

HARC Project H87 Final Report

Retrospective Simulations of TexAQS II-2006 Pollution Events

Investigators:

Daewon Byun (PI)
Soontae Kim, Hyun-Cheol Kim, Fong Ngan, Beata Czader,
Xiangshang Li, In-Bo Oh, Dae-Gyun Lee, Fang-Yi Cheng, and Peter Percell

Institution:

University of Houston

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 NO_x 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, NO_x 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 NO_x 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.

LIST OF CONTENT

Project Summary.....ii

1. INTRODUCTION..... 1

2. SUMMARY OF AIR QUALITY FORECASTING RESULTS FOR THE SECOND TEXAS AIR QUALITY STUDY (TEXAQS-II)..... 1

3. SUMMARY OF ASSIMILATED MM5 SIMULATIONS 4

4. IMPROVEMENT OF CMAQ SIMULATION RESULTS WITH ASSIMILATED MM5 RESULTS..... 9

5. UPDATED 2006 SUMMER EMISSIONS INVENTORIES FOR AIR QUALITY SIMULATIONS 16

 5.1 THE 2006 TEXAS POINT SOURCE SPECIAL INVENTORY (TPSI2006) 17

 5.2 TCEQ BIOGENIC EMISSIONS..... 20

 5.3 COMPARISON OF THE BASE AQF AND UPDATED EMISSIONS..... 21

6. AIR QUALITY SIMULATIONS WITH UPDATED EMISSIONS INVENTORIES 25

7. CMAQ AND HDDM SIMULATIONS WITH THE BASE AND UPDATED EMISSIONS..... 29

8. CONCLUDING REMARKS..... 34

9. REFERENCES..... 37

1. Introduction

The initial objectives of this project were first to perform air quality simulations of 2006 Second Texas Air Quality Study (TexAQS-II) air pollution events, and second to attribute high ozone observed during these events to specific sources. During the TexAQS-II study period, University of Houston (UH) Institute for Multidimensional Air Quality Studies (IMAQS) operated air quality forecasting systems to support experimental planning. After identifying some shortcomings of the forecast simulations, new meteorological and emissions input data for air quality modeling were prepared. Using these inputs, Community Multiscale Air Quality (CMAQ) (Byun and Ching, 1999; Byun and Schere, 2006) model simulations for 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.

In this report we document the results of the research tasks that have been performed to achieve the project objectives. They include: (1) 2006 air quality forecasting (AQF) results for TexAQS-II, (2) assimilated MM5 simulation results for August 16-September 15, 2006, (3) CMAQ simulation results with the assimilated MM5 inputs, (4) processing of the 2006 updated special Texas point-source inventories, (5) comparison of CMAQ simulation results with the AQF and 2006 updated special emission inventories, and finally, (6) source attribution analysis results from the CMAQ/HDDM (High-order Direct Decoupled Model) (Cohan et al., 2005) method with both AQF and TPSI2006 emission inputs.

2. Summary of Air Quality Forecasting Results for the Second Texas Air Quality Study (TexAQS-II)

This section summarizes performance of the two air quality forecasting systems operated by the University of Houston IMAQS. Two East Texas Air Quality (ETAQ) forecasting systems, ETAQ F1 and F2, were made during the TexAQS-II experiment period. We performed daily operation of two-day air quality forecasting simulations at the 12-km resolution for the Eastern Texas regional domain and at the 4-km resolution for the Houston-Galveston-Brazoria (HGB) and Dallas-Fort Worth domains, respectively. The results of individual runs were stored and the analysis graphics were made available to the research community and to State and local officials via the Internet, "<http://www.imaqs.uh.edu/aqfmain.htm>." Detailed evaluation information can be found in the final report, HARC Project H45C Final Report. East Texas Air Quality (ETAQ) Forecasting, Task 1 Operation of 2006 ETAQ Forecasting System (Byun et al., 2007a). Also an alternative air quality forecast was provided utilizing MM5 meteorological output from Texas A&M University (ETAQ-F3) but because the simulation results were close to ETAQ-F2, we did not pursue further evaluation of ETAQ-F3.

Because all these meteorological simulations utilized the same configurations and initialization procedures with the same input data, they produced quite similar meteorological forecasts except for some limited differences in precipitation events and cloud distributions. As reported in the H45C Final Report, the MM5 meteorological forecasting utilized the forecasting output of the NCEP WRF/NMM, which occasionally caused very strong northeasterly flows into the Houston region due to overly intensified low pressure systems in the Gulf of Mexico. Moreover, recent modifications in the MM5 and MCIP code led to very low stable boundary layer heights, mostly set to the middle height of the lowest MM5 layer.

The forecast differences between the ETAQ-F1 and F2 systems are mostly due to the different anthropogenic emissions inputs used for the forecasting simulations. For ETAQ-F1, we utilized TCEQ's Texas Emissions Inventory (TEI) for base year 2000 (<ftp://ftp.tceq.state.tx.us/pub/OEPAA/TAD/Modeling/HGMCR/EI/>). The TEI inventory may overestimate emissions of ozone precursors for the 2005 episodes because several emissions control measures have been implemented since 2000. Thus, For ETAQ F2, the emissions inventory was projected to year 2005 utilizing growth and control factors (http://www.tceq.state.tx.us/assets/public/implementation/air/sip/sipdocs/2005-09-BPA/ado_BPA_D.pdf). Model-ready emissions for the SAPRC99 mechanism were prepared with the Texas Emissions Inventory Processing System (TEIPS), based on SMOKE (Sparse Matrix Operator Kernel Emissions) and EPS components to process Texas-specific emission inventories (Kim and Byun, 2003; Byun et al., 2005). The National Emissions Inventory for 1999 (NEI99) from U.S. EPA was used as a supplementary emissions without any projections to 2005 to fill in the emissions data for regions and emission species not included in the TEI.

Very similar biogenic emissions inputs, estimated by the selective utilization of GloBEIS3 and BEIS3, were used in both F1 and F2 systems. One of the main reasons for using the hybrid method was to utilize the Texas-specific land use/land cover (LULC) data from TCEQ, which was more suitable for GloBEIS3 (Guenther et al., 1993; Yarwood, 2002) than the EPA's national county-based Biogenic Emission Land-cover Database version 3. On the other hand, meteorological data such as temperature and PAR (Photosynthetically Active Radiation) were used to adjust the biogenic emissions depending on meteorological conditions forecasted by F1 and F2. More detailed descriptions of the AQF emissions can be found from the HARC project H60 final report (Byun et al., 2006)

A performance evaluation of the 2005/2006 ETAQ forecasting showed that the AQF systems were capable of forecasting day-to-day ozone variations in East Texas. The ETAQ forecasting systems showed good performance in predicting averaged (either spatially, temporally or both) ozone. The seasonal ozone cycle was captured well by the model, with a double peak in late spring and fall, and a dip in July. The model performance for predicting daily average ozone did not vary by much throughout the year. The forecasted diurnal cycle was less pronounced than observed, but with the peak ozone time (12-17 CST) well simulated. There was a positive night-time and early morning bias which was quite large in the summer time. The model produced less high ozone (>120 ppb) values although it had a positive day-time bias. We found a few air

quality simulation errors that were caused by the imperfect meteorology forecasting by MM5, especially wind fields. We further traced back the imperfect meteorological simulations to problems in the WRF-NMM/EDAS data from NCEP. There could have been other reasons as well, such as inconsistent use of resolution during downscaling. The model nighttime ozone over-prediction was likely due to the high nighttime wind that significantly reduced the impact of local NO emissions and the high model background ozone from the Gulf provided by the 2002 monthly average GEOS-Chem results. The slow rise of ozone concentrations in the morning was also likely due to the higher early morning winds in the model, which hindered build up of precursor species. The slower drop of ozone at dawn could possibly be attributed to the high background ozone and uncertainties in the predicted mixing height. Figure 1 compares daily maximum ozone forecasted by ETAQ F1 and F2 forecasting systems with CAMS measurements in the Houston-Galveston-Brazoria area. Some high ozone daily maximum ozone concentrations forecasted in F1 have been reduced in F2, demonstrating that the emissions inputs for F2 were more suitable for the 2006 episodes. But a few high ozone days observed were not predicted by both systems.

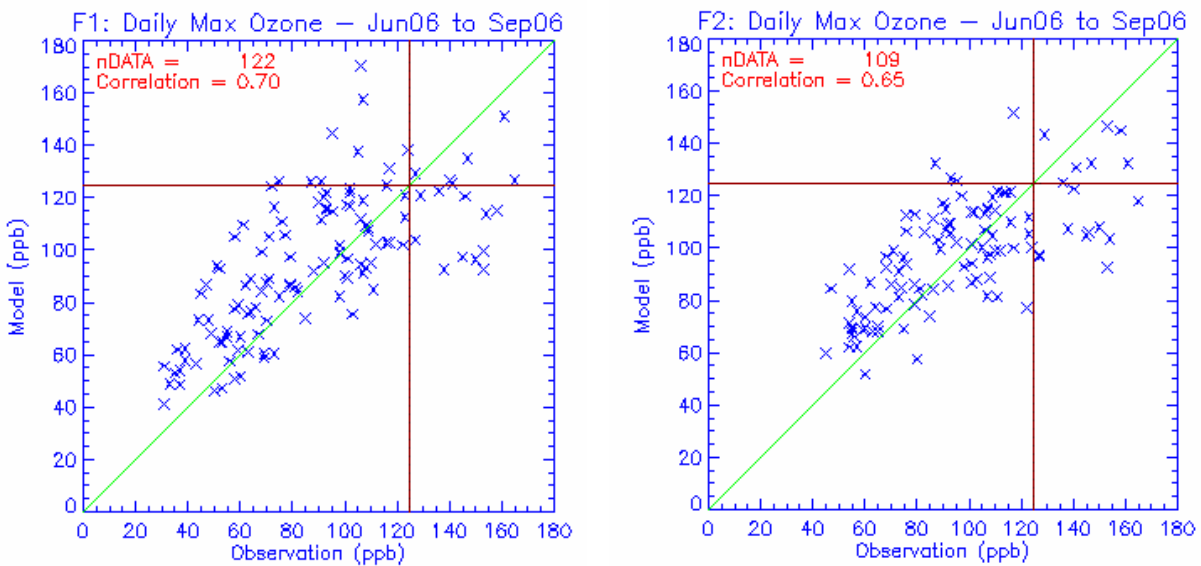


Figure 1. Comparison of daily maximum ozone forecasted by ETAQ F1 and F2 with CAMS measurements in the Houston-Galveston-Brazoria area.

3. Summary of Assimilated MM5 Simulations

As discussed in Section 2 above, there were some difficulties forecasting meteorological conditions for the TexAQS II episodes due to the strong influence of WRF-NMM forecasting inputs, which occasionally predicted too strong development of Gulf Coast low pressure systems. To generate a set of better meteorological inputs representing the TexAQS II air pollution episodes, we performed new meteorological simulations utilizing the UH Regional Data Assimilation System (UH-RDAS) and the Meteorological Assimilation Data Ingest System (MADIS) datasets and CAMS surface measurements together with NOAA WRF-NMM/EDAS inputs. Figure 2 present the processing steps of the University of Houston’s MM5 multiscale nest-down four-dimensional data assimilation (FDDA) scheme utilizing NOAA WRF-NMM/EDAS inputs. The current MM5's nudging implementation is based on Stauffer and Seaman (1990, 1991 and 1994). Figure 3 shows surface observation sites in the extended E12 domain used in the UH nest-down FDDA simulations.

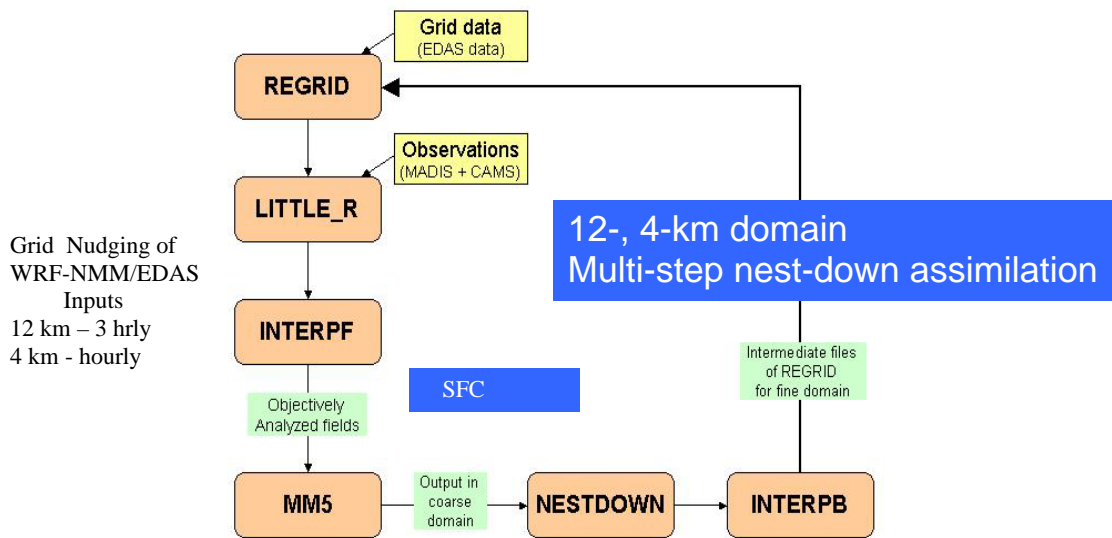
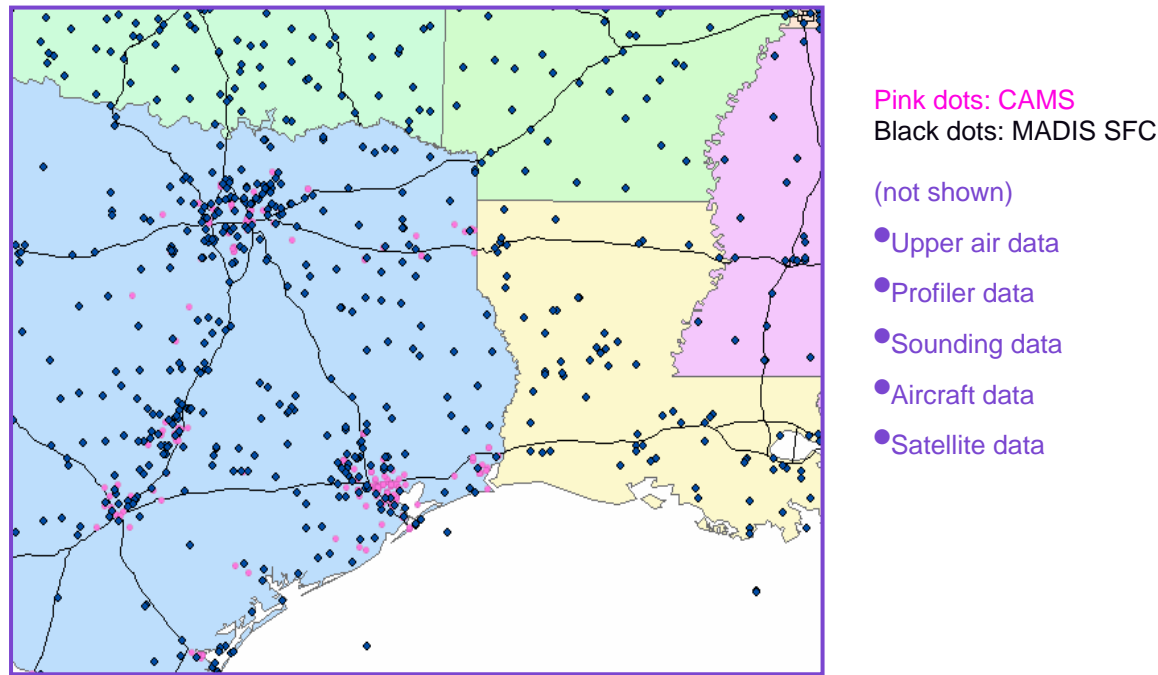


Figure 2. Processing steps of the University of Houston’s MM5 multiscale nest-down four-dimensional data assimilation (FDDA) scheme utilizing NOAA WRF-NMM/EDAS inputs.



n

Figure 3. Surface observations in the extended E12 domain used in the UH nest-down four-dimensional data assimilation (FDDA) simulations. Blue dots indicate MADIS surface data while pink dots represent CAMS sites. Upper air data, profiler data, sounding data were also used in the assimilation. However, the aircraft data and satellite data are not currently used.

