Evaluation of the CMAQ Model with TexAQS 2006 Upper Air Measurements

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INTRODUCTION

Evaluation studies play a critical role in assessing an air quality model's ability to simulate observed pollutant concentrations. Model evaluations are often limited to comparisons of model results against routine surface network sites. However, high ozone pollution plumes emanating from major urban areas can go undetected due to the sparsity of measurement sites in downwind areas under different meteorological conditions. Additionally, model concentrations aloft cannot be evaluated due to a lack of routine concentrations profile measurements.

Intensive experimental field studies often utilize a variety of platforms that acquire a variety of species concentration measurements at the surface, and more importantly, aloft that can be utilized to provide a more rigorous diagnosis of model performance. In particular, instrumented aircraft sampling flights have the capability to collect observations with high temporal and spatial resolution within and above the planetary boundary layer (PBL) allowing for an examination of pollutant transport and chemistry processes.

Preliminary results from selected case studies are highlighted herein from recent CMAQ simulations in the Houston, TX region during the Texas Air Quality Study (TexAQS) 2006 experimental field campaign. Emphasis is placed on comparisons of CMAQ modeled concentrations against upper air measurements obtained by two research aircraft; the NOAA Twin Otter ozone lidar aircraft and the NOAA WP-3 aircraft instrumented to sample a wide array of species concentrations.

MODEL SIMULATION DETAILS

Simulations with CMAQv4.7.1 and CMAQv5.0 were performed on a 4-km domain (171 x 153 x 34) encompassing the greater Houston metropolitan area and eastern TX, which was nested inside a 12-km large eastern regional domain which supplied boundary conditions. The modeling period was from August 1 through October 15, 2006. Simulations with CMAQv5.0 have only been completed for August.

Meteorological fields were generated by the Weather Research and Forecasting (WRFv3.3) model using four-dimensional data assimilation (FDDA). The base case FDDA approach involved nudging of winds, temperature and moisture above the PBL height with 3-D objective analyses (OA) fields that were modified with routine rawinsonde and wind profiles. Also, surface analyses were applied to nudge the lowest model layers. In the updated FDDA approach, additional upper wind data from several boundary layer profiler sites in the greater Houston area were incorporated into the OA fields and surface nudging was also turned off in this WRF rerun simulation.

Hourly gridded area emissions were obtained from the National Emissions Inventory (NEI 2005) and processed by the SMOKE system. On-road emissions were generated by the MOBILE6 model. The Continuous Emissions Monitoring System (CEMS) data and a special inventory were used to specify point source emissions for the modeling period.

AIRCRAFT SAMPLING FLIGHTS AND DATA

The NOAA Twin Otter research aircraft was equipped with a tunable optical profiler for aerosol and ozone (TOPAZ) differential absorption lidar (DIAL) system. Flights were performed on experimental days from August 1 to September 13, 2006. (Senff et al., 2010)

The flight altitude was at about 3-km AGL with the downward-pointing lidar system and horizontal traverses were performed upwind of the city and at several downwind distances to completely sample the entire urban plume. Ozone profiles were processed at 90 m vertical intervals with a horizontal spacing between profiles of nearly 650 m along each traverse.

The NOAA-WP3 research aircraft was deployed with a variety of instruments to collect fast-response (1-s) measurements of gas species including O_3, CO, NO, NO_2, NO_y, HNO_3, PAN, SO_2, and NO_3. Sampling flights included 10 missions during afternoon periods between September 13 and October 6. (Neuman, et al., 2009)

The flights consisted of horizontal traverses at an altitude near 500 m AGL within the afternoon PBL. Flight traverses were made perpendicular to the wind flow and performed upwind of Houston and at several increasingly greater downwind distances to sample across the entire urban plume and background areas on each side of it.

