15 September Preview
Rapid Science Synthesis*

Questions G, H – Regional Background O_3: Satellite, P-3 data
- **Regional influence on Houston air quality**
  (Wallace McMillan, Brad Pierce)

Questions A, C, D, E – Emissions
- **Modeled isoprene concentrations vs. 2000 observations**
  (Elena McDonald-Buller)

Question B – Mixed Layer Height: Moody Tower data
  (Moody Tower team)

Question I – Chemical mechanisms: Moody Tower data
- **Ozone and radical production (Moody Tower team)**

Questions A, C, D, E – Emissions: Moody Tower data
- **Aerosol production (Moody Tower team)**

Questions A, C, D, E – Emissions: RH Brown data
- **VOC measurements vs. inventory (Lori Del Negro)**

***http://esrl.noaa.gov/csd/2006/rss/**

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Questions G, H – Regional Background O_3: Satellite, P-3 data

- Regional influence on Houston air quality
  (Wallace McMillan, Brad Pierce)

Regional Influences During Aug 30 - Sep 02, 2006
Houston Ozone AQ event

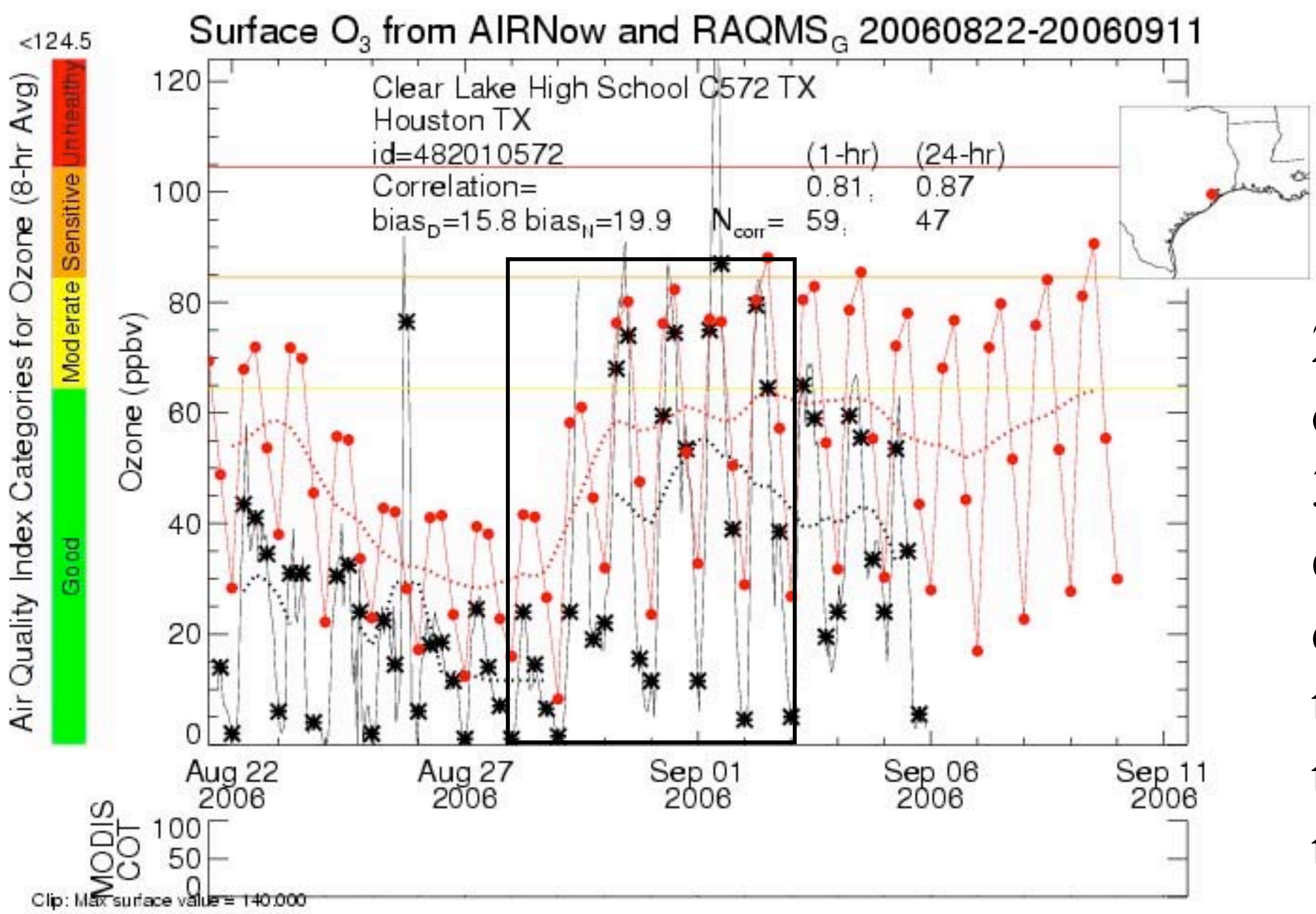
Synthesis of EPA AIRNOW, NOAA P3, NASA AIRS measurements and RAQMS chemical analyses