MM5 simulations with the four-dimensional data assimilation (FDDA) method described above, which is designated as “TMNS11n2,” were performed under the TCEQ modeling project “Improved Modeling Inputs: Analysis of Air Pollution Events in Summer 2006 and Preparation of Model Input Data for the Assessment Study.” Two interim reports of the project, “Interim Report II: MM5/CMAQ Resimulation of TexAQS-II Phase I: Testing Various Nudging Settings - Datasets, Domains, Radius, and Simulation Hours,” (Byun et al., 2007b) and “Interim Report III: MM5/CMAQ Resimulation of TexAQS-II Phase II: Thunderstorm Issues, Nudging with Selected Weather Parameters,” (Byun et al., 2007c) provide detailed description of various modeling results that led to the development of the “TMNS11n2” meteorological inputs.

The highlights of these reports related to the meteorological simulation results for the TexAQS-II summer intensive period are summarized below:

- Identified a few problems with MM5 forecasting results
 - Too strong northwesterly winds simulated
 - Difficulties in simulating thunderstorms and associated cloud and wind fields
 - Too low PBL heights for stable conditions over land and over Gulf Coast areas

- Used a proven MM5/Four-Dimensional Data Assimilation (FDDA) technique to improve meteorological simulations
- Used the IMAQS MM5-based real-time data assimilation framework, with multiple observational datasets from
 - Meteorological Assimilation Data Ingest System (MADIS)
 - CAMS met data
 - Comprehensive surface obs. (SFC – from ASOS by NOAA/NWS)
 - Improved rawinsonde observations (RAOB)
 - Aircraft sounding (ACARS) winds
 - Improved NOAA Profiler Network (NPN) data
- Tested a variety of assimilation configurations
 - Finally arrived at “TMNS11n2”
 - Grid nudging at 36-km using WRF-NMM/EDAS to provide BC for CONUS domain
 - Nest down to 12-km and 4-km with MADIS & CAMS data
 - 3D nudging for (U,V) wind components for everywhere, T & RH nudging in free atmosphere for 36km and 12km domains
 - grid and surface nudging for wind components only for 4-km domain
- Results of MM5/FDDA re-simulation with CAMS and MADIS are:
 - Reduction of wind speed and direction biases to produce more realistic flow variations overall
 - Good temperature predictions
 - Some unwanted flow patterns due to difficulties in simulating thunderstorms at 4-km resolution with the explicit scheme.

To support the present project, we have further evaluated performance of the “TMNS11n2” MM5 simulations for the period of August 16–September 15, 2006 of the TexAQS II experiment period, for which we have received hourly specific point source emissions data (to be discussed later) from TCEQ.

The regional average time series plots (Figure 4–8) are used to identify days with inaccurate MM5 simulation results. Figure 4 compares simulated and observed regional average precipitation amounts (over the CAMS sites). Although the model simulated precipitation events well in general, the precipitation amounts were usually lower and a few hours later than observed. This type of behavior is expected because the temperature and moisture parameters are assimilated only above the boundary layer (i.e., no surface nudging) for the 12-km domain after the real precipitation event, while there is no moisture and temperature nudging at all for the 4-km domain. Also there were a few days (August 23 and September 5 and 9, for example) for which the model failed to predict large precipitation events entirely.

The relative humidity (RH) plot (Figure 5) demonstrates that daytime values, representing synoptic changes, are relatively well simulated. Because the thickness of the lowest model layer used is around 36 m and the measurement height at the CAMS sites is 1.5 m, higher measured RH values at night are expected, in particular for the days with clear skies overnight. Still the RH time series shows that for certain days like during the night of August 29–30, the model overpredicted RH values, while some other days like the night of August 30–31, it severely underpredicted RH. Also, the model underpredicted RH values for September 5, September 9, and September 11 when we had precipitation events in the real world. It seems that the model had a difficult time predicting wind flows during some days, which may explain the underprediction of RH on September 14, a day without precipitation.

The regional average 1.5 m temperature time series plot (Figure 6) shows that the simulation results agree well with observations except for a few days when the model had difficulty simulating precipitation and associated clouds at specific locations. For example, real world precipitation events are not represented or are misplaced in the MM5 simulations on August 23, 26, and 27, and September 5 and 9 at certain CAMS sites.

Time series plots for the wind components and wind speed show again that the meteorological model simulated synoptic changes quite well. Interestingly, there were serious overpredictions of easterlies (i.e., negative U-wind component) and slight overpredictions of northerlies (negative V-wind component) for the period starting on the evening of August 16 and ending at noon August 17, demonstrating that the assimilation could not overcome the strong north-easterlies provided by the EDAS wind fields. There were occasional overpredictions of northerly components on other days (such as September 3, 4, 6, and 7).

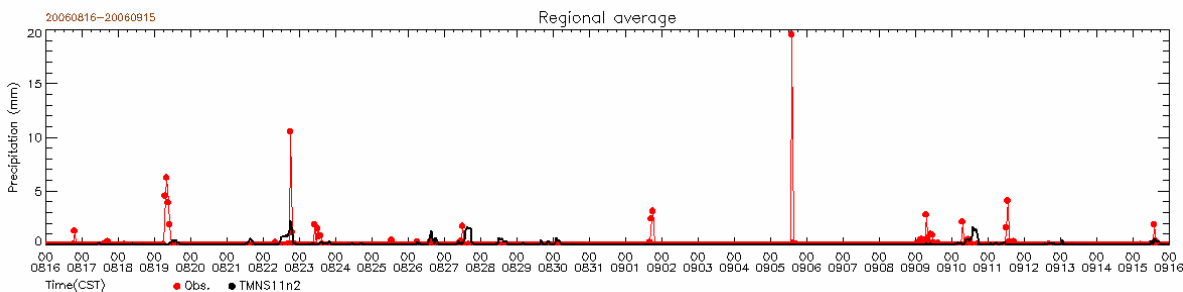


Figure 4. Time series plot of precipitation amounts averaged over the CAMS sites in the HGB domain for the August 16–September 15, 2006 period.

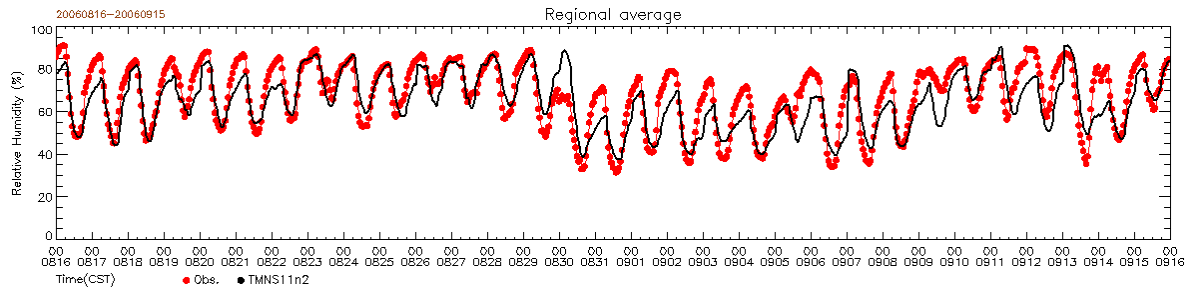


Figure 5. Time series plot of relative humidity averaged over the CAMS sites in the HGB domain for the August 16–September 15, 2006 period.

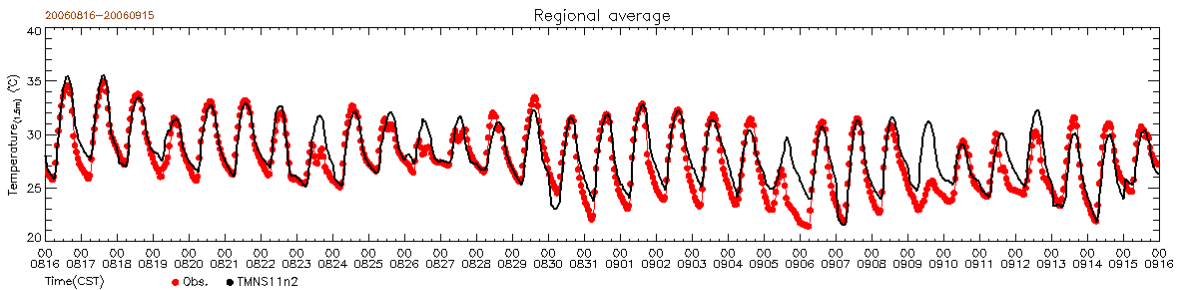


Figure 6. Time series plot of surface (1.5 m) temperature averaged over the CAMS sites in the HGB domain for the August 16–September 15, 2006 period.

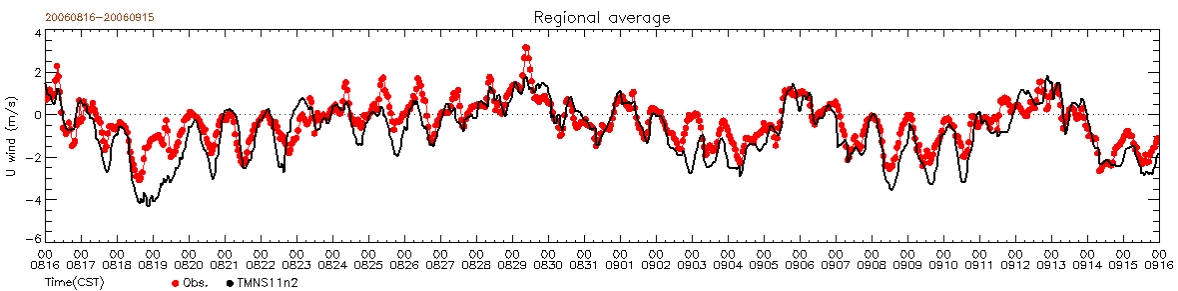


Figure 7. Time series plot of U-wind component averaged over the CAMS sites in the HGB domain for the August 16–September 15, 2006 period.

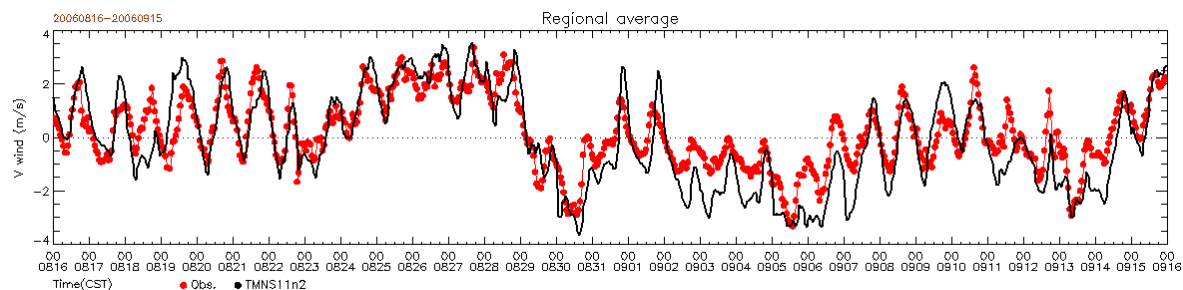


Figure 8. Time series plot of V-wind component averaged over the CAMS sites in the HGB domain for the August 16–September 15, 2006 period.

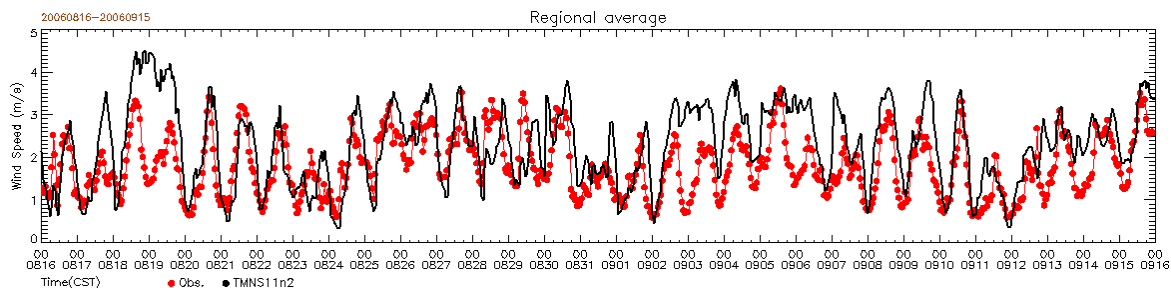


Figure 9. Time series plot of wind speed averaged over the CAMS sites in the HGB domain for the August 16–September 15, 2006 period.

