

1 September Preview - Rapid Science Synthesis

<http://esrl.noaa.gov/csd/2006/rss/>

Questions **F, K** - VOC vs. NO_x Sensitive Photochemistry

- **Model based analysis** (Revisit 25 August discussion)

Questions **A, C, D, E** - Emissions: **Ronald Brown Data**

- **Ship channel industrial emissions revisited**
- **HVROC 2006 vs. 2000**
- **Ethylene, ammonia spatial emission distribution**
- **Ship emission characterization**

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- **Comparison of THOE vs. 8-hour avg. ozone:** (Mark Estes)

Questions **G, H** - Regional Background O₃ and aerosol:

- **Ozone fluxes from NOAA Twin Otter Lidar aircraft**
(Mike Hardesty)
- **Ozone and CO profiles from TES on AURA**
(Kevin Bowman, Jay Al-Saadi)

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Preliminary Data & Analysis

Questions F, K - VOC vs. NO_x Sensitive Photochemistry

- **Model based analysis** (Kim, Frost, Hsie, Trainer, Peckham, Grell)

Compare modeled NO₂ and O₃ levels using emissions from NEI 1999 vs. NEI 1999 updated with 2004 CEMS data

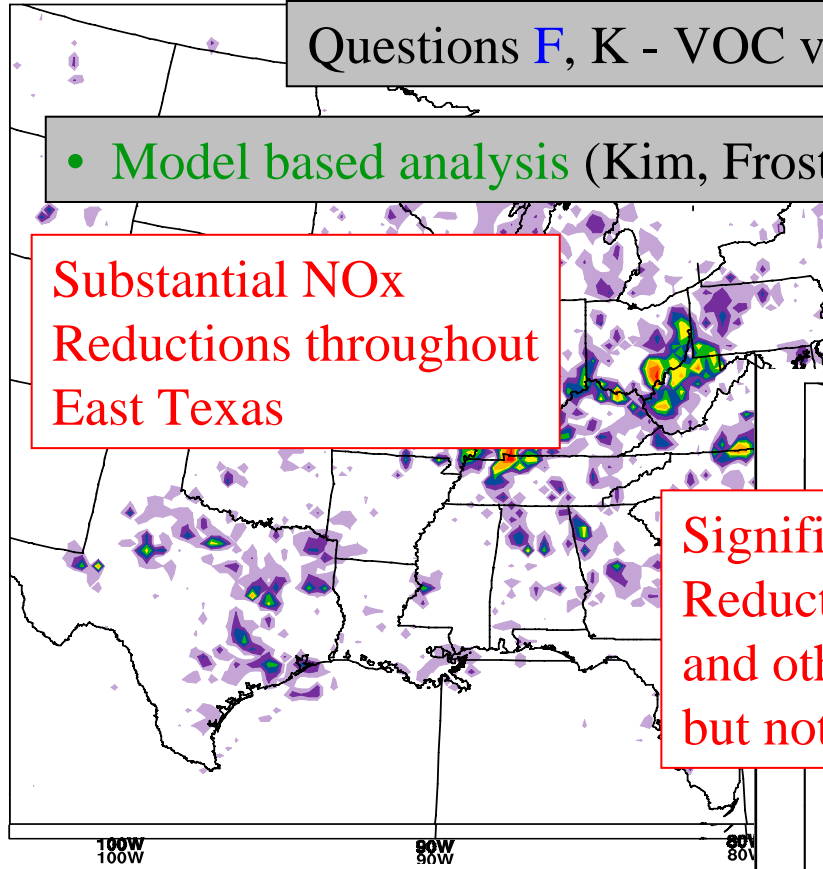
Analysis focused on maximum 8-hour average O₃

Questions F, K - VOC vs. NO_x Sensitive Photochemistry

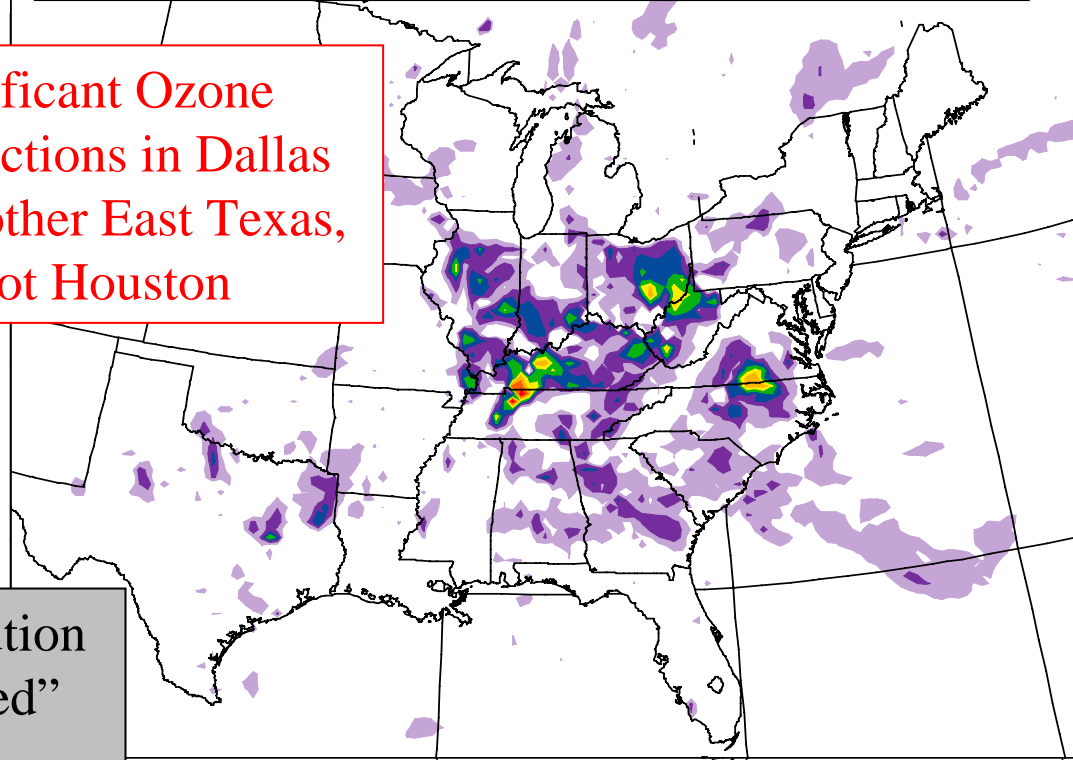
- Model based analysis (Kim, Frost, Hsie, McKeen, Trainer, Peckham, Grell)

Substantial NO_x Reductions throughout East Texas

Compare modeled NO₂ and O₃ levels using emissions from NEI 1999 vs. NEI 1999 updated with 2004 CEMS data



Significant Ozone Reductions in Dallas and other East Texas, but not Houston



Percent surface NO₂ ch
-80 -70 -60 -50 -40 -30

Percent surface O₃ change
-19 -17 -15 -13 -11 -9 -7 -5

WRF-Chem Model: 27 km grid resolution
NEI 1999 without HRVOC “enhanced”
In Houston area, only Parish EGU significant reduction

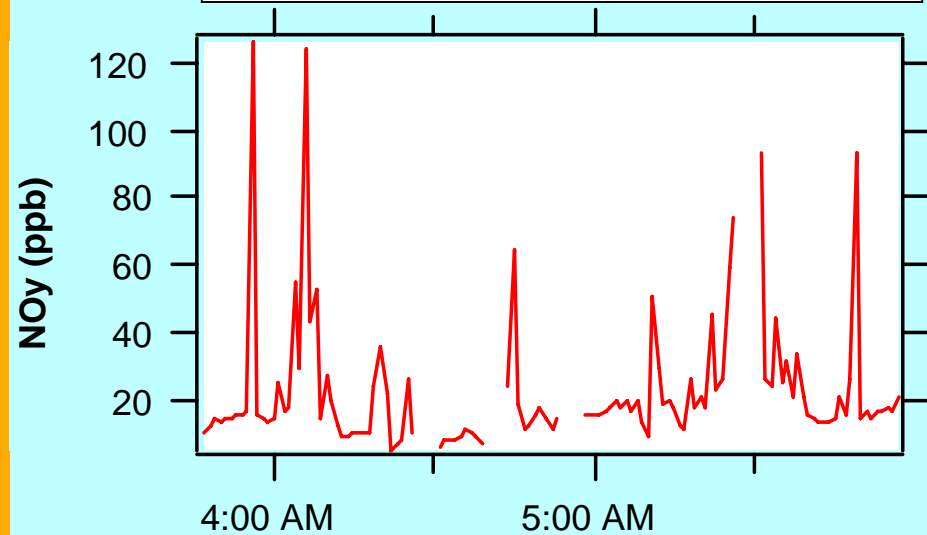
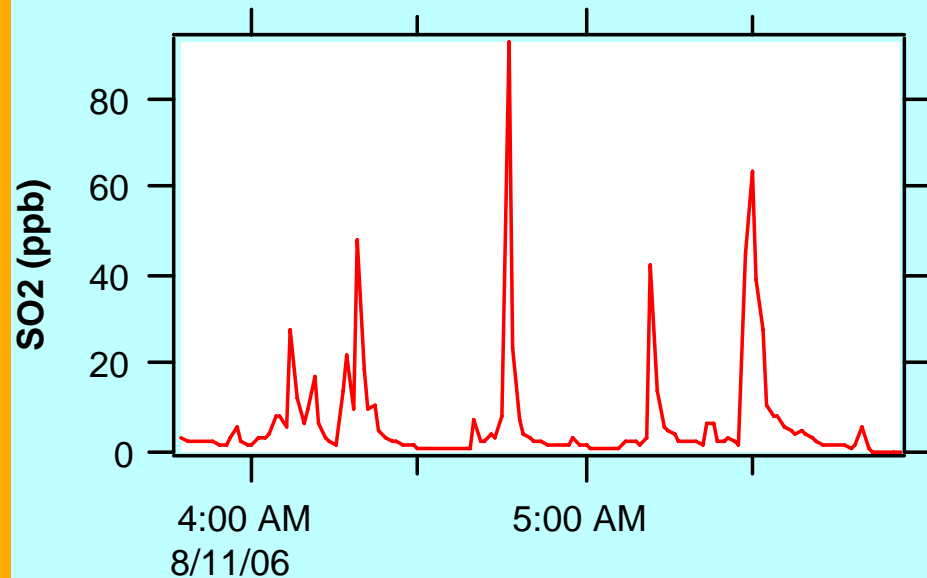
“The devil is in the details”

Questions A, C, D, E - Emissions: Early RHB Data

- **Ship Channel Industrial Emissions**

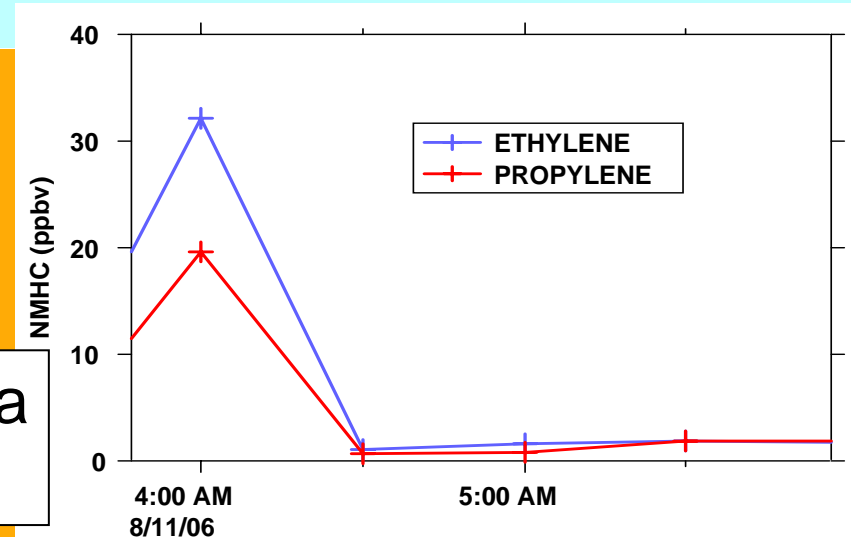
(Eric Williams, Bill Kuster, et al.)

(1 minute average data)

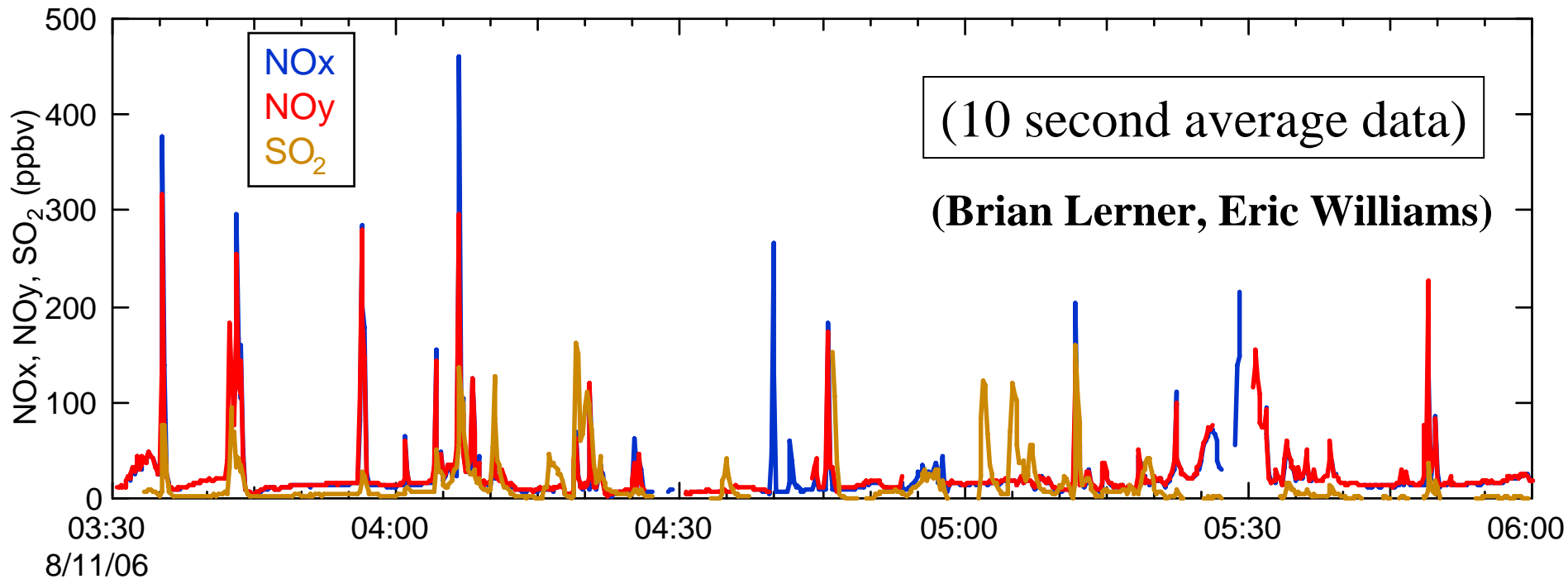


- Many plumes with different emission ratios
- At least some are rich in HRVOC

(5 minute average data every 30 minutes)