Wallace McMillan (U. Maryland Baltimore County)
Brad Pierce (NASA Langley Research Center)
Jassim A. Al-Saadi (NASA LaRC)
Juying Warner (JCET/UMBC)

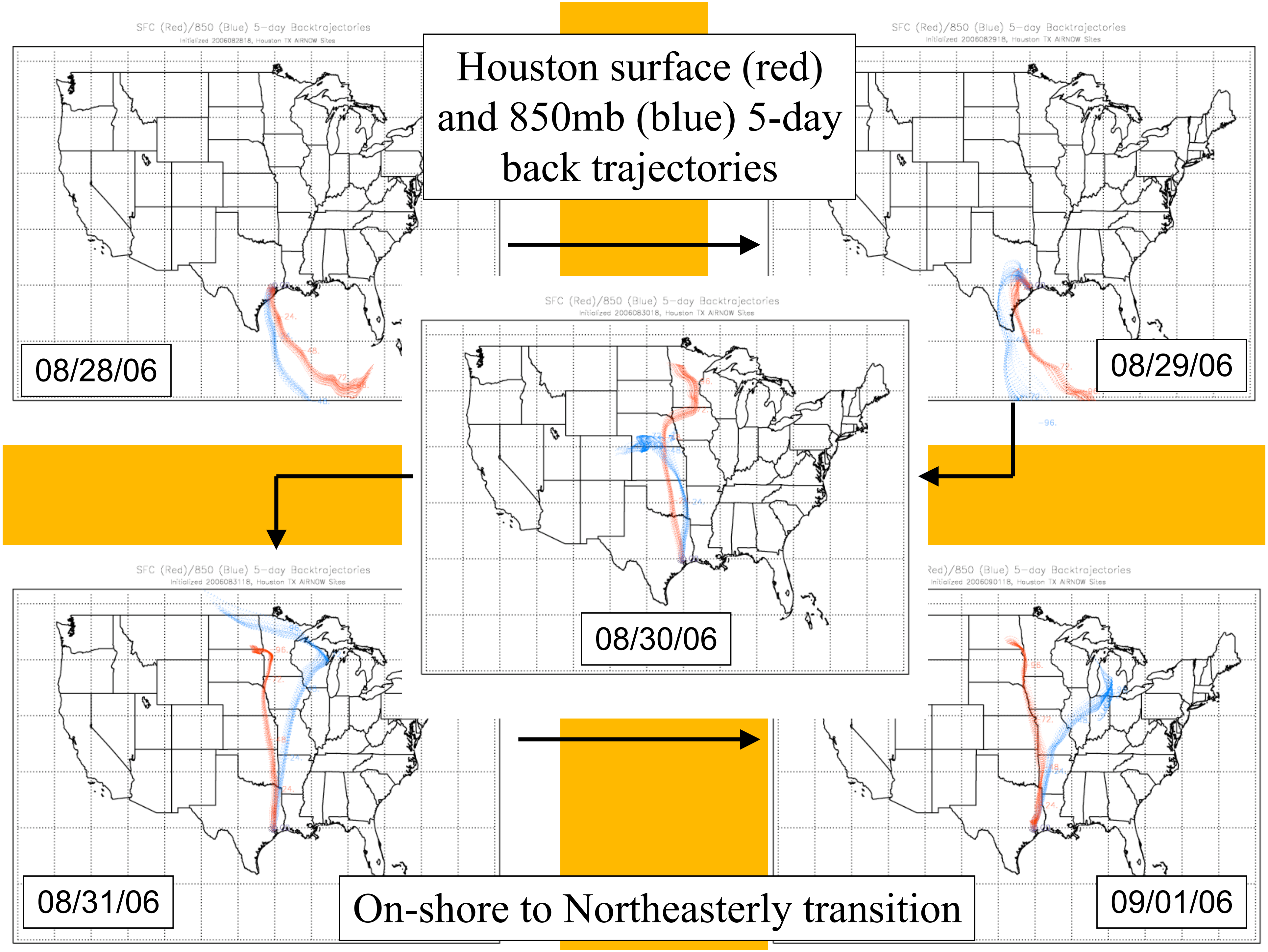
With thanks to
Tom Ryerson, John Holloway, Dirk Richter,
Chris Barnet, Walter Wolf

