Evaluation of CMAQ Results for the Simulation of a High Ozone Episode in the Houston-Galveston-Brazoria Metropolitan Area

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1. INTRODUCTION

Under the Clean Air Act, the Houston-Galveston-Brazoria (HGB) area and several other metropolitan regions in the US are classified as ozone non-attainment areas. These regions must reduce their ozone levels within the next 3 to 5 years through an effective State Implementation Plan (SIP) to comply with EPA standards or they will be penalized with a loss of federal funding and other punitive measures.

Ozone problem is exacerbated when precursor emissions are sent out to the Galveston Bay and Gulf of Mexico by the land breeze in the morning then returned by the sea breeze in the afternoon. To minimize the occurrence of such high ozone events, emissions of volatile organic compounds (VOC) and NO_x (sum of NO and NO_2) from point, mobile and area sources may need to be reduced. Recently, Texas Commission on Environmental Quality (TCEQ) has established a set of input meteorological and emissions data to perform air quality simulations for developing efficient emissions control measures using CAMx model (Environ, 2002) as part of its SIP preparation.

To understand the basic science processes involved in the high ozone events in the HGB area and to provide an independent and objective assessment of the SIP related air quality modeling, the University of Houston (UofH) has been utilizing EPA's Community Multiscale Air Quality (CMAQ) model (Byun and Ching, 1999). The science contents of the two models are similar, but the way inputs are prepared and details of the model implementation are distinctively different. Even with similar inputs, the results from each model are sometimes quite different while at other times close to each other.

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There are several reasons why results of the two models differ. A powerful method to improve our understanding of the atmospheric processes and to help make correct decisions on improving air quality is evaluation of results gained from different modeling systems and compare them against available comprehensive observations. Therefore, one of the main objectives of the present study is to evaluate performance of the CMAQ modeling system to provide an alternative methods for the SIP attainment demonstration modeling in the future. The second objective of the study is to assess if the input dataset prepared for CAMx produces similar air quality simulation results with the CMAQ. To shed light on the factors which make the results different, model simulation results for the Texas Air Quality Study 2000 high ozone episode are compared with the surface and aircraft measurements. In particular, the focus of analysis is to study the multi-species inter-relations to understand the involved physical and chemical processes.

2. TEXAQS 2000 EPISODE

TCEQ, the scientific, environmental, and business community participated in the Texas Air Quality Study during the summer of 2000 (herein called TexAQS 2000) in the Houston-Galveston area to study O_3. Comprehensive datasets were developed from this field program from three radiosonde launch sites, six wind profilers, a Doppler lidar, four instrumented aircraft, and augmented surface measurements. A number of high ozone concentrations occurred between the study period of August 15 and September 15, providing several case studies to develop tentative findings. TexAQS 2000 investigated the causes of rapid O_3 formation and high O_3 concentration events, atmospheric dynamics' influence on these events, the transport of O_3, and the development of air quality modeling capabilities. TexAQS 2000 found that air parcels with very high O_3 had back trajectories from industrial regions. Moreover, the air parcels had chemical compositions representative of industrial sources along the Ship Channel and western shore of Galveston Bay rather than urban areas. This indicates that ozone production in the industrial regions can be very efficient, ranging between 50 ppb/hr and 150 ppb/hr, due to high concentrations of reactive hydrocarbons in the presence of nitrogen oxides (NO_X) (Kleinman et al. 2002). These ozone production rates are higher than most U.S. urban regions, which are almost always less than 40 ppb/hr.

The TexAQS 2000 episode had numerous exceedence days (daily maximum ozone concentration greater than 125 ppb) in the HGB area during the eight-day period, including a period of low ozone in the middle. The episode includes 5 days with the veering wind vectors currently associated with flow reversal and high ozone. Light easterly winds resulted in a maximum ozone concentration at Crawford near the center of the Houston area on August 25th and southeasterly winds carried the maximum level of ozone out of Houston to Conroe (about 40 miles north of Houston) on August 26th. August 27th and 28th were the two low ozone days, with stronger southeasterly sea breeze winds resulting in substantially lower ozone in the HGB by transporting the diluted urban plume to Conroe. August 29, 30, and 31 showed light westerly morning winds followed by afternoon sea breezes which put the ozone pool on the east side of the city at Mt. Belview, La Porte and Deer Park, reflecting the maximum value in that area. A relatively persistent westerly land breeze carried the maximum level of ozone to the Baytown monitor and points further east on September 1st.