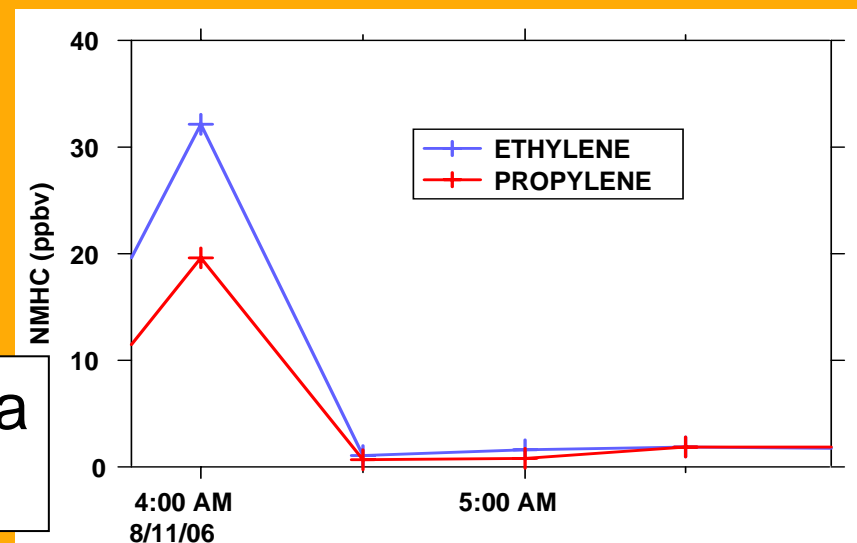


Questions A, C, D, E - Emissions: Early RHB Data

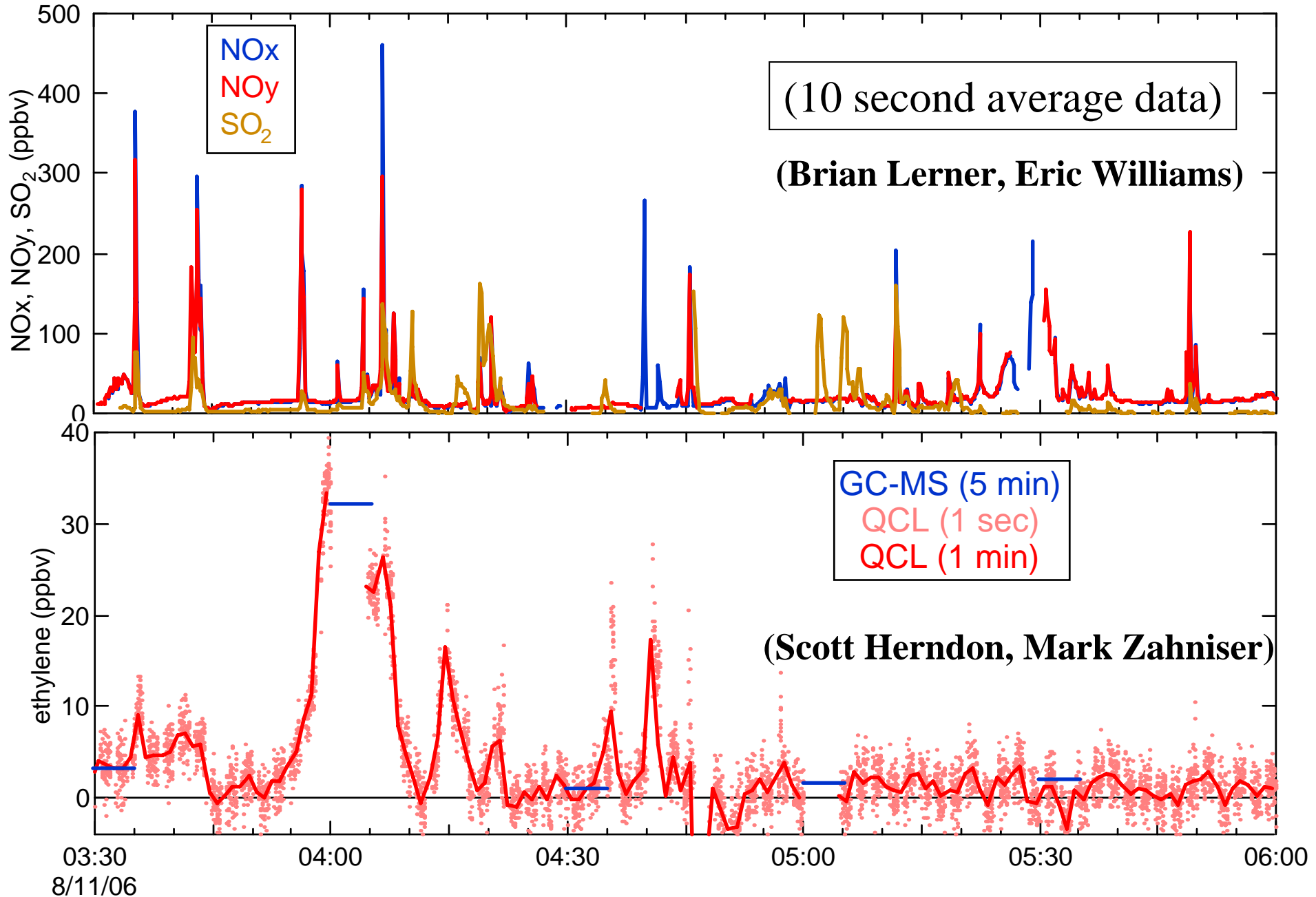


- Many plumes with different emission ratios
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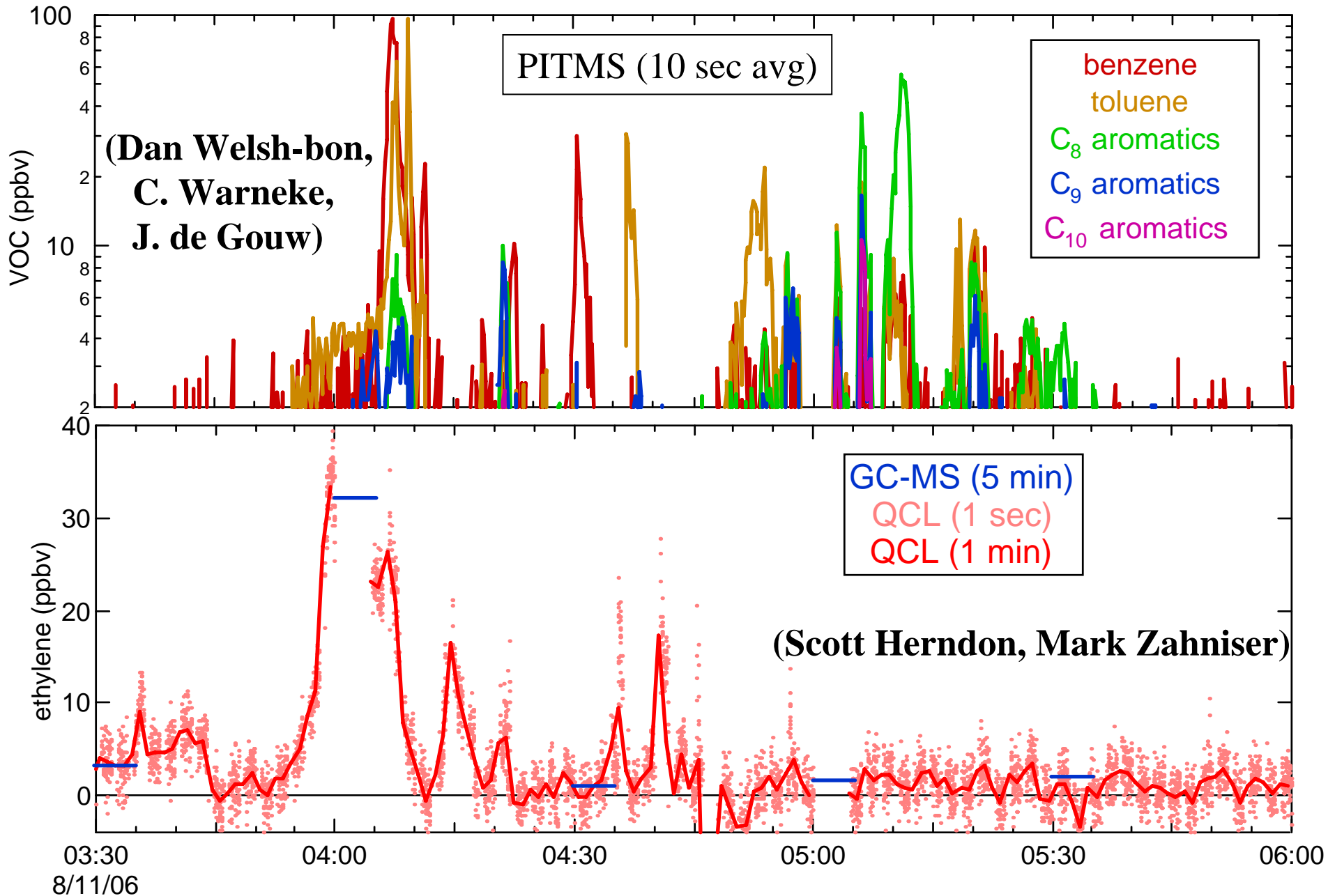
(5 minute average data every 30 minutes)



Questions A, C, D, E - Emissions: Early RHB Data



Questions A, C, D, E - Emissions: Early RHB Data



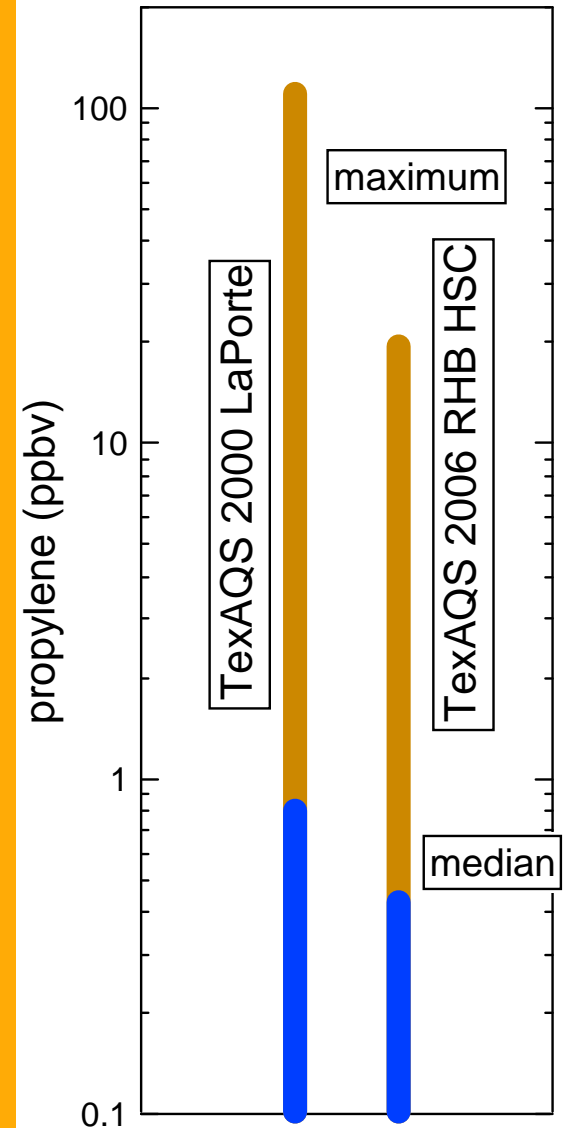
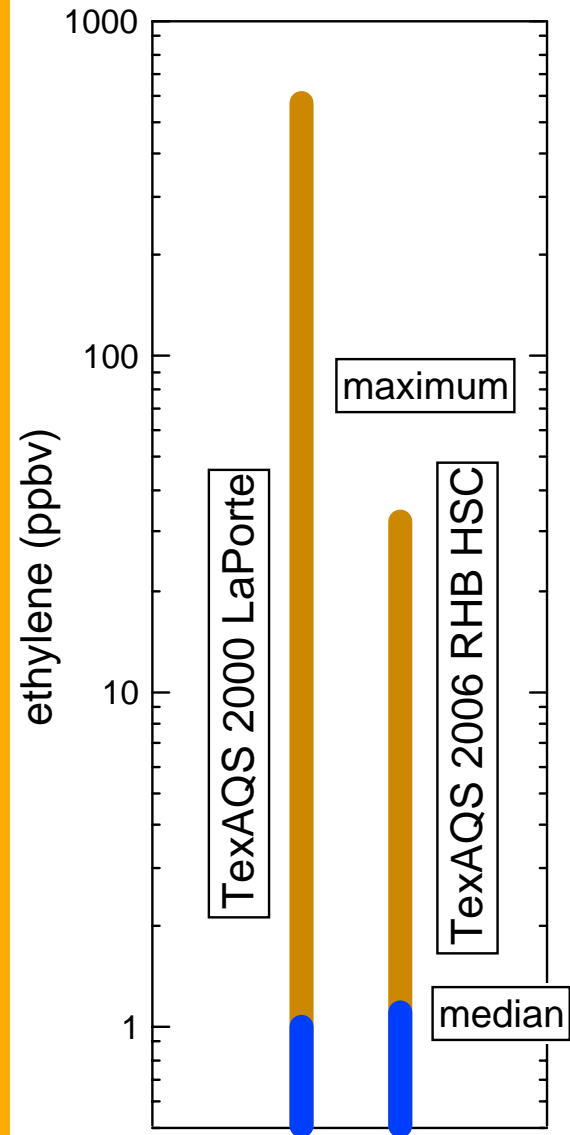
Questions A, C, D, E - Emissions: Early RHB Data

Significant change
in emissions?

High variability
makes significant
comparison
difficult

GC-MS 5 min
Avg. data

(Bill Kuster,
Jessica Gilman)



Ship Position 8/3 - 8/17 2006

UTM Zone 15 (km Northing)

3300
3280
3260
3240



280 300 320 340

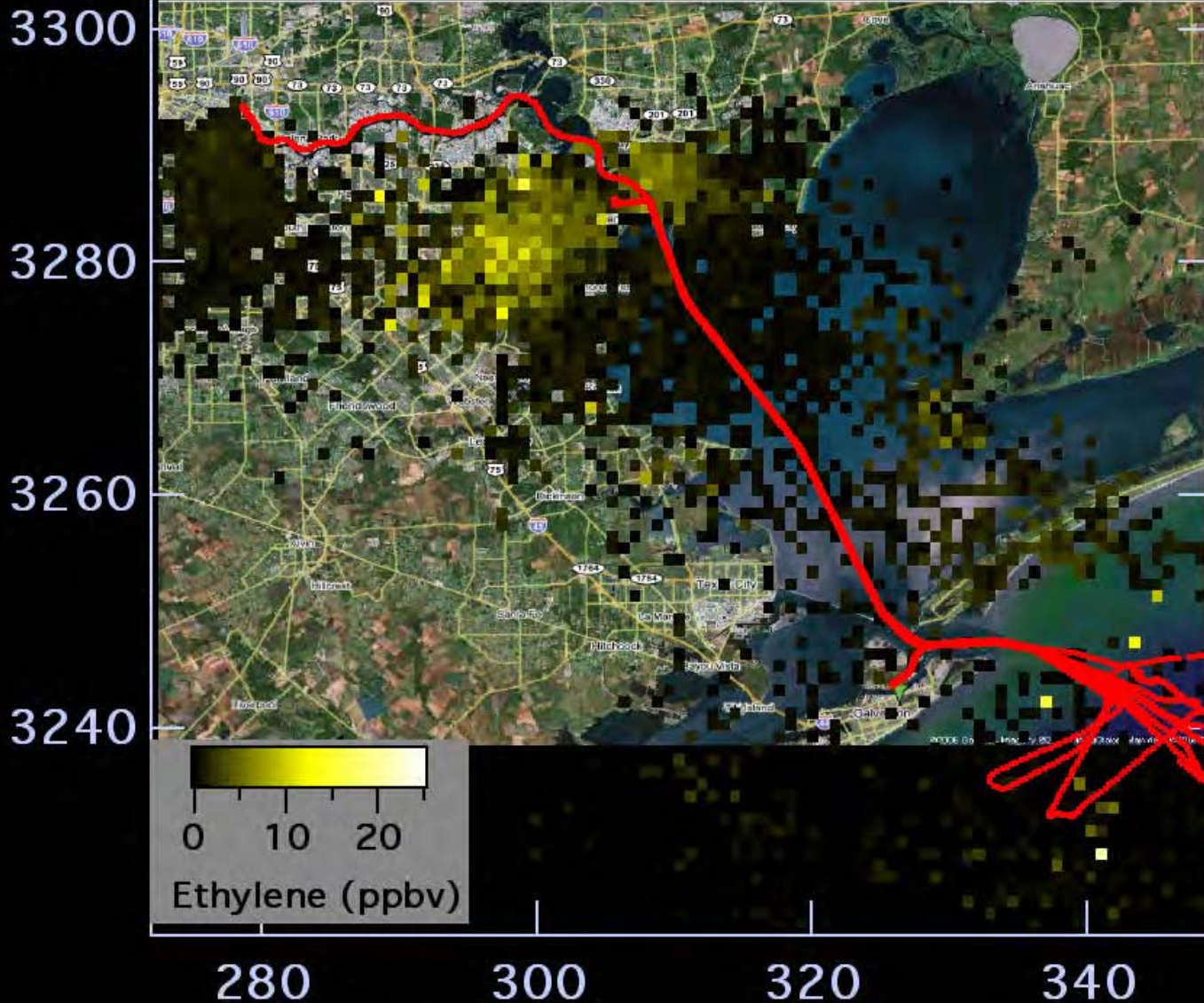
(Scott Herndon)

UTM Zone 15 (km Easting)

(Scott Herndon)

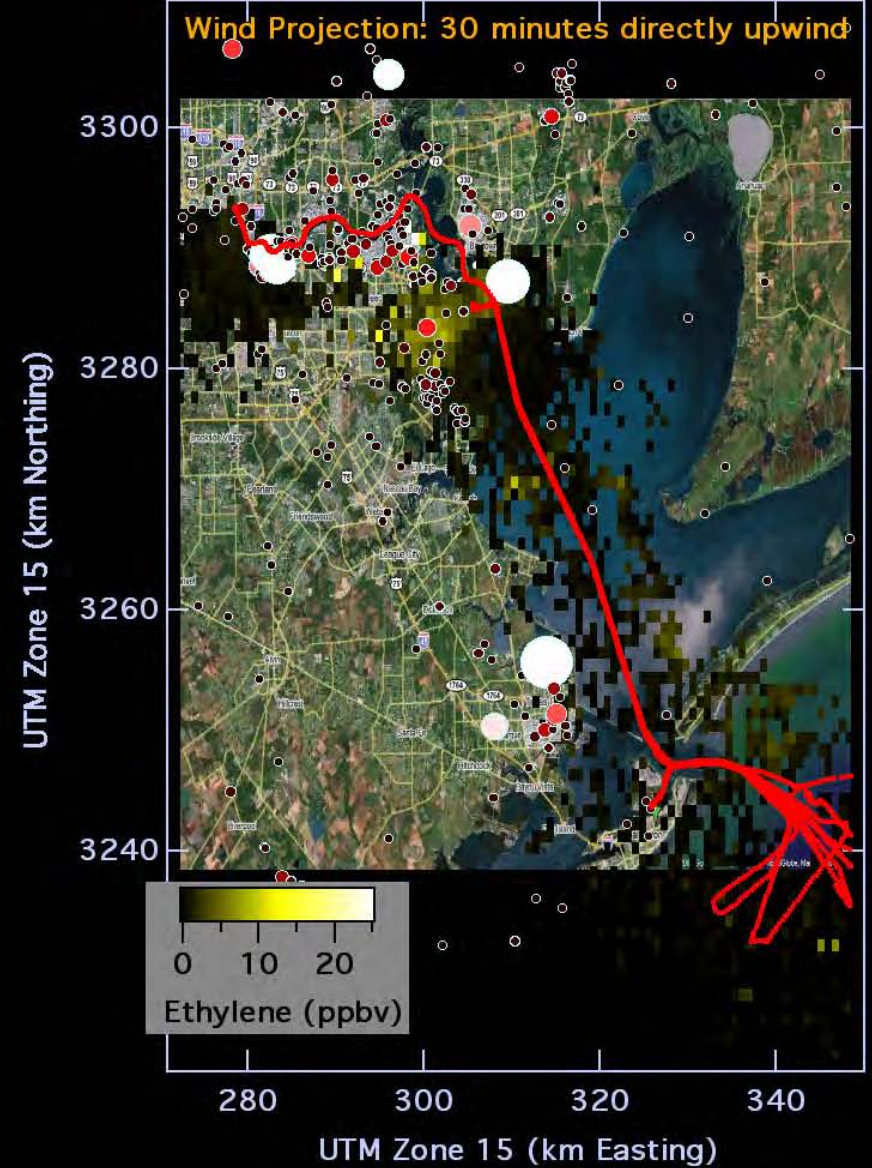
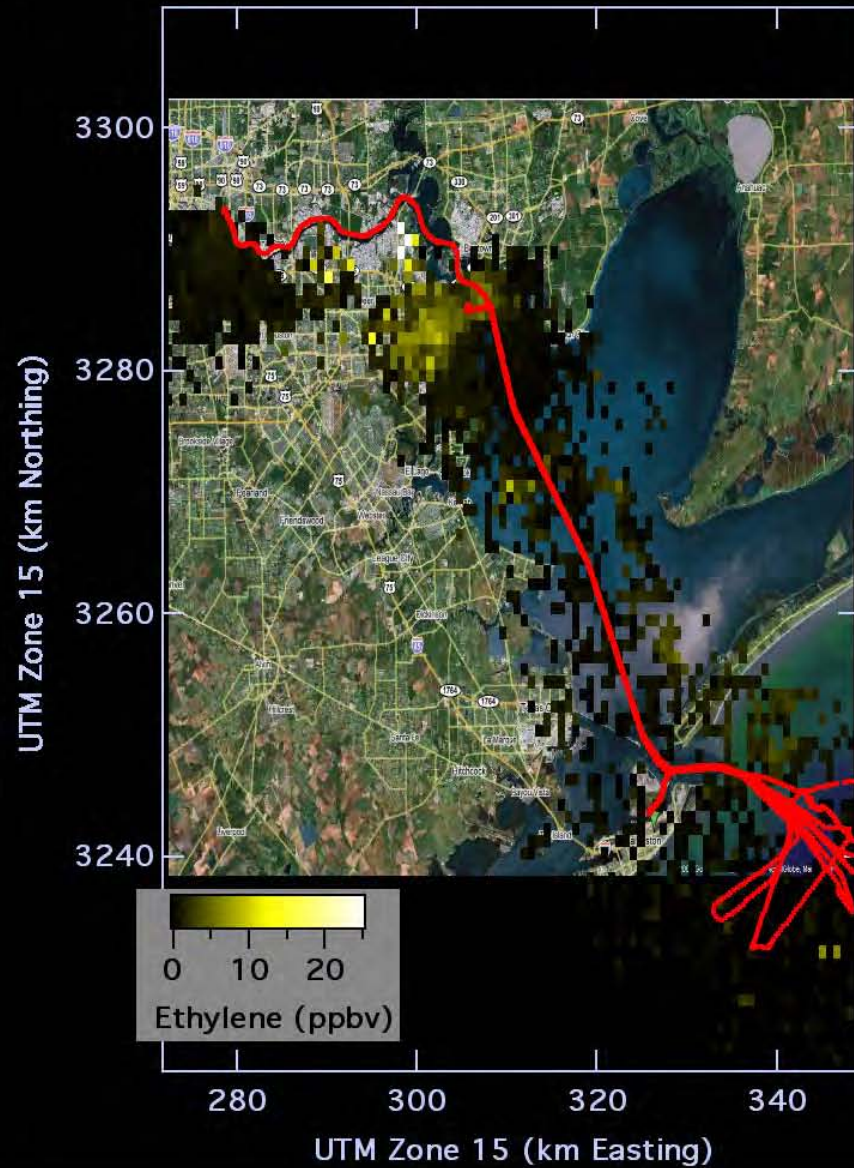
Wind Projection: 1 linear Hour directly upwind

