

Proposed Research: Air Quality Modeling for TexAQS-II

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Air Quality Forecasting Needs

- Better meteorological simulations
- Reliable emissions inventories
- Better initial conditions
- Better boundary conditions

Evaluation AQM with TexAQS-II measurements

- Investigate chemical mechanisms and HCHO issues
- Data assimilation with EnKF – meteorology (by TAMU?)
- CMAQ/adjoint/4D-var applications to estimate IC/BC & EI uncertainty using TexAQS-II data
- Comprehensive chemistry data assimilation – surface, in-situ, remote sensing including satellite chemistry data (long-term)

How sensitive is the result to the chemical mechanism and emissions inventory

CB4

SAPRC99

SAPRC99-Extended

Chemical mechanisms used in Eulerian grid modeling [SAPRC99, CB-4, CB05, RADM2] use simplified set of chemical compounds and reactions to describe atmospheric chemistry occurring in the air.

SAPRC99 [Carter 2000]

for example alkenes (except ethene and isoprene) are represented by

OLE1 – Alkenes (other than ethene) with $k_{OH} < 7 \cdot 10^4 \text{ ppm}^{-1} \text{ min}^{-1}$

OLE2 – Alkenes with $k_{OH} > 7 \cdot 10^4 \text{ ppm}^{-1} \text{ min}^{-1}$

Compound	SAPRC99	SAPRC99 extended
Propene	OLE1	PROPENE
1,3-Butadiene	OLE2	BUTD13
1-butene	OLE1	BUTE1
trans-2-butene	OLE2	BUTE2T
cis-2-butenes	OLE2	BUTE2C
2-methyl-1butene	OLE2	BUTE1_2M
2-methyl-2butene	OLE2	BUTE2_2M
3-methyl-1butene	OLE1	BUTE1_3M
2-methylpropene	OLE2	BUTE_I
1-Pentene	OLE1	PENTE1
1-Hexene	OLE1	HEXENE1
1-Decene	OLE1	DECENE1
PROPANE	ALK2	C3
2-methyl-propane	ALK3	C3_2M
n-Butane	ALK3	C4
n-Pentane	ALK4	C5
2-methyl-butane	ALK4	C4_2M
n-Hexane	ALK4	C6
Cyclohexane	ALK5	CYCC6
Methyl-tert-butyl-ether	ALK3	MTBE
Methyl ethyl ketone	MEK	M_E_KETONE

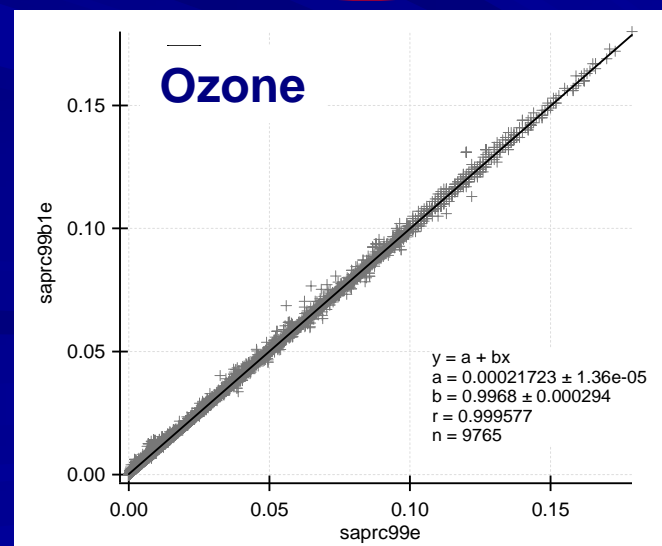
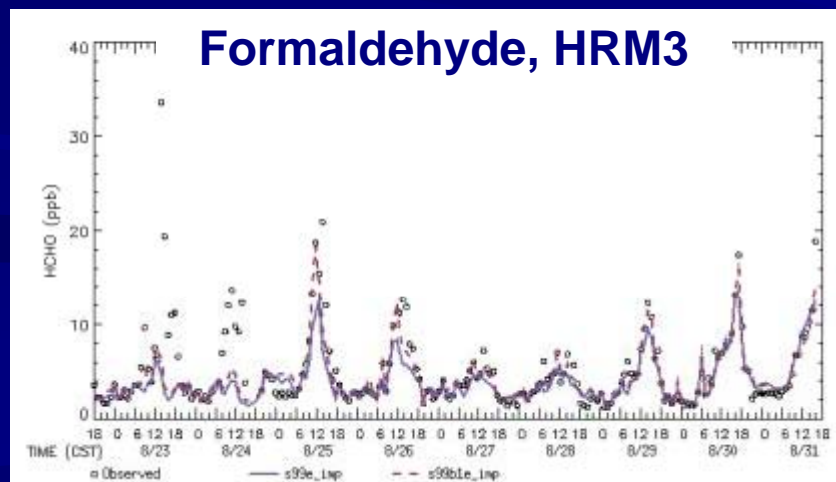
Evaluation of SAPRC99 extended chemical mechanism

