The Second Texas Air Quality Study: Atmospheric Measurement and Modeling to Study Photochemical Processes and Emissions Uncertainties

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TexAQS 2000 has found that

- Houston’s bad air quality is mainly due to very large amount of volatile organic carbons from the regional petrochemical industries, NOx emissions from traffics and power plant.

- The severity of the ozone air quality problem is closely associated with the recirculation flows resulting from the interaction of synoptic weather system and local land-sea breeze

- Large uncertainties in the highly reactive olefin emissions is the key stumbling issues developing efficient emission control measures

- TCEQ “imputed” olefin emissions to develop State Implementation Plan
To assess if the emissions control measures implemented since 2000 were effective and if there are any changes in the significant sources of ozone and aerosol pollution in eastern Texas

Further investigate photochemical and meteorological processes involved in the production, transport, and accumulation of these pollutants

To provide assessment of the adequacy of emissions inventories for both biogenic and anthropogenic sources of ozone and aerosol precursor chemicals

To assess the skill of current air quality modeling and forecasting systems.


-- from Rapid Science Synthesis Report (Cowling et al., 2007)
Air Quality Forecasting for TexAQS-II

**Download**
ETA Forecast

**54 hr forecasting simulation**

**Post-Process**
Visualization
Statistics
Web Display

**MM5 simulations (24 CPUs)**
- 36 km domain
  - 1st day
- 36 km domain
  - 2nd day

**F1=2000 imputed, Houston; F-2=2005 projected, E-Texas**
- 12 km domain
  - 1st day
- 12 km domain
  - 2nd day
- 04 km domain
  - 1st day
- 04 km domain
  - 2nd day

**CMAQ simulations (36 CPUs)**
- 36 km domain
  - 1st day
- 36 km domain
  - 2nd day
- 12 km domain
  - 1st day
- 12 km domain
  - 2nd day
- 04 km domain
  - 1st day
- 04 km domain
  - 2nd day

- MCIP 36 km
  - 1st day
- SMOKE 36 km
  - 1st day
- MCIP 36 km
  - 2nd day
- SMOKE 36 km
  - 2nd day
- MCIP 12 km
  - 1st day
- SMOKE 12 km
  - 1st day
- MCIP 12 km
  - 2nd day
- SMOKE 12 km
  - 2nd day
- MCIP 04 km
  - 1st day
- SMOKE 04 km
  - 1st day
- MCIP 04 km
  - 2nd day
- SMOKE 04 km
  - 2nd day

**Batch mode operation with minimal intervention**

**Multi CPU**

**Data Flow**
What configurations were used for ETAQ-F 2006?

• ETAQ-F 2006  F1 & F2

Meteorology (F1 & F2 used UH MM5)
  * high-resolution Satellite observation based LULC data
  * improved MRF for stable PBL and transition times (under development)
  * cloud; both the subgrid scale explicit scheme at 4-km

Emissions (F1 = 2000 SIP TEI vs. F2 = 2005* projected)
  + 2000 Imputed alkene emissions from Houston Ship Channel
    * 2005 TEI (projected from 2000 (imputed emission) & 2007)
    * 2000 HRVOC (instead of 2005 projected)
    * Mobile projected for 2003
  \* See slides later…..

CMAQ (F1 = HGB 4-km vs. F2 = Extended 4-km (HGB + DFW)
  * CB4 for forecasting and SAPRC99 for evaluation
Modeling Domains – F2, TexAQS-II
Improvement of Meteorological Modeling for Air Quality Assessment

AQF was successfully used for the planning and implementation of TexAQS-II experiment, but we found systematic problems

- Over-prediction of northerly wind caused by inaccurate synoptic input.
- Too strong southerly caused by sea breeze development.
- Discrepancies in max & min temperature for certain days.
- Precipitations & clouds not simulated well occasionally.

For the retrospective meteorological modeling, we applied the “MUltiscale Nest-down Data Assimilation System (MUNDAS)”, which utilized extensive measurements and recursive application of the objective analysis/FDDA method across multiple domains with different resolutions (36-, 12-, to 4-km resolution)
Transition to Assessment Study: MM5
AQF vs. Assimilation

- NCEP NMM (ETA, WRF/NMM)
- CAMS, METARs, NPN profilers, sounding

Ad-hoc tool:
Multi-stage FDDA
12- and 4-km domaina

No time to develop a fancy scheme
Because we need the met data “now”

Intermediate files of REGRID for fine domain

12-, 4-km domains
Multi-step assimilation

Grid data (EDAS data)
Observations (MADIS + CAMS)
In T11, Wind was slow down that convergence ozone could be formed at the afternoon.

Certain days, it improves air quality simulations greatly.