4. Improvement of CMAQ Simulation Results with Assimilated MM5 Results

To determine whether or not the assimilated meteorological inputs would improve air quality simulations for East Texas, we compared two sets of CMAQ simulations, corresponding to the AQF and TMNS11n2 meteorological inputs. To eliminate any differences in the model configurations and operational characteristics, we performed CMAQ simulations with the same AQF emission inputs but with different meteorological inputs (named as “AQFn” and “TMNS11n2”) for the 8-day simulation period, August 14–21, 2006. Again, this activity was supported by the TCEQ modeling project “Improved Modeling Inputs: Analysis of Air Pollution Events in Summer 2006 and Preparation of Model Input Data for the Assessment Study.” The details of the comparison results are summarized in “Interim Report III: MM5/CMAQ Resimulation of TexAQS-II Phase II: Thunderstorm Issues, Nudging with Selected Weather Parameters.”

Here, we provide highlights of the comparison between the two sets of CMAQ simulations, AQFn and TMNS11n2, focusing on the August 16–18 ozone event described below. Figure 10 (a)-(c) are weather charts from NOAA for the ozone event and Figures 11-13 compare air quality simulation results between the two cases.

August 16: Cold front near Dallas, westerly winds; O₃ peak (140 ppb) at NE of Houston

August 17: Affected by front, N/NE'ly winds, O₃ peak (~150 ppb) at Deer Park

August 18: No strong weather system existed, light and variable winds, high background, O₃ (~120 ppb) at W of Harris County.

For all three days, the CMAQ re-simulations with the TMNS11n2 meteorology inputs produce far better peak ozone values and locations than those with the AQFn meteorology inputs when compared with CAMS observations. The spatial ozone plots (Figures 11-13) and scatter plots (Figure 14) all show that TMNS11n2 outperforms AQFn, demonstrating the importance of proper meteorological inputs to simulate ozone levels and spatial distribution patterns correctly.

A high ozone peak of around 140 ppb was observed over North Houston on August 16, while ozone concentrations were kept as low as 60 ppb over the south. TMNS11n2 simulation results show quite a good match of the spatial gradient of ozone concentrations compared to the observations, although regional average ozone was over-predicted during daytime and in the early morning hours. There were significant contributions of ozone and its precursors transported from southerly boundaries, increasing ozone by about 30 ppb. In contrast to the previous day, high ozone peaks were observed and simulated over the southwestern part of Harris County on August 17. NO titration of ozone at night was less than on other days and ozone concentrations remained higher than 40 ppb until midnight. Regional average of ozone observed in early morning of August 18 was as low as 15 ppb. There was a large contribution of transported ozone and its precursors in the morning hours when local NO_x emissions continued to titrate ozone. During the daytime, contributions of local emissions were smaller than on other days. However, the influence of boundary transport increased ozone over the area by 40 ppb.

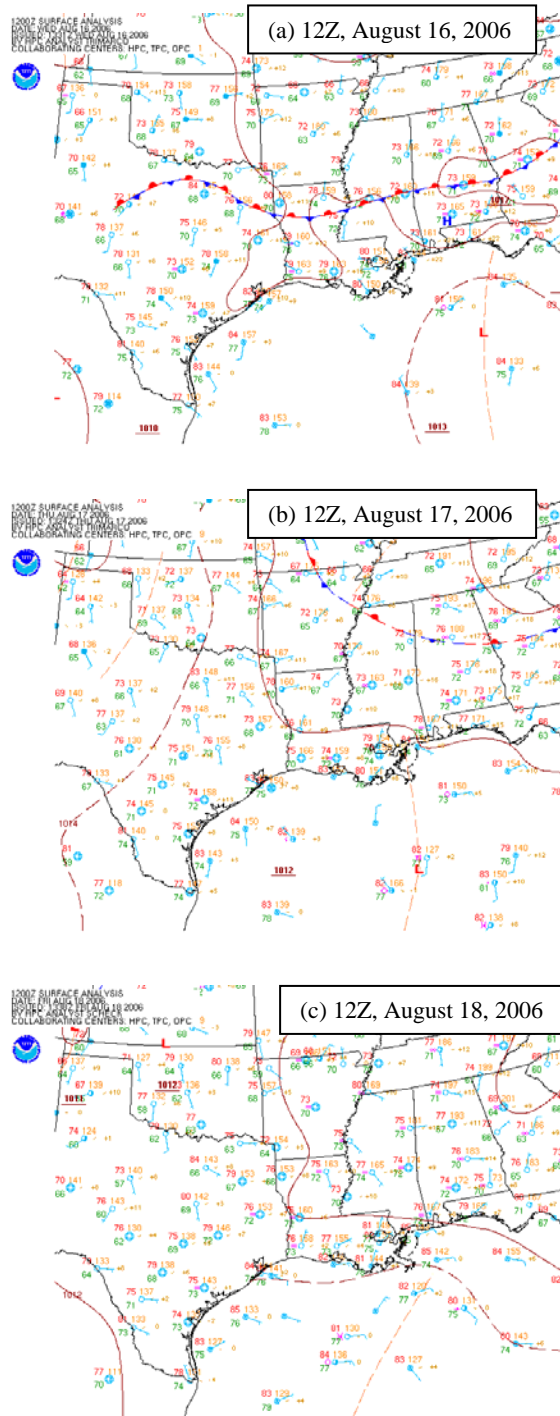
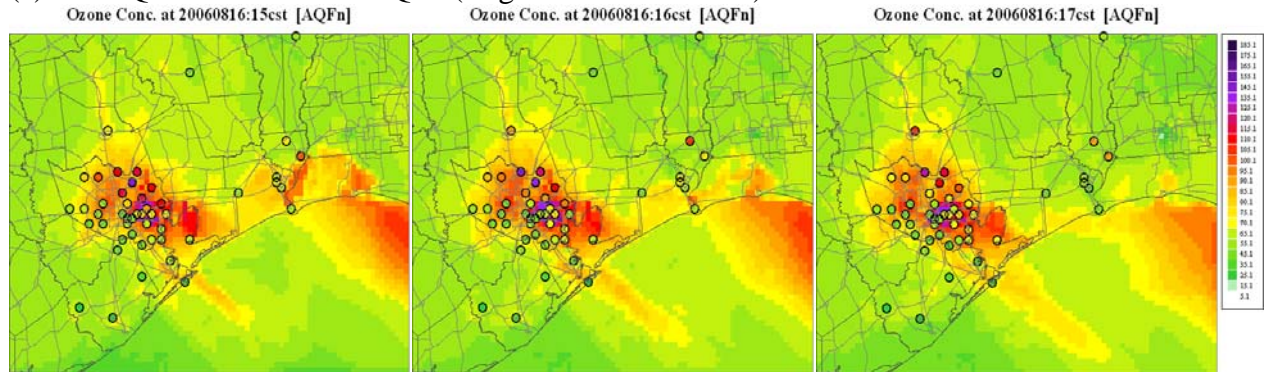


Figure 10 (a)-(c). NOAA surface weather charts for August 16–18, at 12:00 UTC.

(a) CMAQ simulation with AQFn (original MM5 forecast)



(b) CMAQ simulation with TMNS11n2 (MM5/FDDA using UH-RDAS)

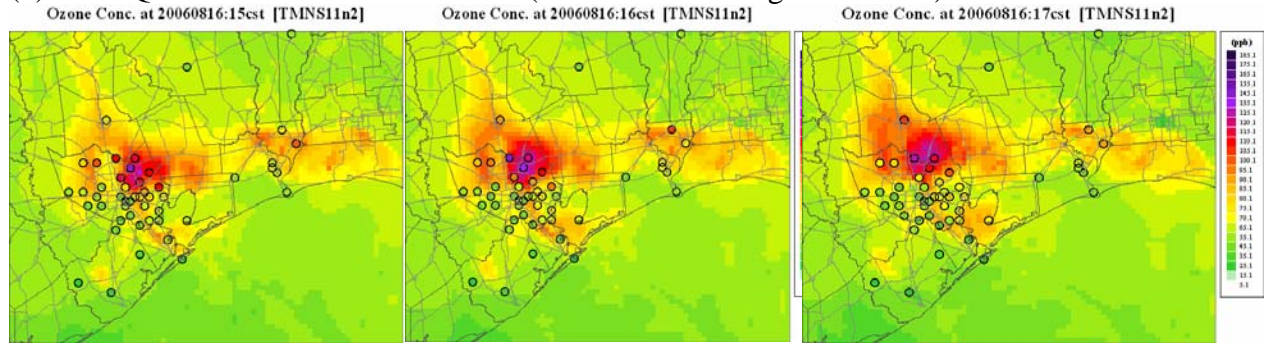
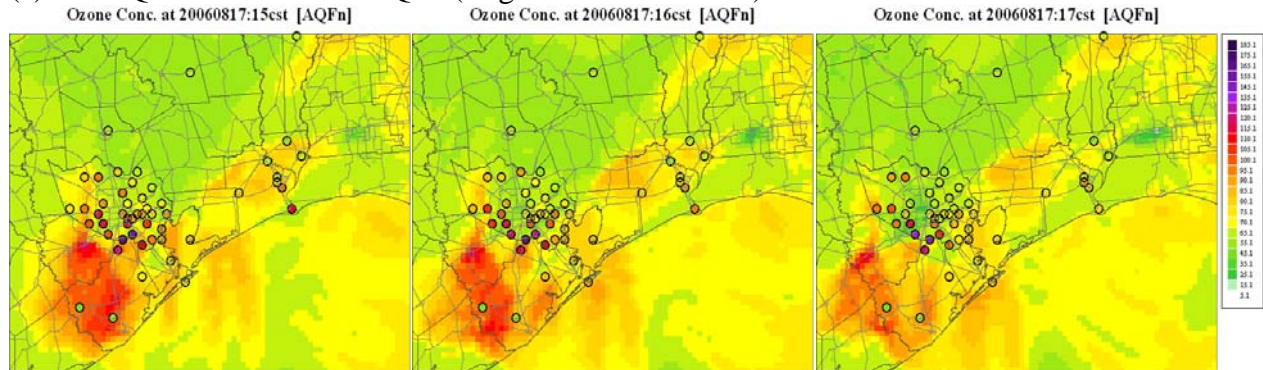


Figure 11 (a) CMAQ simulation with AQFn (original MM5 forecast), and (b) CMAQ simulation with TMNS11n2 (MM5/FDDA using UH-RDAS) for 15-17 CST, August 16, 2006.

(a) CMAQ simulation with AQFn (original MM5 forecast)



(b) CMAQ simulation with TMNS11n2 (MM5/FDDA using UH-RDAS)

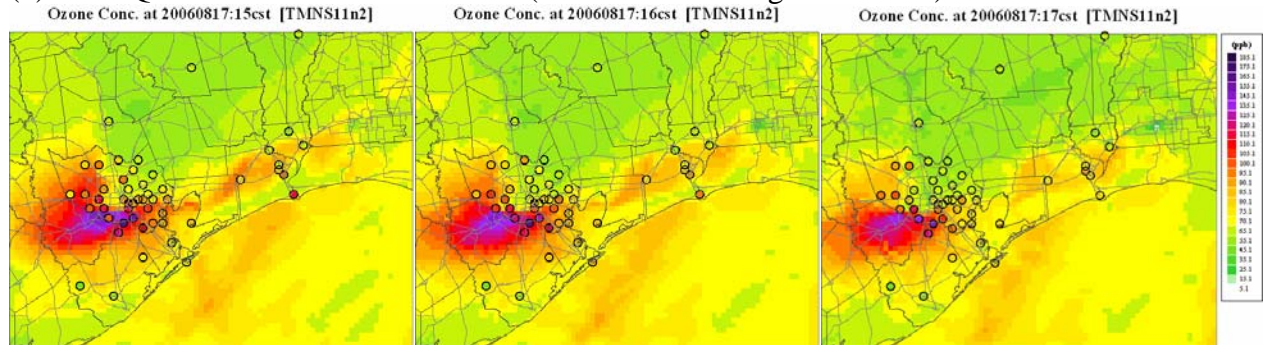
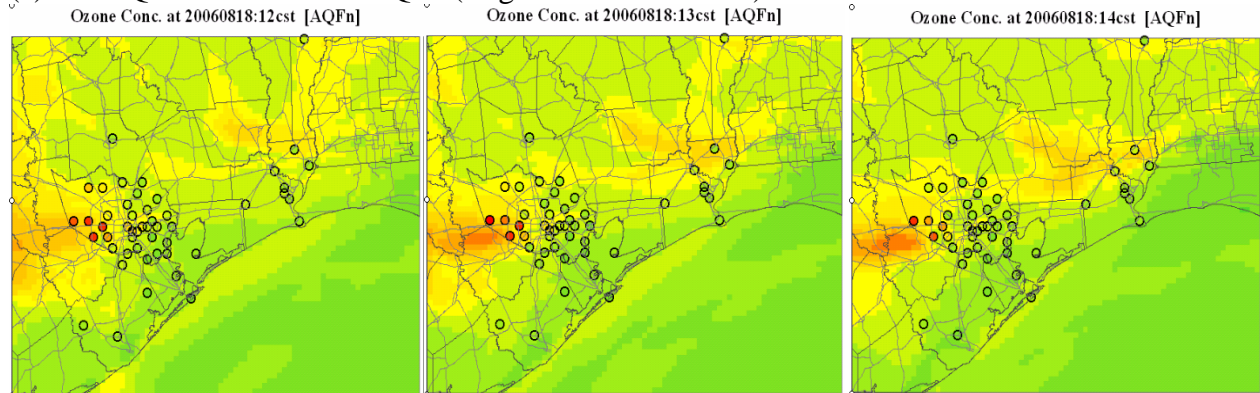


Figure 12 (a) CMAQ simulation with AQFn (original MM5 forecast), and (b) CMAQ simulation with TMNS11n2 (MM5/FDDA using UH-RDAS) for 15-17 CST, August 17, 2006.