SELECTED RESULTS OF THE EVALUATION EFFORT

OBSERVED PBL-AVERAGE OZONE

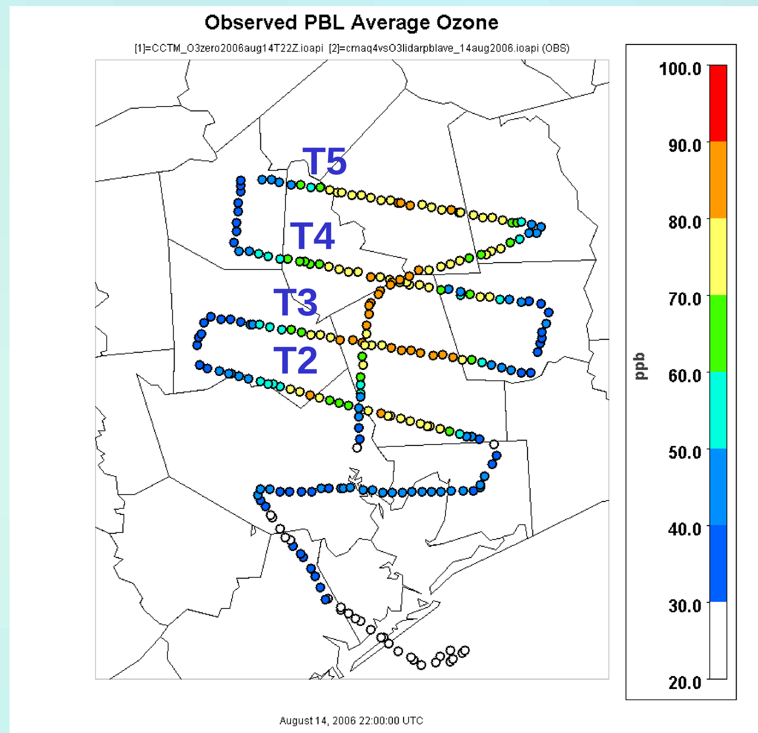

Figure 1. Results of vertically-averaging the high-resolution ozone lidar profile measurements over the PBL within the aircraft traverses during the afternoon of August 14, 2006 in the Houston, TX urban area. Downwind traverses are denoted by T2-T5 and spanned downwind distances from 30 to 115 km and occurred from 1547-1900 local time. Sampling was not done in a Lagrangian mode.

VERTICAL OZONE CROSS-SECTIONS ALONG TRAVERSE 3

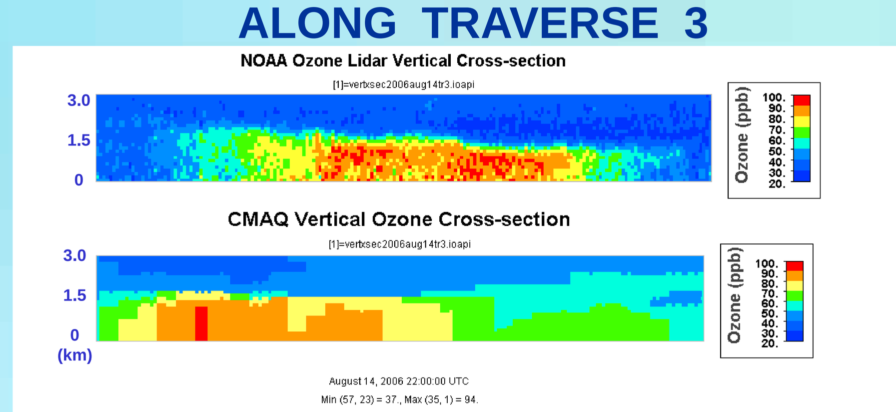

Figure 3. Observed (top) and CMAQv4.7.1 with WRF/base FDDA model results (bottom) along traverse 3 (see Fig. 1) on the afternoon of August 14.