Regional Influences During Aug 30 - Sep 02, 2006 Houston Ozone AQ event

Synthesis of EPA AIRNOW, NOAA P3, NASA AIRS measurements and RAQMS chemical analyses



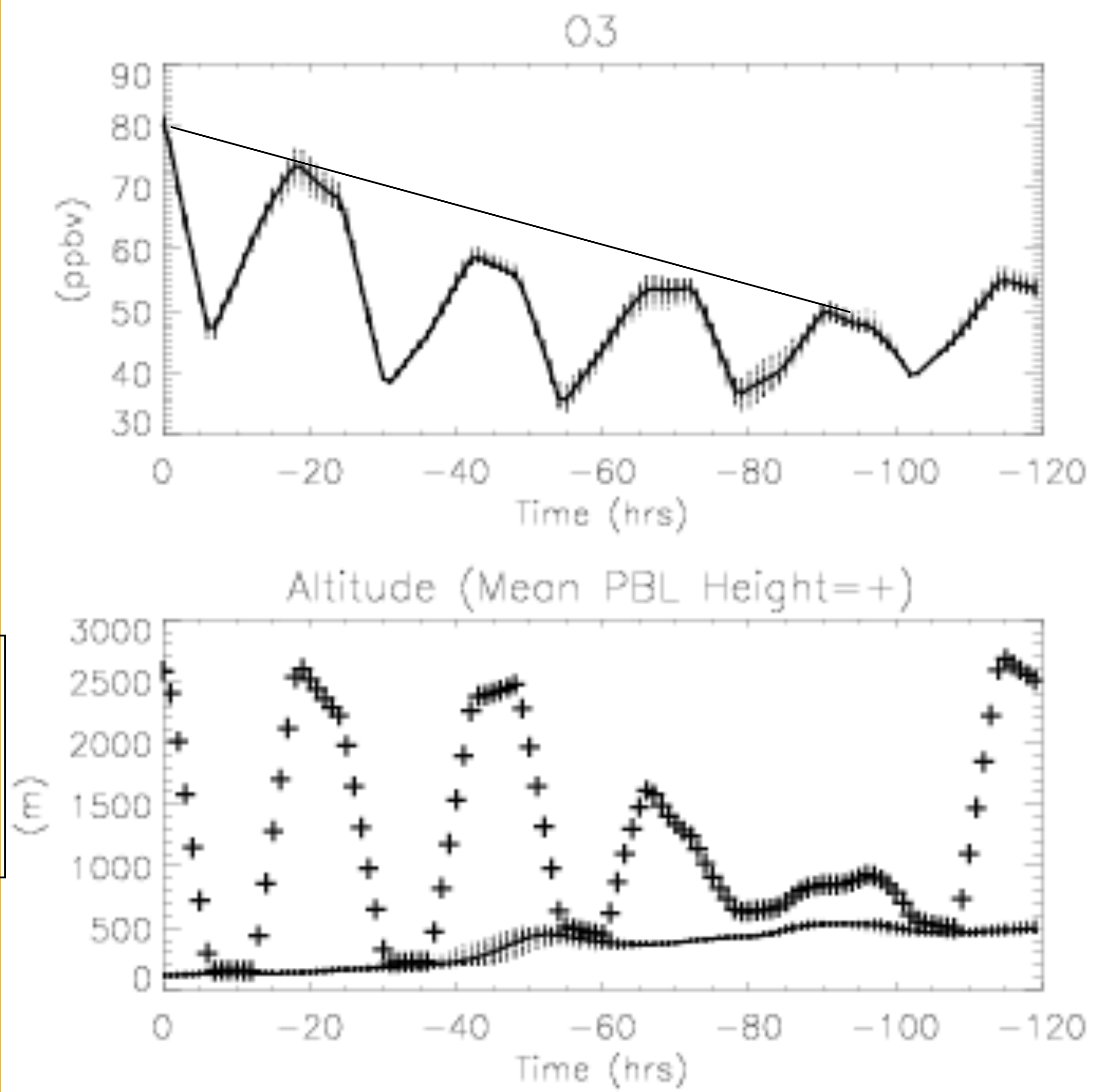
24hr averaged ozone shows 30ppbv enhancement during the period that could be due to regional transport