(a) CMAQ simulation with AQFn (original MM5 forecast)



(b) CMAQ simulation with TMNS11n2 (MM5/FDDA using UH-RDAS)

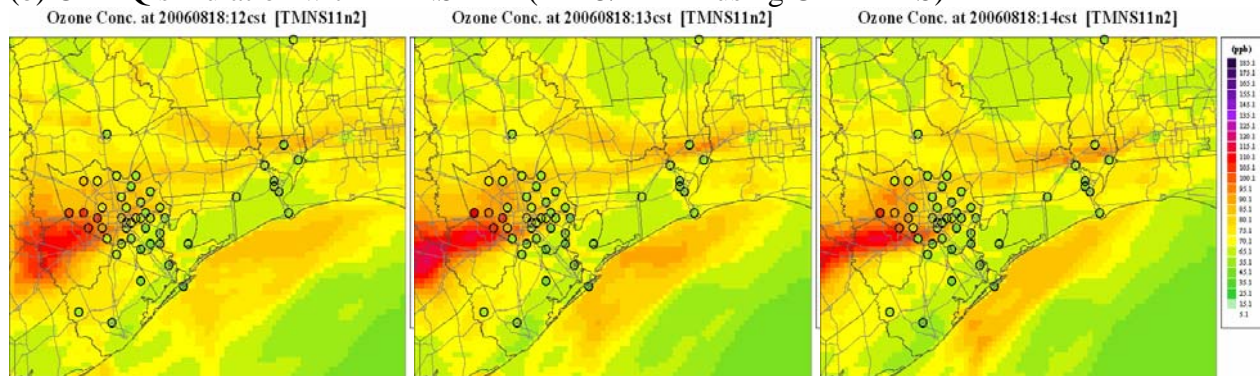


Figure 13 (a) CMAQ simulation with AQFn (original MM5 forecast), and (b) CMAQ simulation with TMNS11n2 (MM5/FDDA using UH-RDAS) for 15-17 CST, August 18, 2006.

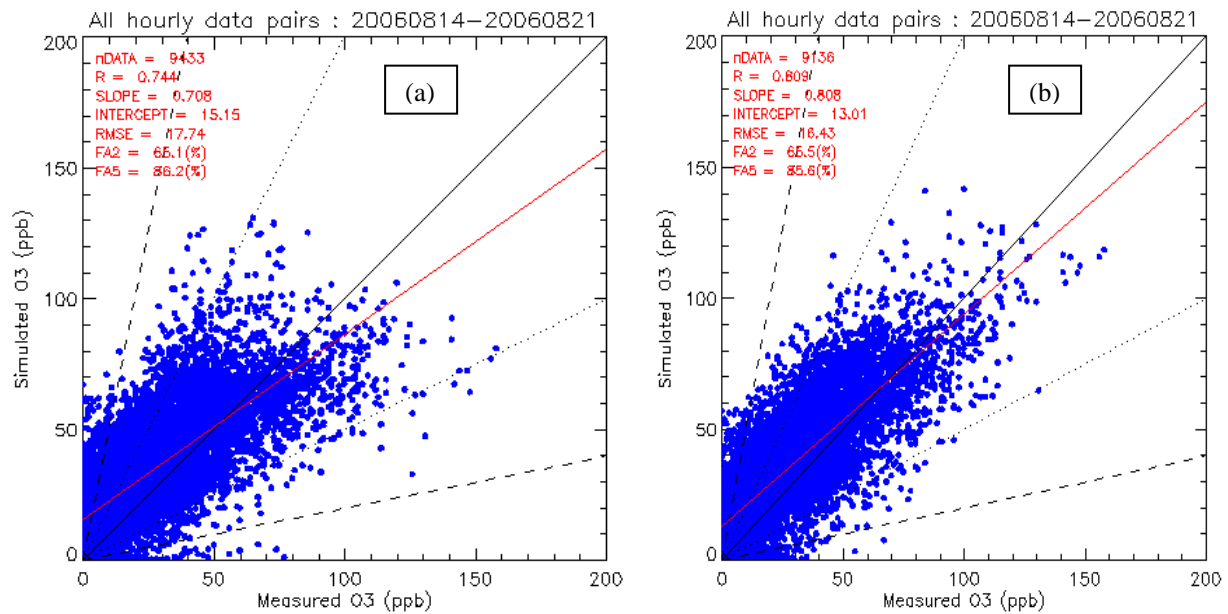


Figure 14 (a) CMAQ simulation with AQFn and (b) CMAQ simulation with TMNS11n2 compared with CAMS surface ozone measurements in the Houston-Galveston-Brazoria domain for August 14-21, 2006 period.

5. Updated 2006 Summer Emissions Inventories for Air Quality Simulations

To perform air quality simulations for the assessment study, we decided to prepare “best-effort model-ready (BEMR) 2006 Texas emissions inputs” first utilizing currently available emissions inventories, projected emissions components such as mobile emissions, and the 2006 special point source emission inventories for summer 2006 TexAQS II from TCEQ and Alpine Geophysics. Because the 2006 Texas special point-source inventories are available for August 15–September 15, the updated inventories are prepared only for this period.

The base-case air quality forecasting (AQF) emissions inputs were processed as follows. The Texas emissions inventory (TEI) was used mainly for the Texas area, while the 1999 National Emissions Inventories (NEI99) was used as a supplementary emissions inventory. For area and non-road sources, TEI base5b for year 2000 was used. MOBILE6 outputs for years 2000 and 2007 were used to interpolate mobile emissions for the base year 2003. For point sources, TEI for year 2000 were projected to year 2005. However, the additional 2000 “imputed” volatile organic compound (VOC) emissions were used without projection. For biogenic emissions, vegetation data from TCEQ was used and then adjusted with the MCIP-processed meteorological data. CMAQ-ready emissions for 36-km, 12-km, and 4-km domains were newly processed with the TMNS11n2 MCIP output for the simulation episode (August 12–October 6, 2006).

For the new BEMR 2006 Texas emissions inventories, we worked with Alpine Geophysics (AG) to prepare the 2006 AFS data sets for SMOKE processing. The 2006 raw point-source special inventories provided by TCEQ had many idiosyncratic features that must be carefully handled. TCEQ provided AG a set of the hourly-specific, speciated as well as aggregated VOC inventories for the point sources that reported during the TexAQS-II intensive period (August 15–September 15, 2006). One of the important questions was how to map TCEQ contaminants to SARAOD (Storage and Retrieval of Aerometric Data) codes to process them with SMOKE. The new BEMR 2006 inventories include the 2002 National Emissions Inventories (NEI2002). Dr. Jerry Lin of Lamar University (LU) provided the IDA format NEI2002 data for the SMOKE system. We conducted additional quality assurance checks of these inventories.

The major changes for the BEMR emissions inputs are; 1) use of the 2006 Texas special point-source emissions inventory (TPSI) for point sources, 2) use of TCEQ’s new biogenic emissions, and 3) replacement of the NEI99 with NEI2002.

Table 1 compares emissions inputs used for the base AQF and the updated BEMR TPSI2006 emissions.

Table 1. Emissions inventories used for the base AQF and the “best-effort model-ready” (BEMR) Texas Emission Inputs.

	Base AQF	BEMR
Area & Non-road	Base5b 2000	Base5b 2007
On-road	Linked-based and HPMS MOBILE6 projected for 2003	Linked-based and HPMS MOBILE6 projected for 2005
Point	Base5b regular emissions projected for 2005 & additional VOC for 2000 imputation	2006 Texas point-source special inventory (TPSI2006)
Biogenic	TCEQ's 2000 LULC and MM5 meteorology	TCEQ's 2006 biogenic emissions
Supplementary	NEI99	NEI2002

5.1 The 2006 Texas Point Source Special Inventory (TPSI2006)

New point source emissions inventory files, which include the speciated VOC emissions, were downloaded from the TCEQ's ftp site (<ftp://ftp.tceq.state.tx.us/pub/OEPAA/TAD/Modeling/HGB8H2/ei/point/2006/>). Table 2 lists the emission files used for the HGB 4-km domain. After converting the formats of the data in these files from the AFS (AIRS Facility Subsystem) to the IDA (Inventory Data Analyzer) format, they were processed with SMOKE to produce the air quality model-ready emission inputs. Emission records in the hourly emission files were first sorted by the times of emissions and then saved on a separate file for each day. To keep the diurnal emission pattern for each emission source, emissions rates and source information such as FIPS, Plant ID, Stack ID, and Point ID were used to generate cross-reference tables and hourly emission factors to perform the temporal allocation. This helped to accelerate the temporal allocation processing in SMOKE, which was designed to work only with a fixed diurnal profile. For point sources not included in the special inventory, we used ozone season daily emissions, temporal allocation for which was performed using the temporal profiles for the relevant source code categories (SCCs) established by the U.S. EPA.

Table 2. Point source emissions files used with the 2006 Texas point-source special inventory

	Name	Description	Filename
Hourly	SI VOC	VOC special inventory	afs.aggVOC_SI_for_15Aug2006_episode_v6
	SI NOX	NOx special inventory	afs.NOx_SI_for_15Aug2006_episode_v5
	ARD	Acid rain division EGUs	afs.ard_minus_SI_for_15Aug2006_episode_v6
	GWEI	the Gulf of Mexico	afs.gwei2000.20000801.3pol.lcp
	LA ARD	Louisiana	afs.Louisiana_ard_15Aug_to_15Sep06_episode_v2
OSD	TX OSD	TX ozone season daily emissions	afs.osd_minus_SI_for_15Aug2006_episode_v5
	States OSD	non-TX ozone season daily	afs.osd_domain_states_minus_TX_and_ARDs_15Aug_to_15Sep06_episode_v2
	Leftover	leftover emissions	afs.osd_n_ard_SI_paths_for_15Aug2006_episode_v5

To generate speciated VOC emissions data for the Carbon Bond Mechanism Version 4 (CB-4) using the special inventories, the TCEQ-provided a cross-reference table (xref.voc.eps3f.stars_2006_vSIb.pt.FACILITY) and VOC profiles (prof.emscvt.stars_2006_vSIb.pt), which were used to match emissions rates for the individual SAROAD species. The chemical split factors for the CB-4 chemical mechanism were then applied to each SAROAD species to calculate an emission rate for each model species. As with the temporal allocation, chemical speciation for other VOC emission data was performed for each SCC and each emission source.

Locations of point sources were provided in a Lambert Conformal Conic (LCC) map projection. We converted them into the latitude-longitude (LL) coordinates for the spatial allocation in SMOKE. Figure 15 shows the spatial distribution of the TPSI VOC emissions in the HGB area.

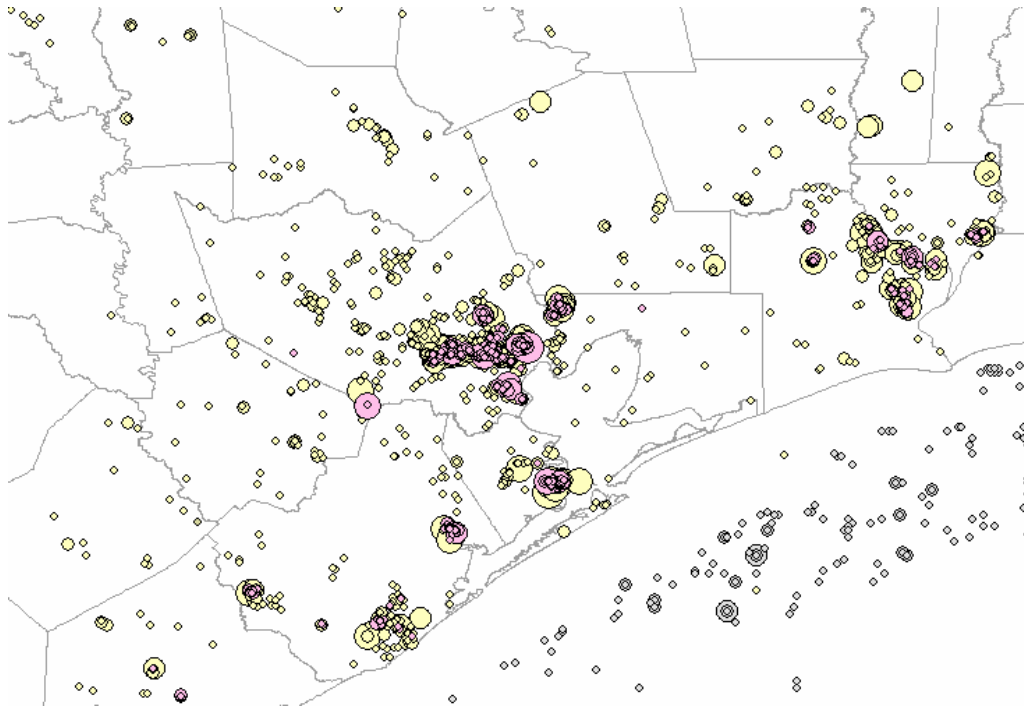


Figure 15. Emissions of volatile organic compounds (VOCs) from the Houston-Galveston-Brazoria (HGB) point sources. Pink and yellow circles represent the 2006 Texas Point-source Special Inventory (TPSI2006) VOC and Texas ozone-season day (OSD) emissions, respectively.

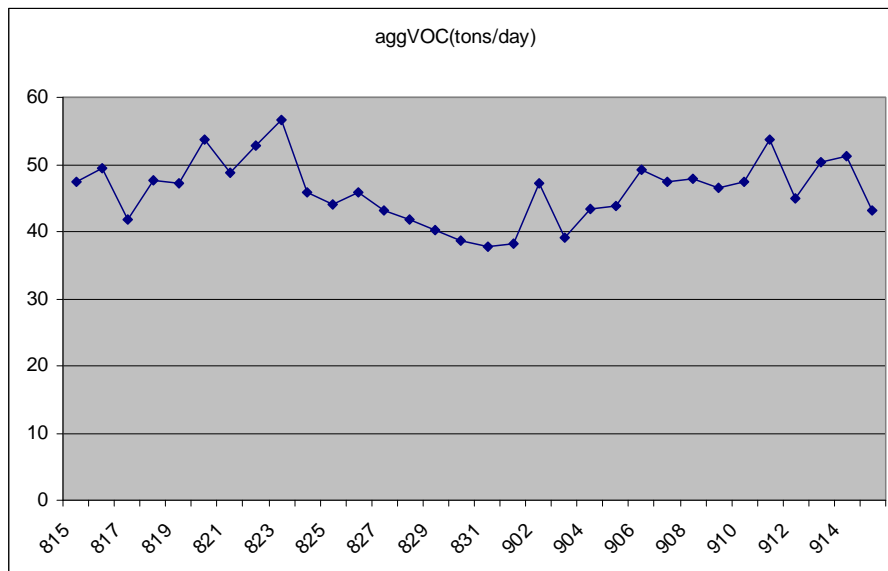


Figure 16. Daily VOC emission rates from the Texas point source special inventory.

