Performance Summary of the 2006 Community Multiscale Air Quality (CMAQ) Simulation for the AQMEII Project: North American Application

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Abstract

The CMAQ modeling system has been used to simulate the CONUS using 12-km by 12-km horizontal grid spacing for the entire year of 2006 as part of the Air Quality Model Evaluation International Initiative (AQMEII). The operational model performance for O_3 and $PM_{2.5}$ for the simulation was assessed. The model underestimates O_3 mixing ratios in the winter, which is likely due to low O_3 mixing ratios in the middle and lower troposphere from the lateral boundary conditions. $PM_{2.5}$ performance varies seasonally and geographically, with $PM_{2.5}$ overestimated in the winter and fall, while performance in the spring and summer is generally good, especially in the summer. $PM_{2.5}$ concentrations are systematically higher in the AQMEII CMAQ simulation than in previous CMAQ simulations, primarily due to higher concentrations of TC and unspeciated $PM_{2.5}$ mass, which may also be due to differences in the lateral boundary conditions.

Keywords: CMAQ; Ozone; Particulate Matter; Air Quality Modeling; Model Evaluation

1. Introduction

The Air Quality Model Evaluation International Initiative (AQMEII) is a model evaluation project involving numerous research groups from North American and Europe with the goal of advancing the way regional scale air quality modeling systems are evaluated. As part of the AQMEII project, the Atmospheric Modeling and Analysis Division (AMAD) of the U.S. Environmental Protection Agency (USEPA) has performed an annual 2006 Community Multiscale Air Quality (CMAQ; Foley et al., 2010) simulation for the continental U.S. (CONUS).

The CMAQ simulation performed for this project is unique compared to previous CMAQ simulations performed by AMAD in the past for several reasons. First, the simulation was performed over a single domain that covers the entire CONUS and a large portion of Canada using 12-km by 12-km horizontal grid spacing. In the past, two separate simulations covering the eastern and western U.S. have been used instead of single, continuous domain. Second, the simulation utilizes meteorology provided by the latest version of the Weather Research and Forecasting (WRF) model, whereas previous CMAQ annual simulations have typically utilized meteorology provided by the 5th Generation Mesoscale Model (MM5; Grell et al., 1994). Finally, the CMAQ simulation utilizes boundary conditions provided by the Global and regional Earth-system Monitoring using Satellite and in-situ data (GEMS) product.

2. Data

2.1 Model Inputs and Configuration

The CMAQ model requires gridded meteorological and emissions data to simulate the formation, transport and fate of numerous atmospheric pollutants, including ozone (O_3) and fine particulate matter ($PM_{2.5}$). Meteorological data for the simulation are provided by the Weather Research and Forecast (WRF) model with a domain covering the CONUS and portions of Canada and Mexico using 12-km by 12-km horizontal grid spacing and 34-vertical layers extending up to 50 hPa. Boundary conditions for the WRF simulation were provided by the North American Model (NAM). Outputs from the WRF simulation were preprocessed for input in the CMAQ model using v3.6 of the Meteorology-Chemistry Interface Processor (MCIP).

The emission dataset used for the AQMEII modeling was based on a 12-km national U.S. domain with speciation for the CB05 mechanism. The emission inventory and ancillary files were based on the 2005 emission modeling platform (http://www.epa.gov/ttn/chief/emch/index.html#2005). The fire emissions were based on 2006 daily fire estimates using the Hazard Mapping System Fire detections and Sonoma Technology SMARTFIRE system. Continuous Emission Monitoring (CEM) data from 2006 was used for the Electric Generating Units (EGU) sector. Plume rise was calculated within the CMAQ model. Temporal allocation was done monthly for each day of the week with all holidays ignored. Emissions were preprocessed for the CMAQ model using the Sparse Matrix Operator Kernel Emissions (SMOKE).