Houston surface (red) and 850mb (blue) 5-day back trajectories
SFC (Red)/850 (Blue) 5-day Backtrajectories
08/28/06
08/29/06
08/30/06
08/31/06
09/01/06
On-shore to Northeasterly transition

5-day Lagrangian mean ozone mixing ratio, altitude, and pbl height Houston AIRNOW sites 09/01/06

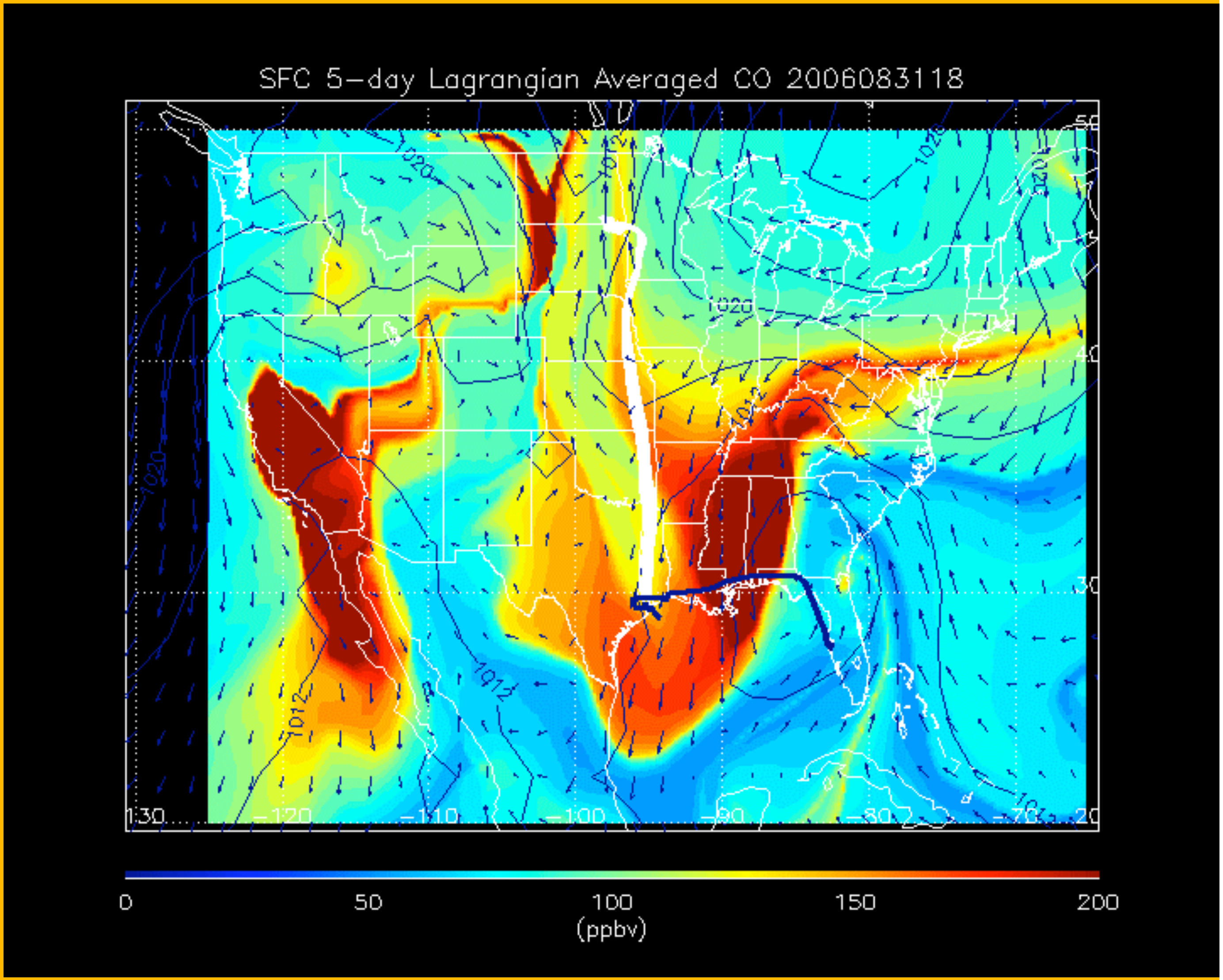
Daily ozone production along back trajectories results in Lagrangian mean ozone increase of nearly 30ppbv during previous 4 days

