PROJECT SUMMARY: Retrospective Simulations of TexAQS II-2006 Pollution Events

Meteorological and air quality simulations of the intensive experimental period of the Second Texas Air Quality Study (TexAQS-II) in summer 2006 were conducted with the goal of improving our understanding of the processes associated with formation and transport of ozone and regional haze in East Texas.

The research conducted under the present project was built upon the previous air quality modeling studies by the University of Houston, such as (1) the 2006 air quality forecasting (AQF) project for TexAQS-II, (2) multiple MM5/FDDA simulations to improve meteorological inputs for air quality modeling, and (3) corresponding CMAQ simulations to test performance of the assimilated MM5 inputs. To improve emission inputs, we processed the updated 2006 Texas point-source special inventories to generate the "best-effort model ready" (BEMR) emissions. We performed CMAQ simulations with these meteorological and emissions inputs. The results were compared with CMAQ simulations with the base AQF emissions and also with CAMS surface measurements. Moreover, source attribution analysis was performed with CMAQ/HDDM to identify contributions of different components to regional and local ozone concentrations.

The assimilated meteorological inputs have significantly improved air quality simulations. The CMAQ re-simulations with the MM5/FDDA inputs better predict locations and magnitudes of peak ozone than those with the AQF meteorology inputs. CMAQ simulations with AQF emissions and MM5/FDDA meteorological inputs compare well with observations, although the regional averages show some overprediction of ozone during the morning hours. There were large contributions of ozone and its precursors transported from boundaries with southerly flows, which led to some overpredictions of regional ozone.

The 2006 Texas BEMR emissions inputs were prepared by utilizing currently available emissions inventories, projected emissions components such as mobile emissions, and the Texas point-source special inventories for the summer 2006 (TSPI2006) TexAQS II period. We worked with Alpine Geophysics (AG) to prepare the 2006 inventories in the AFS data format for processing with SMOKE. TCEQ provided AG sets of speciated and aggregated point source VOC emission inventories reported during the TexAQS-II intensive period (August 15–September 15, 2006). The 2006 raw inventories provided by TCEQ had many idiosyncratic features that must be carefully handled, such as mapping the TCEQ contaminants to the specific SARAOD codes. Major changes for the BEMR emissions inputs are; 1) use of the 2006 Texas point-source special inventory (TPSI2006) for point sources, 2) use of TCEQ's new biogenic emissions, and 3) replacement of NEI99 with NEI2002.

Daily VOC emission rates from the special inventory range from 40 to 50 tons/day. The total point source VOC emission amount is around 210 tons/day for the HGB 8 counties, which is similar to the 2000 Base5b regular inventory (~230 tons/day). The 2006 special inventory includes around 35 tons/day of speciated VOC emissions, while the Texas ozone-season day

(OSD) emissions, which apply to point sources outside the special inventory, include about 165 tons/day of VOC emissions. In addition to incorporating the 2006 point source special inventory, the updated mobile emissions were projected to 2005 (whereas the base MOBILE6 emissions were projected to 2003), resulting in reductions of NOx and CO emissions. Olefin and ethylene emissions in the updated TPSI 2006 emissions are about one third of those in the base emissions. Note that additional VOC emissions used for the imputation in the base emissions is ~170 tons/day, while no imputation was applied to the updated TPSI2006 emissions. Similar to NO emissions, the updated formaldehyde emissions are reduced by ~15% compared to the base emissions. The new biogenic inventory shows a reduction of isoprene emissions over the northern part of the domain.

We have compared the simulation results of CMAQ with TPSI2006 and those with the base AQF emissions. The regional average NO and NO2 time series plots show a general underprediction (overprediction) of NO (NO2) for the nighttime and early morning hours. These biases are expected because the thickness of the model bottom layer is not fine enough to resolve the rapid titration reaction of O3 with emitted NO forming NO2 at nighttime. Because of the wide range of changes in the NO and NO2 concentrations, it is difficult to relate the model-observation bias to specific meteorological events. Considering the daytime values, NOx concentrations predicted by CMAQ with TPSI2006 seem closer to the observations than those predicted with the base AQF emissions. CMAQ simulations with base and updated emission inputs produce comparable general patterns of hourly ozone distributions. But the base emissions predict higher ozone concentrations during the daytime than the updated emissions, possibly due to the additional VOC from the imputation. When compared with the measurements at the University of Houston Moody Tower, CMAQ with the base emissions significantly over-predicted olefin and ethylene concentrations, while simulation with the updated BEMR/TPSI2006 emissions showed smaller biases.

These analyses suggest that the updated TPSI2006 inventories represent the 2006 conditions better than the base AQF emissions, although emissions of highly reactive species for upset events may need to be added. CMAQ-HDDM simulations with the base AQF emissions show higher contributions of anthropogenic VOC emissions to ozone than those with the updated TPSI2006 emissions. Reduced contributions of point source VOCs in the updated emissions, as well as reduced NOx from mobile emissions, led to a decrease in simulated ozone. More detailed studies comparing air quality simulation results with the CAMS data and other special air quality measurements available during the TexAQS-II period will be necessary to verify the TPSI2006 emissions data.