Simulating Ozone: A Comparative Analysis of CMAQ and WRF/Chem

Jerold A. Herwehe, Tanya L. Otte, Rohit Mathur, and S.T. Rao

U.S. EPA/ORD/NERL, Atmospheric Modeling and Analysis Division
Research Triangle Park, North Carolina, U.S.A.

Introduction

The interaction of chemistry and meteorology is a fundamental part of any air quality (AQ) modeling system. The Community Multiscale Air Quality modeling system (CMAQ) is an online chemical transport model driven by meteorological dynamics from weather prediction models such as the Weather Research and Forecasting model (WRF). In contrast, the WRF with Chemistry model (WRF-Chem) is offline coupled, solving the meteorology and chemistry together each time step, thereby allowing bidirectional feedbacks between the chemistry, aerosols, radiation, cloud microphysics, and meteorology during the simulation.

Objective

The purpose of this study is to conduct a comparative analysis between CMAQ and a modified version of WRF/Chem, focusing on simulated ozone (O₃) and selected processes responsible for any differences between the model predictions.

Approach

- To increase compatibility of the models for intercomparison, the CB05 chemical mechanism was implemented into WRF-Chem v3.0.1.1 and coupled to the MADE/SORGAM aerosol scheme.
- Additional model compatibility was achieved by converting CMAQ-ready emissions, initial and boundary conditions for WRF-Chem use.
- Ran a one-month simulation (August 2006, with July 29-31 spin-up) using the modified WRF-Chem for comparison with an available WRF-driven CMAQ v4.7 air quality simulation of the same period.

Simulation configuration similarities:

- Eastern U.S. domain with 12 km grid spacing and 34 layers up to 100 hPa; initial/boundary conditions from NAM (for meteorology) and a CMAQ 36 km simulation for chemistry; CB05: emissions based on 2001 NEI projected to 2006, BEIS Ver. 3.13, and Mobile6; RRTM longwave radiation; grid analysis; FDDA surface updates to SST, albedo, and vegetative fraction; USGS land use; effects of topographic slope and shading on radiation; horizontal Smagorinsky first-order closure; and subgrid convective chemistry transport.

Simulation configuration differences:

- Model Feature: WRF and CMAQ
  - WRF-Chem
    - Microphysics: WSM 6-class (Lin et al.)
    - Shortwave Radiation: Dudhia
    - Sfc. Layer Physics: Pleim-Xu (P-X)
    - Land Surface Model: Pleim-Xu
    - Boundary Layer: ACM2
    - Cumulus Pamm.: Kain-Fritsch
    - w damping: no
    - Positive-Def. Adv. moisture, chemistry scales, chemistry
    - Photolysis: JPROC
    - Aerosols: AE4 with updated MADE/SORGAM
    - NOₓ2 gamma pamm.

- CMAQ

Note: P-X and ACM2 are currently incompatible with WRF-Chem, so recommended alternatives were chosen. Other options are available in WRF-Chem, but the model documentation was chosen to allow feedbacks from the aerosols and convective parameterization to the radiation and photolysis schemes. Also, WRF-Chem in this configuration had only a partial, experimental scheme for aqueous phase chemistry.

- Conducted statistical analyses of the month-long WRF/Chem and WRF-driven CMAQ simulations using the Atmospheric Model Evaluation Tool (AMET) and additional custom-built analysis tools.

Evaluation of Simulated Ozone

Ozone Production Efficiency (OPE) (10-17 LST) for August 2006 at Birmingham, Alabama (urban, industrial region) (top plots) and Yorkville, Georgia (rural, forest-agricultural) (bottom plots).

A comparison of IONS06 ozonesonde observations with corresponding simulated O₃ profiles averaged over available daylight launch times during August 2006 (shown at right) show that both models underestimate O₃ above the PBL and can be either positively or negatively biased within the PBL. At these two IONS06 sites, WRF-Chem has noticeably more O₃ within the boundary layer than CMAQ, though this is not always the case (per other IONS06 sites).

Max. 8-h avg. statistics and hourly boxplot for O₃ reveal both models have a positive bias, especially at night. WRF-Chem is more biased, and it has slightly larger error and lower correlation to AQS observations than CMAQ.

Examination of Associated Processes

WRF-Chem has a deeper PBL, remarkable considering its greater O₃ deposition partition explaining simulated O₃ differences. Differences in O₃ deposition partially explain simulated O₃ differences.

Ozone Production Efficiency (OPE) (10-17 LST) for August 2006 at Birmingham, Alabama (urban, industrial region) (top plots) and Yorkville, Georgia (rural, forest-agricultural) (bottom plots).

Conclusions

- Both CMAQ and WRF/Chem overestimate surface ozone during August 2006, mainly in the South and Ohio River Valley.
- WRF-Chem produces more ozone than CMAQ despite having the same chemical mechanism, emissions, and initial/boundary conditions, plus a generally deeper boundary layer of more aged air.
- Over regions where simulated ozone is biased high, WRF-Chem builds and maintains a 10% greater reservoir of O₃ aloft than CMAQ.
- Differences in land surface model and boundary layer physics, dry deposition, clouds, and especially photolysis rates contribute to the presence of more ozone in WRF-Chem than in CMAQ. Chosen model options are important factors in determining AQ simulation results.

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Jerold A. Herwehe | herwehe.jerry@epa.gov | 919-541-0166