On the Use of a Dynamic Evaluation Approach to Assess Multi-year Change in Modeled and Observed Urban NO_x Concentrations

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Abstract Model results and measurements were analyzed to determine the extent of change in concentrations of nitrogen oxides (NO_x) during morning weekday high traffic periods from different summer seasons that could be related to change in mobile source emissions. The dynamic evaluation technique was applied to compare the relative (%) changes in modeled and observed 3-hour morning NO_x at numerous urban locations. The average changes in modeled and observed NO_x levels between 2002 and 2005 were -16% and -15%, respectively, which are close to the decline (-17%) in NO_x emissions estimated by a mobile emissions model.

1. INTRODUCTION

Since nitrogen oxides ($NO_x = NO+NO_2$) are key precursor species in the photochemical production of tropospheric ozone, numerous control programs have been implemented to reduce NO_x emissions from various source types (USEPA, 2005). The major source categories of anthropogenic NO_x emissions include the electrical utility sector, industrial point sources, on-road and non-road mobile sources. However, in populated areas, on-road mobile emissions are the dominant source of NO_x. It is important from an accountability viewpoint to determine whether emission reductions achieve improvements in air quality. To investigate whether recent estimated reductions in mobile emissions have translated into changes in NO_x concentrations, observed and modeled NO_x concentrations during high traffic weekday 6:00-9:00 periods are analyzed from different summer years. The emerging dynamic evaluation approach was applied to focus on the model's ability to simulate concentration response to emission changes and how well it compares to changes in observations. In this regard, selected results of the relative (%) changes in modeled and observed morning NO_x concentrations between the summers of 2002 and 2005 are highlighted.

2. STUDY DESCRIPTION

2.1 Model Overview and Scenarios

The Community Multiscale Air Quality (CMAQv4.5) chemical transport model (Byun and Schere, 2006) was applied in this study using the CB-IV photochemical mechanism. Simulations were performed for the same 3-month summer period (June 1 – August 31) in 2002, 2004, and 2005. The modeling domain covered the eastern United States (US) and southeastern Canada with a 12 km horizontal grid cell resolution. There were 14 vertical layers with a layer 1 thickness of 40 m. Gilliland et al. (2008) provides details about these model simulations and results of a prototype application of the dynamic evaluation approach involving an assessment of the impact on modeled maximum 8-hour O_3 concentrations in the eastern US due to major point source NO_x emission reductions over these periods.

Meteorological fields were generated by the Penn State/NCAR fifth-generation mesoscale model (MM5v3.6.3) with a four-dimensional data assimilation (FDDA) technique. The CMAQ Meteorology-Chemistry Interface Processor (MCIP v3.1) was exercised to post-process MM5 output into compatible input data sets with hourly 2-D and 3-D meteorological parameter fields for the CMAQ simulations. Specific details about the MM5 simulations are given in Gilliland et al. (2008).

The 3-D emissions were generated by the Sparse Matrix Operator Kernel Emissions (SMOKE v2.2) processing system. Anthropogenic emissions from the EPA 2001 National Emissions Inventory (NEIv3) were used to generate surface and elevated point source emissions with complete details in Gilliland et al. (2008). The MOBILE6 model generated gridded on-road vehicle emissions based on projections of vehicle-miles-traveled (VMT) and fleet factors for a reference county in each state for each summer period. The typical temporal variation in average weekday mobile emissions (Figure 1) shows a rapid early morning ramp up due to increasing traffic with the peak rush period emissions from 7:00-8:00 AM. Figure 1 also indicates mobile NO_x emissions declined between these two summer seasons in this grid cell encompassing Washington, DC. In fact, mobile NO_x emissions in the modeling domain decreased by close to 18% between summers 2002 and 2005 from the MOBILE6 model (Gilliland et al., 2008).

2.2 Measurements

Hourly NO_x measurements at numerous sites in the eastern US were analyzed in this study. Data for different years were obtained from US EPA's Air Quality System data base (http://www.epa.gov/ttn/airs/airsaqs/detaildata/).

3. RESULTS AND DISCUSSION

The hourly average modeled NO_x concentrations in the grid cell covering Washington, DC and at an urban monitoring site in Figure 2 depict the typical temporal variation found at numerous locations with the highest concentrations occurring from 6:00-9:00 AM. Peak concentrations are clearly associated with the highest mobile emissions displayed in Figure 1. The dramatic decrease in modeled and observed NO_x concentrations during the late morning period is primarily attributed to a combination of meteorological processes, (i.e., greater vertical mixing and increasing horizontal transport) associated with the growth of the convective mixing layer and increasing photochemical activity which converts NO_x to other nitrogen products. The temporal pattern of hourly modeled concentrations (Fig. 2a) closely resembles the observed results in Figure 2b indicating CMAQ captures the dynamic and chemical processes governing concentrations during this time period. Modeled and observed results indicate lower NO_x concentrations in summer 2005.