UTM Zone 15 (km Northing)



UTM Zone 15 (km Easting)

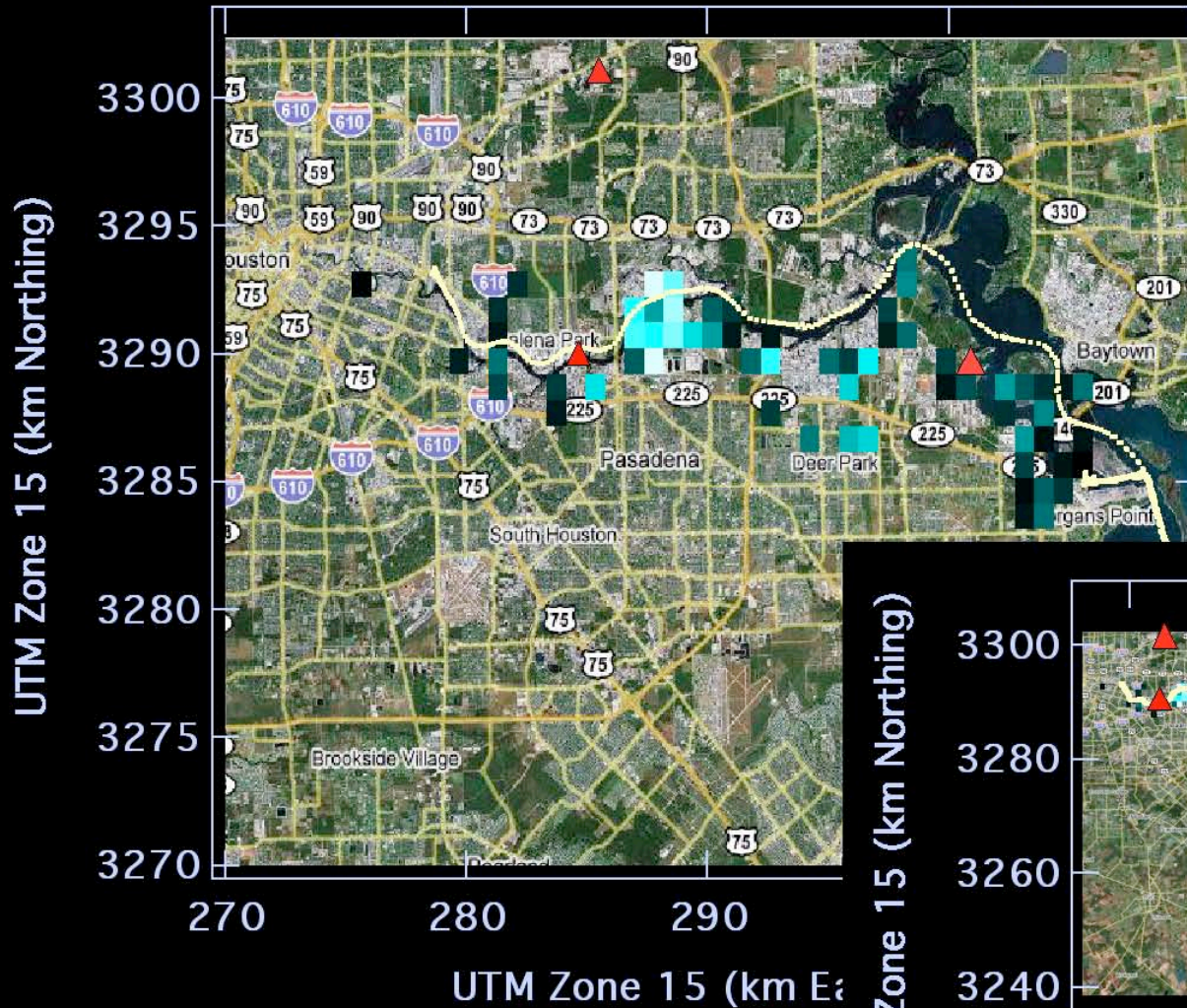
Comparison with Point Source Inventory



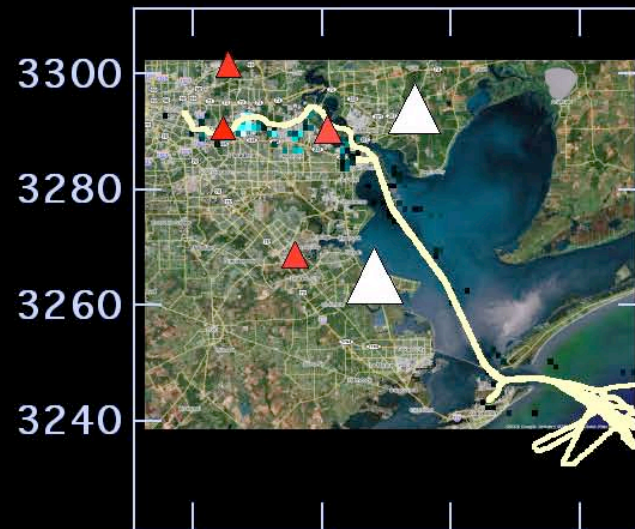
(Scott Herndon)

Ammonia Analysis

Wind Projection: 10 minutes directly upwind



UTM Zone 15 (km Northing)

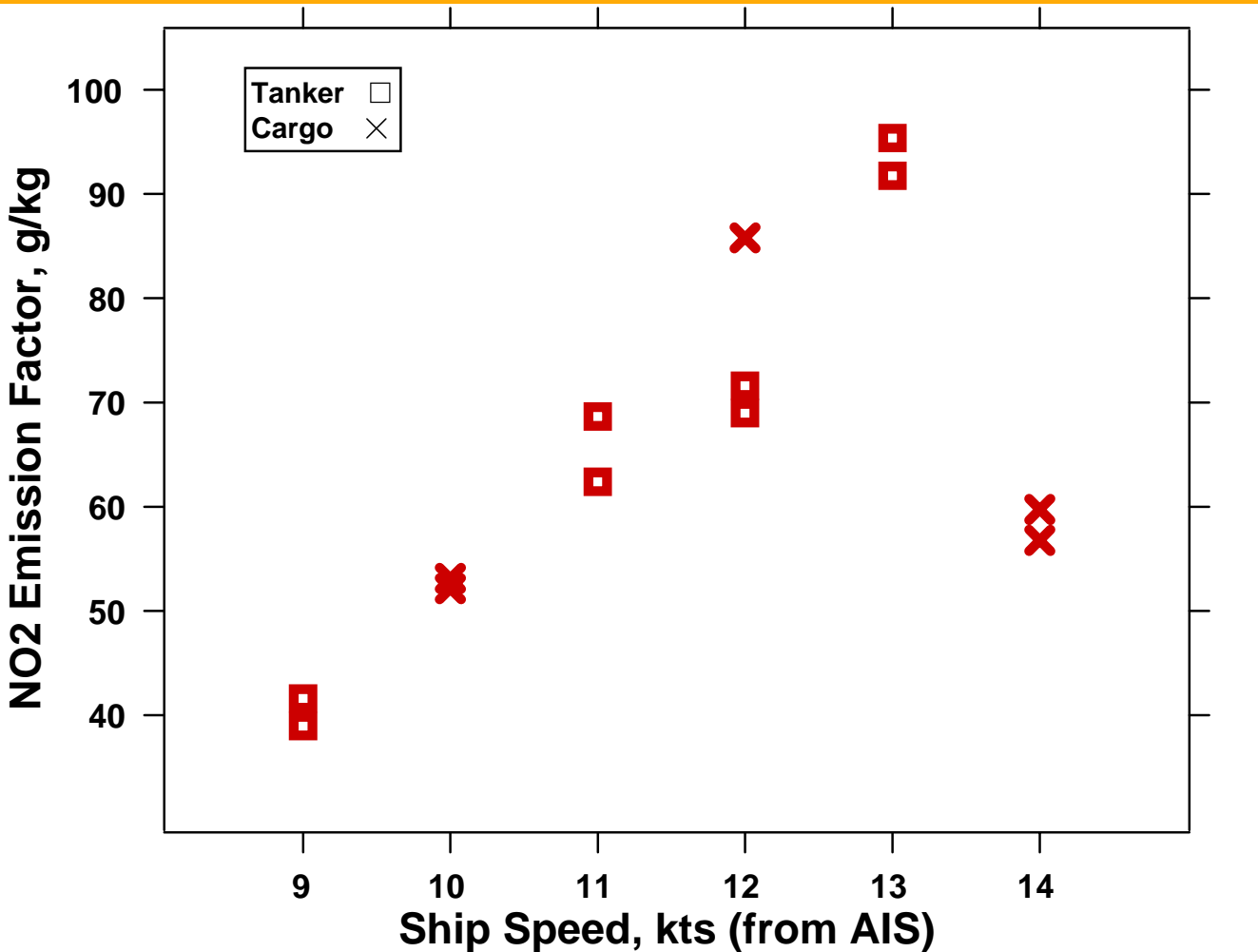


UTM Zone 15 (km Easting)

(Scott Herndon)

Ship emission characterization

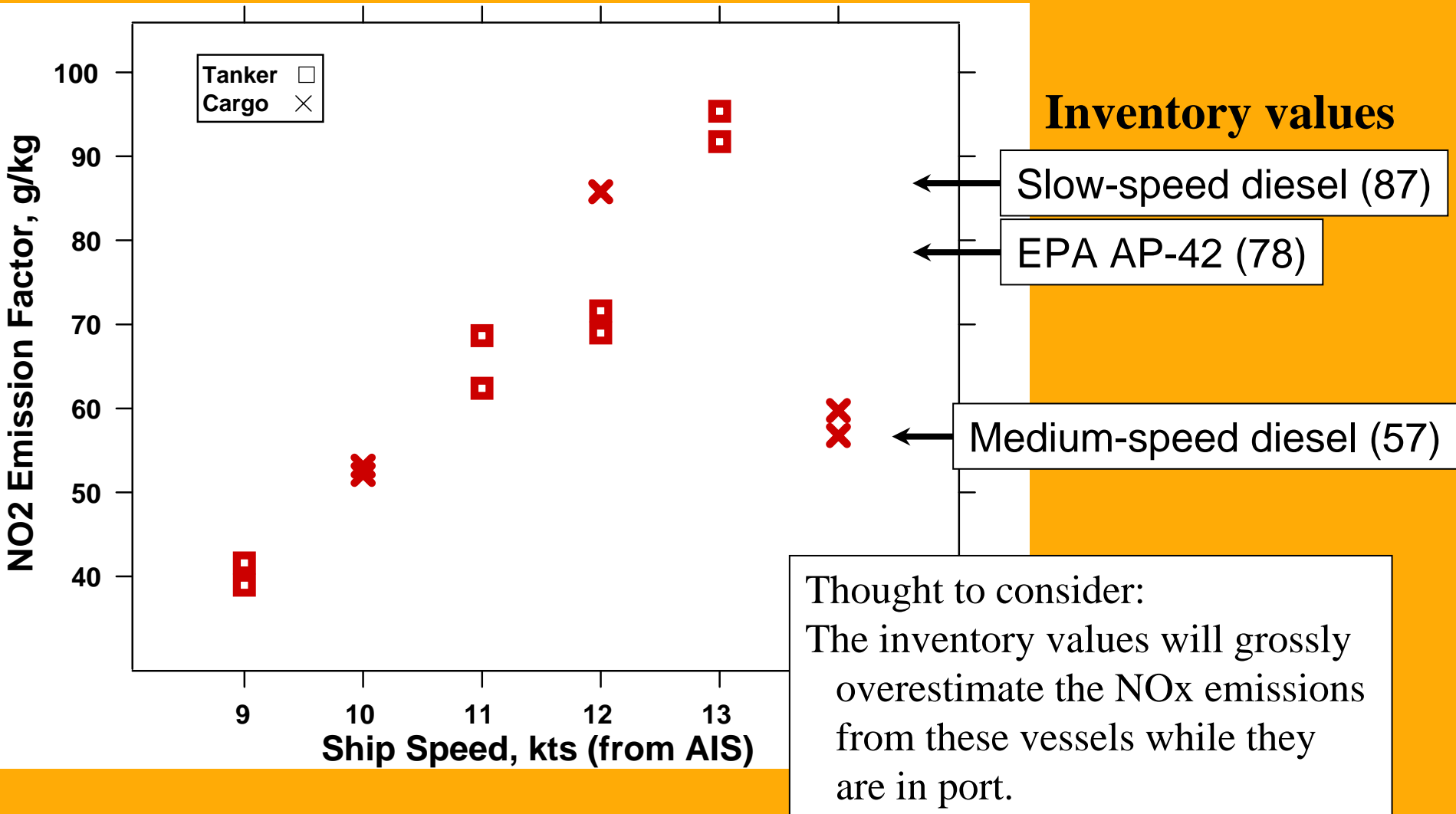
(g NO_x emitted per kg fuel burned determined from measured NO_y/CO₂ ratio)



(Eric Williams)

Ship emission characterization

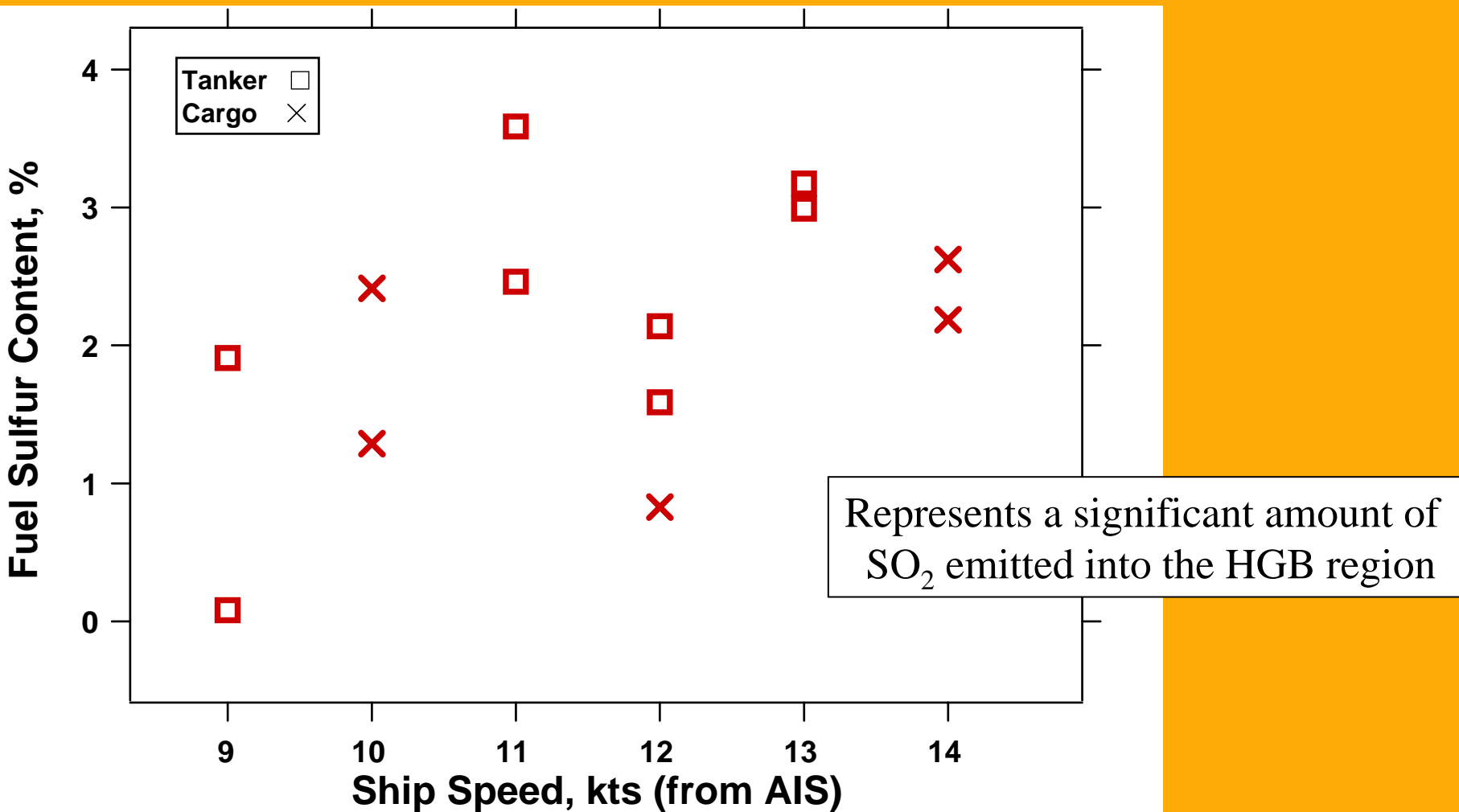
(g NO_x emitted per kg fuel burned determined from measured NO_y/CO₂ ratio)



