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Diagnostic analysis of ozone concentrations simulated by two regional-scale air quality models

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ABSTRACT

Since the Community Multiscale Air Quality modeling system (CMAQ) and the Weather Research and Forecasting with Chemistry model (WRF/Chem) use different approaches to simulate the interaction of meteorology and chemistry, this study compares the CMAQ and WRF/Chem air quality simulation results for a month-long retrospective study period (August 2006) over the eastern United States, including comparisons with data from several observation networks. To help improve the comparability of the two models, the 2005 Carbon Bond chemical mechanism (CB05) was implemented into WRF/Chem. In addition, the same emissions, initial and boundary conditions have been used in both models to intercompare simulated ozone (O_3) from the WRF-driven CMAQ and WRF/Chem models. Results reveal that ground-level O_3 from both models is biased high, especially in the central South and Ohio River Valley; however, WRF/Chem predicts roughly 10% more O_3 aloft (1000–2500 m AGL) than CMAQ. Different model configurations due to the choice of land surface model (LSM), planetary boundary layer (PBL) physics scheme, and convective cloud parameterization contributed to the differences seen in simulated O_3, but most important were the different treatments of the radiative effects of clouds by their respective photolysis schemes.

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1. Introduction

For the past decade, the Community Multiscale Air Quality modeling system (CMAQ; Byun and Schere, 2006) has been an offline chemical transport model driven by meteorological fields from models such as the Weather Research and Forecasting model (WRF; Skamarock and Klemp, 2008). During this decade, CMAQ has built a worldwide community of several thousand users who have successfully employed the modeling system for a variety of research, regulatory, forecasting, and climate applications. However, offline chemistry does not allow aerosol feedbacks from the chemical transport model to affect the radiation budget, cloud microphysics, and precipitation in the meteorological model. Such feedbacks are particularly important in light of the increased focus on the interactions of air quality and climate change. An alternative approach is to use an online coupled chemistry and dynamics model, such as the WRF with Chemistry model (WRF/Chem; Grell et al., 2005) or the coupled WRF–CMAQ system (Mathur et al., 2010) because they treat the physical and chemical feedback processes. However, regional-scale online modeling is relatively new (Zhang, 2008), and there are still many unresolved issues related to the simulation of aqueous chemical processes in an online system. This deficiency affects the online system's ability to properly handle the physical feedback mechanisms. In addition, online systems require increased computational resources to run both the meteorology and chemistry modules concurrently, which may render the online systems impractical for some research and regulatory groups. Thus, both offline and online modeling systems will continue to be used for various applications for some time.

This study presents a diagnostic analysis of Eulerian (i.e., grid-based), limited-area offline and online meteorology and chemistry modeling systems. Here, the WRF-driven CMAQ modeling system and the WRF/Chem model are compared by analyzing simulated ozone (O_3) for a summer month (August 2006) and selected physical and chemical processes that are responsible for differences in modeled O_3 at the surface and aloft. The object of this intercomparison is not to determine which modeling system (offline WRF–CMAQ versus online WRF/Chem) is most skillful in reproducing the observations. Rather, it is to diagnose and understand the differences between the two modeling systems, to identify strengths and weaknesses of the systems, and to inform future development to improve the simulation of air quality (AQ) by both systems.

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2. Modeling configuration and approach

The 2008 versions of the two air quality modeling systems were used for this intercomparison study. CMAQ v4.7 was driven by WRF-ARW v2.2 (WRF-for-CMAQ in this paper) which included additional physics packages that were later released in v3.0 (Gilliam and Pleim, 2010). The 2005 update to the Carbon Bond mechanism (CB05; Yarwood et al., 2005) was implemented into WRF/Chem v3.0.1.1 to conduct a more compatible comparison of gas phase chemistry results with the CMAQ modeling system. In addition, CB05 was coupled to WRF/Chem's Modal Aerosol Dynamics model for Europe (MADE; Ackermann et al., 1998) and Secondary Organic Aerosol Model (SORGAM; Schell et al., 2001) schemes to allow direct and indirect aerosol feedback to the shortwave (SW) radiation and cloud microphysics. Specialized software converted CMAQ-ready initial and boundary conditions (ICs/BCs) and CB05-speciated emissions for WRF/Chem to enable both systems to use the same initial, lateral boundary, and emissions forcing. Hourly meteorological input data for offline ingestion by CMAQ were prepared from the WRF output by the Meteorology–Chemistry Interface Processor (MCIP; Otte and Pleim, 2010). CMAQ then linearly interpolated the hourly meteorological input data for each model time step (e.g., every five minutes) during the CMAQ simulation. In contrast, the online coupled WRF/Chem drove its chemistry with meteorological values from every model time step (every minute for this study), thereby allowing temporally nonlinear changes in the meteorology within each hour to more realistically affect the transport, mixing, and effective reaction rates of the chemical species.