Reaction constant of alkenes and OH radical has changed ($\text{cm}^3 \text{ molec}^{-1} \text{ s}^{-1}$)

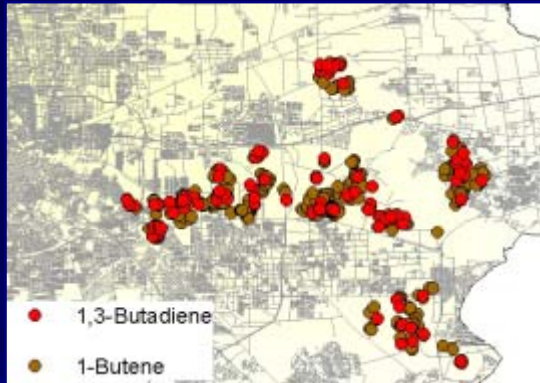
OLE1	saprc99	
propene		$32.3 * 10^{-12}$
1-butene		$26.3 * 10^{-12}$
3-methyl-1butene		$31.4 * 10^{-12}$
1-pentene		$31.4 * 10^{-12}$
1-hexene		$37 * 10^{-12}$

OLE2	saprc99	
1,3-butadiene		$63.1 * 10^{-12}$
trans-2-butene		$66.6 * 10^{-12}$
cis-2-butenes		$64.0 * 10^{-12}$
2-methyl-1-butene		$56.4 * 10^{-12}$
2-methyl-2-butene		$61 * 10^{-12}$
2-methylpropene (isobutene)		$86.9 * 10^{-12}$

Propene reaction with hydroxyl radical in SAPRC99 and SAPRC99 extended. Explicit representation of propene results in increased formaldehyde (HCHO) yield.