(Eric Williams)

Ship emission characterization

(Fuel Sulfur content determined from measured SO_2/CO_2 ratio)



(Eric Williams)

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**“Transient high ozone events”,
rapid ozone formation, and ozone
exceedances in Houston and
Dallas**

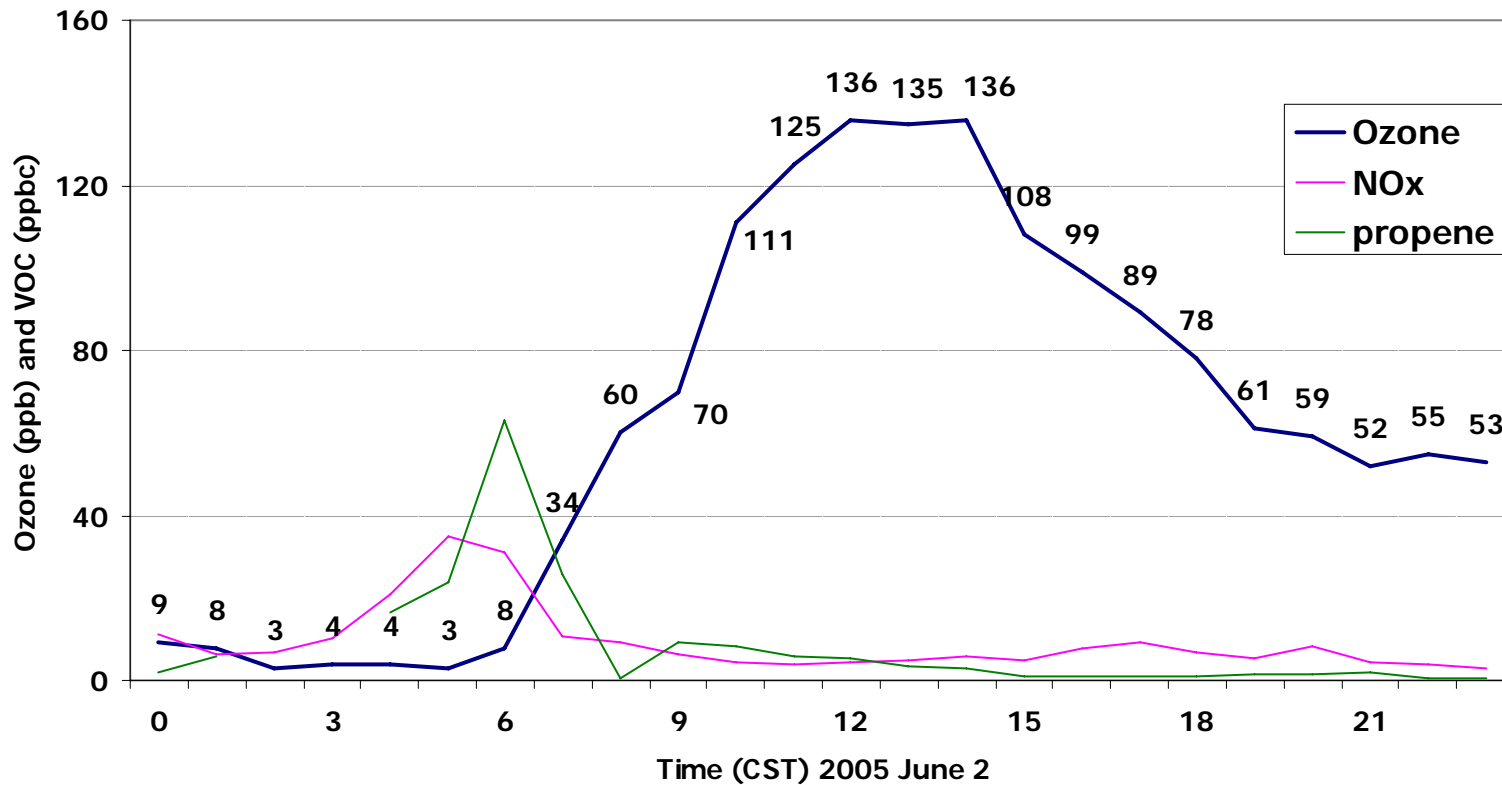
TCEQ Air Modeling and Data Analysis Section,
Rapid Synthesis Briefing, September 1, 2006

Definitions

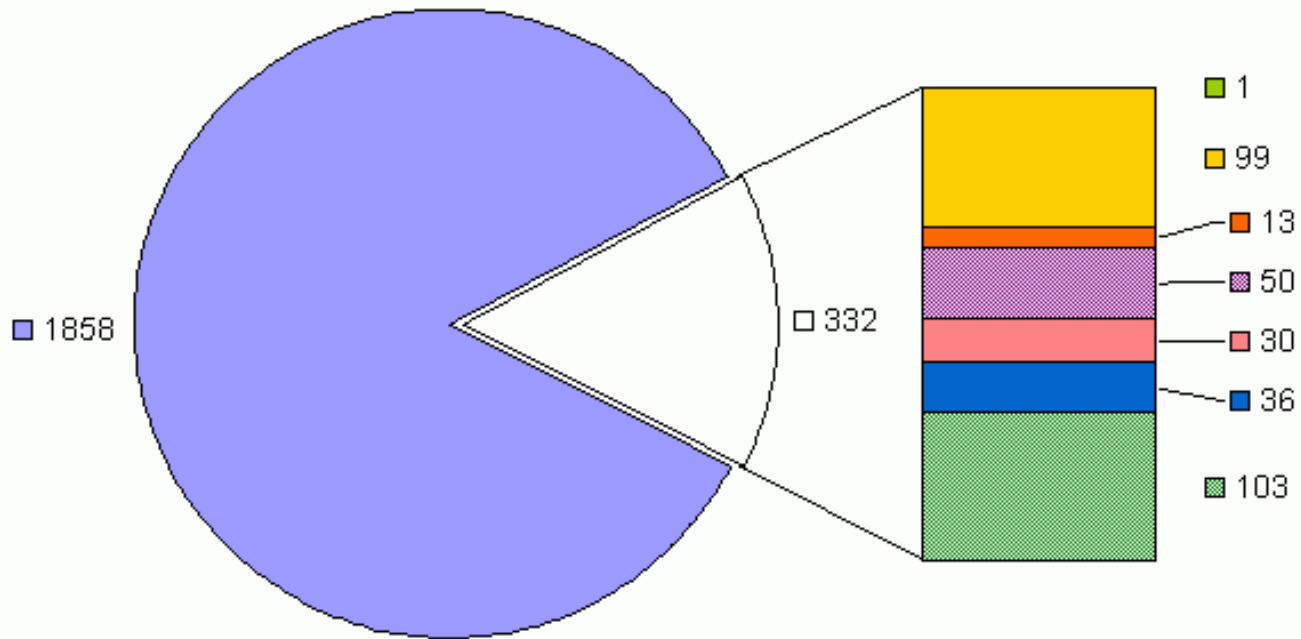
- Transient High Ozone Event (THOE) = increase of ≥ 40 ppb O₃ in one hour. Arbitrary, but customary.
- 8-hour ozone exceedance = ≥ 85 ppb O₃, averaged over 8 hours
- 1-hour ozone exceedance = ≥ 125 ppb O₃, averaged over 1 hour

EXAMPLE of all three phenomena

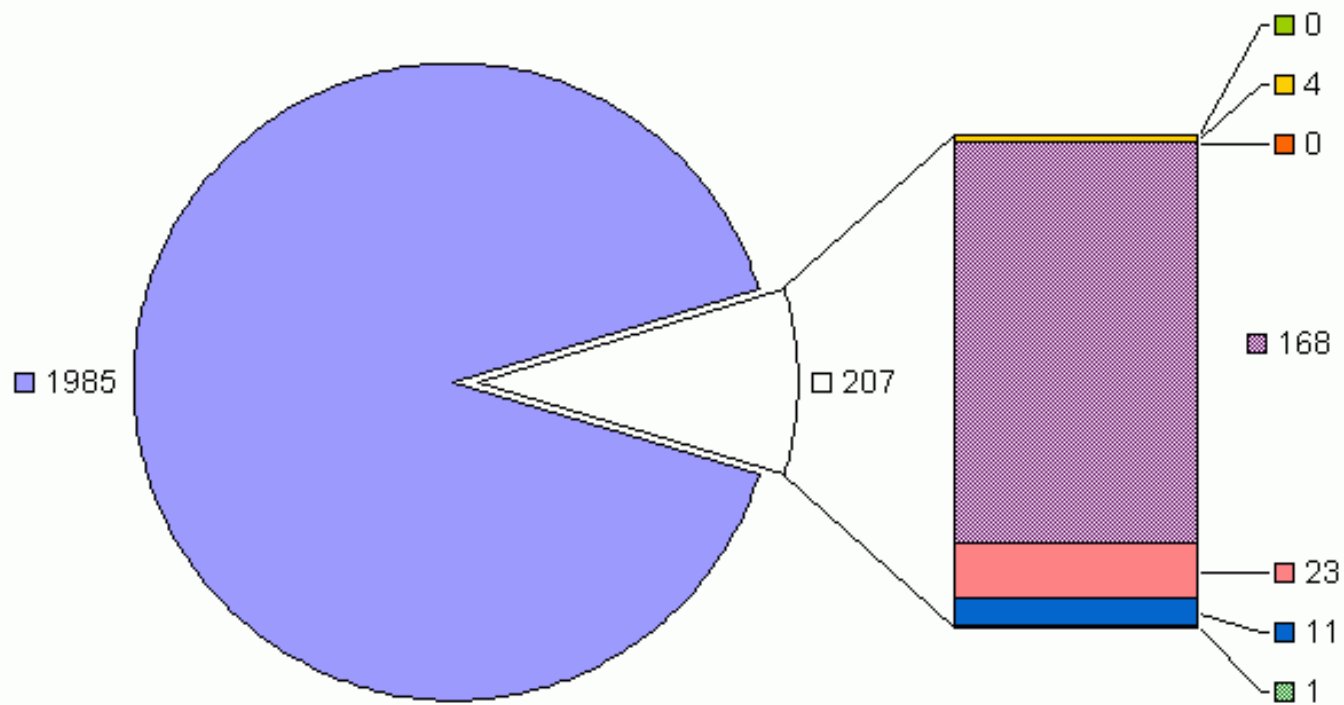
Wallisville Road CAMS 617
"Transient" High Ozone Event, 8-hr exceedance, and 1-hr exceedance
2 June 2005



Houston 2000-2005



DFW 2000-2005



~8Hr, ~THOE, ~1Hr	~8Hr, ~THOE, 1Hr
~8Hr, THOE, ~1Hr	~8Hr, THOE, 1Hr
8Hr, ~THOE, ~1Hr	8Hr, ~THOE, 1Hr
8Hr, THOE, ~1Hr	8Hr, THOE, 1Hr;

Comparison between Houston and Dallas

- Between 2000-2005, Houston had 219 eight-hour ozone exceedance days, and Dallas had 203 days.
- Houston had 251 days with THOEs, whereas Dallas had 16 days.
- In Houston, 63% of the 8-hr exceedance days were accompanied by THOEs, but in Dallas, only 6% were.

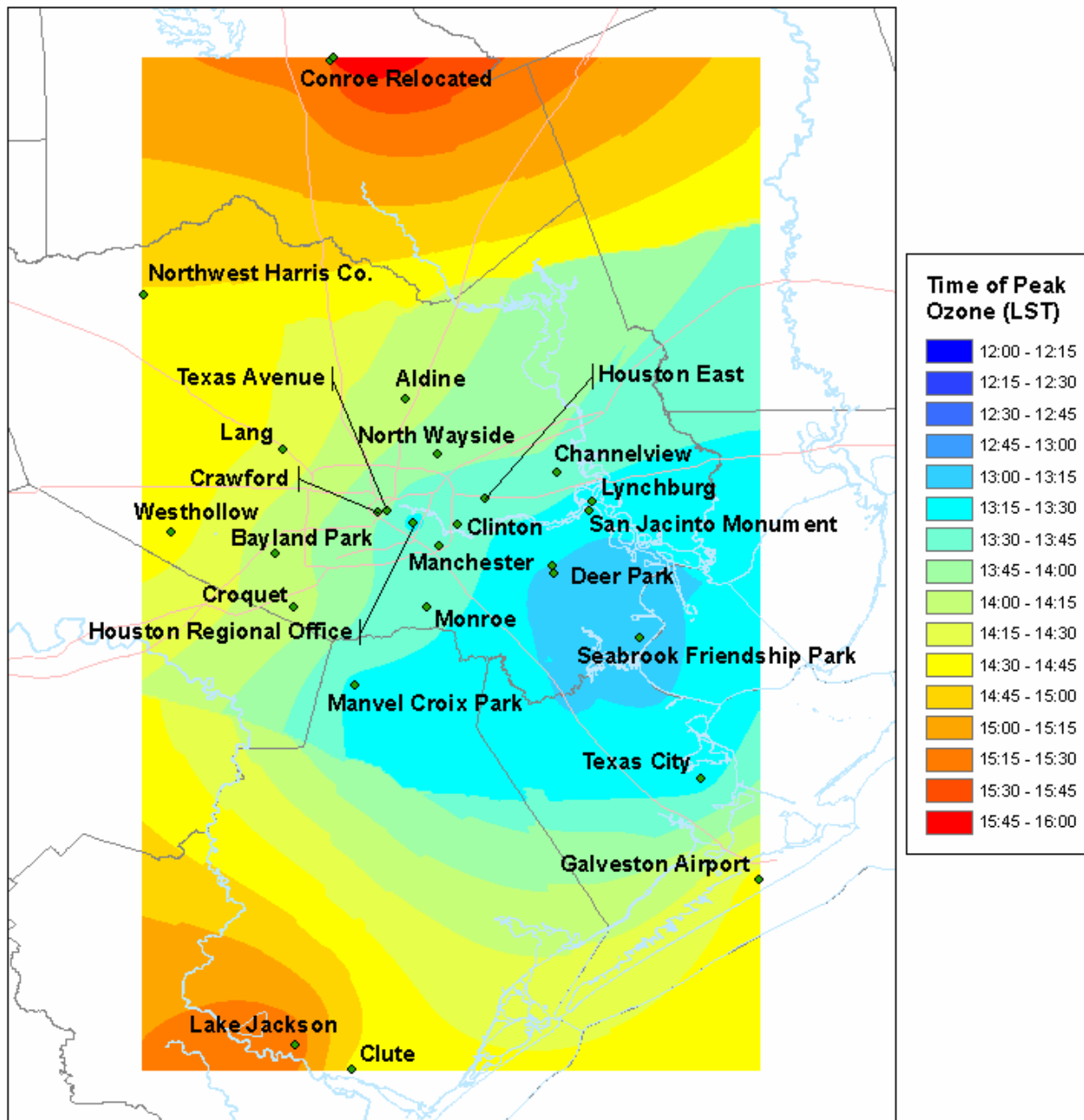
Comparison between Houston and Dallas

- 61% of Houston 8-hr exceedance days were accompanied by 1-hr exceedances, but only 12% were in Dallas.
- In Houston, 99 THOE days (39%) were not accompanied by ozone exceedances.
- Caveat: Ozone networks are not perfect, and do not sample all events.

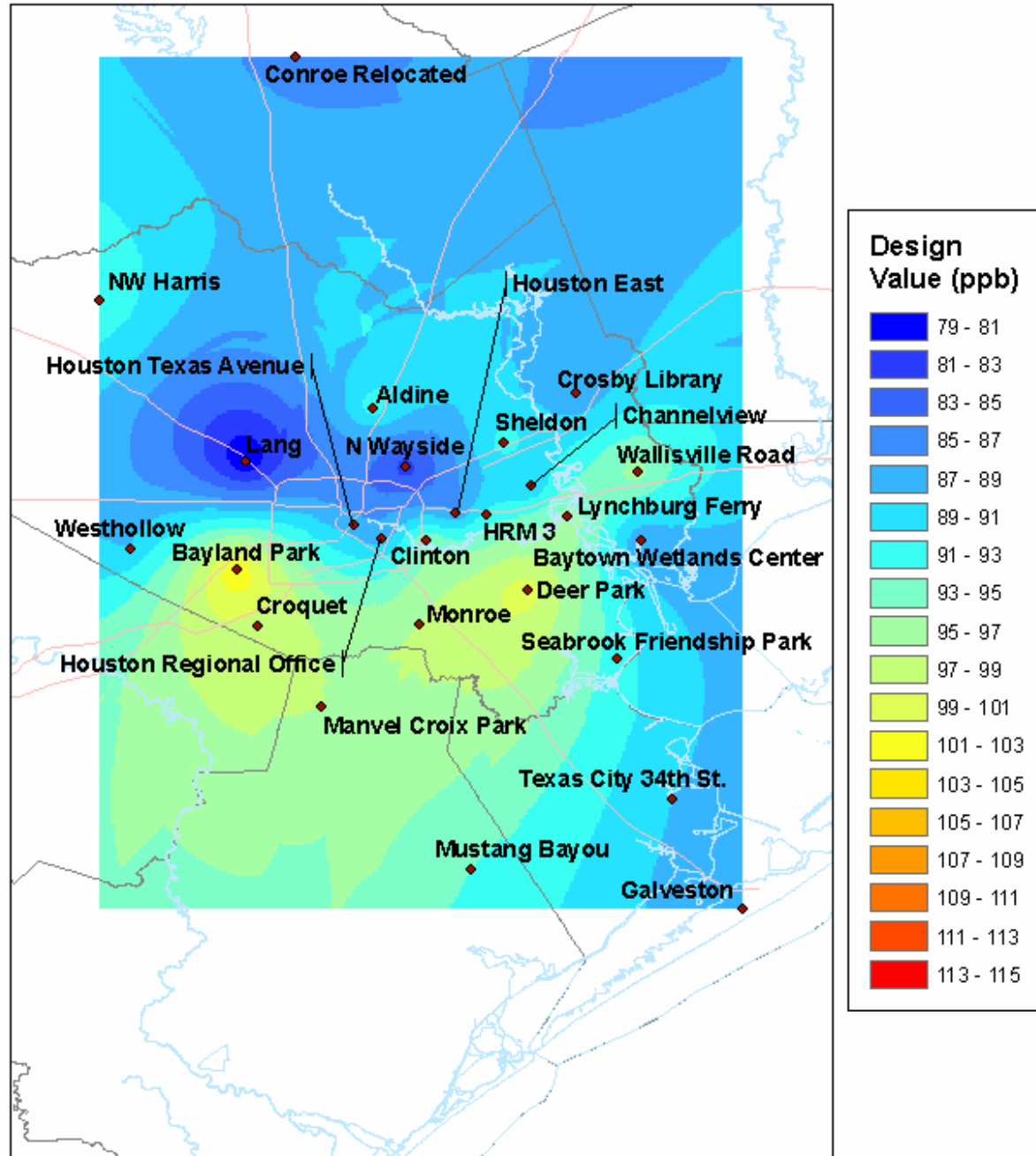
Hypotheses to explain different ozone behavior in Dallas and Houston

- Rapid ozone formation from HRVOCs and NO_x emitted by point sources in Houston create relatively narrow, intense plumes of ozone, and these strong ozone gradients are carried through the city by winds that shift direction.
- Shift in wind direction in Houston due to the bay breeze/coastal oscillation pushes moderately high ozone into an area with low ozone, resulting in a strong ozone gradient.
- Neither of these phenomena occur in Dallas.

