Representing the Effects of Long-Range Transport and Lateral Boundary Conditions in Regional Air Pollution Models

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Abstract The Community Multiscale Air Quality (CMAQ) modeling system was applied to a domain covering the northern hemisphere; meteorological information was derived from the Weather Research and Forecasting (WRF) model run on identical grid and projection configuration, while the emission inputs were derived from global inventories. The ability of the model to represent long-range transport of pollutants is analyzed through comparisons with aircraft measurements from the 2006 INTEX-B field campaign, ozonesonde profiles, and remotely sensed observations of aerosol optical depth. Time varying lateral boundary conditions from these hemispheric scale calculations were used to drive regional-scale air quality simulations over a finer resolution domain covering the continental United States. Comparison of model predictions with surface O₃ and PM_{2.5} measurements indicate comparable or better performance relative to other approaches (e.g., other global models, static profiles). The successful expansion of CMAQ to the hemispheric scales now provides a conceptual framework to examine interactions between atmospheric processes occurring at various spatial and temporal scales in a consistent manner.

1. Introduction

Both observational and modeling studies have demonstrated that pollutants near the Earth's surface can be convectively lofted to higher altitudes where strong winds can efficiently transport them from one continent to another, thereby impacting air quality on intercontinental to global scales. Changes in emission patterns over different regions of the world are likely to exacerbate the impacts of long-range pollutant transport on background pollutant levels in other regions, which may then impact the attainment of local air quality standards. Thus, strategies for reduction of pollution levels of the surface air over a region are complicated not only by the interplay of local emissions sources and several complex physical, chemical, dynamical processes in the atmosphere, but also hemispheric background levels of pollutants. Consistent modeling frameworks that can represent the interactions between various physical and chemical atmospheric processes at the disparate space and time scales are thus needed.

2. Model Setup

The Community Multiscale Air Quality (CMAQ) modeling system (Byun and Schere, 2006) was applied over a domain encompassing the northern hemisphere. The horizontal domain, set on a polar stereographic projection was discretized using grid cells with a 108 km resolution (see Figure 1), while the vertical extent ranging from the surface to 50mb was discretized with 44 layers of variable thickness with a 20 m deep lowest layer. 3-D meteorological fields were derived from the Weather Research and Forecasting (WRF) modeling system operating on the exact same projection and grid configuration as CMAQ. Observations from NCAR's global upper air observation data set combined with the GFS 1-degree analysis provided the reanalysis fields every 6 hours for grid nudging in the WRF simulations. CMAQ v4.7.1 was configured with CB05 chemical mechanism and the AER05 aerosol module. In addition, O₃ mixing ratios in the top most model layer (~50mb) were modulated based on scaling to the spatially and temporally varying potential vorticity fields to represent possible effects associated with stratosphere-troposphere exchange (Mathur et al., 2008). Emissions of NO_x, SO₂, CO, volatile organic compounds, and particulate matter from anthropogenic and biomass burning sources were derived from the ARCTAS global emission inventory (http://www.cgrer.uiowa.edu/arctas/emission.html). Monthly varying biogenic emissions of isoprene and terpene were based on the Precursors of Ozone and their Effects on the Troposphere (POET) inventory.

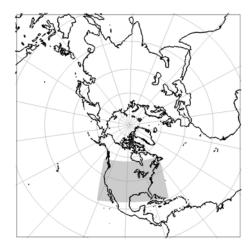


Fig. 1 The northern hemisphere modeling domain discretized using a 108km resolution grid. The shaded region shows the extent of the Continental U.S. nested domain discretized using a 12km resolution horizontal grid.

3. Results and Discussion

Model simulations were conducted for the entire 2006 calendar year with a 20 day spin-up. Previous comparisons of 3-dimensional model estimates of O_3 against ozonesonde profiles and aircraft measurements over the Pacific demonstrated the feasibility of extending CMAQ to the hemispheric scale (Mathur et al., 2012). To further investigate the ability of the model to capture the variability in daily maximum 8-hr O_3 levels at the surface, Figure 2 compares distributions of modeled and observed (at CASTNET sites) max-8 hr. O_3 for the spring season when transport across the Pacific and from the stratosphere influence O_3 mixing ratios in the surface air over the U.S.; these comparisons suggest that the model is able to capture the dynamic range of the observations.

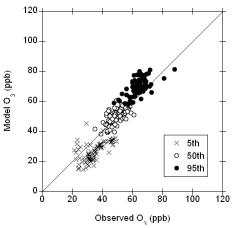


Fig. 2 Comparisons of modeled and observed (CASTNET) daily maximum 8-hr. O₃ mixing ratio distributions during Spring (March-May, 2006). At each observation location the time-series of modeled and observed daily maximum -8-hr. O₃ is examined and percentiles of the distributions are computed.

The ability of the hemispheric model to provide spatially and temporally varying and consistent lateral boundary conditions (LBCs) to limited area finer resolution calculations was examined through nesting a 12km grid over the Continental U.S. within the hemispheric domain. During the late July – early August period, particulate matter levels over large portions of the southeastern U.S. were influenced by long-range transport over the Atlantic of dust from the Sahara, as evidenced by the increase in measured $PM_{2.5}$ concentrations at monitors in Florida (Figure 3a). Also shown in Figure 3, are comparisons of simulated $PM_{2.5}$ levels in the regional calculations driven with LBCs derived from the hemispheric model with those in which the LBCs were based on GEOS-Chem. As illustrated, the regional calculations with LBCs derived from hemispheric-CMAQ show comparable or better performance (reduced bias, Fig. 3b) relative to other approaches, further illustrating that the extension of CMAQ to hemispheric scales provides a conceptual framework to examine interactions between processes occurring at various spatial and temporal scales in a consistent manner.

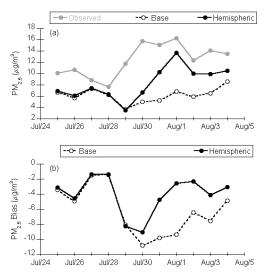


Fig. 3 Comparison of regional average (across 31 sites in Florida) (a) modeled and measured daily average $PM_{2.5}$ concentrations, and (b) corresponding model bias. The Base calculation used LBCs derived from GEOS-Chem, while the Hemispheric calculation used LBCs derived from CMAQ calculations over the northern hemisphere.

Disclaimer: Although this paper has been reviewed by EPA and approved for publication, it does not necessarily reflect EPA's policies or views.

References

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Questions and Answers

Questioner Name: M. Astitha

- **Q**: Given the very good correlation of the modeled vs. observed O_3 at the flight tracks using 108 km horizontal resolution, did you test different setups of the vertical layers to get the optimal one?
- A: We conducted tests with 2 different vertical layer configurations: a 35-layer and a 44-layer configuration. Both configurations have comparable resolution within the nominal daytime boundary layer (~3km); the latter configuration better resolves the atmosphere between 3-20 km, especially near the tropopause. The comparisons shown were based on the 35-layer configuration results. The 44-layer simulated distributions within the lowest 10km (examined in these comparisons) are similar. However, as expected much larger differences between the two configurations are seen in the upper troposphere.

Questioner Name: M. Astitha

- **Q**: About the dust transport towards the U.S., you mentioned $PM_{2.5}$ measurements were used. Maybe PM_{10} would be most likely associated to dust particles?
- A: Yes, wind-blown dust emissions influence both ambient $PM_{2.5}$ and PM_{10} levels and our simulation results also show that. In future analyses we will also examine the influence of this transport event on coarse PM levels in the region.