MODELED PBL-AVERAGE OZONE CONCENTRATIONS

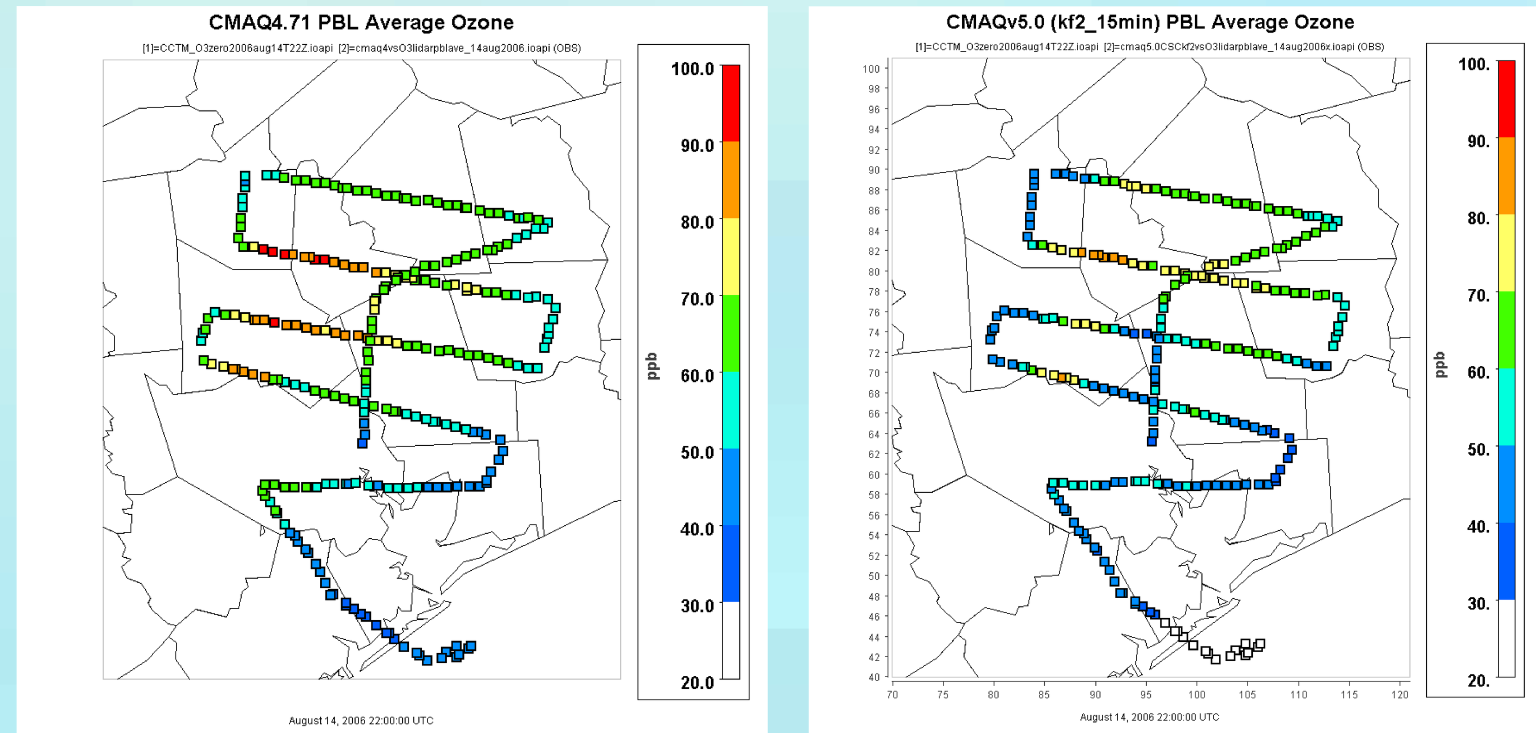

Figure 2. CMAQv4.71 (left) and CMAQv5.0 (right) O_3 concentrations vertically-averaged over the PBL corresponding in time and space to the observed flight pattern in Figure 1.

