

## 1. Executive Summary

This document is University of Houston's Final Report in accomplishment for the Houston Advance Center/Texas Environmental Research Consortium (TERC) Contract Number H98, "Air Quality Modeling of TexAQS-II Episodes with Data Assimilation." This is an omnibus modeling project involving various institutions. The prime goal of the project is to synthesize key observational findings of the 2006 Texas Air Quality Study-II (TexAQS-II) experiment through enhanced air quality modeling studies with intense meteorological and chemical data assimilations. The objectives of the research are: (1) to improve model inputs affecting air pollution chemistry using satellite-derived quantities, such as cloudiness and sea-surface temperature, in addition to various surface and upper meteorological observations and updated emissions inventories; (2) to synthesize and analyze meteorological and chemical data from various observations including Continuous Air Monitoring Stations (CAMS) the University of Houston Moody Tower and other in-situ and remote-sensing measurements through model sensitivity studies; (3) to assess uncertainties in model inputs for emissions of selected air pollutants and model boundary conditions through four dimensional variational (4D-VAR) chemical data assimilation; (4) to provide continued ozone forecasting for the Houston and Dallas ozone nonattainment areas; and (5) to implement a surface HONO chemistry module in Community Multiscale Air Quality (CMAQ) regional air quality model.

The one overarching hypothesis of this research is that we can enhance air quality simulation capabilities through the improvement of basic databases across the modeling systems. Retrospective meteorological simulations with the Penn State/National Center for Atmospheric Research Mesoscale Model v. 5 (MM5) can be improved by the utilization of accurate and high-resolution databases such as land-use/land-cover and subsoil classification data, and the remaining biases can be considerably reduced through data assimilation of satellite observations (clouds and SST) together with Meteorological Assimilation Data Ingest System (MADIS) and CAMS surface and upper air observations. Application of CMAQ/4D-VAR using comprehensive chemistry measurement datasets with consistent meteorological inputs will reduce uncertainties in the emissions inputs and initial and boundary conditions for different meteorological conditions. Continued forecast modeling of Houston and Dallas air quality for 2008/2009 will help to verify findings of the TexAQS studies, enhance conceptual models, and assist other TERC-supported field studies.

H98 is organized along 5 individual project tasks: Main results of these tasks are listed below:

Task 1: Development of improved air quality model inputs with satellite and in-situ measurements.

- High resolution satellite observation-based land use/land cover (LULC) data for the Southeastern Texas area produced by the University of Texas Center for Space Research (UT-CSR) was converted to fit with the land use categories used in the MM5.
- two additional clay sub-soil types were introduced to account for the different "dampness" of clay soil in the river and lake basins.
- A method was developed to estimate sea surface temperature (SST) by reconstructed daily SST from monthly data and adjustment of observed SSTs from GOES satellite data.
- The updated land surface inputs and satellite-based SST were applied to MM5 simulation at 12-km resolution. The high bias of the surface temperature is reduced due to more accurate land surface inputs used in the MM5 model. Also, spatial distribution of PBL heights was affected.
- A retrospective meteorological simulation for TexAQS-II period utilizing the MM5 model showed improvements in modeling surface temperature, relative humidity, and wind flows. Still problems are associated with precipitation events.
- Gridded emissions were derived with SMOKE using NEI2002 and Texas inventory, as well as

Texas 2006 special emissions inventories.

- Apart from NH<sub>3</sub>, the values for NEI2002 are mostly lower than the corresponding values for NEI1999. This trend is generally true for each source category except for NO<sub>x</sub> in the area and nonroad mobile category as well as for PM10-PRI in the area category.
- CMAQ simulations showed that fire emissions caused a significant increase in PM2.5 and CO concentrations close to the fire locations, while ozone concentrations were only a little enhanced.
- For the area emission source, the Lamar-processed NEI2002 values are in general close to EPA-released values with CENRAP values being substantially lower, especially for CO, NH<sub>3</sub>, PM10-PRI and PM25-PRI. For the nonroad mobile source, the three EIs are similar with the EPA-released NEI2002 being slightly higher for most species especially NO<sub>x</sub>. For the point emission source, the three EIs show similar values with the CENRAP values being slightly higher, especially for NH<sub>3</sub>, PM10-PRI, and PM25-PRI.
- CMAQ-HDDM simulations showed that first-order responses of daytime ozone to NO<sub>x</sub> are typically positive in downwind regions, but are negative in the core region of the HGB area. Ozone responses to VOC emissions have a smaller spatial extent, but are important to ozone formation in key portions of the HGB region where ozone concentrations are high. Daytime ozone in Brazoria and Galveston Counties is most sensitive to HGB Point NO<sub>x</sub> and domain-wide biogenic VOC emissions, and daytime ozone in Harris County is most sensitive to HGB Area and mobile NO<sub>x</sub> and domain-wide biogenic VOC emissions.
- MM5 using the Grell cumulus scheme tends to simulate more clouds than the Kain-Fritsch scheme.
- CMAQ running with MCIP which adjusted by satellite cloud information yields ozone results which match better the observations than CMAQ with the original MCIP which uses cloud information based on MM5 simulations.