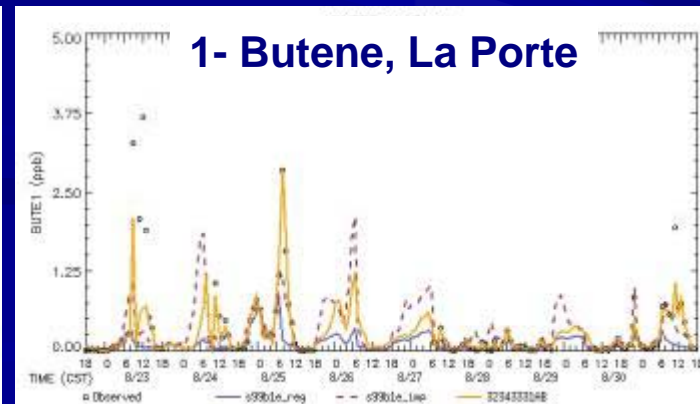
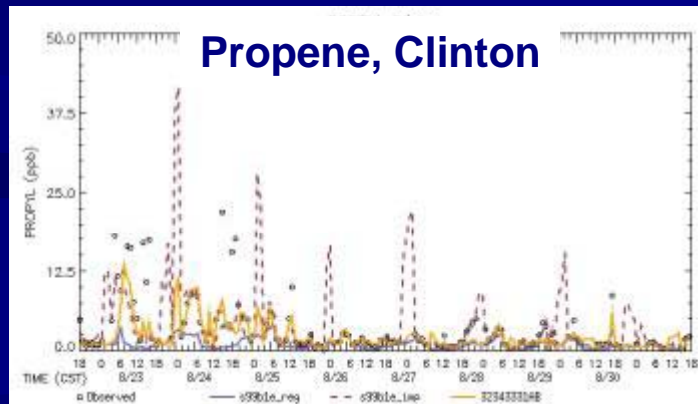
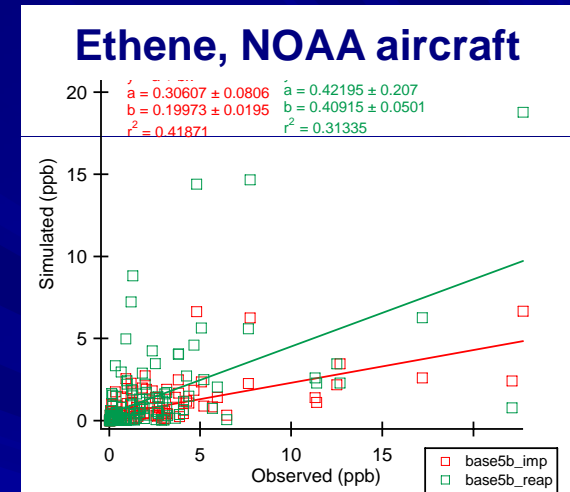
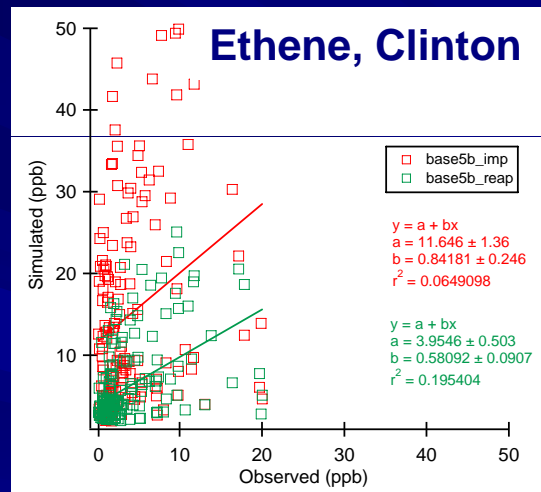