Figure 16 shows that daily VOC emission rates from the special inventory range from 40 to 50 tons/day for the period of August 15–September 15, 2007. Total point source VOC emissions in the HGB 8-county area are around 210 tons/day, similar to the total point source VOC emissions in 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) portion of the inventory includes about 165 tons/day of VOC emissions. These VOC emissions are speciated depending on the SCC for the target chemical mechanism and gridded for the domain to generate the model-ready emissions data.

Table 3. VOC emissions from HGB 8 counties for August 15, 2007

County	SI VOC	ARD	TX OSD	Leftover	Total
Brazoria	4.1	0.0	16.1	0.0	20.2
Chambers	1.5	0.7	9.3	0.0	11.6
Fort Bend	0.0	0.8	2.5	-	3.4
Galveston	3.5	0.0	28.9	0.0	32.5
Harris	24.1	1.4	103.4	6.5	135.4
Liberty	-	-	2.7	-	2.7
Montgomery	-	0.2	2.2	-	2.4
Waller	-	-	0.3	-	0.3
8-County total	33.3	3.1	165.4	6.6	208.4

5.2 TCEQ Biogenic emissions

New biogenic emissions for the HGB 4-km domain in an ASCII format were downloaded from TCEQ's ftp site (<ftp://ftp.tceq.state.tx.us/pub/OEPAA/TAD/Modeling/HGB8H2/ei/bio/>). Split factors from GloBEIS were used to derive model-ready emissions for a selected chemical mechanism. Table 4 shows the split factors for the CB-4 mechanism applied to emissions of terpenes and other VOC species.

Table 4. Split factors of monoterpenes and other VOC emissions for the CB-4 chemical mechanism

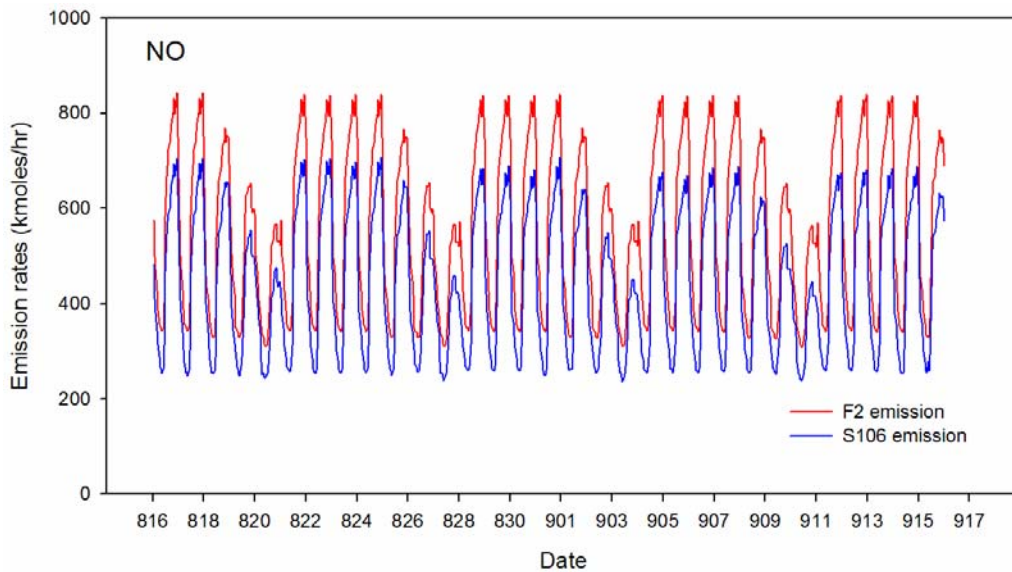
SPECIES	MONO	OVOC
OLE	7.401	3.09
PAR	53.198	16.451
XYL	0.329	0
FORM	0	1.667
ALD2	6.195	2.778
ETH	0	2.083
MEOH	0	41.667
ETOH	0	2.5
NR	0.311	2.646

5.3 Comparison of the Base AQF and Updated Emissions

Figures 17(a) and 17(b) show that NO and CO emissions rates in the updated emissions are reduced by 10-15 % compared to the AQF base emissions. It should be noted that in addition to the use of 2006 point special inventory, the updated BEMR emissions data include mobile emissions projected for 2005. Because the base AQF emissions data uses MOBILE6 emissions projected for 2003, the BEMR NO_x and CO emissions are lower than the corresponding base AQF emissions.

In Figures 17(c) and 17(d), olefin (OLE) and ethylene (ETH) emissions in the updated emissions are about one third of those in the base emissions. Additional imputed VOC emissions (~170 tons/day) are used for the base AQF emissions, while no imputation is applied to the updated point-source special inventory. Note that the early morning peaks in ETH emissions that are repeated for the week days (Monday-Thursday) in the base AQF emissions data are absent in the BEMR/TSPI emissions data (see Figure 17(d)). These peaks were originally present in the 2000 daily imputed ethylene inventory. Similar to NO, the updated emissions show a reduction of formaldehyde (FORM) emissions by ~15% compared to the base emissions (Figure 17(e)). When biogenic emissions are compared, isoprene in the updated BEMR emissions data is apparently reduced over the northern part of domain due to the use of different land use and land cover data in the two datasets. Figure 17(f) shows that total isoprene emissions in the HGB 8 counties are also reduced in the updated emissions data.

(a) NO



(b) CO

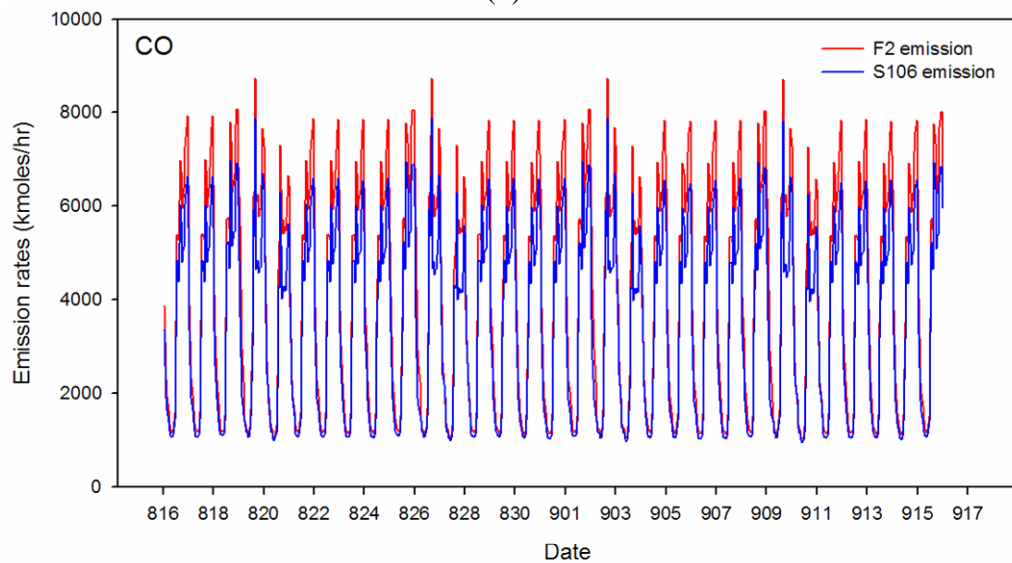


Figure 17. Comparison of hourly emissions rates of (a) NO, (b) CO, (c) OLE, (d) ETH, (e) FORM, and (f) ISOP between the base and updated emissions for the HGB 8-county area during the August 15–September 15, 2006. Red and blue lines represent the base AQF (designated as “F2”) and updated BEMR/TSPI2006 (designated as “S106”) emissions respectively.

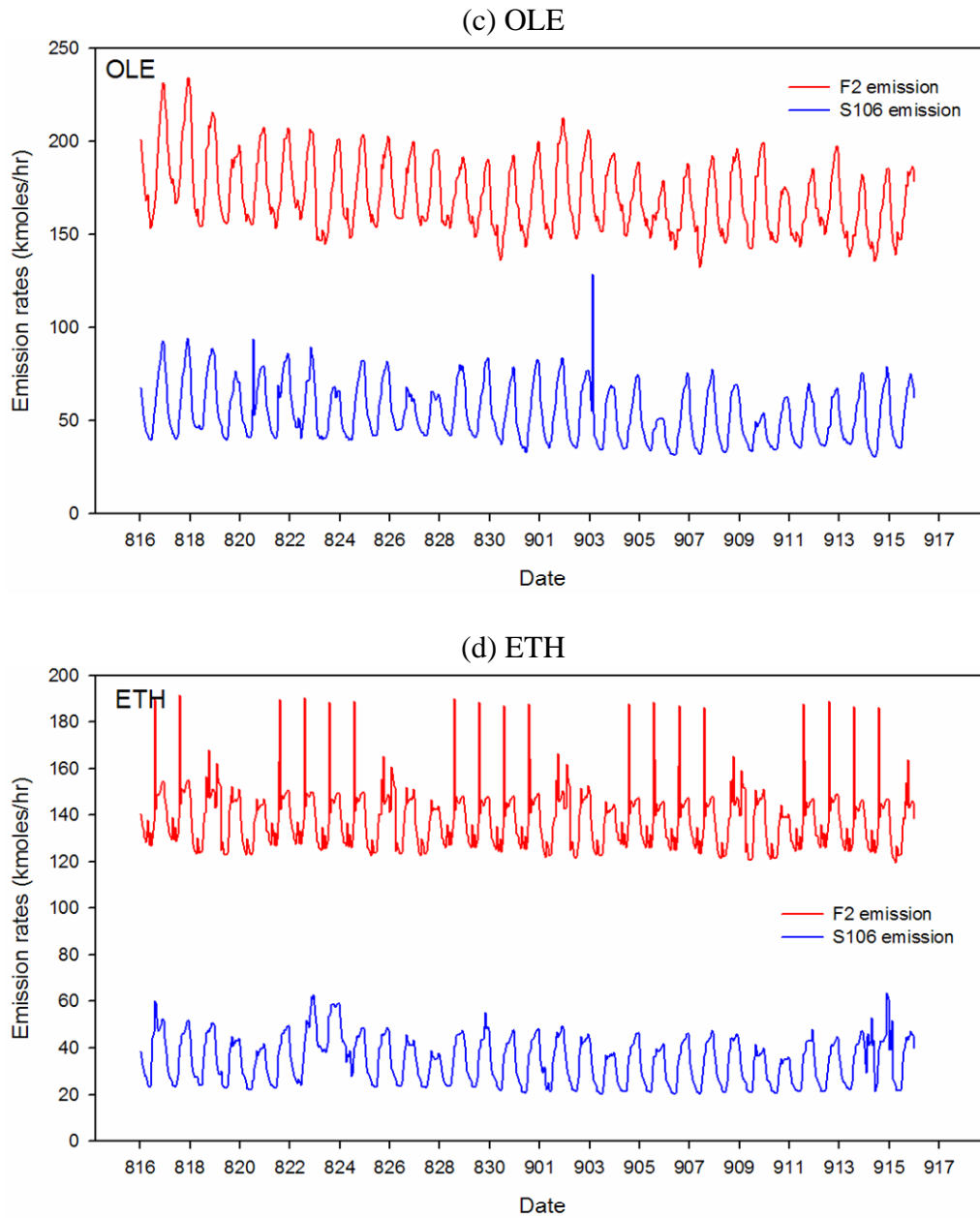


Figure 17. *continued*

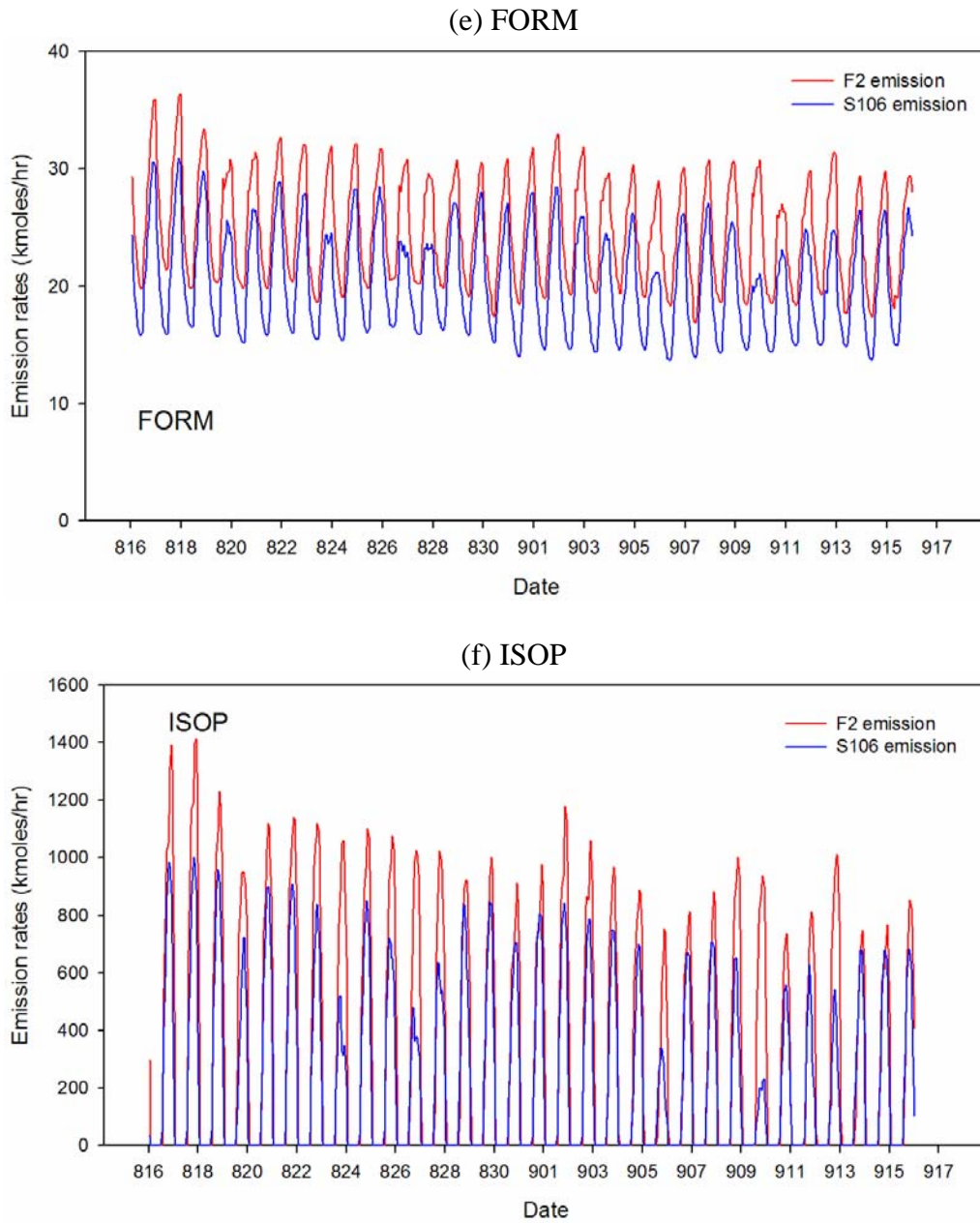


Figure 17. *continued*

6. Air Quality Simulations with Updated Emissions Inventories

We compared the results of a CMAQ simulation using the “best-effort model-ready” (BEMR) emissions to those from a CMAQ simulation using the base AQF emissions. Both simulations utilized the assimilated MM5 inputs, TMNS11n2, described above. During this process, we found several quality assurance issues with the newly prepared emissions, and therefore the final simulation set used here was named as the “corrected and cleared version three” (cc_03). For identification purposes, the two simulations are referred to as follows:

- (a) TMNS11n2: TMNS11n2 MCIP + Geos-Chem BC + base AQF F2 level emission with imputed HRVOC
- (b) cc_03: TMNS11n2 MCIP + Geos-Chem BC + BEMR/TPSI2006, no imputed HRVOC

In Figures 18–22, the results of the two simulations are compared with CAMS surface measurements.