Trajectories remain within boundary layer during previous 5 days



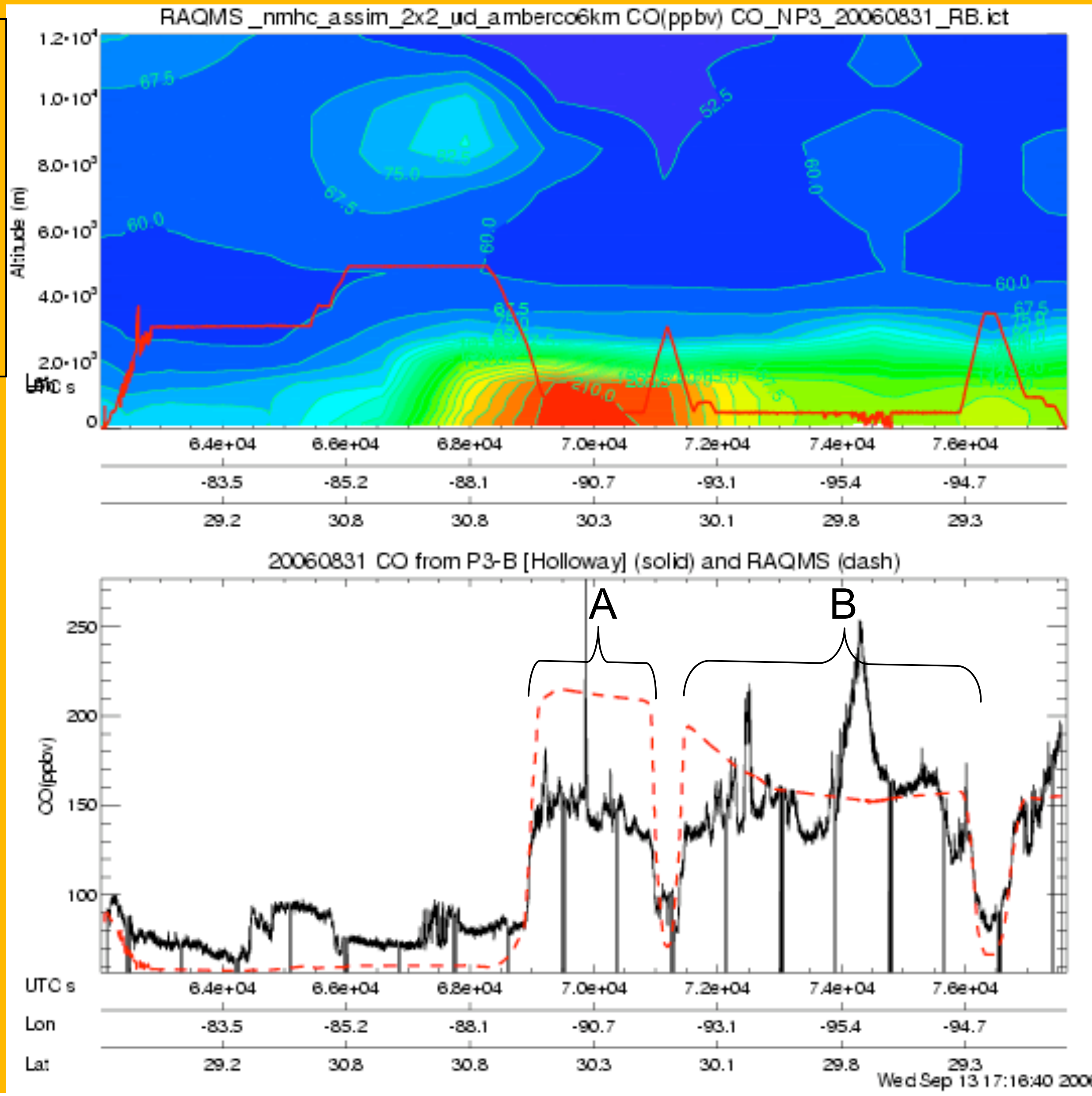
NOAA P3 measurements are used to assess model predictions

08/31 NOAA P3 transit flight sampled the airmass that was impacting Houston air quality during this period.