Reapportioned inventory



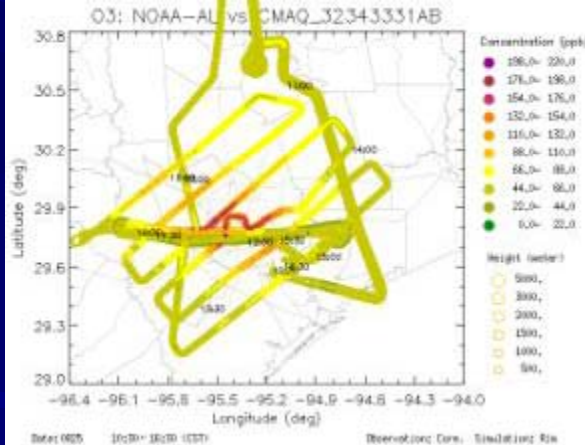
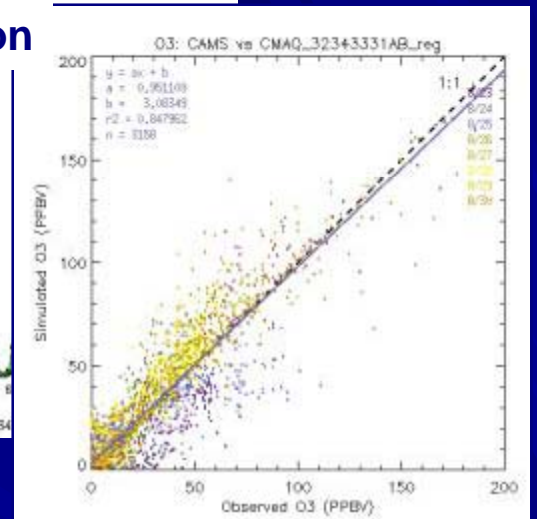
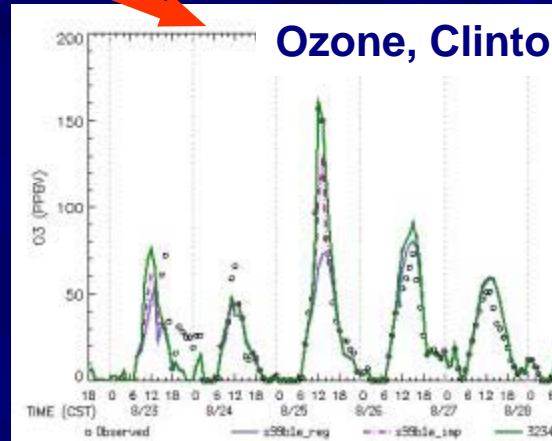
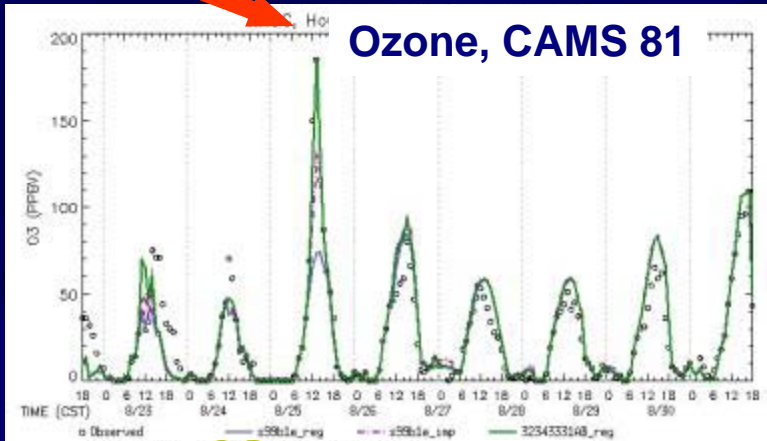
Additional emissions of individual compounds were estimated based on the **reapportioned inventory** from the Texas Commission on Environmental Quality (TCEQ). They were added to the regular base5b inventory.

TCEQ 2000 “imputed”
vs.
2000 “reapportioned”
inventories

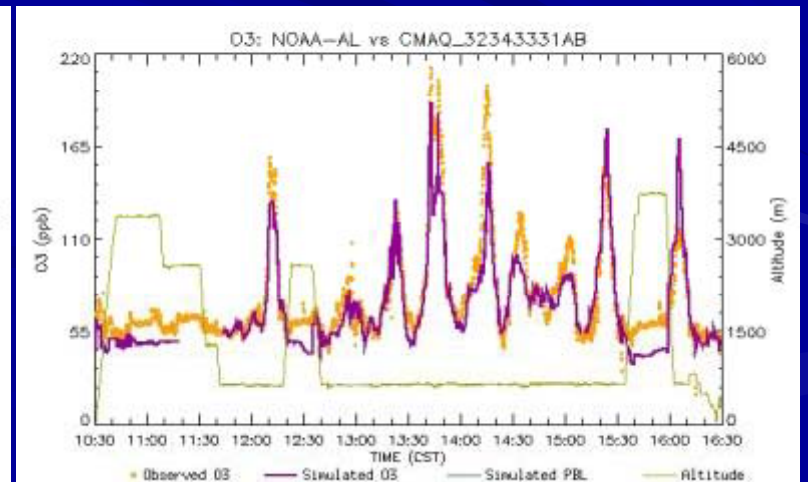
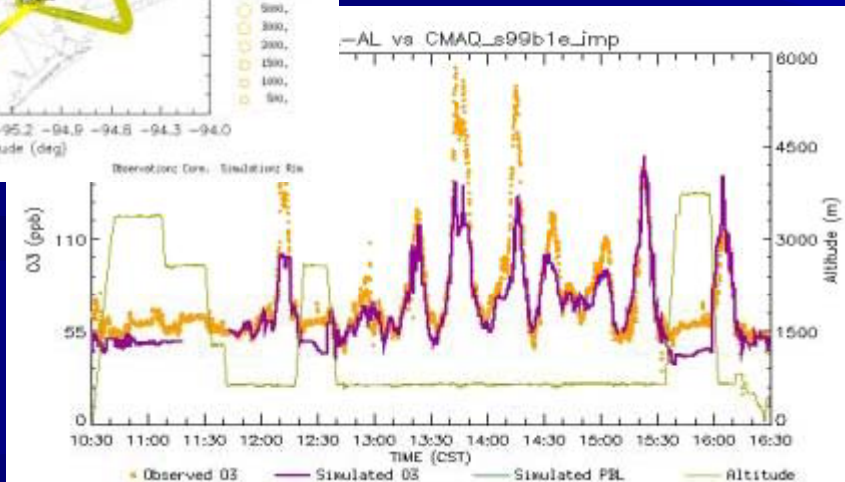