Average Time of Peak 1-Hour Ozone on 8-Hour Ozone Exceedance Days in the HGB Area (1995-2005)



2005 8-Hour Ozone Design Values in the HGB Area



Do emission events explain THOEs?

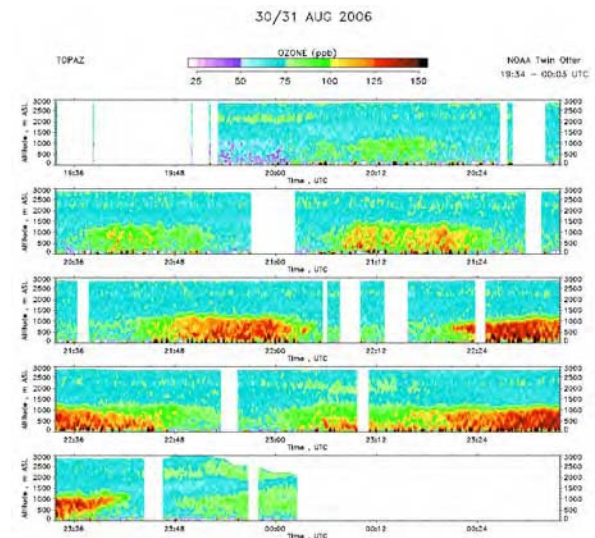
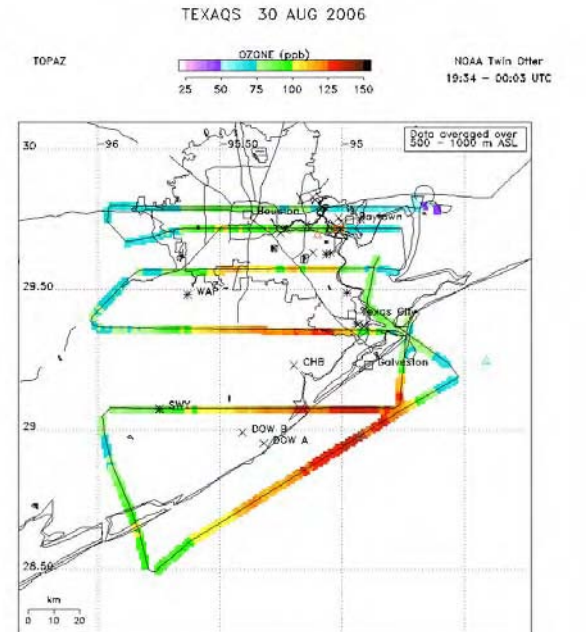
- Murphy and Allen (2005) found 455 emission event reports in TCEQ records for 2003. Of these, Nam et al. (2006) found that only 1.5% of these were large enough to make 10 ppb of additional O₃, and only 0.5% could make 70 ppb.
- Suppose 1% of 2003 emission events made 40 ppb O₃, i.e., ~5 events.
- From 2000-2005, there were an average of 42 THOE days per year, and 37 eight-hour ozone exceedances per year.
- Therefore, the *reported* emission events apparently cannot explain the THOE phenomenon.

Conclusions

- Strong ozone gradients have been observed 15 times more often in Houston than in Dallas.
- Two possible explanations: Presence of strong point sources; wind shifts on high ozone days.
- Nonetheless, DFW still has about the same number of eight-hour ozone exceedances as Houston.
- Maybe need a new acronym, since “Transient High Ozone Events” often aren’t transient, don’t have high ozone, and aren’t driven by emission events. How about Strong Ozone Gradients (SOGs)?

Estimating ozone fluxes

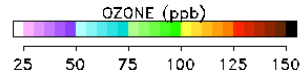
- Measure ozone profiles in a curtain transverse to the wind on several legs downwind of the source
- Define extent of the plume
- Integrate to compute the total ozone in the plume
- Interpolate profiler observations to estimate wind speeds at all points within the plume
- Compute flux at each point within the curtain
- Subtract background to get “flux above background”
- Best when wind speed and direction are relatively steady



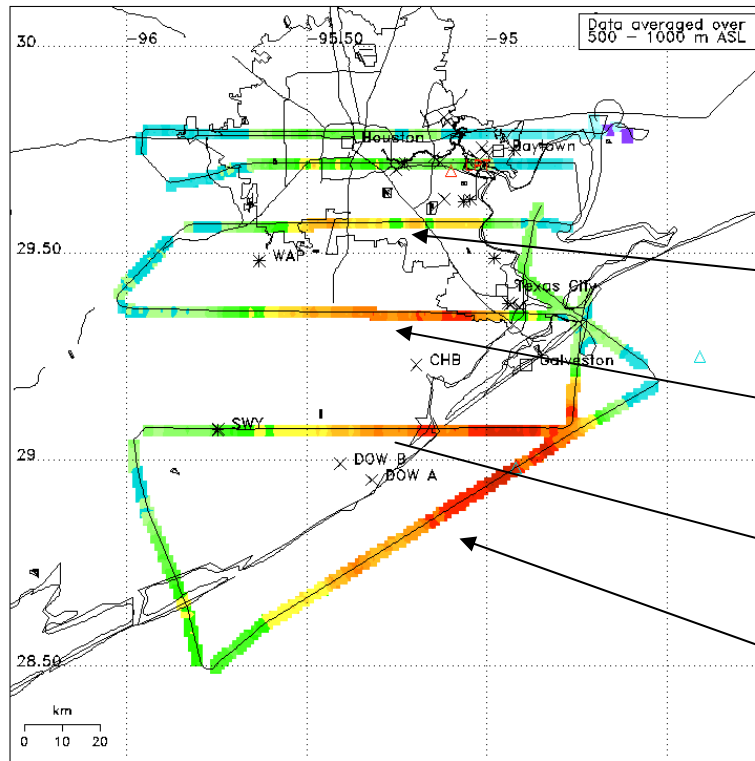
August 30 – Northerly flow

TEXAQ3 30 AUG 2006

TOPAZ

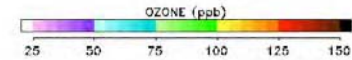


NOAA Twin Otter
19:34 – 00:03 UTC

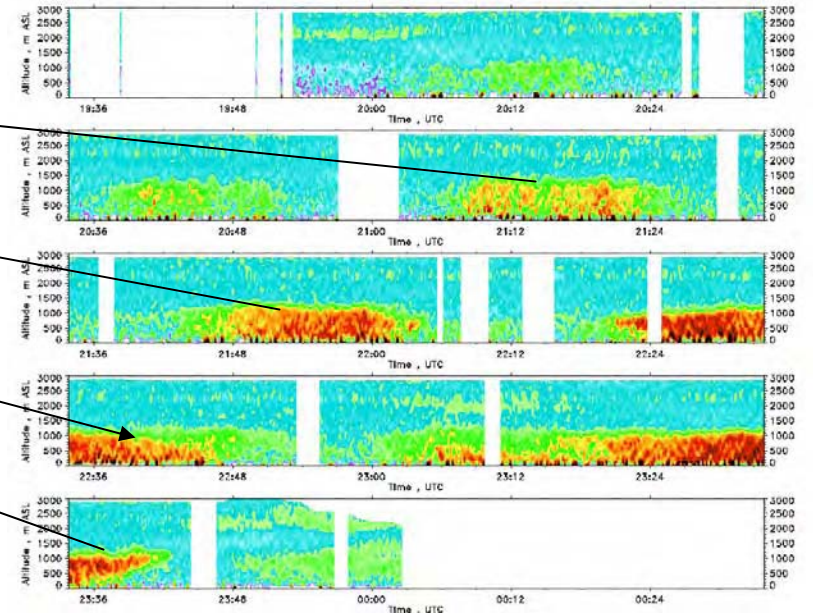


30/31 AUG 2006

TOPAZ



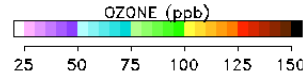
NOAA Twin Otter
19:34 – 00:03 UTC



August 30 southerly ozone fluxes

TEXAQS 30 AUG 2006

TOPAZ

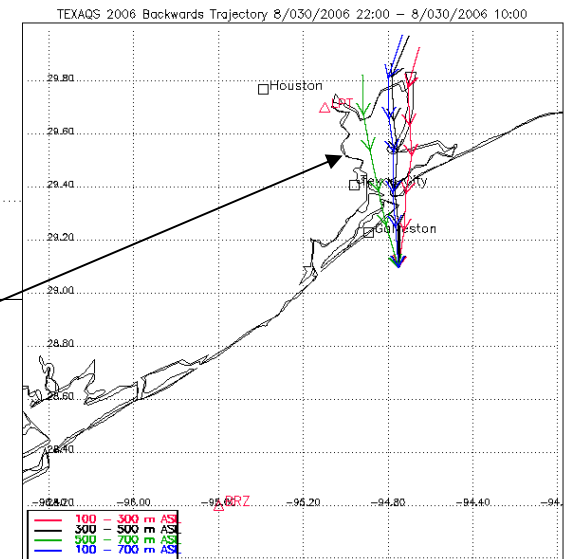
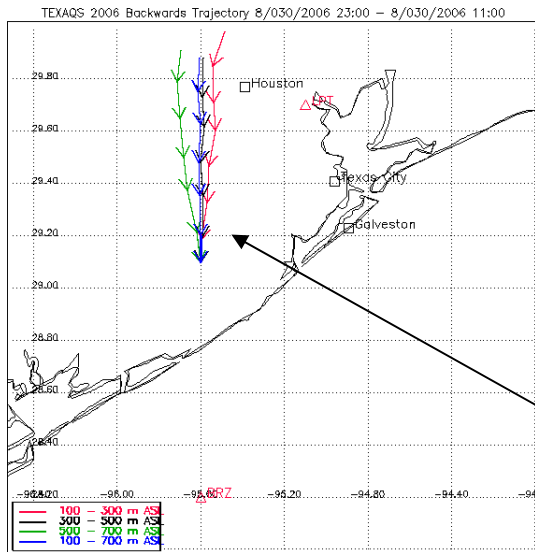
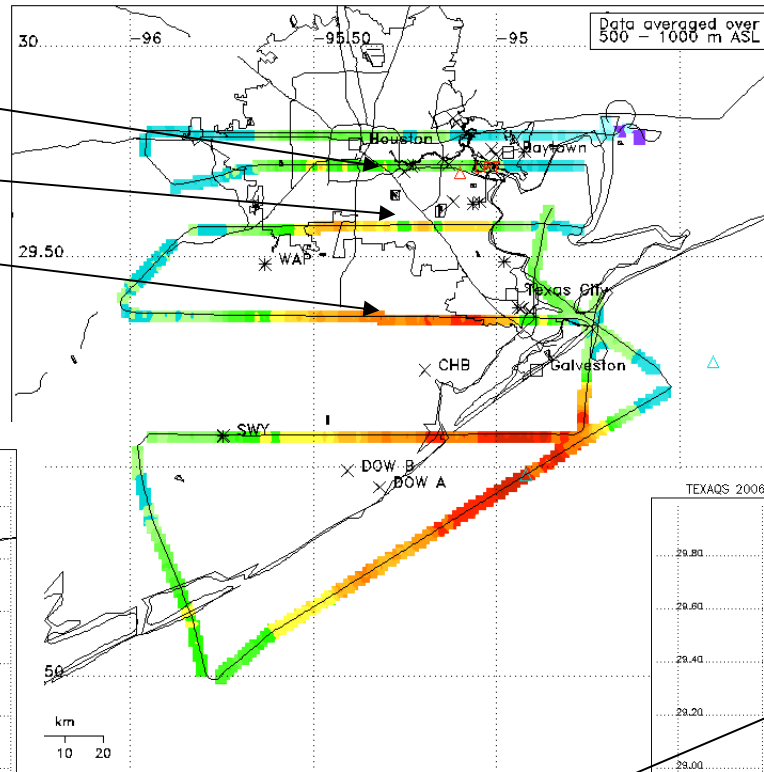