The CMAQ model simulation utilized version 4.7.1 of the model (Foley et al., 2010) with 34 vertical layers and 12-km by 12-km horizontal grid spacing covering the CONUS, southern Canada and northern Mexico. The CB05 chemical mechanism and AERO5 aerosol module were also used. Boundary conditions for the CMAQ simulation were provided by the GEMS product, which combines modeled data and observations (surface and satellite) to provide data for meteorology and atmospheric gases including greenhouse gases, global reactive gases and global aerosols.

2.2. Observed Data

The observed data used to assess the CMAQ model estimates are obtained from several observational networks available across the U.S. that measure a combination of gas, aerosol, dry and wet deposition and meteorological variables. The primary source of ground level ozone (O_3) and federal reference method (FRM) daily average $PM_{2.5}$ mass measurements is the EPA's Air Quality System (AQS). The O_3 and $PM_{2.5}$ networks in AQS are geographically diverse and span the entire U.S. and are an excellent source of quality assured air quality measurements. Assessment of the model performance was accomplished using the Atmospheric Model Evaluation Tool (AMET; Appel et al., 2010), which can perform a vast number of different analyses and produce many different plots useful for assessing model performance.

3. Results

3.1. Ozone

Operational model performance was generally consistent with previous CMAQ simulations performed for the same time period, with several notable exceptions. Performance of maximum 8-hr average O_3 for the eastern U.S. (east of 110°W longitude) in the winter (January - March) underperformed previous CMAQ simulations, with the simulation demonstrating a large underestimation of O_3 in the winter. The underestimation was largest in the Northeast and Great Lakes regions of the U.S., with smaller underestimations in the southern U.S. This is a significant deviation from previous CMAQ simulations for the same time period, where O_3 performance was generally good and not significantly underestimated. Figure 1 presents a time series comparison of results from the CMAQ simulation using WRF/GEMS data with those from a previous CMAQ simulation for the same time period that utilized GEOS-CHEM model generated boundary conditions and MM5 meteorology.

The large underestimation of O_3 in the current simulation that was not present in previous CMAQ model simulations is likely due to several differences between the current simulation and previous simulations. First, the boundary conditions used in previous CMAQ model simulations of 2006 used were provided by the GEOS-CHEM model, unlike the current simulation which utilizes boundary conditions provided by GEMS. Estimates of O_3 mixing ratios in the mid to lower troposphere are much higher in the GEOS-CHEM boundary conditions than in the GEMS boundary conditions. It is likely that the lower O_3 mixing ratios in the troposphere in the GEMS boundary conditions result in lower ground-level O_3 mixing ratios, particularly in the winter when the O_3 provided from the boundaries comprises a significant portion of the CMAQ estimated ground-level O_3.

The CMAQ model estimates of maximum 8-hr average O_3 for the rest of the year are relatively good overall, with similar performance to previous CMAQ model simulations (Fig. 1). The CMAQ model typically overestimates O_3 mixing ratios from approximately 20 ppbV to 50 ppbV and underestimates the very highest O_3 mixing ratios. During the summer (June through August), O_3 mixing ratios are significantly overestimated in the lower mid-western U.S. The exact cause of the overestimation in that region is still under investigation; however it may be related to several large NO_x point sources in that region.