Comparison of Ozone Predictions

Surface, now even better than before,,,,,

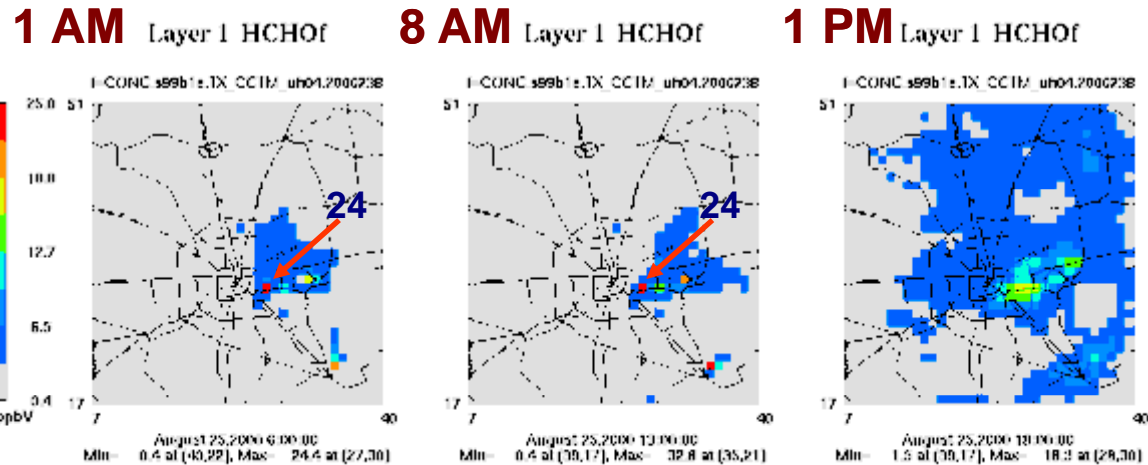


Aloft -- explicit mechanism & newer inventory improves the O3 prediction – will it reduce HCHO bias too?