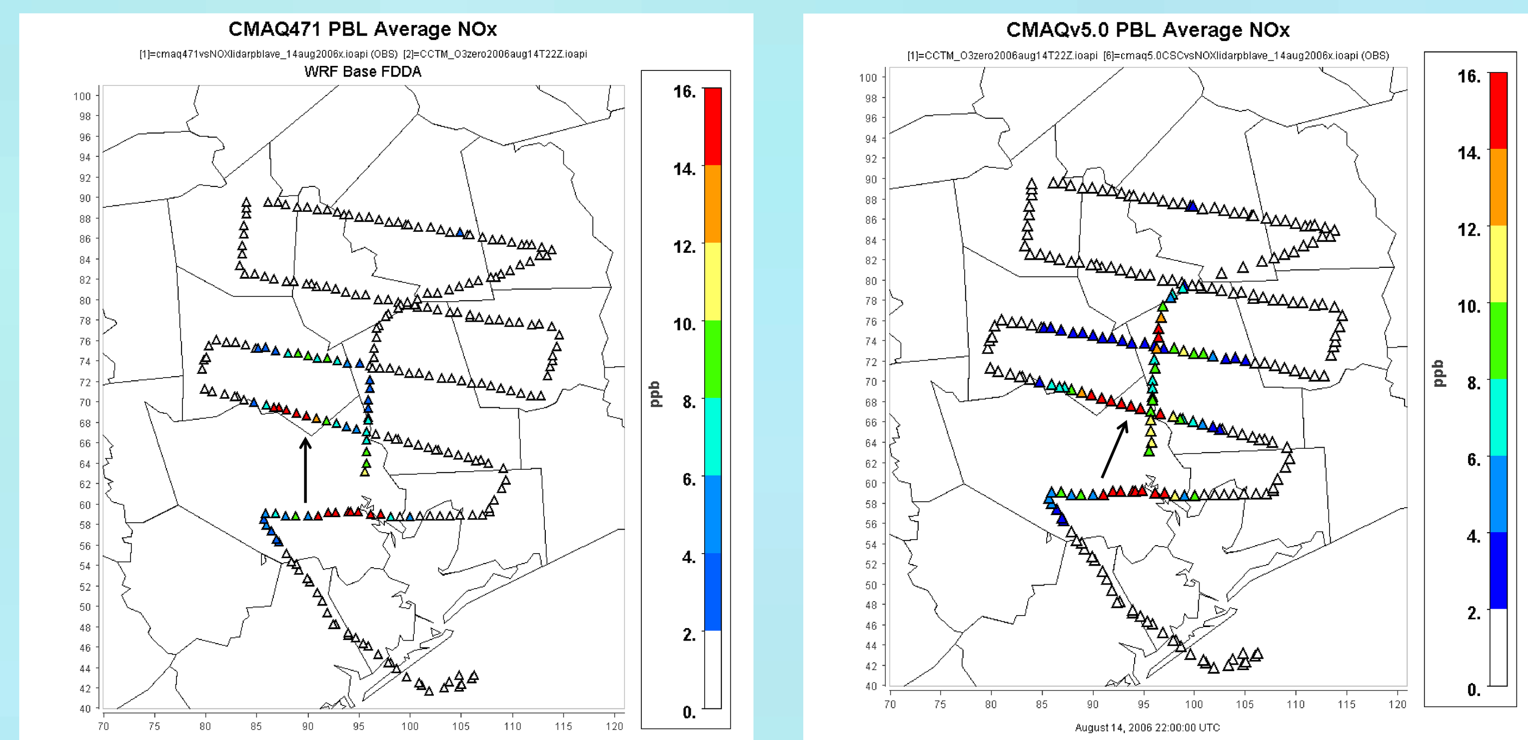

Figure 4. Modeled NO_X concentrations from CMAQv4.71 (left) and CMAQv5.0 (right) vertically-averaged over the PBL along the same flight pattern as modeled ozone in Figure 2 above with the wind flow depicted by the arrow in each simulation.

► CMAQv4.7.1 driven by WRF/base FDDA meteorology appears to transport the ozone plume to the left of the observed plume and background values are overestimated (see Fig. 2, 3)

► CMAQv5.0 results using WRF/updated FDDA meteorology (see R. Gilliam presentation) reveals a closer match to the urban plume position, however, there is considerable ozone titration (Fig. 2) due to the relatively high NO_X concentrations that depressed ozone formation (Fig. 4)