Weekday morning periods from 6:00–9:00 are of particular interest since the high NO_x concentrations are strongly governed by mobile emissions. Observed and modeled 3-hour average NO_x concentrations were computed from hourly concentrations for each weekday. Cumulative frequency distributions (CFDs) of modeled 3-hour NO_x concentrations from an urban grid cell displayed in Figure 3 depict the range in concentrations and the differences between these two summer periods. A notable decrease in NO_x is apparent across a broad range of concentrations which was also evident at other urban locations (not shown). A weekday mean concentration was computed from values over the 50^{th} to 95^{th} percentiles in each CFD to focus on change in the upper portion of the modeled and observed distributions for each urban site. A comparison of modeled results from summer 2002 versus summer 2005 in Figure 4a reveals that, with few exceptions, NO_x in 2005 was lower than in 2002 at sites exhibiting a broad range of NO_x concentration levels. Figure 4b displays similar results from the urban measurement sites. These results are also in agreement with the overall decline reported in 3-hour average morning observed NO_x concentrations in this region spanning a more extended set of years (NESCAUM, 2006). Results based on 34 urban sites reveal the average changes in modeled and observed weekday morning NO_x concentrations between summers 2002 and 2005 were $-16\% \pm 6\%$ and $-15\% \pm 9\%$, respectively, which are close to yet slightly less than the mobile NO_x emissions decline of $-17\%\pm1\%$ generated by the MOBILE6 model at these locations. Although mobile emissions represent a majority ($\approx 70\%$ or more) of NO_x emissions in the urban areas, variations in NO_x emissions from other source categories are also likely impacting the relative change in concentrations.

Disclaimer: Although this work was reviewed by EPA and approved for publication, it may not necessarily reflect official Agency policy.

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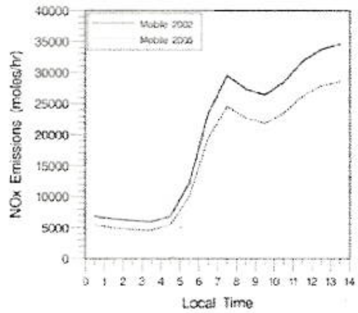

Fig. 1 Modeled mobile NO_x emissions in the grid cell of Washington, DC during summers 2002 and 2005.

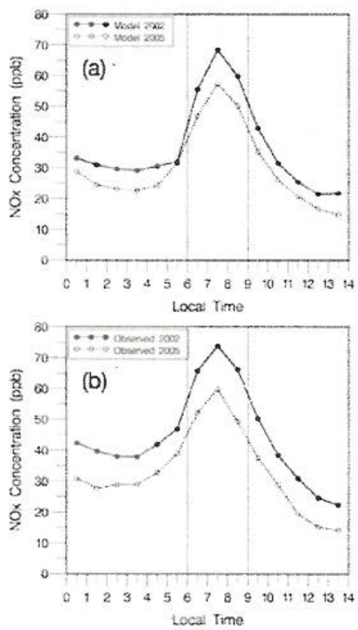

Fig. 2 Temporal variation of a) modeled and b) observed weekday average NO_x concentrations at the same location as in Figure 1.

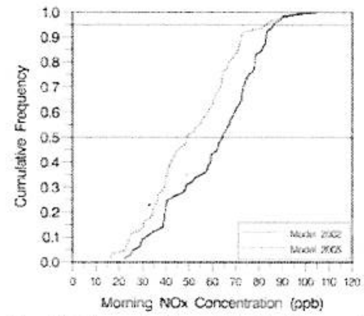

Fig. 3 Cumulative distributions of modeled morning NO_x concentrations from summer 2002 and 2005 in the Washington, DC grid cell.

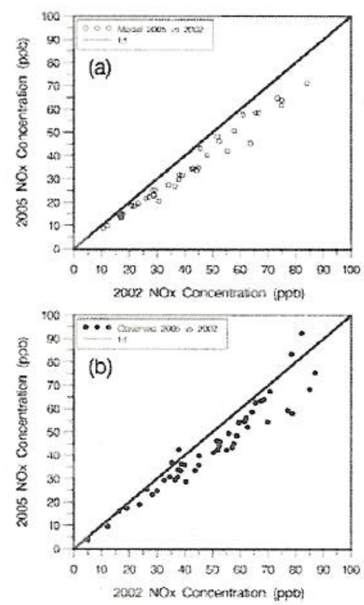

Fig. 4 Results of a) modeled and b) observed mean NO_x concentrations averaged over the 50^{th} to 95^{th} percentiles of CFDs for the summer of 2002 versus 2005.