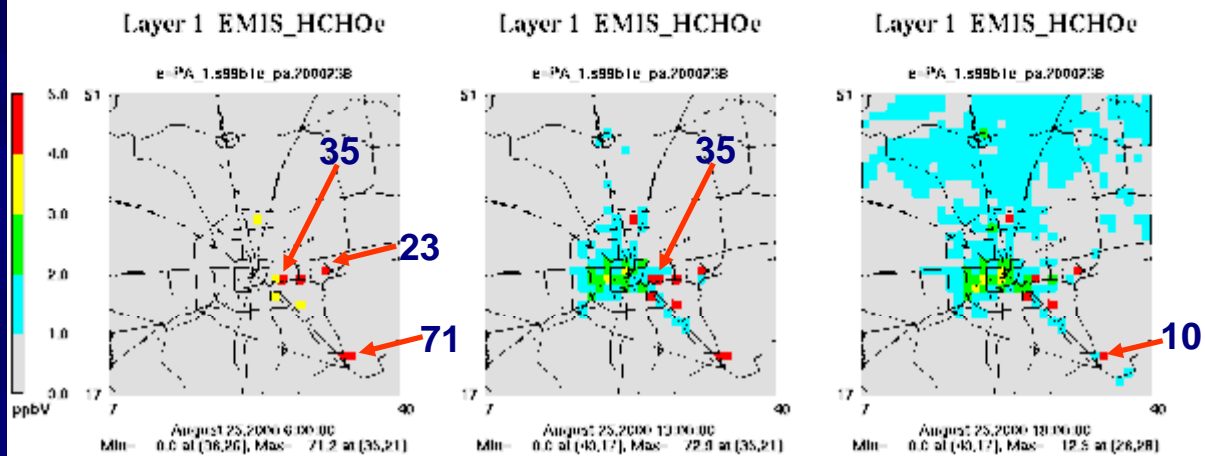


Aug. 25, 2000

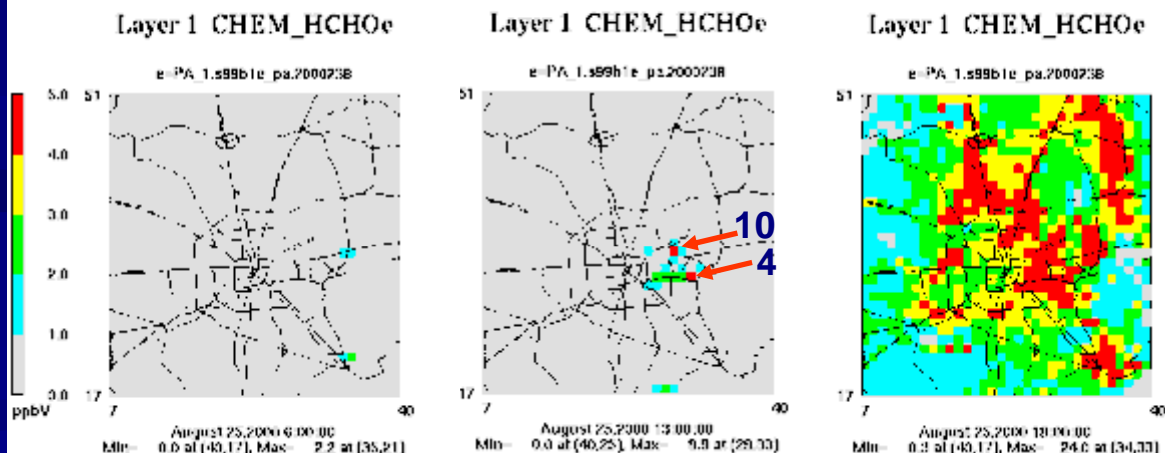
CONC



EMIS



CHEM



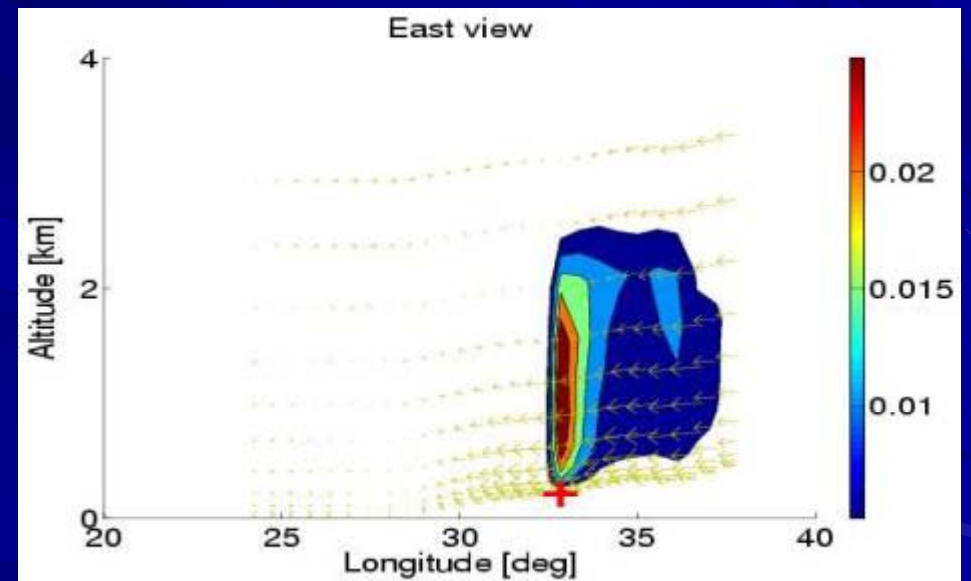
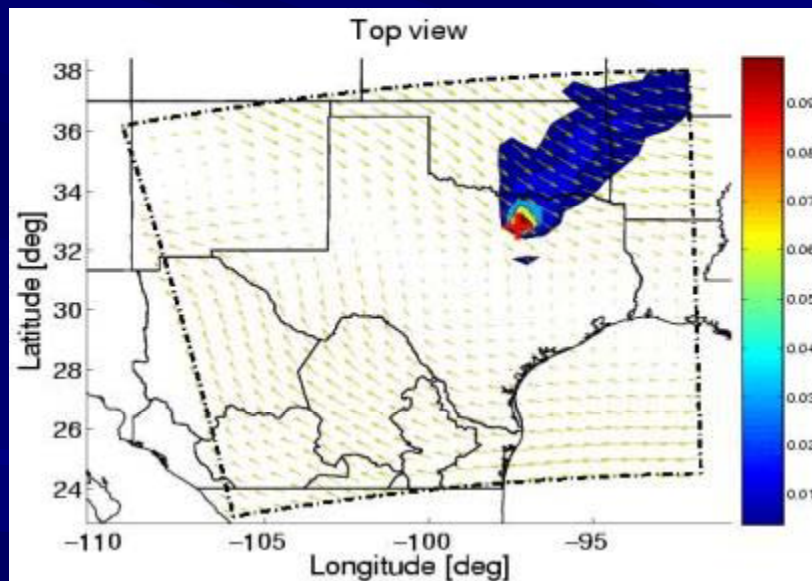
Using TexAQS-II measurements, this part of research will study

- Study the impact different chemical mechanisms simulating HGA air quality and how to “fix” deficiencies in the SAPRC for low NOX conditions
- Study the direct HCHO emissions influence on early morning O3 increase near the Ship Channel and other part of HGA