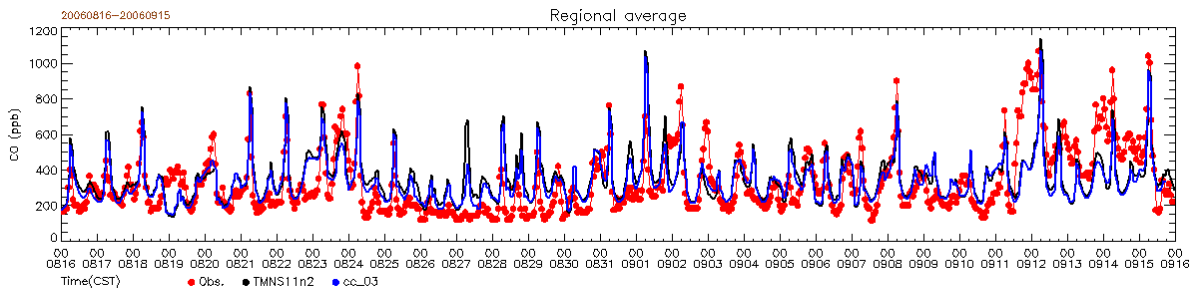


Figure 18. Time series plot of CO concentrations averaged over the CAMS sites in the HGB domain for the August 16-September 15, 2006 period.

CAMS CO measurement data usually show some peculiar jumps in the values either due to the machine response problem or calibration issues. However, when regionally averaged, we hope they still provide some useful information regarding the CO emissions and meteorological conditions of the region (Figure 18). The CO at surface represents mostly contributions from traffic emissions. As expected from the previous analysis of meteorological time series, we had problems in simulating CO on August 23 and 26, and September 5, 9, and 11 stemming from the poor simulation of precipitation events); on August 27 and 28 due to misrepresentation of morning planetary boundary layer (PBL) growth and overnight cloudiness; and on September 14 due to wind pattern errors. But there are other days with large differences between model predictions and measurements (such as the nights of September 1–2 and September 12–13) that cannot be readily attributed to the analyzed meteorological conditions. Either additional meteorological measurements or other issues such as real emission events and/or CO measurement problems must be considered. During the daytime hours, the simulated CO concentrations by both emission scenarios were slightly higher than the observations.

The regional average NO and NO₂ time series plots (Figures 19 and 20) show a general underprediction (overprediction) of NO (NO₂) for the nighttime and early morning hours. These biases are expected because the thicknesses of the lowest model 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 NO and NO₂ concentrations, it is difficult to relate the model-observation bias to specific meteorological events. Considering the daytime values, NO_x from “cc_03”, i.e. with BEMR/TPSI2006 emission inventory, seems closer to the observations.

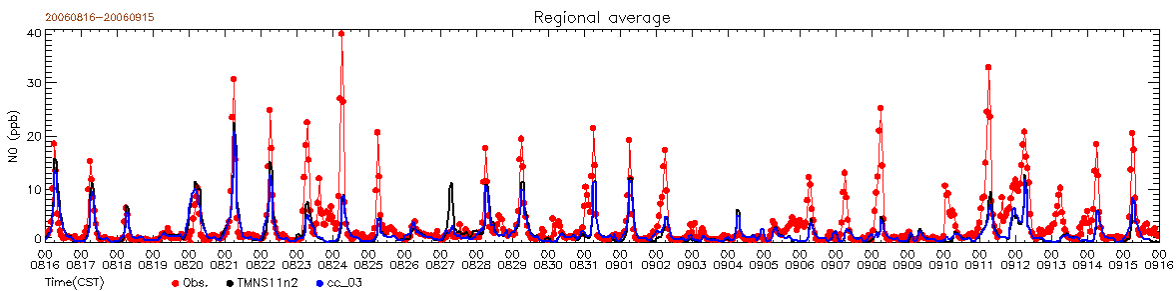


Figure 19. Time series plot of NO concentrations averaged over the CAMS sites in the HGB domain for the August 16–September 15, 2006 period.

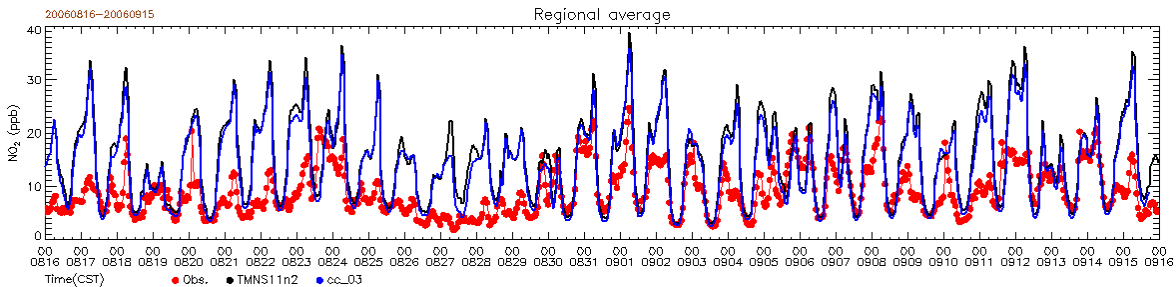


Figure 20. Time series plot of NO₂ concentrations averaged over the CAMS sites in the HGB domain for the August 16–September 15, 2006 period.

The regional average ozone time series plot is presented in Figure 21. The model shows serious overprediction of peak ozone for August 23–24 and September 9–10 (both sets of days were real precipitation episodes). It shows that incorrect prediction of precipitation events not only skews air quality simulation of the initial precipitation day, but also influences prediction of the following days, because the initial conditions are daisy-chained with the simulation results of the previous day. Interestingly, for the southerly wind days (i.e., positive V-wind component days,

such as August 24-29), the model overpredicted ozone by around 10 to 15 ppb. This suggests that the model boundary ozone concentrations, which were provided through downscaling of year 2002 monthly average GEOS-Chem model output using 36-km and 12-km nested CMAQ simulations, are set too high to represent the air from the Gulf of Mexico. Overprediction of ozone during September 9–12 are attributed to both the missing precipitation and some weaker southerly flows in the MM5 simulations compared to the observations. Although peak ozone concentrations for August 16, 17, 20, 30, September 2-5, September 8, 14, 15 are well predicted, there were significant underpredictions of ozone peaks for days such as August 29, 31, September 1, 6, and 7. Additional analysis of meteorology and emission events is needed to understand these discrepancies.

In general, the “cc_03” simulations show slightly lower ozone peak concentrations than the “TMNS11n2” simulations. The former simulates lower ozone days better than the latter, but is worse when simulating peak ozone events. Detailed comparison of the air quality simulations with the observations at each CAMS site and other special air quality measurements will be necessary to further verify the TPSI2006 emissions data.

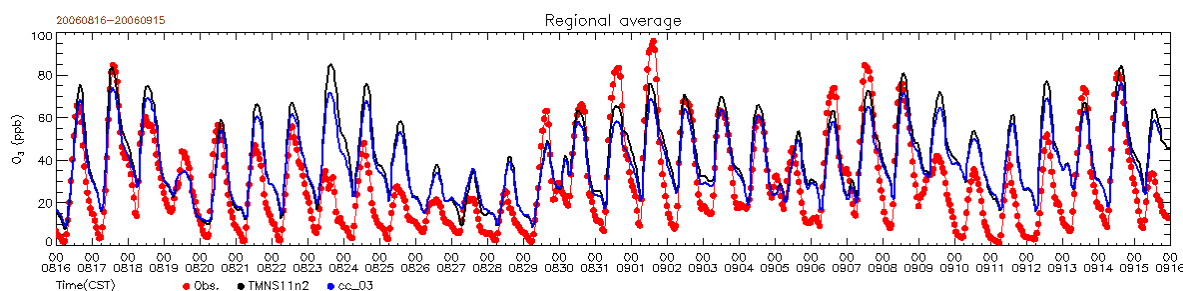


Figure 21. Time series plot of ozone concentrations averaged over the CAMS sites in the HGB domain for the August 16-September 15, 2006 period.

Scatter plots comparing simulated hourly ozone and corresponding CAMS observations during the one-month period are presented in Figure 22. Simulations with the BEMR/TPSI2006 emissions show slightly less scatter than those with the base AQF emissions, especially on the days with missed precipitation events and less accurately predicted wind patterns. We suspect that the morning peak ETH emissions present in the imputed emissions inventory for weekdays might have made the model more sensitive to meteorological errors, thus causing much larger discrepancies in the predicted ozone. However, simulations with the BEMR/TPSI2006 emissions failed to predict ozone peaks over 100 ppb. The high biases of ozone concentrations in the lower range are evident in both simulations, indicating the effects of high ozone background values used under southerly wind conditions. These results again call for further in-depth analysis of

the meteorological and emissions inputs, and of various measurements during the TexAQS-II period to isolate the causes of these model biases.

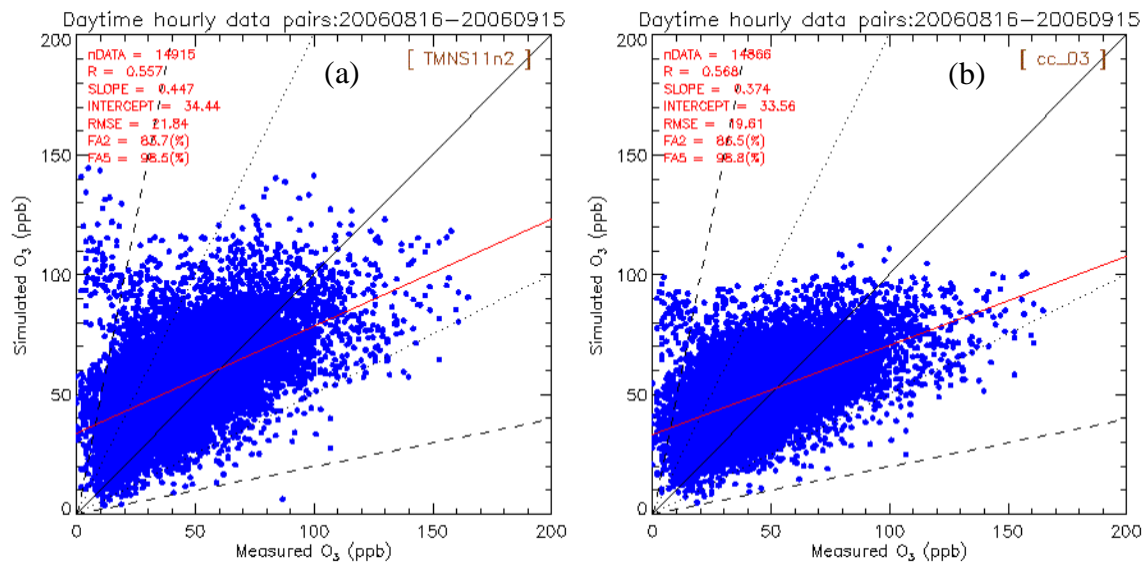


Figure 22. Scatter plots of the simulated ozone concentrations averaged over the CAMS sites in the HGB domain for the August 16-September 15, 2006 period. (a) CMAQ with base AQF emissions and (b) with best-effort model-ready emissions with 2006 Texas special point source inventories (BEMR/TSPI2006).

7. CMAQ and HDDM Simulations with the Base and Updated Emissions

A set of CMAQ-HDDM simulations for the HGBPA 4-km domain were conducted to study the contributions of local emissions and model boundaries to ozone concentrations predicted over the HGB 8-county area for August 17–18, 2006. The targeted contribution sources are as follows:

- Domain-wide anthropogenic NO_x emissions (Dark blue bars in contribution plots)
- Domain-wide anthropogenic VOC emissions (Purple)
- Cross-term of a) and b) (Orange)
- Domain-wide biogenic NO_x (NO) emissions (Yellow)
- Domain-wide biogenic VOC emissions (Green)
- Cross-term of d) and e) (Light orange)
- Ozone from boundaries (Red)
- Ozone precursors from boundaries: Summed contributions of NO_x, NO_z, and VOC from boundaries (Light blue)

The same meteorological data for the TMNS11n2 case were used for this CMAQ-HDDM simulations. The base AQF and updated TPSI2006 emissions were used to drive CMAQ (i.e., Q150 and Q149 in Figure 23) and CMAQ-HDDM, and the results were compared with observations at CAMS sites in the HGB area. Figure 23 shows that CMAQ simulations with the base AQF and the updated BEMR emission inputs (TPSI2006) produce generally comparable distribution patterns of hourly ozone. However it is seen that CMAQ with the base emissions predicts higher ozone concentrations during the daytime than with the updated emissions, possibly due to the imputed highly reactive VOCs in the base emissions. Table 5 compares general model performance with the base and updated emissions for the period of August 16–24, 2006. The CMAQ simulation with the updated TPSI2006 emissions predicted lower ozone peaks than the base emissions. Simulations with the updated emissions show better agreement with the observations for the August 16-September 15 episode in general, but not for peak ozone values. When compared with OLE and ETH concentrations measured at the University of Houston Moody Tower (Figure 24), CMAQ simulation with the base emissions significantly over-predicted the observations while simulation with the updated TPSI2006 emissions showed lower OLE and ETH concentrations and under-predicted observations from time to time. These analyses suggest that the updated TPSI2006 inventories represent the 2006 conditions better than the base AQF emissions, although inclusion of additional emissions of highly reactive species for upset events may be necessary to obtain the peak ozone values.