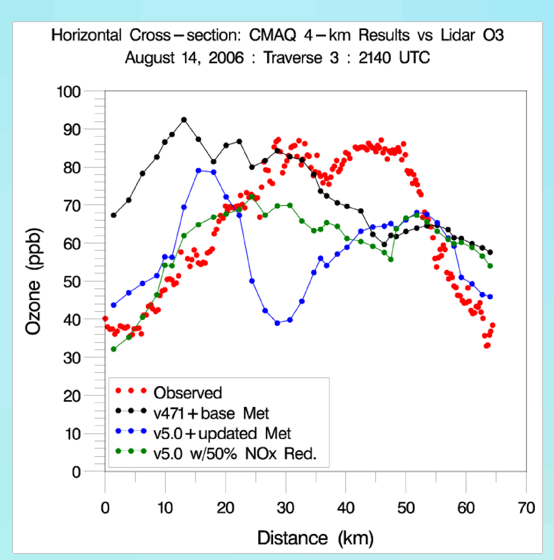

Figure 5. Observed (red) and modeled PBL-averaged ozone concentrations with distance from West to East along traverse T3 (see Fig. 1, 2) during afternoon of August 14.

► The observed ozone plume (red) is a combination of urban and adjacent Ship Channel emission sources with the excess ozone about 40 ppb above surrounding background levels in this case.

► CMAQv5.0 with the updated WRF/FDDA (blue) reveals the impact of substantial titration of O_3 due to the high NO_X evident in Figure 3, however, this feature occurs where the observed high O_3 exists indicating more accurate transport of the urban emissions downwind

► CMAQv4.7.1 results (black) with WRF/base FDDA exhibit a noticeable spatial displacement as is evident in Figure 2 and observed background values are overestimated compared to the CMAQv5.0 results in this case.

► The CMAQv5.0 results from a 50% NO_X emissions reduction simulation (green) display an ozone recovery and magnitudes are beginning to approach observations.

COMPARISONS OF CMAQ VS NOAA-WP3 DATA ALOFT

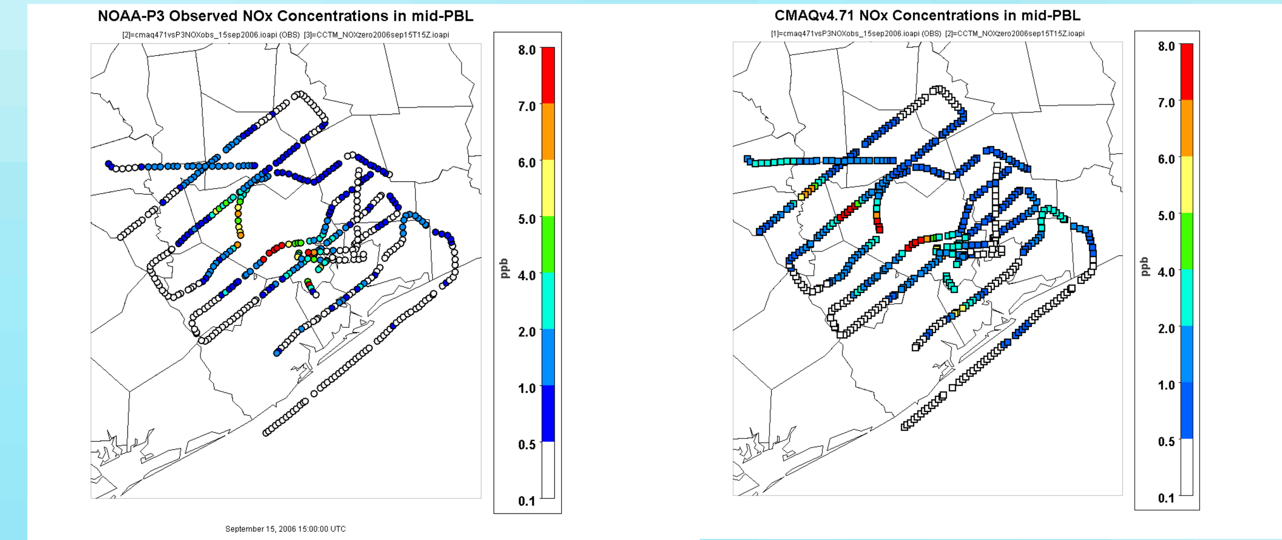

Figure 6. Observed (left) and modeled (right) NO_X concentrations during the afternoon of September 15, 2006 are depicted along the horizontal traverses by the WP3 aircraft at a single altitude of ≈ 500 m AGL over the Houston area.