- Study causes of the large discrepancy in HCHO compared to aircraft data
- Reduce significant under-representation of elevated secondary HCHO sources – possibly from ethylene, propylene

Next item: CMAQ/adjoint/4Dvar applications to estimate IC/BC & Emissions uncertainty (collaboration with Adrian Sandu, Virginia Tech)

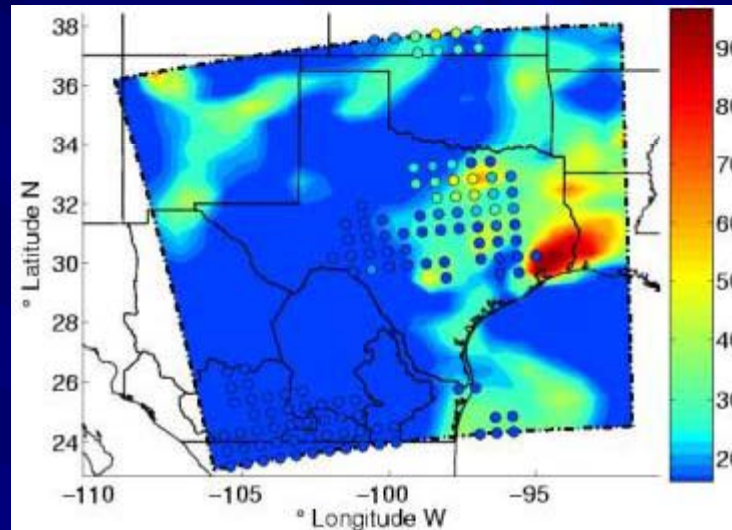
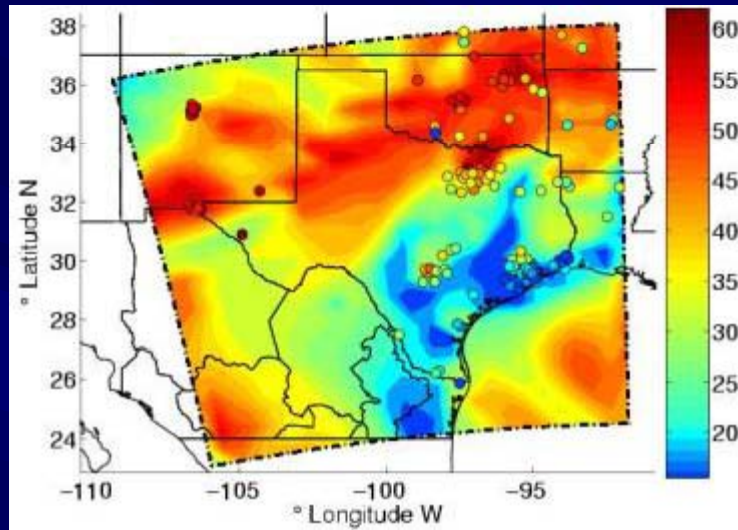
CMAQ/Adjoint for IC/BC/EI improvement for AQM