NOAA Twin Otter
19:34 - 00:03 UTC

4.9×10^{25} mol/s

1.2×10^{26} mol/s

1.7×10^{26} mol/s

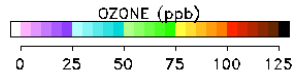


Speed = 3.05 m/s

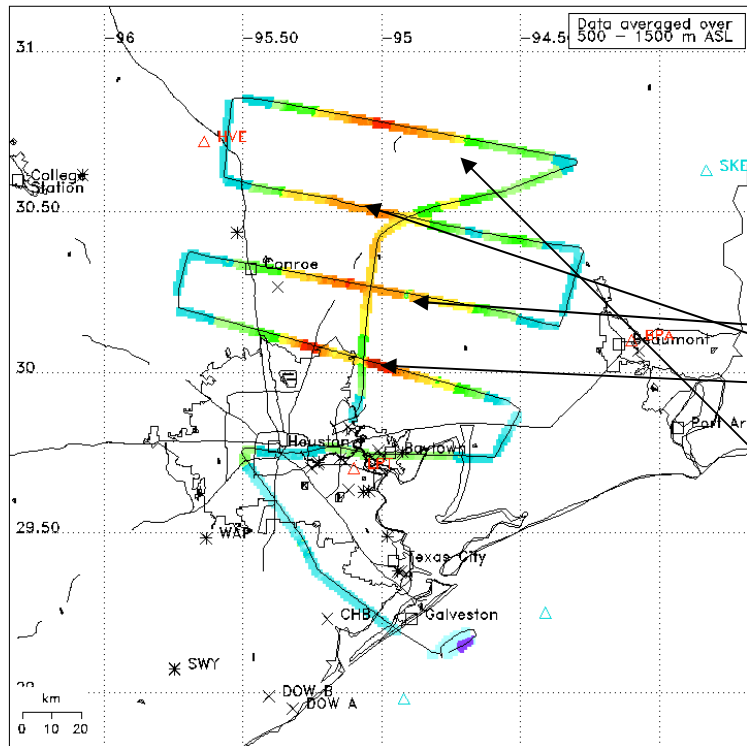
August 14 – southerly flow

TEXAQS 14 AUG 2006

TOPAZ

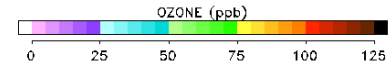


NOAA Twin Otter
20:06 – 00:00 UTC

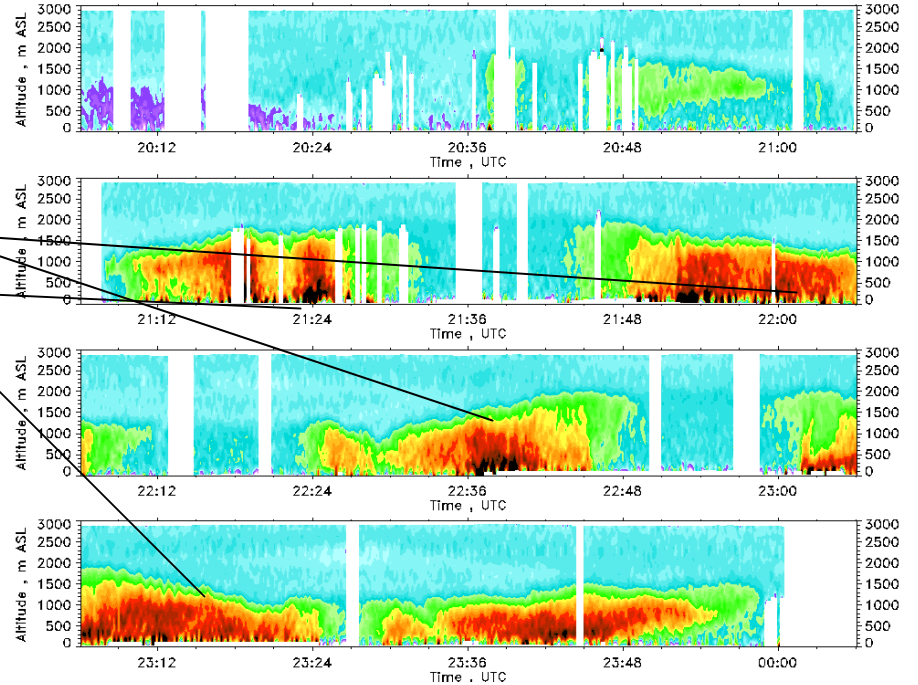


14/15 AUG 2006

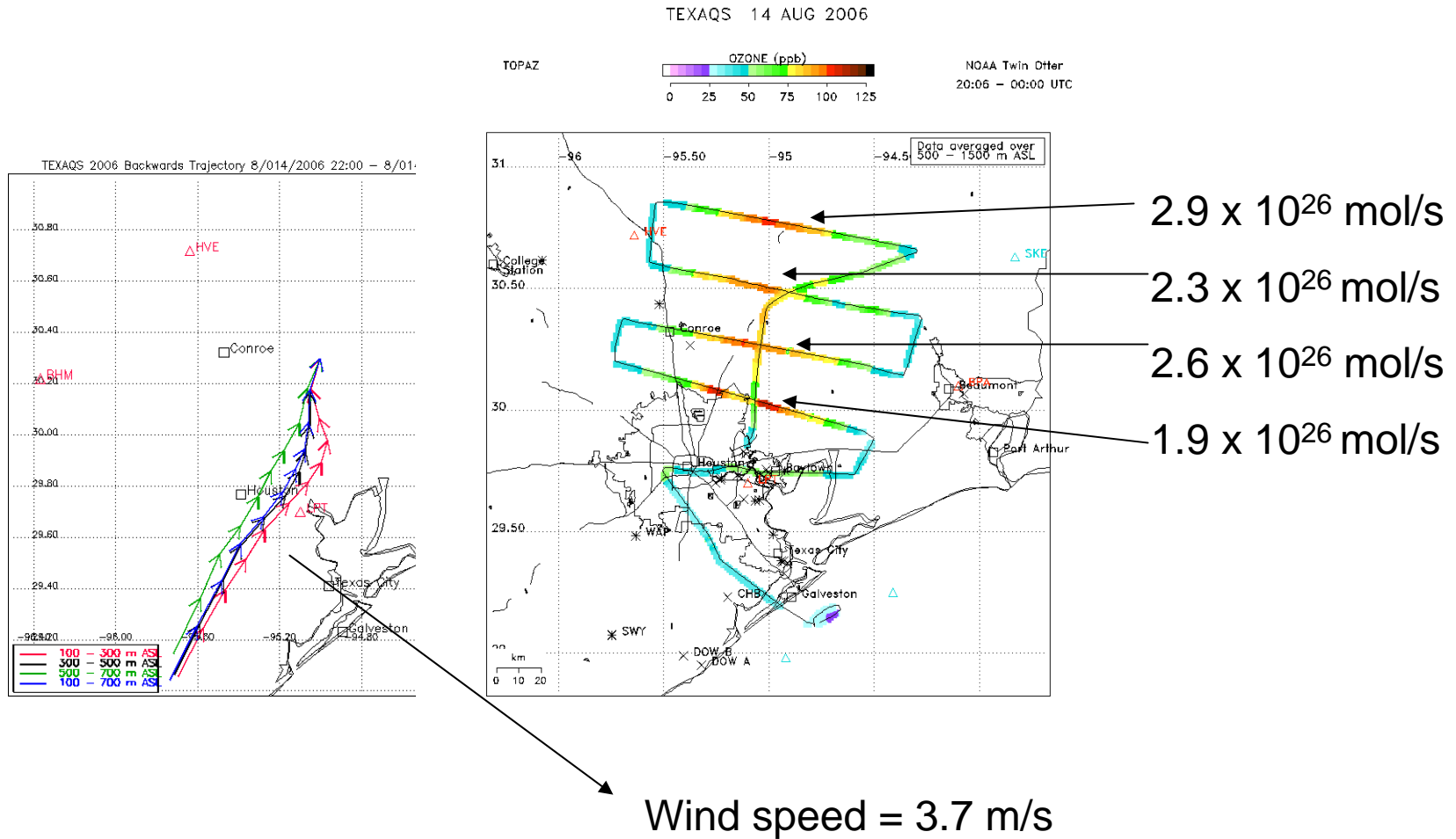
TOPAZ



NOAA Twin Otter
20:06 – 00:00 UTC



August 14 – Northerly ozone fluxes



Detailed analysis (later)

- Better quality checking of ozone data
- Interpolate profiler data at each point within the curtain
- Compute ozone production downwind within each leg
- Compare with model outputs



Assessing the impact of distant sources of ozone on the Houston area using the RAQMS global chemical model and TES satellite observations: a test case for August 23rd 2006

Kevin W. Bowman (JPL), Jassim Al-Saadi (LaRC), and Brad Pierce (LaRC)



TCEQ High Priority SIP-Relevant Science Questions

- G: How do emissions from local and distant sources interact to determine the air quality in Texas? What meteorological and chemical conditions exist when elevated background ozone and aerosol from distant regions affect Texas? How high are background concentrations of ozone and aerosol, and how do they vary spatially and temporally?
- H: Which areas within Texas adversely affect the air quality of non-attainment areas within Texas? Which areas outside of Texas adversely affect the air quality of non-attainment areas within Texas?



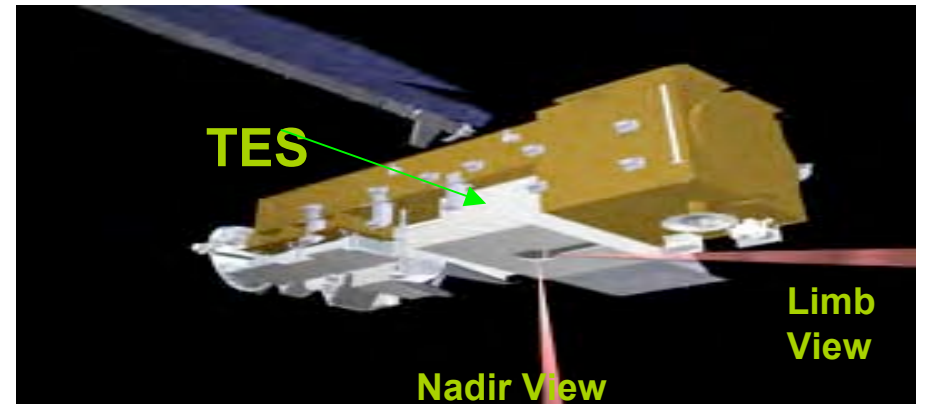
Synthesis of satellite observations, *in-situ* measurements, and chemistry and transport models

- Observations of ozone and carbon monoxide profiles in the free troposphere from TES can provide critical information for studying boundary layer exchange.
- Ground *in-situ* observations such as AIRNow are the standard for boundary layer measurements of ozone and its precursors
- Chemistry and transport models such as the real-time air quality modeling system (RAQMS) are the critical link between these two observations
- The integration of these assets can provide valuable input into the science objectives for TexAQS.

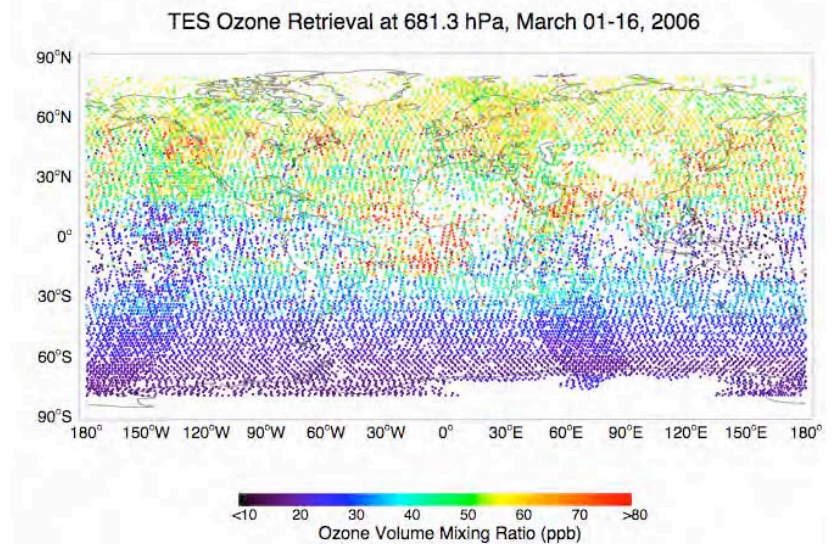


TES is a Fourier transform spectrometer specifically designed to measure tropospheric ozone and its precursors

- .1 cm⁻¹ spectral resolution (apodized)
- 650 to 3050 cm⁻¹ (3.2 to 15.4 microns)
- 0.5 x 5 km (nadir) spatial resolution
- 3 observation modes
 - Global survey (72 obs/orbit, 16 orb/day, ~1.3 deg lat)
 - Step and stare (~.4 deg lat)
 - Transect (near-continuous)
- Estimates vertical profiles from the surface to .01 mb of temperature, H₂O, ozone, carbon monoxide, HNO₃ as well as emissivity, surface temperature, and effective cloud parameters
- Estimates made both for day and night

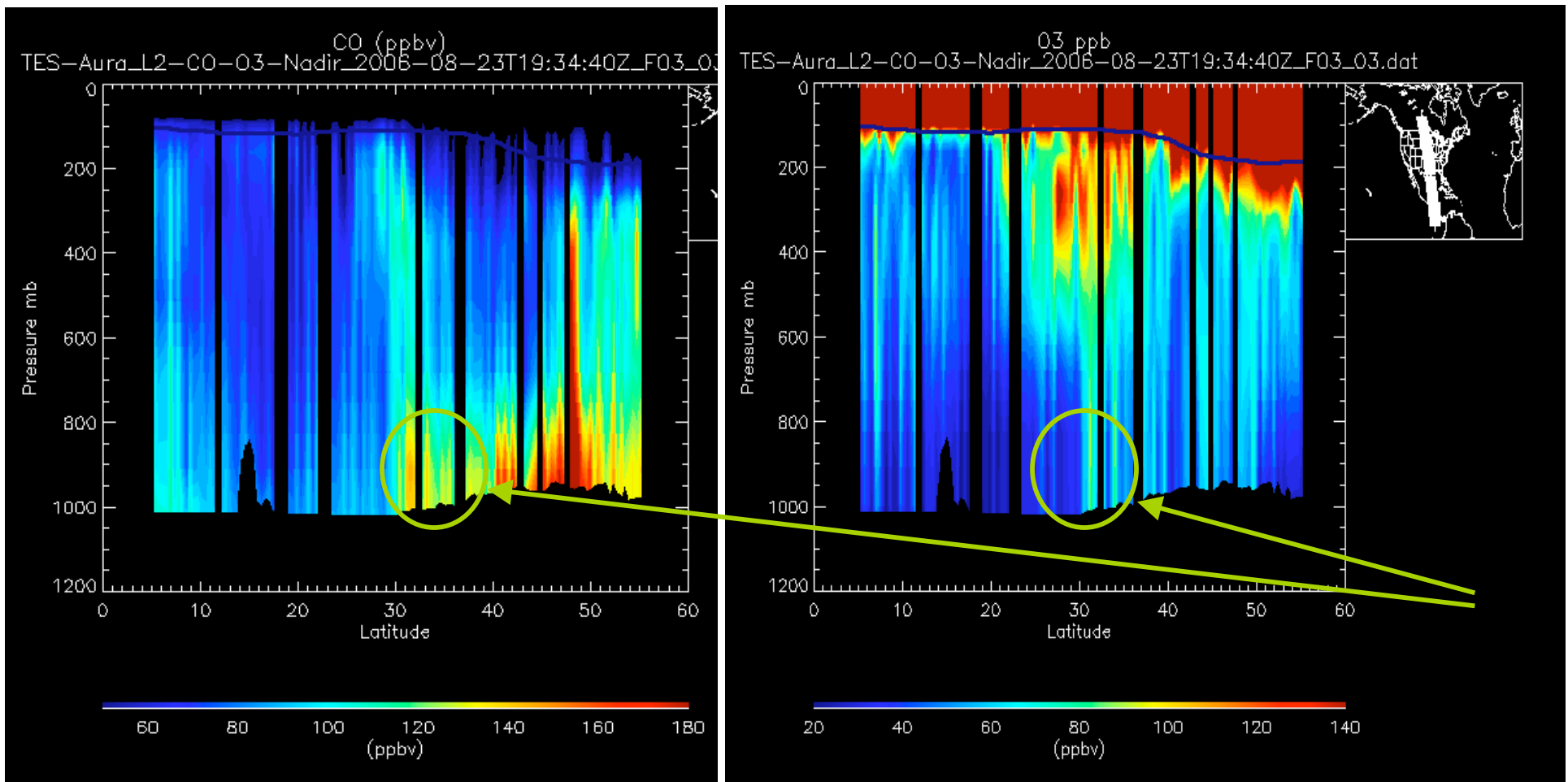


TES “global survey” mode



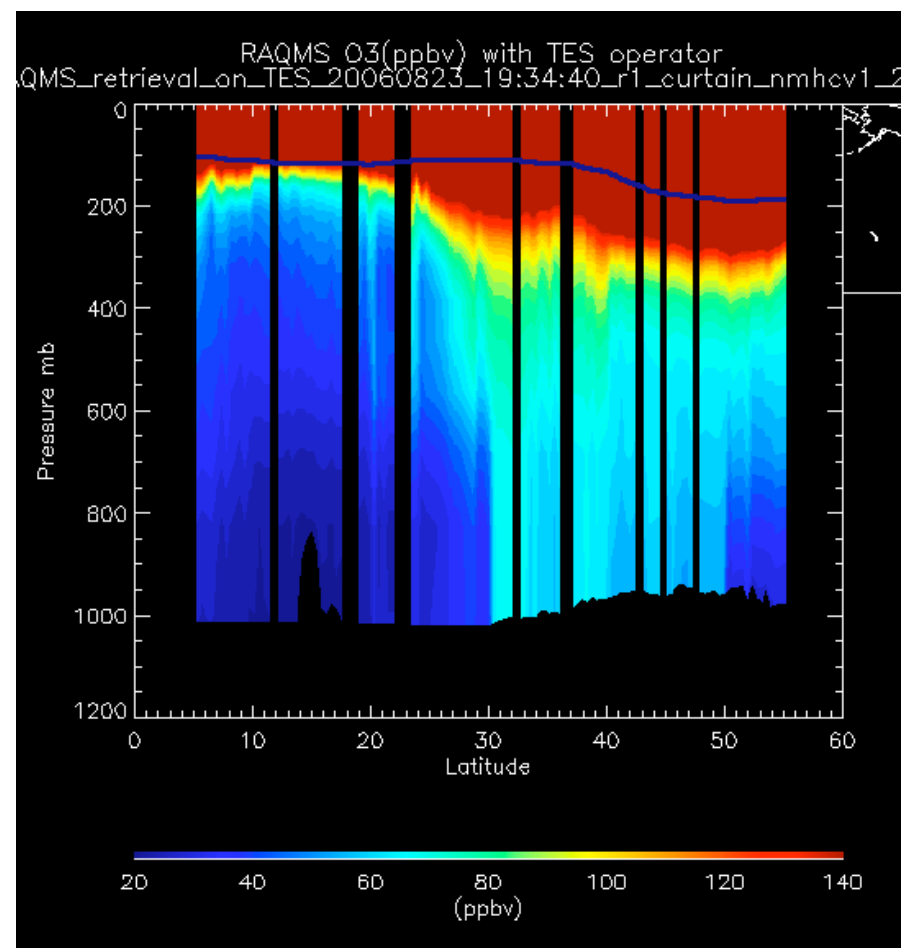
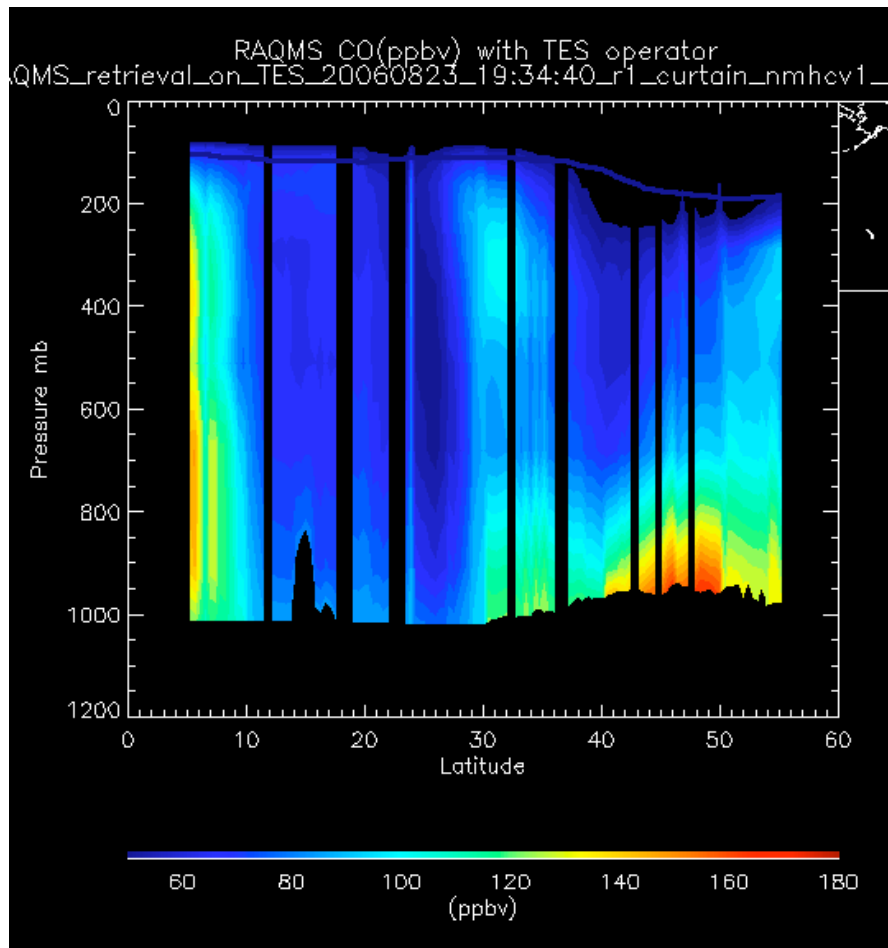


Elevated CO and ozone over Houston region observed from TES "special observations" Aug 23rd, 2006