The input fields and geophysical dimensions of the offline and online modeling systems were set to be as similar as possible (Table 1), but each modeling system was allowed to use the physics options in the meteorological module that are typically recommended by the developers of the AQ models (Table 2). The modeling domain covered the eastern United States with 12-km horizontal grid cells with vertical extent to 100 hPa using 34 terrain-following layers and the lowest layer is 35-m thick. A month-long period was chosen for this study to permit robust statistical analyses on the regional scale. August 2006 was selected because of expected summer season high O_3 values and a partial overlap with the observational period of an intensive field campaign conducted around Houston, Texas. Meteorological ICs/BCs originated from the National Centers for Environmental Prediction (NCEP) North American Mesoscale model (NAM), which also provided fields for four-dimensional data assimilation (FDDA), as documented by Gilliam and Pleim (2010). Chemical ICs/BCs were created from a CMAQ simulation for the same period but which used 36-km horizontal grid spacing (Foley et al., 2010).

Table 1
Air quality simulation configuration similarities.

Feature	Selected for both AQ simulations
Domain	Eastern U.S. on 12-km grid with 34 layers
Domain top	100 hPa
Initial and boundary conditions	NAM for meteorology; CMAQ simulation on 36-km grid for chemistry
Chemical mechanism	CB05 (Yarwood et al., 2005)
Emissions	USEPA 2001 NEI projected to 2006, BEIS Ver. 3.13, and Mobile6
Longwave radiation	RRTM (Mlawer et al., 1997)
Nudging	Grid (analysis) FDDA
Surface updates	SST, albedo, vegetative fraction
Land-use classification	USGS
Topographic effects	Slope and topographic shading on radiation
Eddy coefficient	Horizontal Smagorinsky first-order closure
Subgrid transport	Subgrid convective chemistry transport

Table 2
Air quality simulation configuration differences.

Feature	WRF and CMAQ	WRF/Chem
Microphysics	WSM 6-class (Hong and Lim, 2006)	Purdue Lin (Tao et al., 1989)
Shortwave radiation	Dudhia (Dudhia, 1989)	Goddard (Chou and Suarez, 1994)
Surface layer physics	Pleim (Pleim, 2006)	Monin–Obukhov (Skamarock et al., 2008)
Land surface model	Pleim–Xiu (Xiu and Pleim, 2001)	Noah (Chen and Dudhia, 2001)
Planetary boundary layer	ACM2 (Pleim, 2007)	YSU (Hong et al., 2006; Hong, 2010)
Cumulus parameterization	Kain–Fritsch (Kain, 2004)	Grell–Dévényi (Grell and Dévényi, 2002)
Vertical velocity damping	No	Yes
Positive-definite advection	Moisture, chemistry	Moisture, scalars, chemistry
Photolysis	JPROC/PHOT (Roselle et al., 1999)	Fast-J (Wild et al., 2000)
Aerosols	AE4 with updated N_2O_5 gamma parameterization (Binkowski and Roselle, 2003; Davis et al., 2008)	MADE/SORGAM (Ackermann et al., 1998; Schell et al., 2001)

Anthropogenic emissions were projected to 2006 from the 2001 U.S. Environmental Protection Agency's (USEPA's) National Emissions Inventory (NEI; http://www.epa.gov/ttn/chief/net/critsummary.html) and include mobile emissions from the Mobile6 emissions model (http://www.epa.gov/otaq/m6.htm). The biogenic emissions were processed using the Biogenic Emissions Inventory System (BEIS) v3.13. WRF, CMAQ, and WRF/Chem were initialized at 00 UTC 29 July 2006 to allow for a three-day spin-up period for the chemical processes, and this spin-up period is not used in the analyses described later in this paper.

Table 2 also lists differences in the recommended near-surface physics options for each modeling system. WRF-for-CMAQ and CMAQ utilized the Pleim–Xiu (PX) LSM, the Pleim surface layer scheme, and the Asymmetric Convective Model version 2 (ACM2) PBL scheme, while WRF/Chem used the NCEP – Oregon State University – Air Force – Hydrologic Research Laboratory (Noah) LSM, Monin–Obukhov surface layer, and Yonsei University (YSU) PBL schemes. The important effects of these choices are described later as appropriate during the discussion of the results and analyses.

The Rapid Radiative Transfer Model (RRTM) used in both modeling systems for longwave (LW) radiation processes considers cloud optical depth; and distributions of water vapor, O_3, carbon dioxide (CO_2), and other trace gases, such as methane (CH_4) and nitrous oxide (N_2O), if available. Neither modeling system treats the effects of prognostic aerosols on LW radiation. However, both modeling systems simulate the direct effects of scattering and absorption on SW radiation and photolysis due to resolved water vapor and cloud droplets. In addition, WRF/Chem allows for direct feedback effects from parameterized subgrid convective precipitation and prognostic aerosols on the SW radiation and the photolysis rates. WRF/Chem also allows some indirect feedbacks on radiation and cloud microphysics by computing a prognostic cloud droplet number, though there are no aerosol indirect effects from the MADE/SORGAM scheme in this version of WRF/Chem.

Photolysis in CMAQ is a two-step process. First, an offline preprocessor ("JPROC") computes clear-sky climatological photolysis rates as a function of zenith angle, latitude, altitude, and chemical mechanism using prescribed aerosol and interpolated seasonal O_3 profiles. Second, an online routine ("PHOT") then dynamically corrects the preprocessed photolysis rates according to