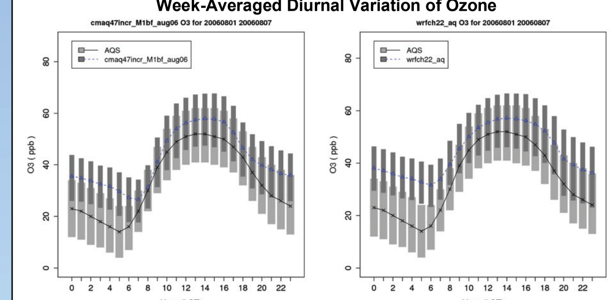
Despite apparent problems with O_3 predictions, the modified WRF/Chem v3.0.1.1 model simulated $PM_{2.5}$ for August 2006 as well as CMAQ v4.7 when compared to IMPROVE observations.

AMET Ozone Evaluation, 1-7 August 2006

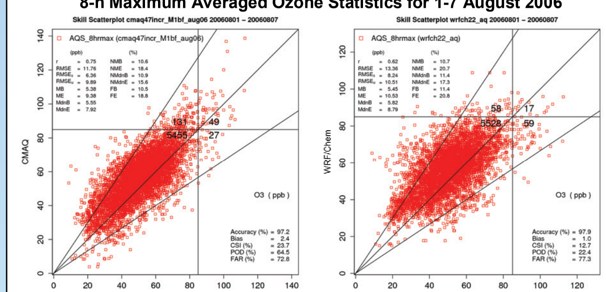
In 2008, CB05 was implemented into WRF/Chem v2.2 (but not coupled to an aerosol scheme) and an AQ simulation of 29 July – 7 August 2006 was completed. AMET was used to analyze this available older simulation in order to help diagnose the current O_3 problem in the modified WRF-Chem v3.0.1.1 model.

CMAQ v4.7 (left figures) | **Modified WRF/Chem v2.2 (right figures)**

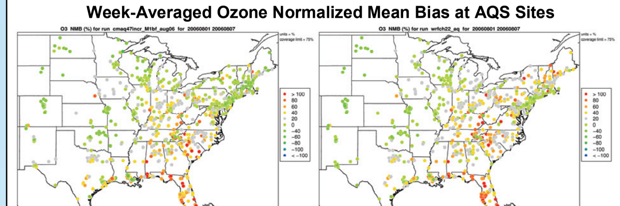
Week-Averaged Diurnal Variation of Ozone



8-h Maximum Averaged Ozone Statistics for 1-7 August 2006



Week-Averaged Ozone Normalized Mean Bias at AQS Sites



The WRF/Chem v2.2 simulation did not use the same chemical IC/BCs as CMAQ, nor was FDDA specified. Nevertheless, the WRF/Chem v2.2 O_3 predictions are generally comparable to those from CMAQ for the first week of August 2006.

Further Discussion

Other differences in physics options for these simulations were that WRF/Chem v3.0.1.1 employed Lin microphysics, Goddard short-wave radiation, and the new Grell 3D ensemble cumulus scheme, while WRF for driving CMAQ utilized Thompson microphysics, Dudhia SW radiation, and the Kain-Fritsch cumulus scheme. WRF/Chem v3.0.1.1 also specified 6th-order horizontal diffusion and positive-definite TKE advection. These WRF/Chem options are recommended by experts to enable such processes as convective transport of chemistry, and feedbacks from aerosols and the cumulus parameterization to the radiation schemes. The WRF/Chem v2.2 simulation, coming from an older version of WRF, used WSM 6-class microphysics, Dudhia SW, Monin-Obukhov surface layer, NOAH land-surface model, YSU boundary layer, Grell-Devenyi ensemble cumulus, and no FDDA, resulting in different meteorology.

Conclusions

WRF/Chem v3.0.1.1 was modified to include CB05 coupled to the MADE/SORGAM aerosol scheme and used to simulate August 2006 for the eastern U.S. Results were evaluated using the AMET analysis package and compared against a relevant CMAQ simulation and observations. Principal findings include:

- the modified WRF/Chem v3.0.1.1 currently produces too much O_3 in afternoons near metropolitan areas, with a significant high bias;
- CMAQ compares reasonably well against observational data;
- though most aerosol statistics have not yet been analyzed, the $PM_{2.5}$ predictions from the modified WRF/Chem v3.0.1.1 were less biased than those produced by CMAQ;
- and the older simulation from the modified WRF/Chem v2.2 performed better than WRF/Chem v3.0.1.1, but this may be fortuitous.

Immediate Plans

Several numerical experiments with different physics options are planned to diagnose the O_3 overprediction problem in the modified WRF/Chem v3.0.1.1 model. Of particular interest is the 6th-order diffusion and whether it is compatible with the P-X and ACM2 options. Once a solution to the O_3 problem is found, these AMET analyses will be revisited to produce new statistics and a more consequential model intercomparison.

References

Appel, K. W., and R. C. Gilliam, 2008: The Atmospheric Model Evaluation Tool. Presented at the 7th Annual CMAS Conference, Chapel Hill, NC, October 2008. [Available online at http://www.cmascenter.org/conference/2008/slides/appel_amet_cmas08.ppt]

Byun, D., and K. L. Schere, 2006: Review of the governing equations, computational algorithms, and other components of the Models-3 Community Multiscale Air Quality (CMAQ) modeling system. *Appl. Mech. Rev.*, **59**, 51-77.

Gilliam, R. C., W. Appel, and S. Phillips, 2005: The Atmospheric Model Evaluation Tool: meteorology module. Presented at the 4th Annual CMAS Conference, Chapel Hill, NC, September 2005. [Available online at http://www.cmascenter.org/conference/2005/abstracts/6_1.pdf]

Grell, G. A., S. E. Peckham, R. Schmitz, S. A. McKeen, G. Frost, W. C. Skamarock, and B. Eder, 2005: Fully coupled "online" chemistry within the WRF model. *Atmos. Environ.*, **39**, 6957-6975.

Sarwar, G., D. Luecken, G. Yarwood, G. Z. Whitten, and W. P. L. Carter, 2008: Impact of an updated carbon bond mechanism on predictions from the CMAQ modeling system: Preliminary assessment. *J. Appl. Meteor. Clim.*, **47**, 3-14.

Skamarock, W. C., J. B. Klemp, J. Dudhia, D. O. Gill, D. M. Barker, M. G. Duda, X.-Y. Huang, W. Wang, and J. G. Powers, 2008: A description of the Advanced Research WRF version 3. NCAR Technical Note, NCAR/TN-475+STR. [Available online at http://www.mmm.ucar.edu/wrf/users/docs/arw_v3.pdf]

Yarwood, G., S. Rao, M. Yocke, and G. Whitten, 2005: Updates to the carbon bond chemical mechanism: CB05. Final report to the U.S. EPA, RT-0400675. [Available online at http://www.camx.com]

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