With T11 met., O3 was able to build up & location of peak stayed south of downtown.
Phase III: 8/14 – 10/5 (54 days)

Regional average of observed and model 1.5 m temperature

No T & RH nudging at both SFC & upper level

T11 better generated max & min temp than AQF for certain days

Precip. had strong impact on variation of SFC temp.
Phase III: 8/14 – 10/5 (54 days)

Regional average of observed and model 1st wind speed

(a) T11 wind matches better to OBS than AQF

(b)

9/1

9/10

9/21
Reduce O3 model biases by improving meteorology through data assimilation

O3 averaged over the CAMS sites in the HGB domain for Aug. 16-Sept. 14, 2006 (upper) and Sept. 15 – Oct. 6, 2006 period (lower).
Warm sector – southerly and cloudy – low ozone
September 23
Warm sector – southerly and cloudy – low ozone

06 CST

September 24
Frontal passage
Cloudy, rainy

September 25

September 26
CMAQ, CB-4, F2 Projected with 2000 Imputed vs. Reduced Imputation to 2005 level

September 19, 2006

Ozone Conc. at 20060919:12cst [TMNS11n2]

Ozone Conc. at 20060919:15cst [TMNS11n2]

September 20, 2006

Ozone Conc. at 20060920:12cst [TMNS11n2]

Ozone Conc. at 20060920:15cst [TMNS11n2]
CMAQ, CB-4, F2 Projected with 2000 Imputed vs. Reduced Imputation to 2005 level

September 25, 2006

September 26, 2006
Highlights of O3 simulation

• Model generally captured the daily ozone cycle well, although there were some night-time overprediction.

• 08/23, model overpredicted the low ozone values in the daytime due to the MM5’s failure of simulating precipitation events in HGB. High bias continued to linger (08/24, 08/25) due to the daisy-chained I/Cs used.

• Overpredicted ozone by around 10 to 15 ppb during southerly wind days (08/26-27, 09/16 – 17, 09/21 – 23) when erroneous high ozone drift problem LA.

• Overprediction of ozone during 9/9 – 9/12 are also attributed to both the missing precipitation and some weaker southerly flows in the MM5 simulations compared to the observations.

• Significant overprediction of regional average ozone concentrations on 9/30 – 10/01 is probably caused by the much less cloud cover simulated by MM5.
# Updated Emission Inventory for 2006 Summer

TCEQ collected 2006 raw hourly point-source special inventories from industry.

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

<table>
<thead>
<tr>
<th>Emission Type</th>
<th>Base AQF</th>
<th>BEMR</th>
</tr>
</thead>
<tbody>
<tr>
<td>Area &amp; Non-road</td>
<td>Base5b 2000</td>
<td>Base5b 2007 (TCEQ)</td>
</tr>
<tr>
<td>On-road</td>
<td>Linked-based and HPMS MOBILE6 projected for 2003</td>
<td>Linked-based and HPMS MOBILE6 projected for 2005</td>
</tr>
<tr>
<td>Point</td>
<td>Base5b regular emissions projected for 2005 &amp; additional VOC for 2000 imputation</td>
<td>2006 Texas point-source special inventory (TPSI2006)</td>
</tr>
<tr>
<td>Biogenic</td>
<td>TCEQ's 2000 LULC and MM5 meteorology</td>
<td>TCEQ's 2006 biogenic emissions</td>
</tr>
<tr>
<td>Supplementary</td>
<td>NEI99</td>
<td>NEI2002</td>
</tr>
</tbody>
</table>
Updated Emission Inventory for 2006 Summer

TCEQ collected 2006 raw hourly point-source special inventories from industry.

Emissions of volatile organic compounds (VOCs) from the Houston-Galveston-Brazoria (HGB) point sources. Pink and yellow circles represent TPSI2006 and VOC and Texas ozone-season day (OSD) emissions, respectively.
Updated Emission Inventory for 2006 Summer
TPSI 2006 vs. AQF2 (NO, CO and Isoprene)

Biogenic emissions between 2000 vs. 2006 inventories (from TCEQ)
Updated Emission Inventory for 2006 Summer

TPSI 2006 vs. AQF2/imputed emissions
Air quality simulations with BEMR 2006 and AQF2

TPSI 2006 vs. AQF2/imputed emissions (regional average)
Air quality simulations with BEMR 2006 and AQF2

TPSI 2006 vs. AQF2/imputed emissions

Regional average do not represent different emissions impact properly for O3 !
(dominated by the boundary flux)

Comparison with for all the Individual CAMS sites:
BEMR/TPSI shows less scatter
But lacks reactivity significantly!
→ Need HRVOC emissions for 2006 as well
Summary

◆ MM5/FDDA re-simulation with CAMS, MADIS, others
- Reduction of WD & Speed biases and more realistic flow variations overall
- But, some unwanted flow patterns due to difficulties in T-Storm simulations

◆ Emissions
- AQF1 (2000 TEI) with 2000 TCEQ imputed alkene too high NOx and VOC....
- AQF2 (2005* projected) with 2000 TCEQ imputed alkene ~ OK
- BEMR/TPSI2006 – lower NOx, CO, and VOC than AQF2

◆ CMAQ re-simulation results
- Used of TMNS112n meteorology quite successful
  But not always improves met & air quality simulation results
  - Shows effects of evening mixing and wind speed bias

Used of BEMR/TPSI
- Less scatter
- lacks some O3 reactivity…
- Need substantial amount of additional HRVOC emissions over TPSI2006
- Upset event simulation issues existing for certain days

http://www.imaqs.uh.edu/          Acknowledgement: HARC, TCEQ, EPA, NOAA, NASA