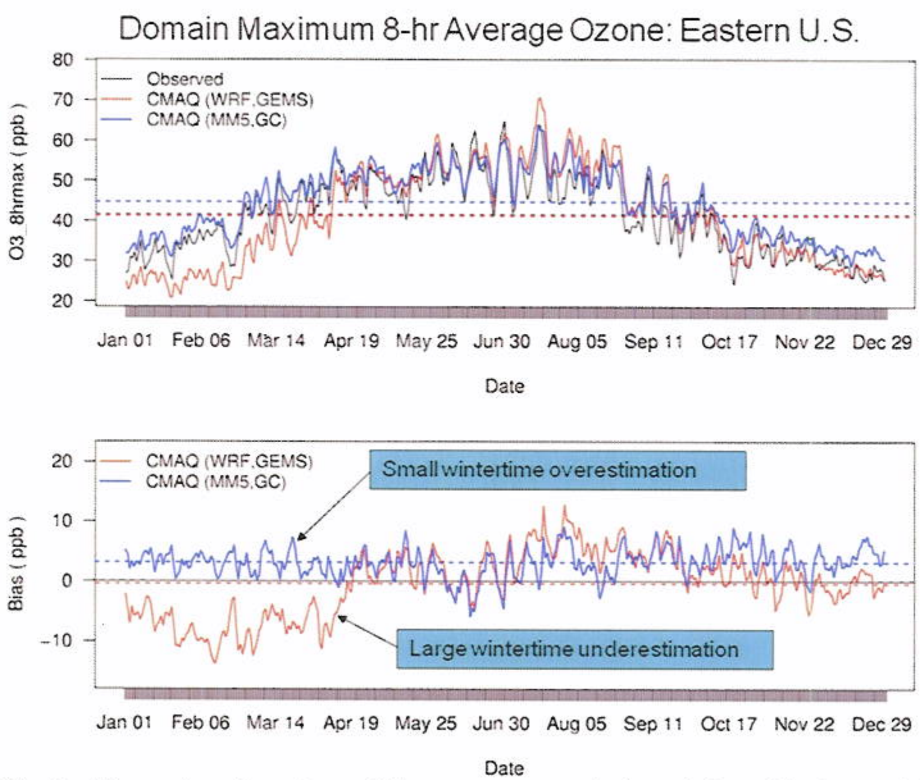

Fig. 1. Time series of maximum 8-hr average ozone (ppb; top) for AQS observed (black), CMAQ using WRF and GEMS data (red) and CMAQ using MM5 and GEOS-Chem data (blue). The bottom time series plot shows the corresponding bias (ppb) for each simulation.

3.2. Particulate Matter

For the winter, $PM_{2.5}$ is typically overestimated in the eastern U.S., while in the spring (March – May) the model still overestimates $PM_{2.5}$ but to a lesser extent than in the winter

(Fig. 2). For the summer, CMAQ estimated $PM_{2.5}$ concentrations generally compare well with observations in the eastern U.S. This is a significant improvement over previous CMAQ model simulations for the same time period, where $PM_{2.5}$ was underestimated across the entire eastern U.S. In the fall (September – November), $PM_{2.5}$ is once again overestimated in both the eastern and western U.S., with worse performance than previous CMAQ simulations for the same time period.

The CMAQ model estimated $PM_{2.5}$ is higher in all seasons and regions in the current simulation compared to previous simulations. The primary source of the higher $PM_{2.5}$ concentrations in CMAQ is higher concentrations of EC and OC (herein referred to as TC) and higher concentrations of unspeciated particulate matter (PM_{other}). The higher TC and PM_{other} concentrations in the current simulation are likely due to differences in both the meteorology and boundary conditions used. Previous studies have shown that CMAQ estimated $PM_{2.5}$ concentrations are higher in simulations using WRF meteorology as compared to MM5 driven CMAQ simulations (Appel et al., 2010).

The GEMS boundary conditions used are year-specific and capture large sources of TC and PM_{other} (e.g. wildfires), particularly during the summer and fall periods as detected by satellite sensors. Previous CMAQ simulations for the same period utilized climatological boundary conditions, which would not have captured wildfire events. The result is systematically higher total $PM_{2.5}$ mass throughout the year, which results in improved comparisons to observations when $PM_{2.5}$ is underestimated and degraded performance when $PM_{2.5}$ is overestimated.

