A Comparison of Modeled Pollutant Profiles with MOZAIC Aircraft Measurements

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Abstract In this study, we use measurements performed under the MOZAIC program to evaluate vertical profiles of meteorological parameters, CO, and ozone that were simulated for the year 2006 with several versions of the WRF/CMAQ modeling system. Model updates, including WRF nudging strategies, boundary conditions, lightning NO emissions, and vertical transport were found to affect the simulated profiles. MOZAIC descent/ascent pairs provide a unique dataset to investigate PBL structure and its representation in regional-scale models during afternoon and early evening hours. Other data sources (e.g. ozonesondes, field studies such as DISCOVER-AQ) can be used to complement MOZAIC measurements in evaluating upper air predictions by regional-scale models over various airsheds.

Keywords: Model Evaluation, MOZAIC, CMAQ, AQMEII, ozonesondes

Introduction

While it is well known that ozone concentrations aloft affect the magnitude and temporal evolution of ground-level ozone concentrations through vertical mixing and entrainment, most comparisons of air quality model predictions with ambient measurements utilize surface data only. In this study, we use aircraft measurements performed under the MOZAIC (Measurements of OZone, water vapor, carbon monoxide and nitrogen oxides by in-service AIrbus airCraft, http://mozaic.aero.obs-mip.fr/web/) program to evaluate vertical profiles of meteorological variables, CO, and ozone simulated for the year 2006 over North America. MOZAIC was started in 1993 as a joint effort involving European scientists, aircraft manufacturers, and airlines and consists of five long-haul aircraft equipped with instruments to measure meteorological variables and chemical species. More than 100 measured profiles were available at each of the following North American airports during 2006: Portland, Oregon (KPDX), Dallas/Fort Worth, Texas (KDFW), Atlanta, Georgia (KATL), and Philadelphia, Pennsylvania (KPHL).

Database and Methods

Most commercial aircrafts carrying MOZAIC instrumentation arrive from Europe at their North American destination during early to mid afternoon and depart for Europe during mid afternoon to early evening. For Portland, Dallas and Atlanta, inbound flights typically occur around 2-3 pm local time while outbound flights typically occur around 4-5 pm local time. The typical timing of the Philadelphia inbound and outbound flights (3-4 pm and 6-7 pm local time, respectively) allows the analysis of vertical profiles during the evening PBL transition period.

To assess the impact of recent updates to the WRF/CMAQ modeling system on model performance aloft, we compared observed MOZAIC profiles to the following four CMAQ simulations: CMAQ4.7.1-AQMEII, CMAQ4.7.1-Reference, CMAQ5.0-Beta, and CMAQ5.0-Final. The CMAQ4.7.1-AQMEII simulation was described in detail by Appel et al. (2012). The CMAQ4.7.1-Reference simulation was based on CMAQ4.7.1-AQMEII with slight updates to the emission inputs as well as updated boundary condition. It served as a reference case for the development cycle of CMAQ5.0. The CMAQ5.0-Beta simulation incorporated many of the science updates of the CMAQ5.0 release such as NO emissions from lightning and updated treatment of photolysis (Pleim et al., 2011) but used the same meteorological and emission inputs as the CMAQ4.7.1-Reference case. The main changes from the CMAQ5.0-Beta to the CMAQ5.0-Final simulation were the introduction of an additional vertical layer near the ground, the use of a new nudging approach in the WRF simulations used to drive CMAQ, and an updated treatment of vertical advection in CMAQ. As described in Gilliam et al. (2012), the new nudging approach incorporates observations from wind speed profiles above the boundary layer to improve the treatment of overnight pollutant transport. The two WRF simulations are hereafter referred to as WRF_OLD and WRF_NEW. All simulations were performed for January – December 2006 over the continental U.S. at a horizontal grid spacing of 12 km with a model top at 50mb. The first three simulations used 34 vertical layers with a ~40m first layer height, while the last simulation used 35 vertical layers with a ~20m first layer height.

MOZAIC observations and CMAQ simulations were matched using the Remote Sensing Information Gateway (RSIG). RSIG automatically aligns information from various spatial positions and temporal scales into a unified structure. Additional information can be found at http://www.epa.gov/rsig. Unless noted otherwise, the analysis of simulated and observed vertical profiles was performed by averaging over all individual profiles to create annual averages.

Results and Discussion

The differences in nudging strategies between the WRF_OLD and WRF_NEW simulations caused temperature differences of 0.5 C or less in the PBL and negligible differences above the boundary layer at all four airport locations considered in this study. Most of the temperature differences in the PBL were negative, i.e. the revised nudging strategy led to slightly cooler temperatures. Wind speed values simulated by WRF_NEW are higher by about 0.5 m/s throughout the PBL at all airports compared to WRF_OLD. Both the WRF_OLD and WRF_NEW simulations tend to overpredict wind speeds observed by MOZAIC aircraft near the ground and underpredict wind speeds observed above ~1.5 km.

Analysis of simulated and MOZAIC-measured CO profiles showed that updated boundary conditions had the largest impact on simulated CO profiles. The CMAQ4.7.1-AQMEII simulations utilizing the boundary conditions derived from GEMS (Schere et al., 2012) showed closer agreement with observations above the PBL during all seasons at all airports compared to all the other CMAQ simulations that used boundary conditions derived from GEOS-Chem. The better performance of CMAQ using the GEMS-based boundary conditions for CO likely reflects the use of CO data assimilation by GEMS.

Results for ozone show that updated boundary conditions, the updated treatment of photolysis and introduction of lightning NO emissions and the updated treatment of vertical advection, as well as updated meteorological fields, all had a pronounced impact on simulated mid- to upper level ozone, while the impact of these updates tends to be smaller for the lowest 2.5 km. Agreement with observed MOZAIC profiles varied between seasons, different airports and model versions. One common feature during spring and summer at all the airports was that while all the simulations overestimated ozone above 8km, the overestimation was least pronounced for the CMAQ5.0-Final simulation that utilized an updated vertical advection scheme and the WRF_NEW meteorological fields (Pleim et al., 2011). The overprediction of ozone above 8km was also present when comparing CMAQ simulations to ozonesonde observations at Trinidad Head and Wallops Island during August 2006, though CMAQ5.0-Final was not always the simulation showing closest agreement with observed ozonesonde profiles. Note that in addition to the spatial mismatch between the location of MOZAIC profiles and ozonesonde observations, there also is a temporal mismatch since MOZAIC flights and ozonesonde launches typically do not occur on the same date and at the same time. Analysis of model-to-MOZAIC differences for individual flights showed that model performance in the lower and mid-troposphere is more variable during summer than winter, likely due to more active photochemistry and stronger convective activity.

As mentioned above, the typical timing of the Philadelphia inbound and outbound flights (3-4 pm and 6-7 pm local time, respectively) enables the analysis of vertical profiles during the evening PBL transition period. When computing differences between these ascents and descents, it was found that the MOZAIC observations often show an increase of O_3 and CO concentrations between 4pm and 7pm for altitudes between ~1000m and ~2500m; this effect is not captured by any of the model simulations. Additional analyses using longer time periods, back trajectories and complementary measurements from other platforms are needed to determine the physical and chemical processes causing the observed increases and the reason this phenomenon is not captured by these model simulation. Examples of such additional datasets of interest are the NASA P3 aircraft spirals performed over Maryland during the DISCOVER-AQ campaign in July 2011.

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