Table 5. Statistics of 1-hour ozone simulations with the base and TPSI2006 emissions.

	Base	Updated
NDATA	8425	8425
Observed Max (ppb)	158.0	
Simulated Max (ppb)	141.6	108.2
Observed Mean (ppb)	27.9	
Simulated Mean (ppb)	35.9	34.2
R2	0.4923	0.5284
G_BIAS	7.9	6.3
G_ERR	14.6	13.5
G_RMSE	20.5	18.0
G_SDE	20.1	18.3
IOA	0.81	0.83

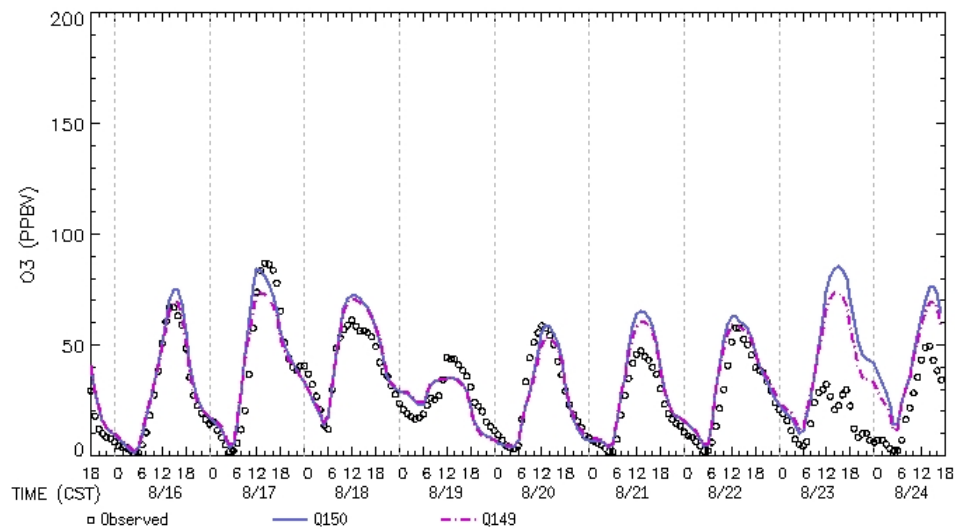
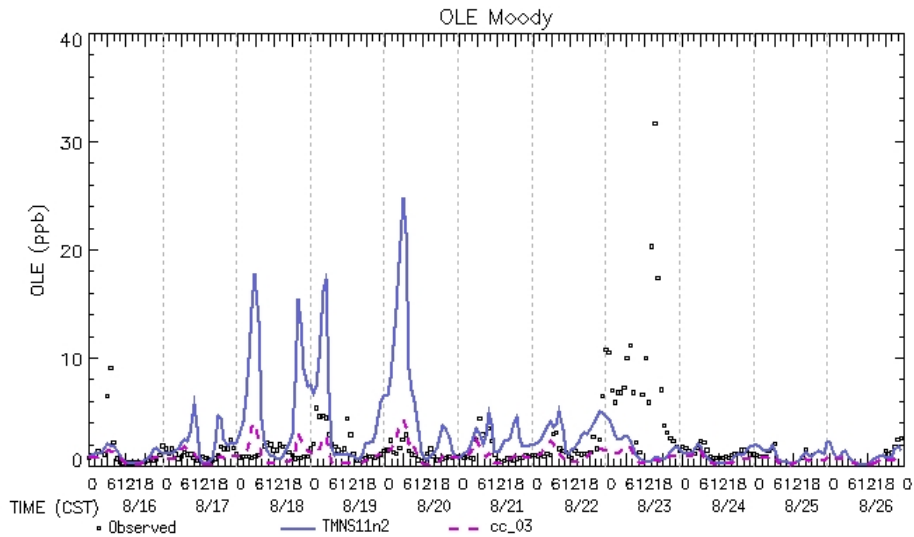


Figure 23. Hourly ozone concentrations simulated with the base (blue, Q150) and updated TPSI2006 (red, Q149) emissions for the period of August 16–24, 2006. Observed and simulated ozone concentrations are averaged over the CAMS sites inside the HGB area.

(a) olefins (OLE)



(b) ethylene (ETH)

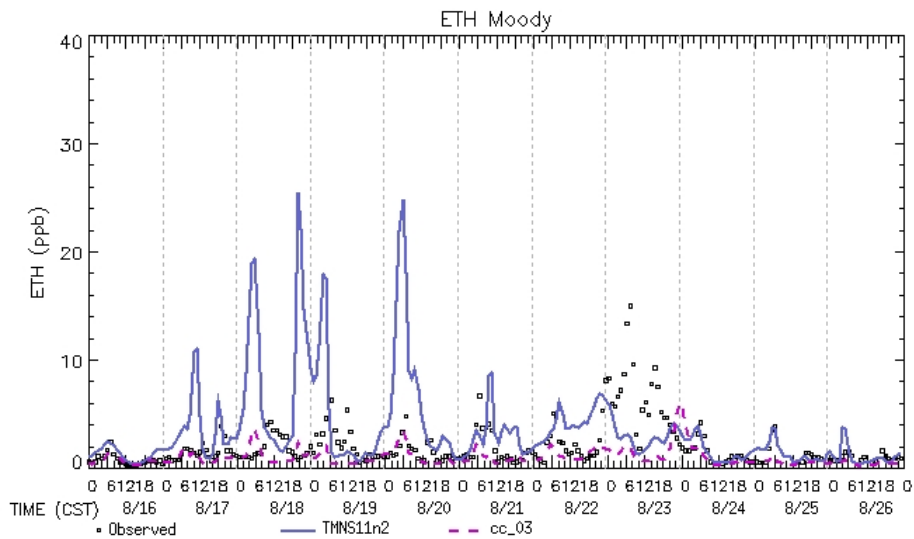
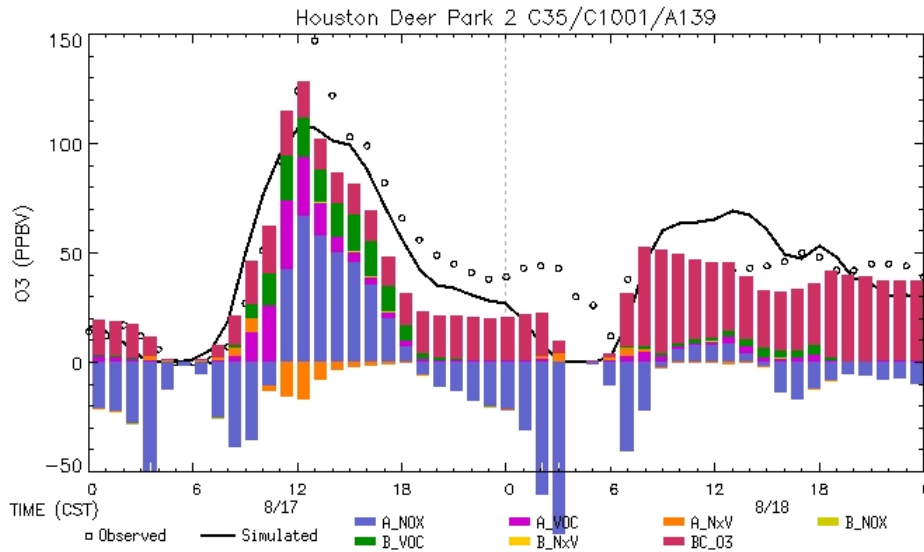


Figure 24. Hourly (a) olefin (OLE) and (b) ethylene (ETH) concentrations compared to the Moody tower measurements for the period of August 16–26, 2006. Blue and red lines represent simulations with base and updated emissions, respectively.

Figures 25 and 26 provide the source contribution characteristics from the CMAQ-HDDM simulations with the base and updated emissions. The former shows higher contributions of anthropogenic VOC emissions to ozone than the latter. For example, anthropogenic VOC in CMAQ with base emissions contributed around 60 ppb of ozone for August 17 at 12 PM at the Clinton Site, while the corresponding contribution from the updated emissions was less than 20

ppb. The major changes in anthropogenic VOC emissions resulted from use of the 2006 special inventory. It is therefore likely that reduced point source VOCs in the updated emissions led to a decrease in the ozone simulated.

(a) Base AQF emissions



(b) TPSI2006 emissions

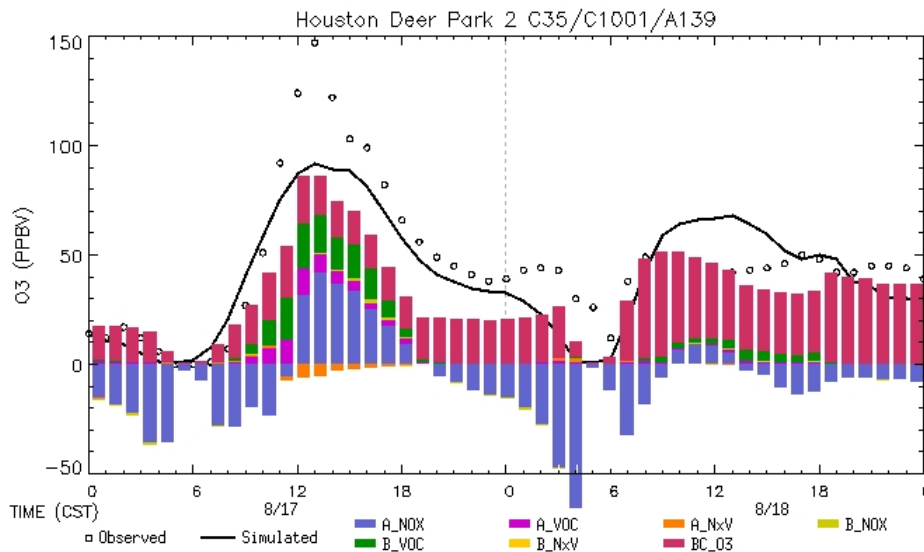
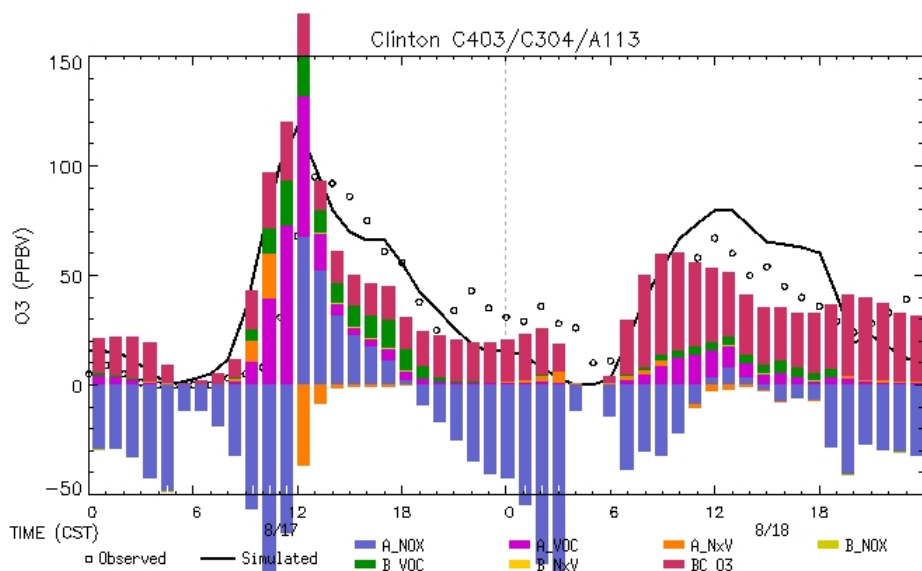


Figure 25. Ozone concentrations and source contributions simulated (a) the base and (b) updated emission at Deer Park for August 17th and 18th, 2006. Domain-wide anthropogenic ('A') and biogenic ('B') NOx and VOC emissions, and the cross-term ('NxV') were used. 'BC_O3' represent ozone transported from boundaries.

(a) Base emissions



(b) Updated emissions

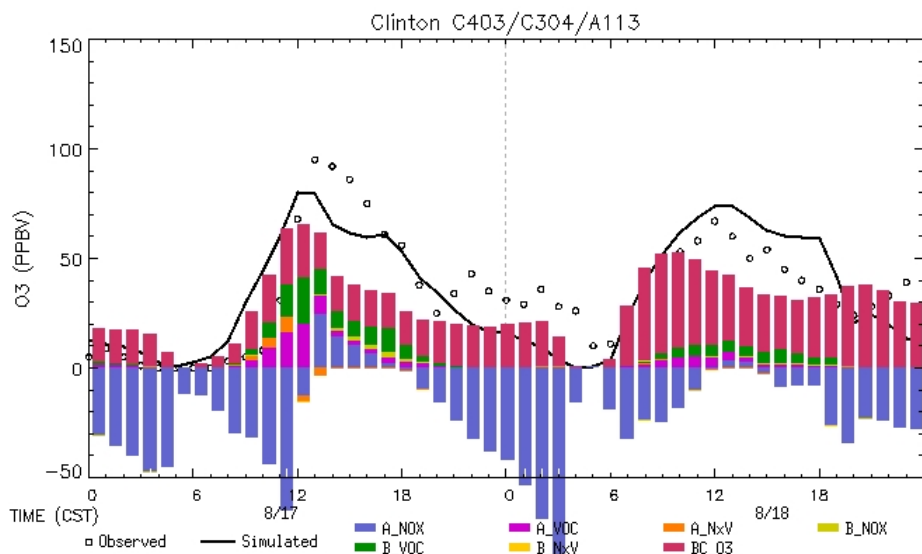


Figure 26. Ozone concentrations and source contributions simulated (a) the base and (b) updated emission at Clinton for August 17th and 18th, 2006. Domain-wide anthropogenic ('A') and biogenic ('B') NO_x and VOC emissions, and the cross-term ('NxV') were used. 'BC_O₃' represent ozone transported from boundaries.