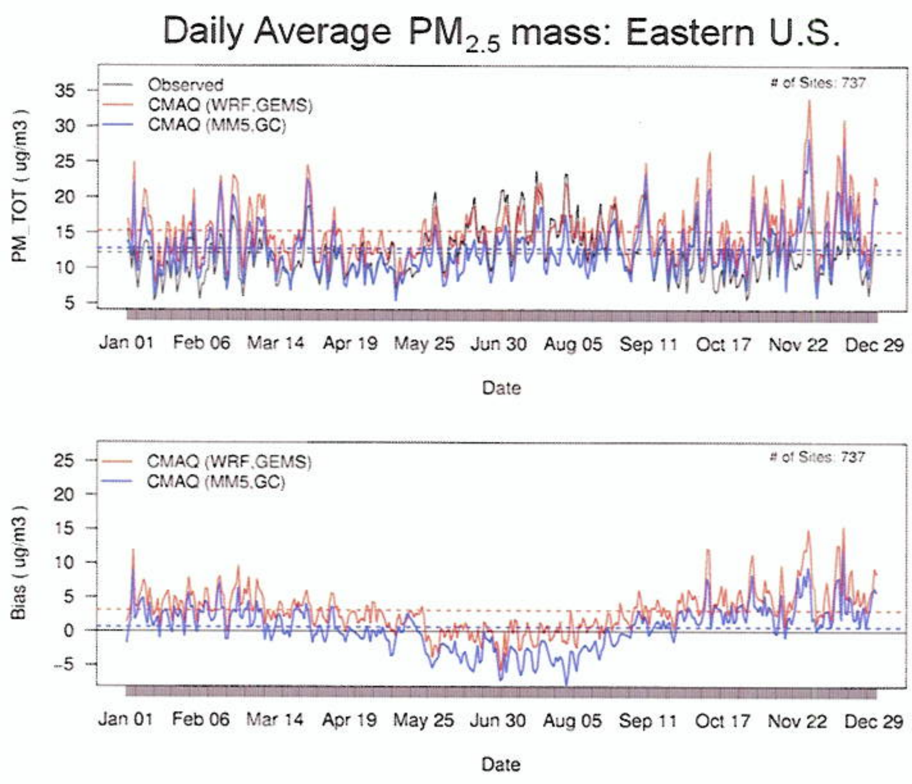

Fig. 2. Time series of daily average $PM_{2.5}$ ($\mu g/m^3$; top) for observed (black), CMAQ using WRF and GEMS data (red) and CMAQ using MM5 and GEOS-Chem data (blue). The bottom time series plot shows the corresponding bias ($\mu g/m^3$) for each simulation.

4. Conclusions

The CMAQ modeling system has been used to simulate the CONUS using 12-km by 12-km horizontal grid spacing for the entire year of 2006. The operational model performance for O_3 varies seasonally, with the model largely underestimating O_3 mixing ratios in the winter. Performance for the other seasons is generally good, with the model overestimating O_3 mixing ratios at low observed levels and underestimating O_3 mixing ratios at high levels. The underestimation of O_3 mixing ratios in the winter represents a significant departure from previous CMAQ simulations, which generally showed little winter bias. It is believed that lower O_3 mixing ratios in the middle and lower troposphere from the GEMS generated boundary conditions as compared to GEOS-CHEM generated boundary conditions are primarily responsible for the lower ground-level O_3 mixing ratios.

As with O_3, $PM_{2.5}$ performance varies seasonally and geographically, with $PM_{2.5}$ overestimated in the winter and fall, while performance in the spring and summer is generally good, especially in the summer. $PM_{2.5}$ concentrations are higher in the current simulation than in past simulations, primarily due to higher concentrations of TC. The higher TC concentrations are due to differences in the WRF meteorology versus MM5 (winter) and higher concentrations coming in from the GEMS generated boundary conditions (summer).

References

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Audience Questions

Q: Henk Eskes - "Does the capping of ozone in the stratosphere influence radiation and reaction rates in the troposphere?"

A: "No, the capping of ozone in the upper troposphere and stratosphere in these simulations has no impact on the radiation or reactions rates in the model."

Q: Jaako Kukkonen - "There are some PM2.5 source categories that are poorly known, such as residential combustion and non-exhaust vehicular sources. How did you allow for those sources? The residential combustion emissions have a substantial seasonal variation, which could potentially have an influence on the agreement of predictions and data seasonally?"

A: "These emissions sources are included in the emission inventory used in the simulations. The seasonable variability in residential combustion is accounted for in the emissions inventory."