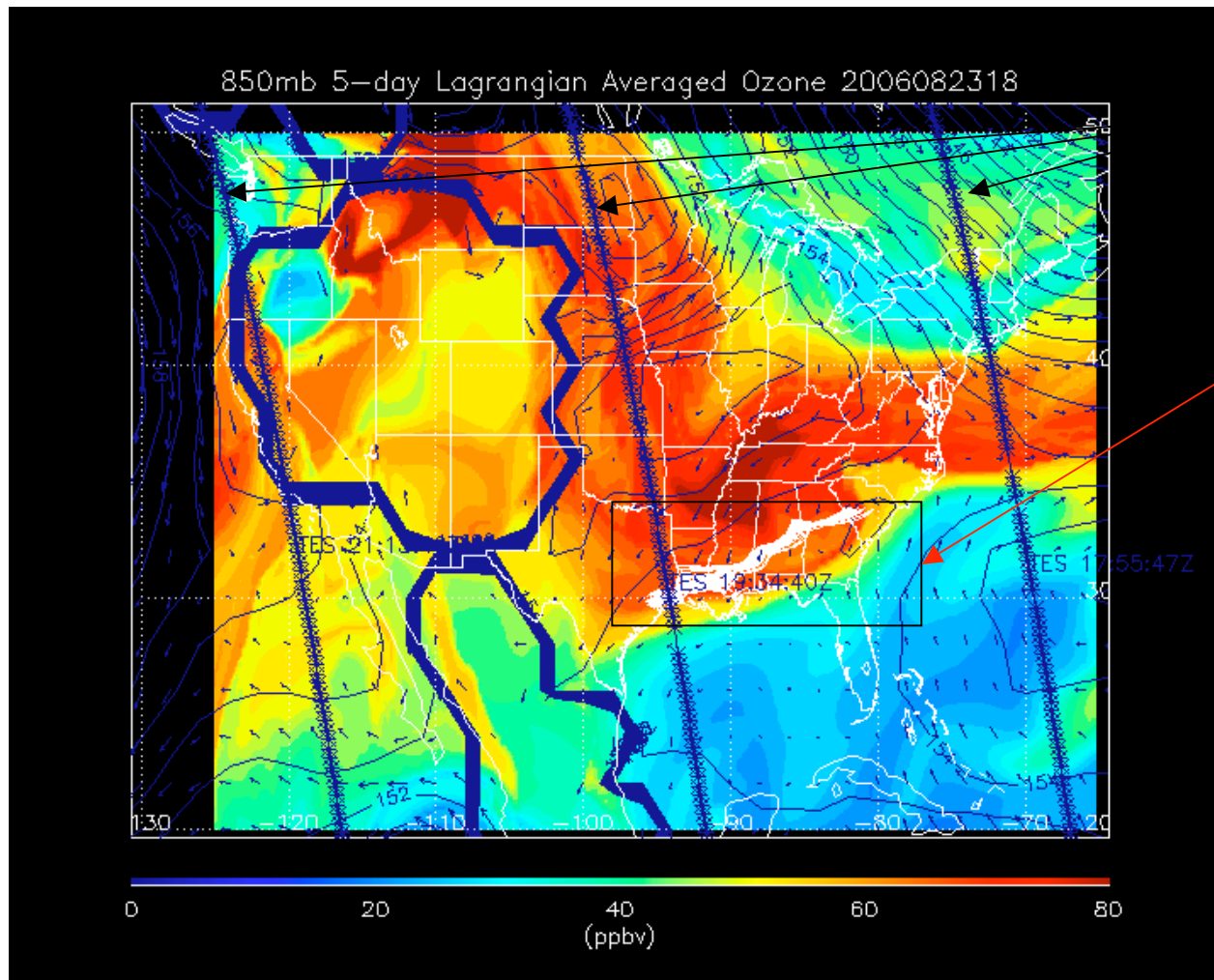


RAQMS with the TES *observation operator*





What is the origin of the ozone and CO enhancement?



TES orbits

White lines represent 5-day back-trajectories emanating from Houston AIRNow Metropolitan statistical area (MSA) sites

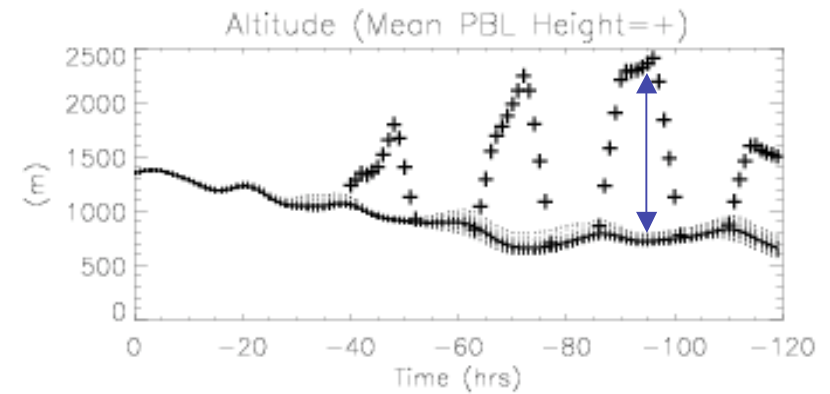
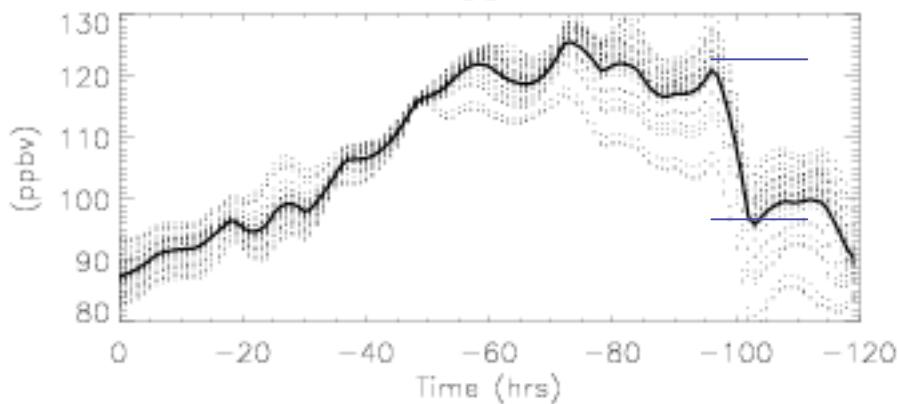
Each point represents ozone averaged over a 5-day back-trajectory

Moderate values (60-70ppb) over Houston, but high values over Tennessee, Kentucky, Alabama, and Arkansas (~80 ppb)



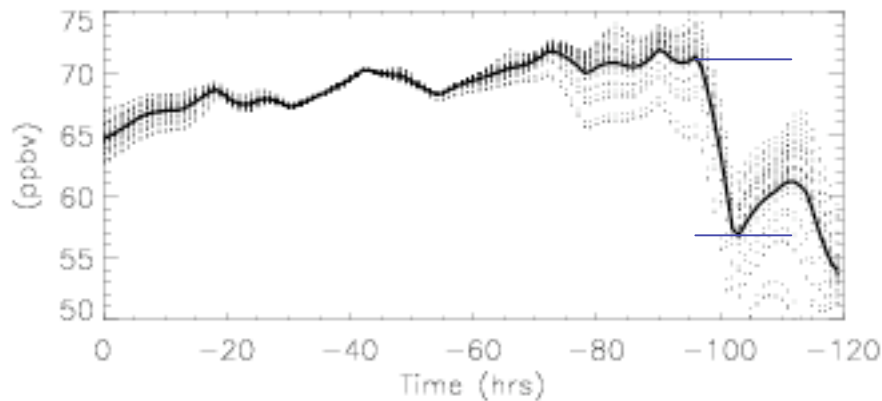
Process history of ozone and CO

850mb Houston Backtrac
CO

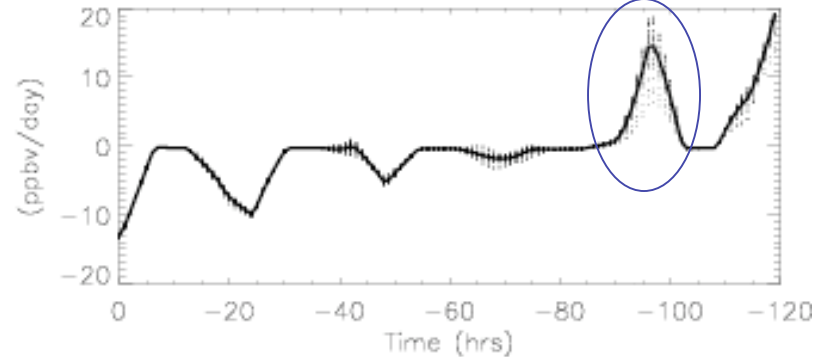


Ozone production in the boundary layer about 4 days prior to arrival in Houston

O3



O3 P-L





Conclusions

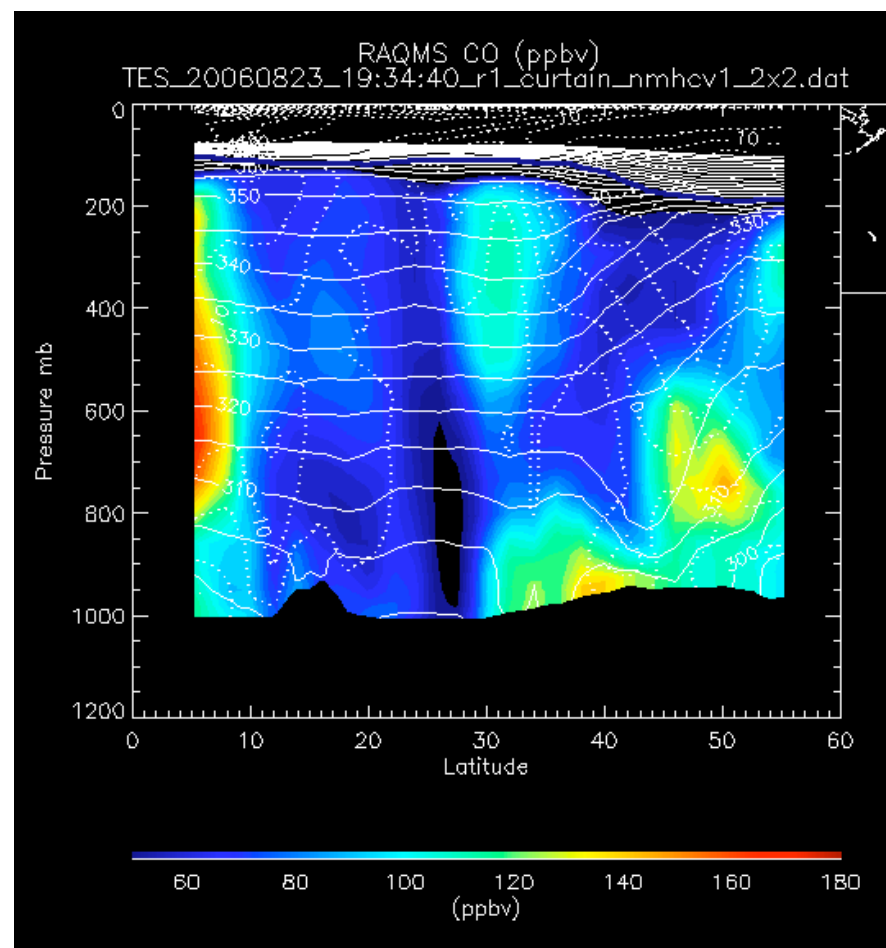
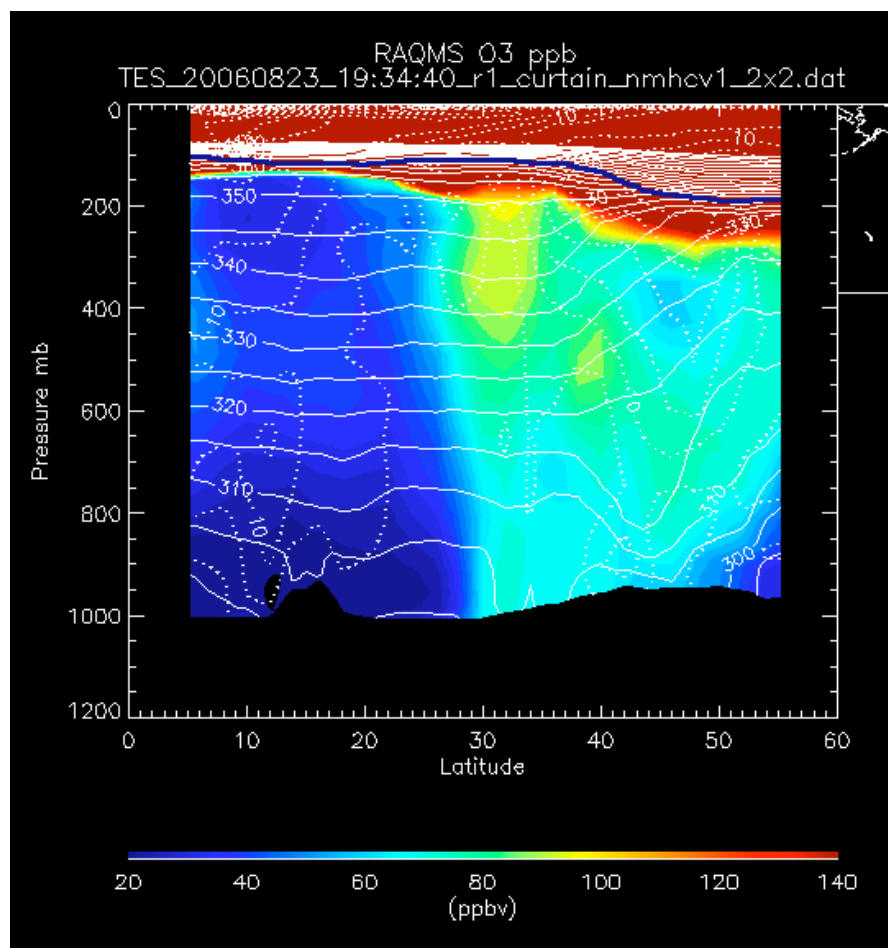
- TES retrievals of CO and ozone vertical profiles in conjunction with the RAQMS global model provide a means of investigating the impact of distant sources on the background concentrations over Texas.
- Enhancement observed from TES east of the Houston area in both CO and ozone, slightly higher than RAQMS fields.
- Model analysis suggests anthropogenic production of ozone from surface emissions at -90 hrs.
- Ozone at 850 mb on Aug 23rd, 2006 is above the boundary layer and therefore will have minimal impact on Houston air quality.
- Validation of TES estimates with respect to IONS ozone sonde measurements will be performed.
- Additional information for RAQMS (<http://rossby.larc.nasa.gov/RAQMS/>) and TES (http://tes.jpl.nasa.gov/TexAQS_2006/main_SS_TEXAQS_2006.html)



Back-up slides



RAQMS CO and ozone model fields



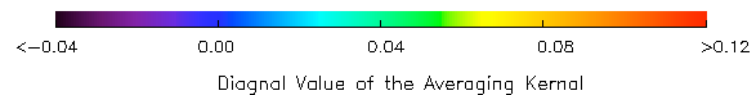
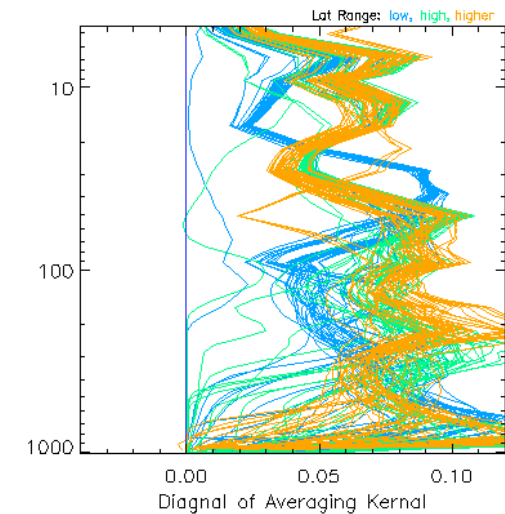
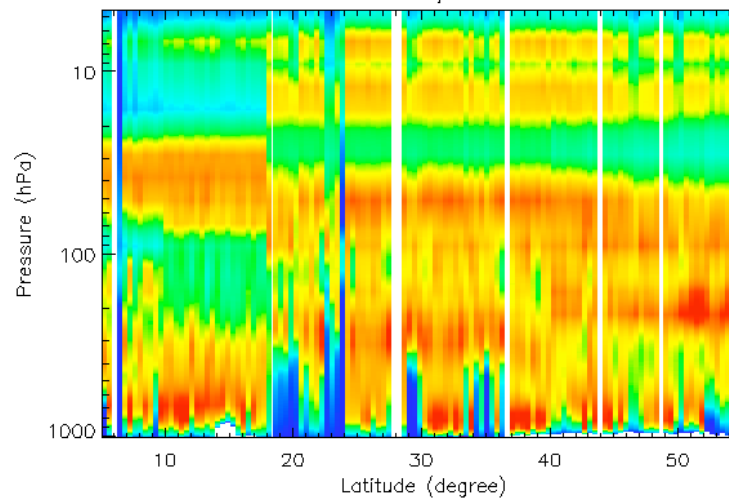
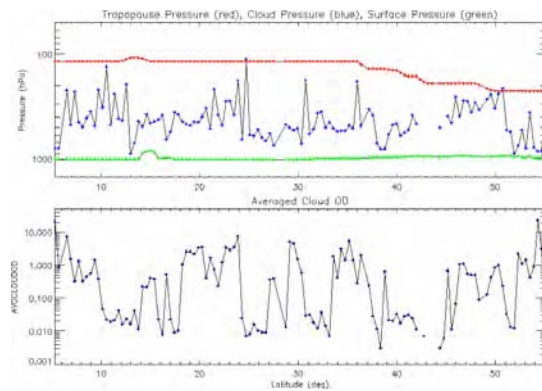