8. Concluding Remarks

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.

Although the University of Houston's ETAQ forecasting systems were capable of forecasting the day-to-day ozone variations in the East Texas in summer 2006, the meteorological predictions were occasionally influenced by strong northeasterly flows due to overly intensified low pressure systems in the Gulf of Mexico. To generate a set of better meteorological inputs representing TexAQS II air pollution episodes, we performed FDDA meteorological simulations utilizing the Meteorological Assimilation Data Ingest System (MADIS) and CAMS data. Performance evaluation led to significant improvement in meteorological inputs to the TexAQS-II air quality simulations. The system predicted precipitation events well in general, but precipitation amounts were usually lower and events occurred a few hours later than observed. Modeled air temperatures agree well with observations except for a few days when the model had difficulties in simulating precipitation events and associated clouds at specific locations. Time series plots for the wind components and speed showed that the meteorological model simulated synoptic changes well, although there were occasional serious overpredictions of easterlies and slight overpredictions of northerlies.

The assimilated meteorological inputs have significantly improved air quality simulations. The CMAQ re-simulations with the TMNS11n2 meteorology inputs predict locations and magnitudes of peak ozone better than those with the AQFn meteorology inputs. The spatial and scatter plots all show that TMNS11n2 meteorology outperforms AQFn. CMAQ simulations with the AQF emissions and TMNS11n2 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 regional average ozone concentrations show serious overprediction of peak ozone for August 23–24 and September 9–10, both sets of days being precipitation episodes. This demonstrates that incorrect prediction of a precipitation event not only skews air quality simulation of the initial precipitation day, but also influences prediction capability on the following days because the initial conditions are daisy-chained with the simulation results of the previous day. The model overpredicted ozone by around 10–15 ppb during southerly wind days suggesting that the boundary ozone concentrations are set too high to represent the air from the Gulf of Mexico. Overprediction of ozone during September 9–12 may be attributed to both the missing precipitation and some weaker southerly flows in the MM5 simulations. Although peak ozone concentrations for August 16, 17, 20, 30, September 2–5, September 8, 14, 15 are well predicted, there are significant underprecipitations for days such as August 29, 31, September 1, 6, and 7.

Additional analyses of meteorology and emission events are needed to understand these discrepancies. In general, lower peak ozone concentrations are predicted by the “cc_03” simulation results compared to TMNS11n2.

To perform air quality simulations for the assessment study, we prepared “best-effort model-ready (BEMR)” 2006 Texas emissions inputs by utilizing the currently available emissions inventories, projected emissions components such as mobile emissions, and the Texas point-source special inventories for the summer 2006 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 a few 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 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) portion of the inventory includes about 165 tons/day of VOC emissions. The updated mobile emissions were projected to 2005 (whereas the base MOBILE6 emissions were projected to 2003) resulting in reductions of NO_x and CO emissions. OLE and ETH emissions in the updated TPSI 2006 emissions are about one third of those in the base emissions. Note that imputed VOCs in the base emissions amount to ~170 tons/day, while no imputation was applied to the updated TPSI2006 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 thicknesses of the lowest model 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, NO_x concentrations predicted by CMAQ with TPSI2006 seem closer to the observations than those predicted with the base AQF emissions.

CMAQ with the base and updated TPSI2006 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 imputed VOCs in the base emissions. When compared with measurements at the University of Houston Moody

Tower, CMAQ simulation results with the base AQF emissions significantly over-predicted OLE and ETH concentrations, while simulation with the updated BEMR/TPSI2006 emissions showed lower values with occasional under-predictions. CMAQ-HDDM source apportionment results with the base emissions show higher contributions of anthropogenic VOC emissions to ozone concentrations than with the updated emissions. Considering that the major changes in anthropogenic VOC emissions resulted from the 2006 special inventory, it is likely that reduced contributions of point source VOCs in the updated emissions led to a decrease in simulated ozone. These analyses suggest that the updated TPSI2006 inventories represent the 2006 conditions better than the base AQF emissions for medium ozone peak days, although emissions of highly reactive species may need to be added to reflect upset events. Further studies targeting detailed comparison of air quality simulations with CAMS and other air quality measurements will be necessary to further verify the TPSI2006 emissions data.

9. References

- Byun, D.W. and J.K.S. Ching, ed., 1999: Science Algorithms of the EPA Models-3 Community Multi-scale Air Quality (CMAQ) Modeling System, EPA Report, EPA/600/R-99/030, NERL, Research Triangle Park, NC. (peer reviewed).
- Byun, D.W., Kim, S.-T, T.C. Ho, and Jerry Lin, 2005: Development of Texas Emissions Inventory Preparation System for SMOKE, Final report for TARC, University of Houston, Houston, TX
- Byun, D.W., S. Kim, F.Y. Cheng, B. Czader, I.-B. Oh, M. Jang, C.-K. Song, H.-C. Kim, P. Percell, F. Ngan, V. Coarfa, and D. Cohan, 2006: HARC Project H60 Final Report. Regional Air Pollution Transport Modeling: Application of CMAQ/HDDM Simulations on Ozone Concentrations over Dallas and Houston Areas, IMAQS, University of Houston, Houston, Texas. (available from <http://files.harc.edu/Projects/AirQuality/Projects/H060/H60UHFfinalReport.pdf>)
- Byun, D.W. and K. L. Schere, 2006: Review of the Governing Equations, Computational Algorithms, and Other Components of the Models-3 Community Multiscale Air Quality (CMAQ) Modeling System. Applied Mechanics Reviews, Volume 59, Number 2, 51-77.
- Byun, D.W., S. Kim, M. Jang, H.-C. Kim, F. Ngan, C.-K Song, X. Li, I.-B. Oh, R. Perna, D.-G. Lee, F. Cheng, B. Czader, and P. Percell, 2007a: East Texas Air Quality (ETAQ) Forecasting: Task 1, Operation of 2006 ETAQ Forecasting System. Final Report for H45C, Houston Advanced Research Center.
- Byun, D.W., F. Ngan, X. Li, D.-G. Lee, and S. Kim, 2007b: Interim Report II: MM5/CMAQ Resimulation of TexAQS-II Phase I: Testing Various Nudging Settings - Datasets, Domains, Radius, and Simulation Hours. Project report for the Texas Commission on Environmental Quality (TCEQ) Grant No. 582-5-64594-FY07-02 "Improved Modeling Inputs: Analysis of Air Pollution Events in Summer 2006 and Preparation of Model Input Data for the Assessment Study".
- Byun, D.W., F. Ngan, X. Li, D.-G. Lee, and S. Kim, 2007c: Interim Report III: MM5/CMAQ Resimulation of TexAQS-II Phase II: Thunderstorm Issues, Nudging with Selected Weather Parameters. Project report for the Texas Commission on Environmental Quality (TCEQ) Grant No. 582-5-64594-FY07-02 "Improved Modeling Inputs: Analysis of Air Pollution Events in Summer 2006 and Preparation of Model Input Data for the Assessment Study".
- Cohan, D., A. Hakami, Y. Hu, A. Russell, 2005: Nonlinear response of ozone to emissions: Source apportionment and sensitivity analysis. Environmental Science & Technology, 39, 6739-6748.
- Guenther, A. B., P. R. Zimmerman, P. C. Harley, R. K. Monson, and R. Fall, 1993: Isoprene and monoterpene emission rate variability: model evaluations and sensitivity analyses. J. Geophys. Res., 98D, 12609-12617.

- Kim, S., and Byun, D.W. , 2003: Prototyping the Texas emissions inventory preparation system for the SMOKE system, 12th International Emission Inventory Conference, San Diego, April 29 - May 1, 2003. (<http://www.epa.gov/ttn/chief/conference/ei12/poster/kim.pdf>).
- Stauffer, D.R., and N.L. Seaman, 1990: Use of Four-Dimensional Data Assimilation in a Limited-Area Mesoscale Model. Part I: Experiments with Synoptic-Scale Data. *Mon. Wea. Rev.*, 118, 1250–1277.
- Stauffer, D.R., N.L. Seaman, and F.S. Binkowski, 1991: Use of Four-Dimensional Data Assimilation in a Limited-Area Mesoscale Model Part II: Effects of Data Assimilation within the Planetary Boundary Layer. *Mon. Wea. Rev.*, 119, 734–754.
- Stauffer, D.R., and N.L. Seaman, 1994: Multiscale Four-Dimensional Data Assimilation. *J. Appl. Meteor.*, 33, 416–434.
- Yarwood, G., Wilson, G., and S. Shepard, 2002: User's Guide to the Global Biosphere Emissions and Interactions System (GloBEIS) Version 3; ENVIRON International Corporation;

List of Figures

Error! No table of figures entries found. Figure 1. Comparison of daily maximum ozone forecasted by ETAQ F1 and F2 forecasting systems with CAMS measurements in the Houston-Galveston-Brazoria area.

Figure 2. Processing steps of the University of Houston's MM5 Multiscale nest-down four-dimensional data assimilation (FDDA) scheme utilizing NOAA WRF-NMM/EDAS inputs.

Figure 3. Surface observations in the extended E12 domain used in the UH Nestdown four-dimensional data assimilation (FDDA) simulations. Blue dots indicate MADIS surface data while pink dots represent CAMS sites. Upper air data, profiler data, sounding data were also used in the assimilation. However, the aircraft data and satellite data are not currently used.

Figure 4. Time series plot of precipitation amounts averaged over the CAMS sites in the HGB domain for the August 16-September 15, 2006 period.

Figure 5. Time series plot of relative humidity averaged over the CAMS sites in the HGB domain for the August 16-September 15, 2006 period.

Figure 6. Time series plot of temperature averaged over the CAMS sites in the HGB domain for the August 16-September 15, 2006 period.

Figure 7. Time series plot of U-wind component averaged over the CAMS sites in the HGB domain for the August 16-September 15, 2006 period.

Figure 8. Time series plot of V-wind component averaged over the CAMS sites in the HGB domain for the August 16-September 15, 2006 period.

Figure 9. Time series plot of wind speed averaged over the CAMS sites in the HGB domain for the August 16-September 15, 2006 period.

Figure 10 (a)-(c). NOAA surface weather charts for August 16-18, at 12:00 UTC.

Figure 11 (a) CMAQ simulation with AQFn (original MM5 forecast), and (b) CMAQ simulation with TMNS11n2 (MM5/FDDA using UH-RDAS) for 15-17 CST, August 16, 2006.

Figure 12 (a) CMAQ simulation with AQFn (original MM5 forecast), and (b) CMAQ simulation with TMNS11n2 (MM5/FDDA using UH-RDAS) for 15-17 CST, August 17, 2006.

Figure 13 (a) CMAQ simulation with AQFn (original MM5 forecast), and (b) CMAQ simulation with TMNS11n2 (MM5/FDDA using UH-RDAS) for 15-17 CST, August 18, 2006.

Figure 14 (a) CMAQ simulation with AQFn and (b) CMAQ simulation with TMNS11n2 compared with CAMS surface ozone measurements in the Houston-Galveston-Brazoria domain for August 14-21, 2006 period.

Figure 15. Emissions of volatile organic compounds (VOCs) from the Houston-Galveston-Brazoria (HGB) point sources. Pink and yellow circles represent the 2006 Texas Point-source Special Inventory (TPSI2006) VOC and Texas ozone-season day (OSD) emissions, respectively.

Figure 16. Daily VOC emission rates from the Texas point source special inventory.

Figure 17. Comparison of hourly emissions rates of (a) NO, (b) CO, (c) OLE, (d) ETH, (e) FORM, and (f) ISOP between the base and updated emissions for the HGB 8-county area during the August 15–September 15, 2006. Red and blue lines represent the base AQF (designated as “F2”) and updated BEMR/TPSI2006 (designated as “S106”) emissions respectively.

Figure 18. Time series plot of CO concentrations averaged over the CAMS sites in the HGB domain for the August 16–September 15, 2006 period.

Figure 19. Time series plot of NO concentrations averaged over the CAMS sites in the HGB domain for the August 16–September 15, 2006 period.

Figure 20. Time series plot of NO₂ concentrations averaged over the CAMS sites in the HGB domain for the August 16–September 15, 2006 period.

Figure 21. Time series plot of ozone concentrations averaged over the CAMS sites in the HGB domain for the August 16–September 15, 2006 period.

Figure 22. Scatter plots of the simulated ozone concentrations averaged over the CAMS sites in the HGB domain for the August 16-September 15, 2006 period. (a) CMAQ with base AQF emissions and (b) with best-effort model-ready emissions with 2006 Texas special point source inventories (BEMR/TPSI2006).

Figure 23. Hourly ozone concentrations simulated with the base (blue, Q150) and updated TPSI2006 (red, Q149) emissions for the period of August 16–24, 2006. Observed and simulated ozone concentrations are averaged over the CAMS sites inside the HGB area.

Figure 24. Hourly (a) olefin (OLE) and (b) ethylene (ETH) concentrations compared to the Moody tower measurements for the period of August 16–26, 2006. Blue and red lines represent simulations with base and updated emissions, respectively.

Figure 25. Ozone concentrations and source contributions simulated (a) the base and (b) updated emission at Deer Park for August 17th and 18th, 2006. Domain-wide anthropogenic (‘A’) and biogenic (‘B’) NO_x and VOC emissions, and the cross-term (‘N_xV’) were used. ‘BC_O3’ represent ozone transported from boundaries.

Figure 26. Ozone concentrations and source contributions simulated (a) the base and (b) updated emission at Clinton for August 17th and 18th, 2006. Domain-wide anthropogenic ('A') and biogenic ('B') NO_x and VOC emissions, and the cross-term ('NxV') were used. 'BC_O3' represent ozone transported from boundaries.

List of Tables

Table 1. Emissions inventories used for the base AQF and the “best-effort model-ready” (BEMR) Texas Emission Inputs.

Table 2. Point source emissions files used with the 2006 Texas point-source special inventory

Table 3. VOC emissions from HGB 8 counties for August 15, 2007

Table 4. Split factors of monoterpenes and other VOC emissions for the CB-4 chemical mechanism

Table 5. Statistics of 1-hour ozone simulations with the base and TPSI2006 emissions.