Task 2: Synthesis datasets for chemical data assimilation.

- Lateral boundary conditions were generated from the results of global model RAQMS with satellite data assimilations. Comparisons with observational data showed the benefits of using fully assimilated RAQMS LBCs to improve regional CMAQ air quality simulations.
- Compared with the 2006 air quality forecasting (AQF) simulations for the TexAQS-II, MM5 with multiscale data assimilation of high-density surface observations improved the prediction of locations and magnitudes of peak ozone for those days that had noticeable large scale flow biases, but not for days with difficulties in simulating precipitation and high cloud areas correctly.
- CMAQ with “best-effort model-ready” (BEMR) emissions simulates lower ozone days better, but is worse when simulating peak ozone events.
- The results of adjusted BEMR emissions show that an increase of emissions resulted in higher ozone concentration which were closer to the observations.

Task 3: Assessment of model input uncertainties with 4D-VAR chemical data assimilation.

- A new CMAQ(v4.5)/4D-Var system has been implemented. It includes CB4 and SAPRC99 chemical mechanisms. Control variables for the optimization include initial conditions, boundary conditions and boundary scaling factors, and emissions and emission scaling factors. The system runs in parallel.
- The “factor of 2” problem has been explained and resolved. The “factor of 2” problem refers to the fact that, in some point to point comparisons, sensitivities obtained by adjoint approach are almost twice as large as the sensitivities obtained by the finite difference approach. The differences appear due to the nonlinearity of the PPM method used to solve advection. As part

of the solution we have developed discrete advection adjoints for both the horizontal and vertical advection processes. These adjoints have been carefully tested in both sensitivity analysis and 4D-Var data assimilation setting.

- To validate the new CMAQ/ADJ system data assimilation tests have been carried out for a chosen domain that covers Texas, and for the period Aug 30-Sept 1 2006. Assimilation of initial ozone conditions greatly improves the agreement between model predictions and observations. The assimilation of boundary scaling factors helps the predictions to a lesser degree.

#### Task 4: Air quality forecasting of Houston and Dallas metropolitan areas

- The UH-IMAQS AQF system has been operated since 2005 with daily operation of two-day air quality simulations. The operation was successful throughout the year of 2009 except for some technical problems in F2 during October.
- The CAMS observations in the HGA show that high 8-hour ozone events are slightly reduced in 2008 and 2009. Model results show similar patterns, but with a high bias. The reason for the change in high ozone frequencies is still unknown and would require further analysis.
- When separating the HGA and DFW regions, ozone fluctuation is much higher in the HGA, most likely due to higher variability in emissions and meteorology found in the HGA.

#### Task 5: Development of surface HONO heterogeneous chemistry parameterization in CMAQ

- CMAQ (v4.7) with SAPRC99 chemical mechanism was used to simulate heterogeneous formation of HONO on different surfaces. Emissions of HONO from mobile sources and several additional variables were derived to simulate HONO heterogeneous formation.
- The highest HONO production occurred in the areas with high NO<sub>x</sub> emissions. The predicted HONO mixing ratios are close to the observed values with maxima reaching 2 ppb.
- The most significant contribution to HONO mixing ratios comes from its formation on urban and leaves surfaces, HONO emissions and formation on particles only slightly increase its concentration. Heterogeneous HONO production and accumulation during nighttime accelerates morning ozone formation with a maximum increase of 4 ppb. The addition of soil as a surface for heterogeneous reaction resulted in only a slight increase of HONO mixing ratio (up to 0.5 ppb) but with little effect on ozone.