- CMAQ/4DVar developed under H59!
- Utilize TexAQS-II measurements
- Perform adjoint sensitivity simulations to compare with DDM results

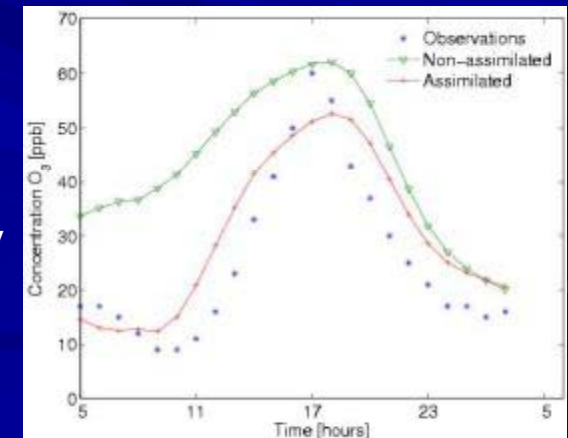


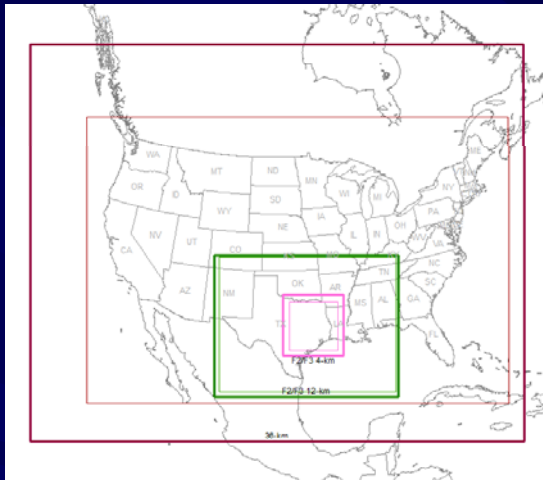
the adjoint sensitivities can be used to calculate the influence of distant and local sources on ozone distributions over Texas for July 25, 2005.

CMAQ/4Dvar example (with STEM)



The data used in the assimilation experiments for July 16, 2004. (a) AIRNow ground level O₃ data and model predictions at 2pm CST, July 16, 2004. (b) SCHIAMACHY NO₂ column data and model predictions at 10am CST, July 16, 2004. (c) Ground level O₃ time series at DFW shows a considerable improvement between model predictions and observations after data assimilation.





Domains to be used
For CMAQ/4Dvar

Objective 1. *Evaluate regional air quality forecasting system through downscale linkage of global model output: Adapt the RAQMS output for the TexAQS-II project period.*

Objective 2. *Estimate of initial conditions, boundary conditions for the modeling using CMAQ/4Dvar*

Objective 3. *Study emissions uncertainty with CMAQ/4Dvar with rich TexAQS-II data*

Objective 4. *Evaluate the overall system performance with TexAQS-II measurements*

Cost:

Research item #1 Investigate chemical mechanisms and HCHO issues ~ 100K

Research item #2 CMAQ/4DVar ~ \$150K (UH: \$80K, VT: 70K) total ~ \$250K