3. MODEL INPUT DATA

Probably, one of the most important findings of the TexAQS 2000 was the reported emissions of light olefins were not consistent with measured atmospheric concentrations. Therefore, key model inputs have been modified substantially to improve CAMx model simulations of high ozone events for the purpose of establishing the base case simulation for the HGB area SIP preparation. They are such as modification of the alkene (ethylene, propylene, 1,3 butadiene, and all butenes) emissions for selective stacks in the HGB area and, probably less important, reduction of the heights of Planetary Boundary Layer (PBL) replacing the base simulation results of the Mesoscale Model Version 5 (MM5). In support of the TCEQ's SIP modeling studies, Dr. John Nielsen-Gammon of Texas A&M University (TAMU) simulated the NCAR/Penn State (National Center for Atmospheric Research/the Pennsylvania State University) Mesoscale Model, Version 5, Release 3.6 (MM5V3.6) for HGA. The MM5 simulation results currently used in the HGA SIP modeling utilized the GOES-satellite skin temperature assimilation technique developed by Dr. McNider of University of Alabama Huntsville. The vertical structure used in the MM5 simulation extended from the surface to the 5000 Pa with 43 sigma levels the frontal circulations. The first layer had a vertical thickness of approximately 34 meters.

The initial and boundary conditions for the MM5 simulation were obtained from three-hourly EDAS analyses, available from NCAR. Sea surface temperature information was extracted from the surface temperatures of the EDAS analyses. The data is available through TCEQ and Texas A&M and details of the model physics options used can be found in Nielsen-Gammon (2001, and 2002). We have used this data as the base meteorological inputs for anthropogenic emissions processing and air quality modeling to provide wind, moisture, and temperature fields, as well as parameters determining atmospheric mixing and deposition characteristics, required.

The TCEQ's emission inventories used for the HGB SIP modeling are prepared in a data format suitable to be processed through the EPS2 (Emissions Preprocessing System Version 2) system. The emissions data are used with the CAMx air quality model to assess the efficacy of the emissions control strategies in the HGB (TCEQ, 2002). While the system has proven its capability providing necessary emissions input for CAMx operated by TCEQ, external organizations or university researchers have been unable to test emissions scenarios. UofH has developed additional processing tools to generate necessary model-ready emissions data for CMAQ (Kim and Byun, 2003).

4. CMAQ SIMULATION RESULTS

CMAQ was set up at 23 vertical layers, which followed the MM5 vertical structure exactly from ground to 1-km, then two or three layers were collapsed. For simulating atmospheric turbulence transport, resolution-dependent horizontal diffusivity and the PBL similarity theory based vertical eddy diffusivity algorithms were used.

Piecewise parabolic methods were used for both horizontal and vertical advection and the CMAQ standard mass adjustment algorithm was applied. Carbon-Bond4 chemical mechanism was used for the gas-phase chemistry. Initial and boundary conditions were provided by the 36- and 12-km resolution regional domain model simulations a few days ahead of the 4-km simulations, which was used for the model evaluation for the August 23-31, 2000 episode.

4.1 Comparison with CAMS measurements

Figure 1 compares CMAQ simulation results with the surface measurements at the Continuous Air Monitoring Stations (CAMS) for the August 23-31st period. Model simulations were quite reasonable except that some peak ozone concentrations were not adequately simulated.

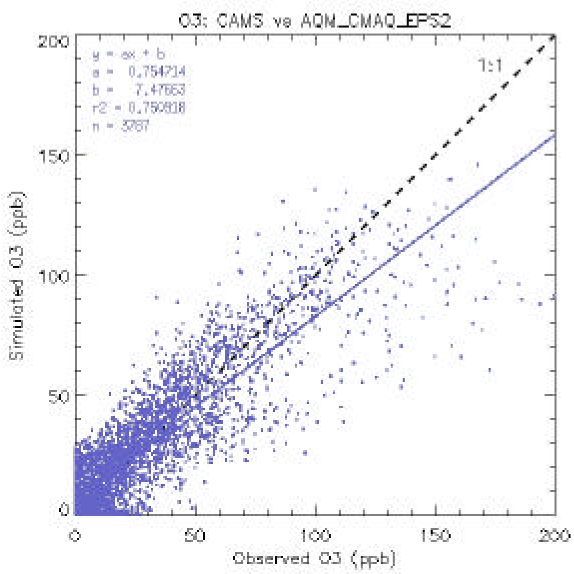

Figure 1. Comparison of CMAQ simulation with surface ozone measurements at CAMS sites.