Model Verification: RAQMS vs P3 (Holloway) CO 08/31/06

NOAA P3 measurements provide verification of regional scale predictions and satellite measurements

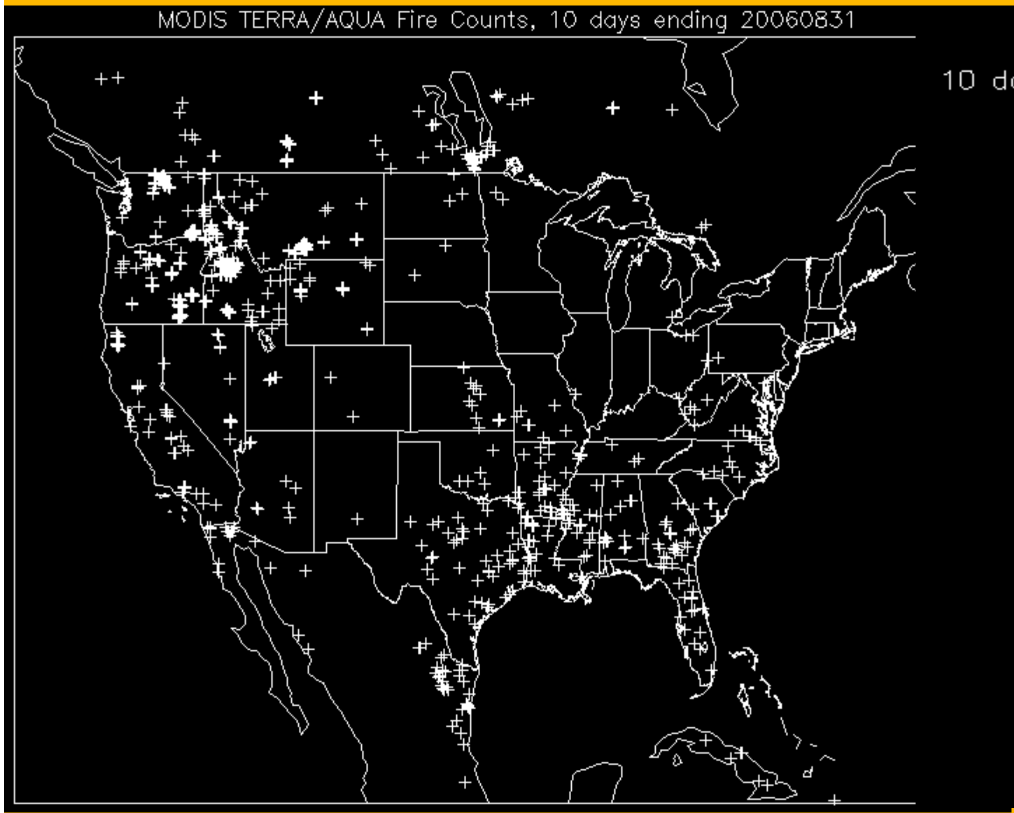


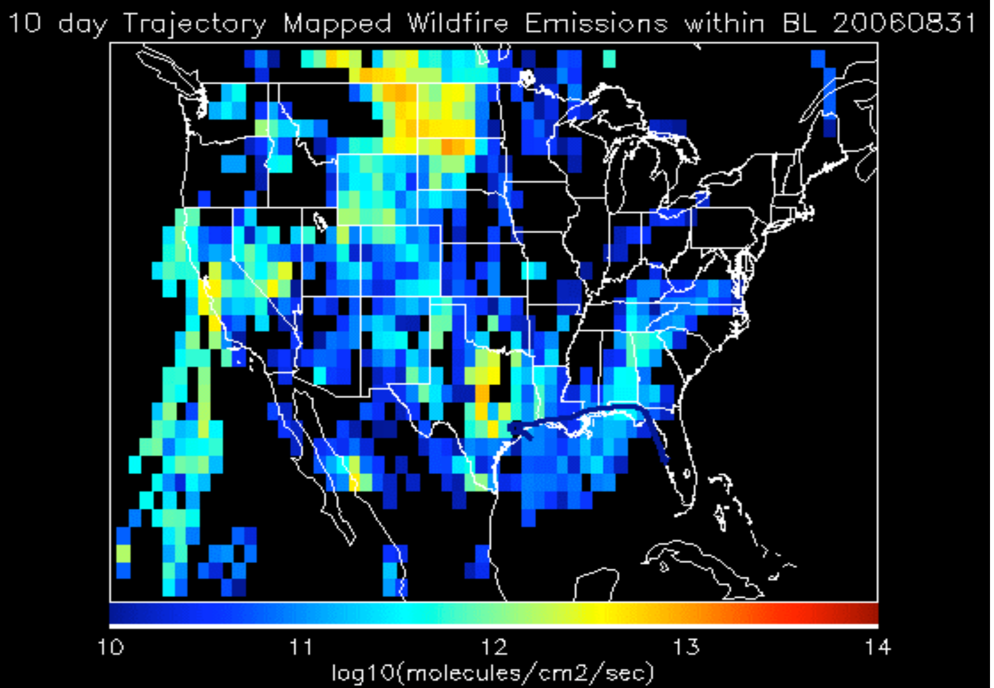
RAQMS overestimates Eastern BL CO enhancement (A) by 50% but does a reasonable job predicting enhancements in background CO on western portion of P3 flight (B).