TES sensitivity metric: the averaging kernel

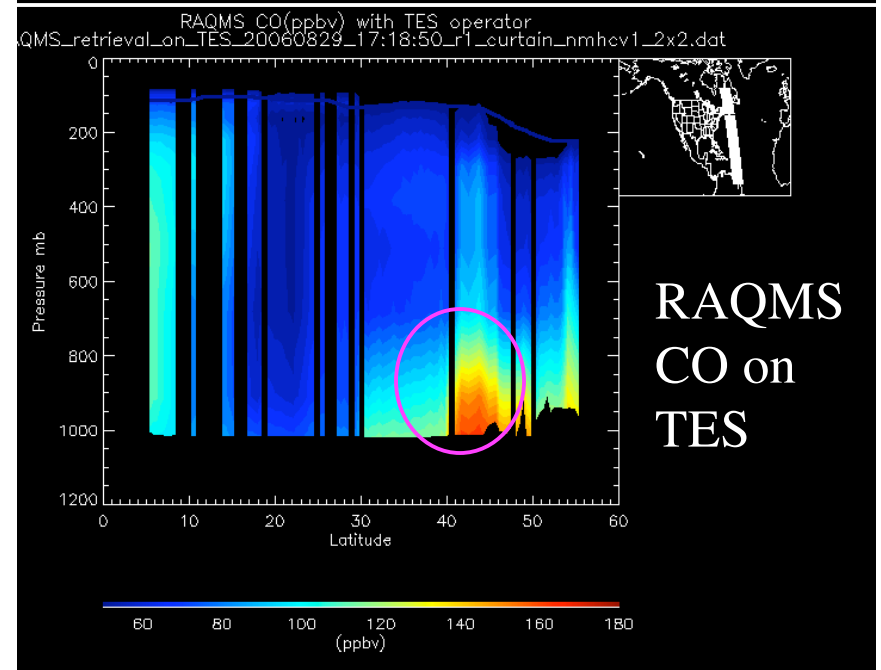
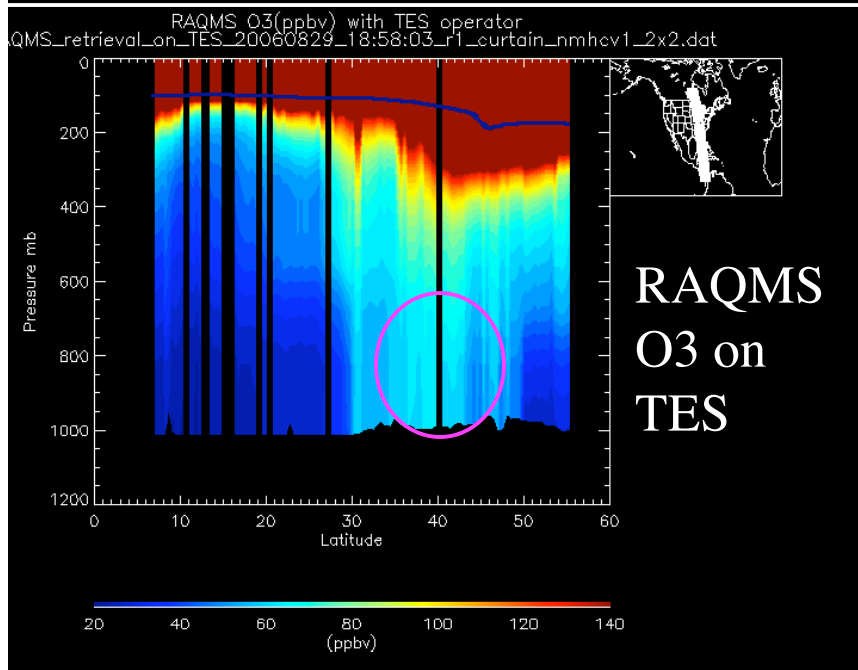
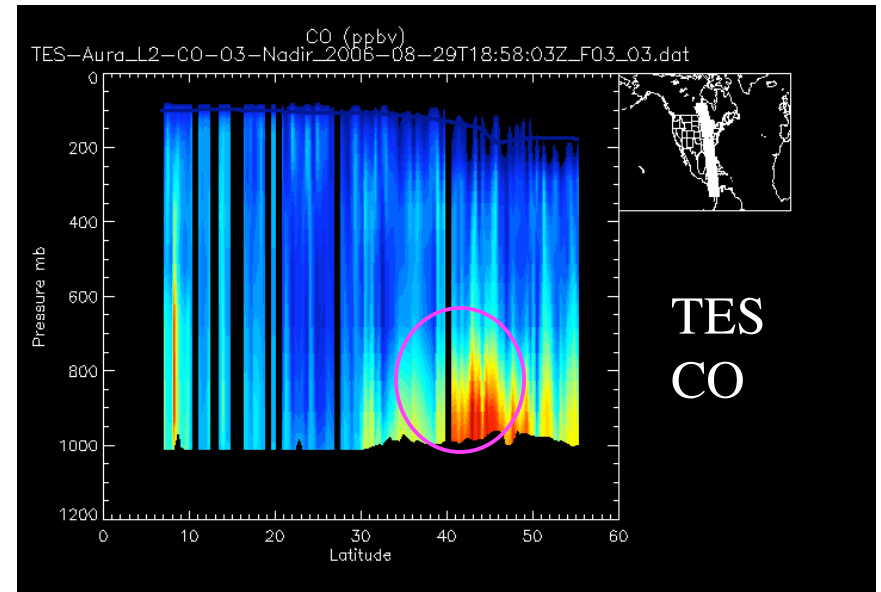
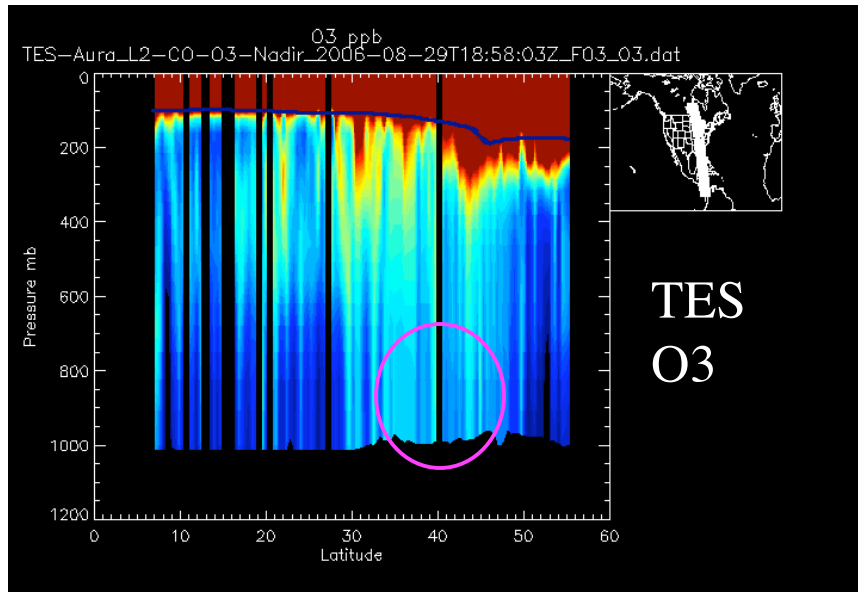
TES Step & Stare Nadir Averaging Kernel Diagonals: Ozone

Cross Section Along Orbit Track: RunID=4911, Seq=1-1, Scan=0-124, UTctime=2006-8-23 19:34:40-19:48:31

min = -0.00302002, max = 0.197352

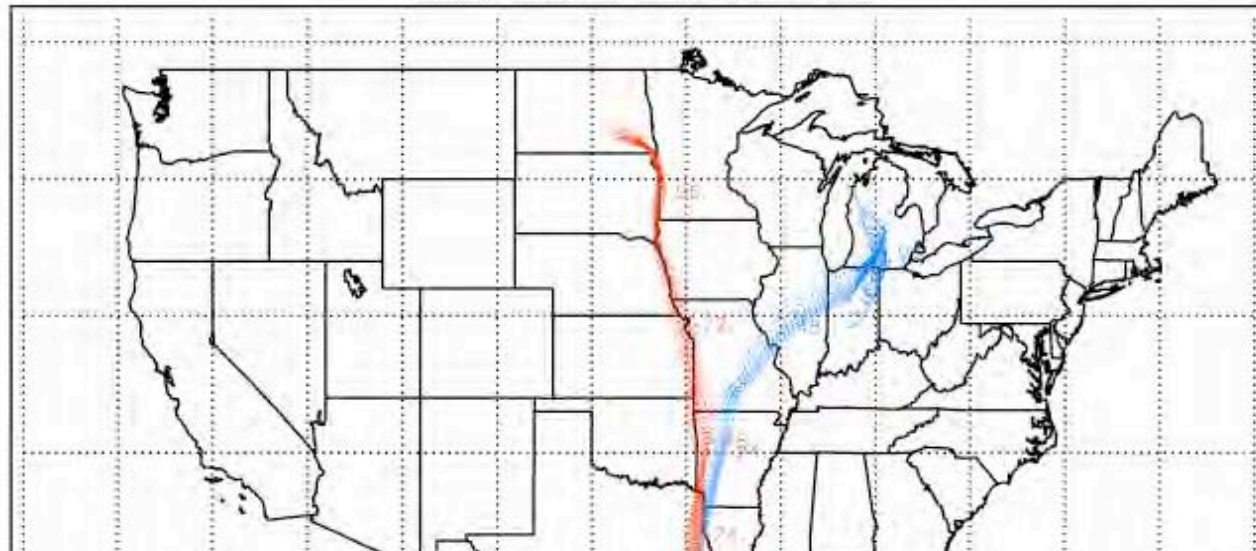


TES special observations Aug 29 2006 and RAQMS curtains on orbit track show moderate enhancements in O3 and CO near 800mb near 40N

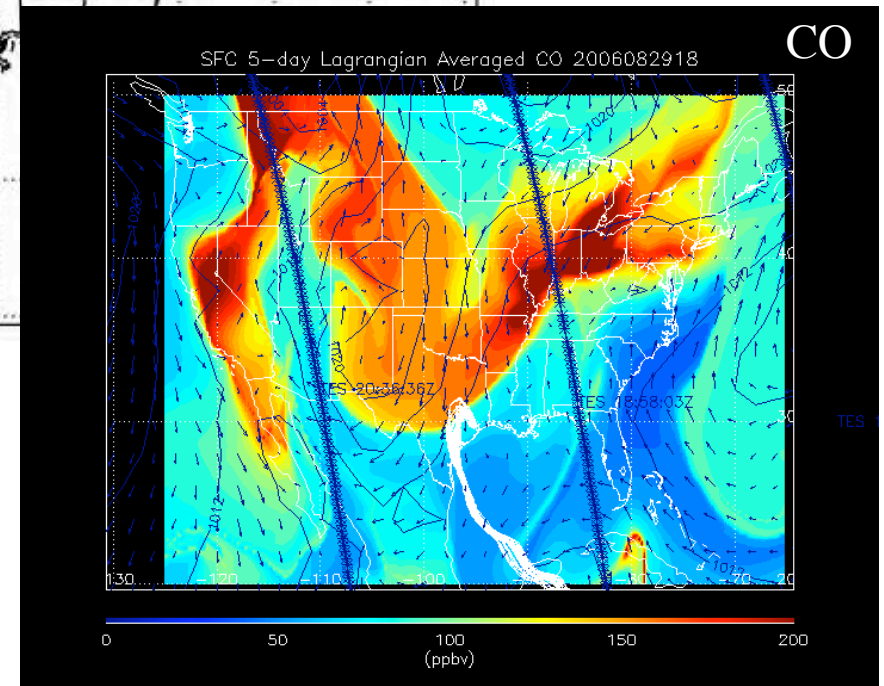
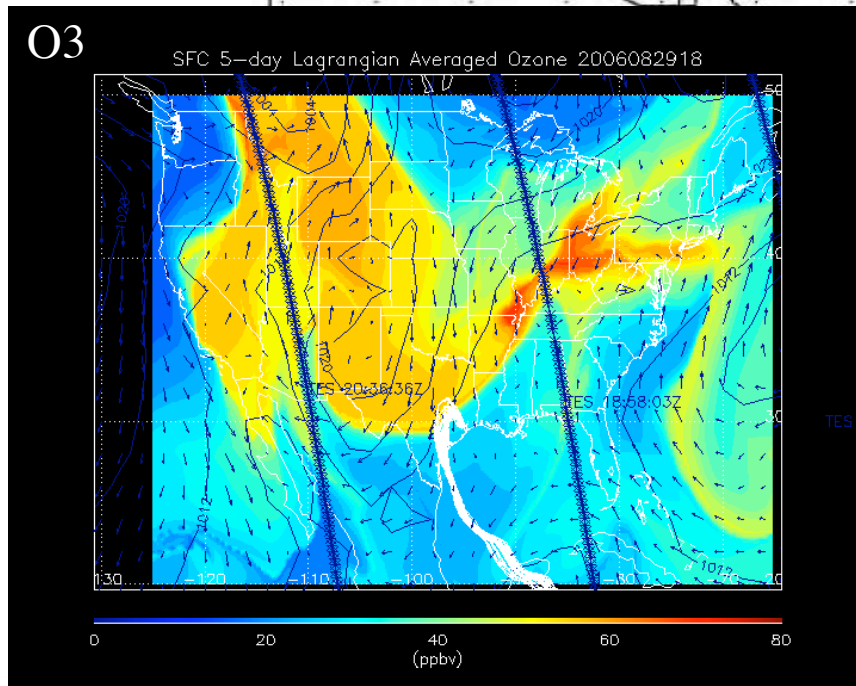


Houston 5-day back trajectories initialized Sep 01 intersect TES orbit ~3 days prior;
similar behavior for Dallas back trajectories

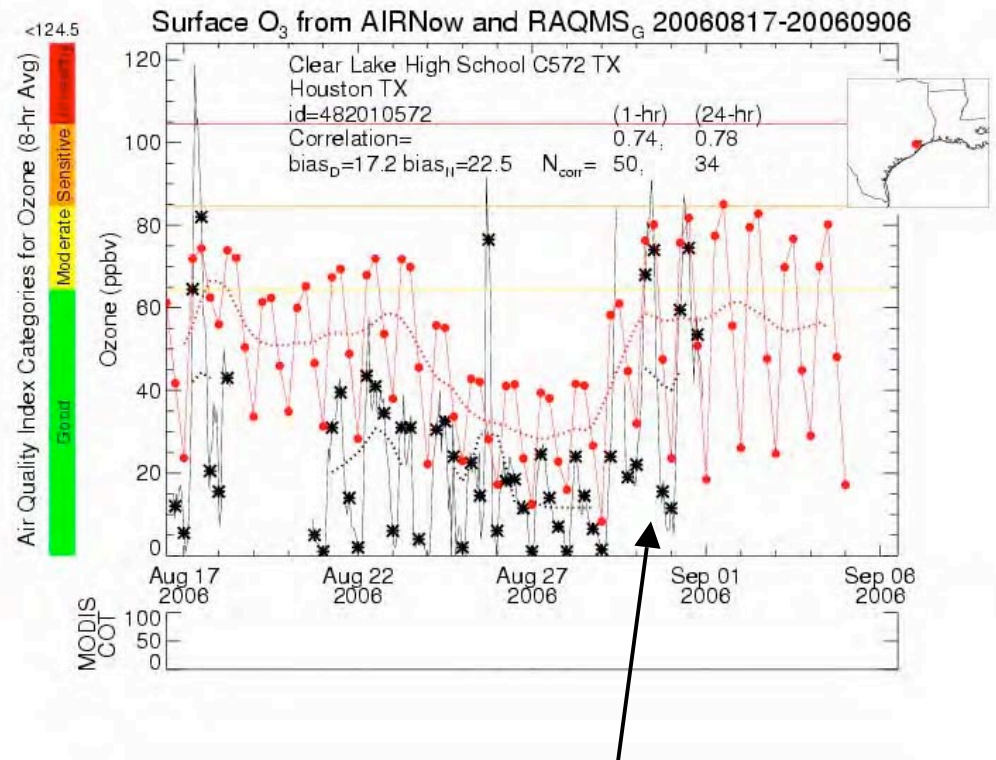
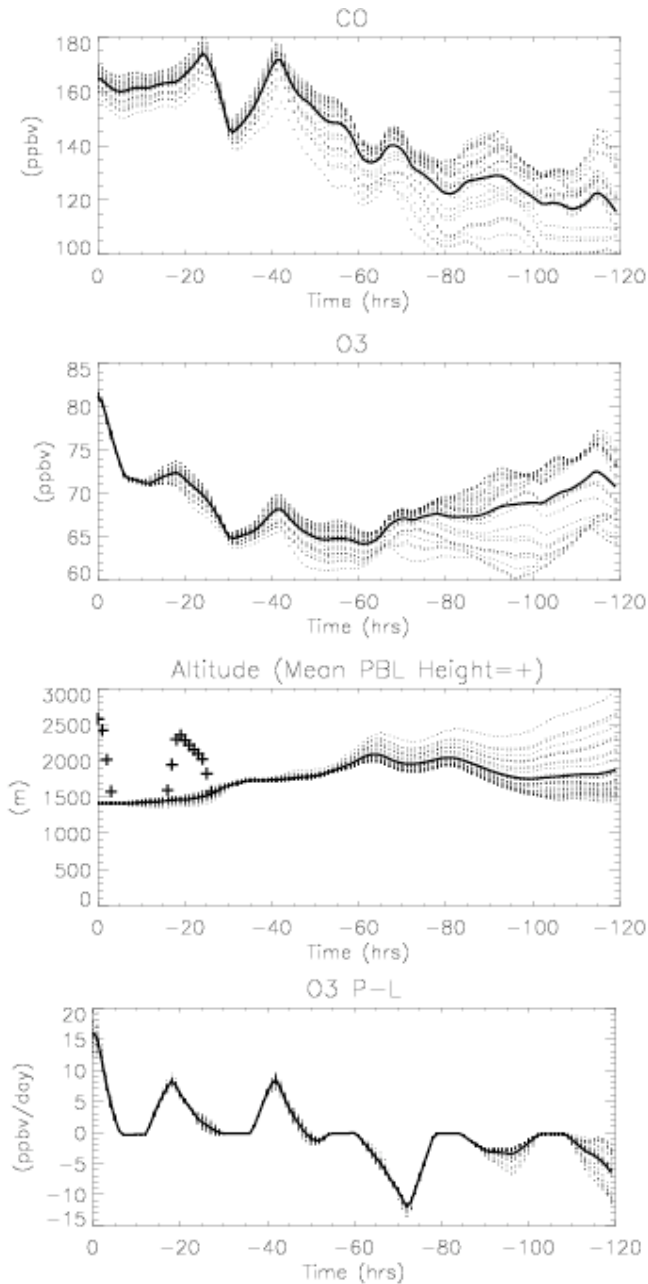
SFC (Red)/850 (Blue) 5-day Backtrajectories
initialized 2006080118, Houston TX AIRNOW Sites



Red: initialized
at surface
Blue: initialized
at 850mb



Back trajectories arriving Houston 850mb show air descending into BL and O₃ building last 72 hrs, suggesting current event is combination of transport from central US and local emissions



RAQMS model has high bias but is capturing temporal evolution of large-scale events well

Similar situation for Dallas but note that long-range contribution appears to be much larger fraction relative to local emissions