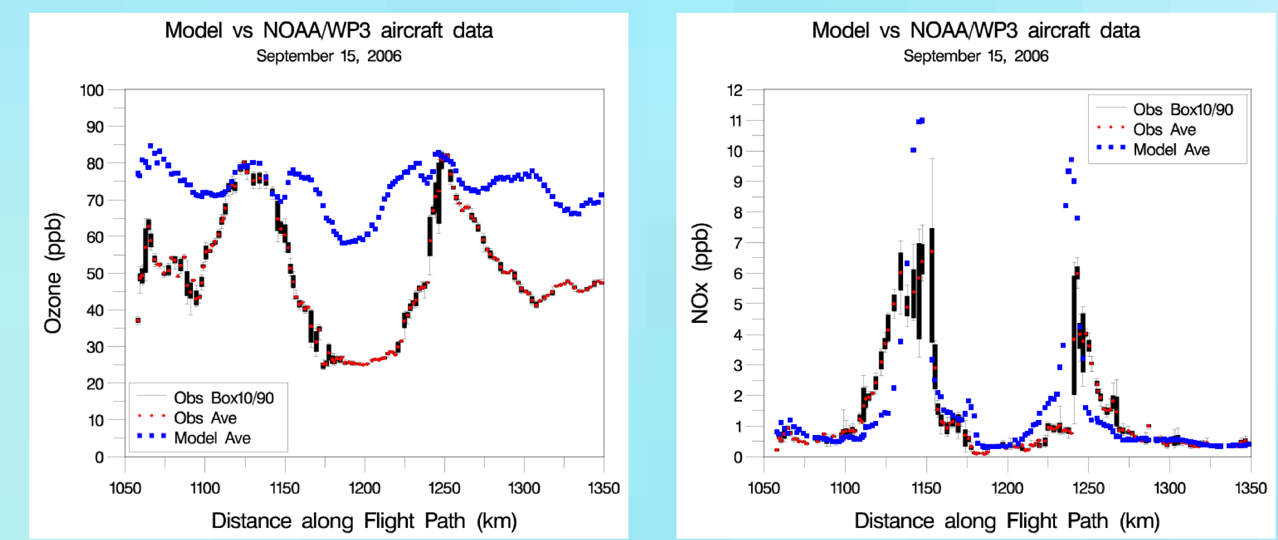

Figure 7. Modeled (CMAQv4.7.1) and observed O_3 (left) and NO_X (right) along two horizontal traverses crossing the urban plume downwind of Houston during the afternoon of September 15, 2006.

► Results of these comparisons between CMAQv4.7.1 concentrations and the WP3 aircraft data, albeit for another case study day from this field experiment, reveal that modeled NO_X concentrations overestimated observed values in the urban plume portions of the horizontal traverses in Figure 7, which is also in agreement with the results found at the surface displayed in G. Sarwar's poster. Some spatial displacement is also evident along the last downwind traverse to the NW of Houston (Figure 6).

► Although ozone concentrations in the model and observations are in close agreement within the urban plume at this time, modeled background values show large overestimates of observed values. CMAQv5.0 runs for the September/October period are pending.

SUMMARY AND PLANS

► Measurements from both research aircraft provide considerable information on the dimensions and concentrations of the ozone plume downwind of Houston and surrounding background values for use in comparisons with CMAQ modeled concentrations on numerous case study days under different flow conditions which cannot be captured from the surface monitoring site network.

► Preliminary results presented here indicate the WRF/updated FDDA meteorology provides more accurate transport of the urban plume. However, modeled O_3 in the near-downwind urban plume was greatly underestimated owing to overestimated modeled NO_X concentrations which may be attributable to overestimated NO_X emissions in the Houston urban area. Additional model runs are planned with CMAQv5.0 for the entire TexAQS 2006 period with evaluation against the full set of aircraft measurements.

REFERENCES

Neuman, et al., 2009: Relationship between photochemical ozone production and NOX oxidation in Houston, Texas. J. of Geophy. Res. (Atmospheres), 114, D00F08, doi:10.1029/2008JD011688.

Senff, C., et al., 2010: Airborne lidar measurements of ozone flux downwind of Houston and Dallas. J. of Geophy. Res. (Atmospheres), 115, D20307, doi:10.1029/2009JD013689.