4.2 Comparison with aircraft measurements

Simulation results were also compared with the NOAA aircraft continuous measurements (Figures 2a-c). Similar to the surface data comparison, CMAQ somewhat under-predicted the peak ozone concentrations. However, CO and NOy compared relatively well with observation. Accompanying studies on the effects of model resolution and of chemical mechanism show that higher ozone concentrations can be achieved either by the use of SAPRC-99 chemical mechanism and higher (say, 1-km) model resolution (Byun et al., 2004, Czader and Byun, 2004). Comparison with the predicted olefin species with the auto GC measurements at the La Porte and Clinton sites showed that the olefin emissions of the input inventory might not have adequate vertical distributions--too high at the surface and too low at higher altitudes where aircraft measurements were taken.

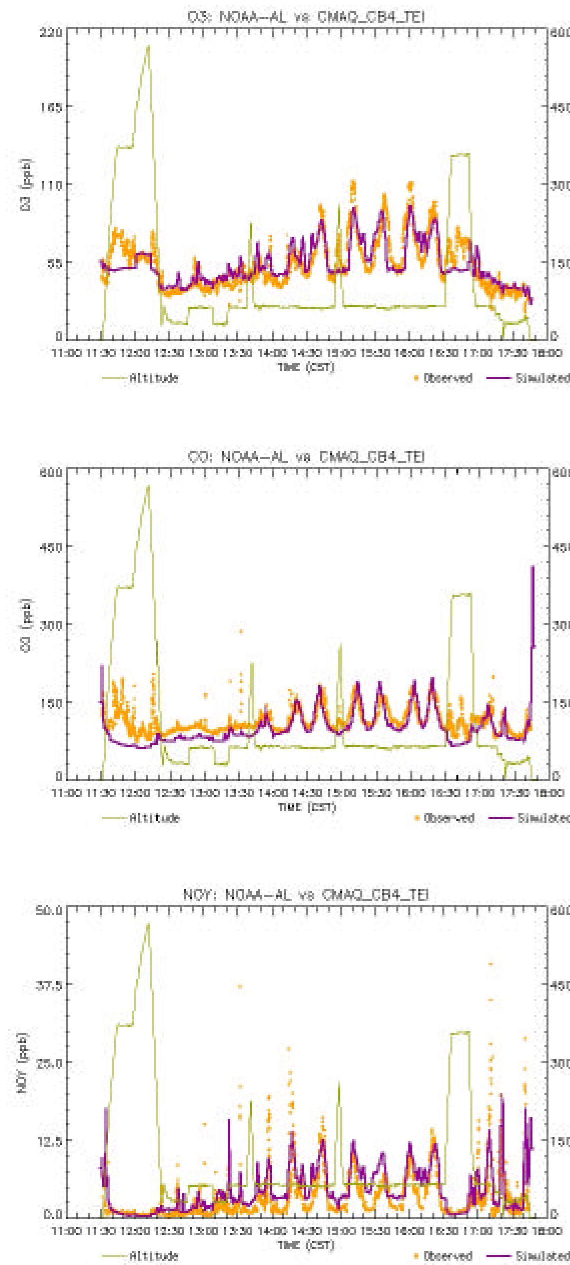

Figure 2. Comparison of CMAQ results for (a) O3, (b) CO, and (c) NOy with NOAA aircraft measurements. Thin lines show aircraft altitudes, observations are orange dots and CMAQ simulation results are blue solid lines.

5. DISCUSSIONS

Performance of a comprehensive air quality model is mostly determined by the accuracy of model formulations, choice of proper model configurations, and validity of the model input data. Utilization of the CAMx model inputs for the CMAQ simulation provided an opportunity to study the validity of the emissions and meteorological inputs used in the Houston SIP modeling.

Based on the present study and other analyses performed by the authors, we present the following hypotheses, which must be verified further sensitivity studies:
(1) Comparison of the precursor species with surface and aircraft data suggests that vertical mixing process in CMAQ seems quite adequate
(2) Problem of lower predicted peak ozone concentrations may be mitigated if the "imputed" olefin emissions are adequately distributed vertically
(3) Application of high vertical and horizontal resolution may improve the ozone productivity caused by the fast reacting olefin species.

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