CO enhancements due to local biomass burning and Houston are not predicted due to coarse model resolution

Boundary Layer Wildfire Influences 20060831

(Ensemble average emission rates computed from 0-10 day wildfire trajectories found within boundary layer)

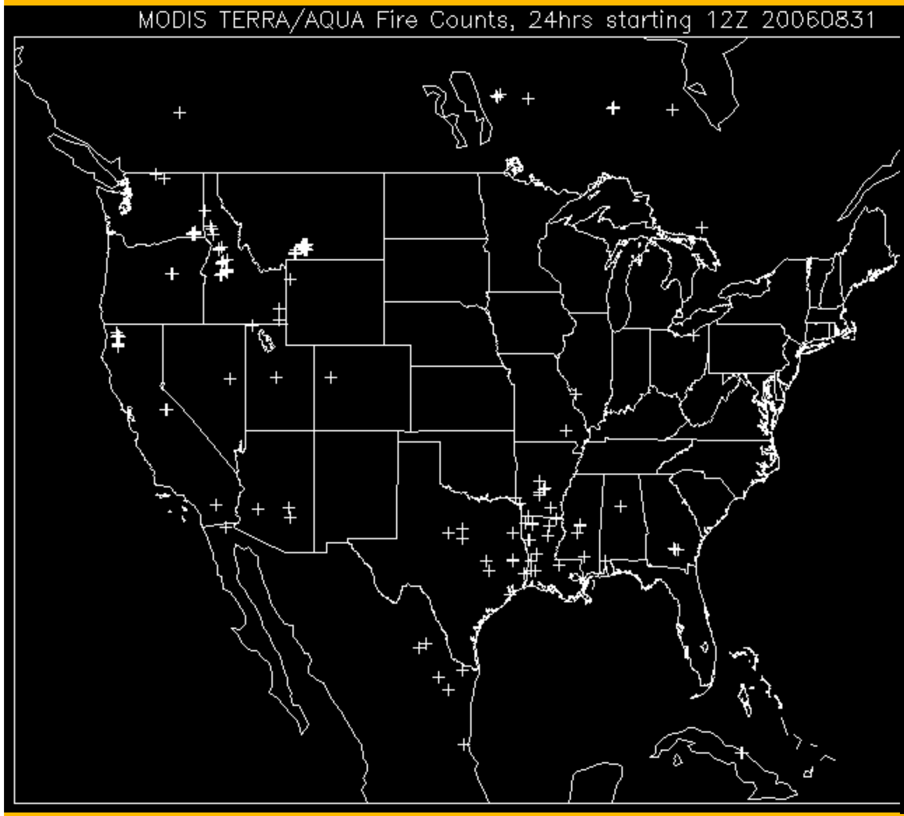


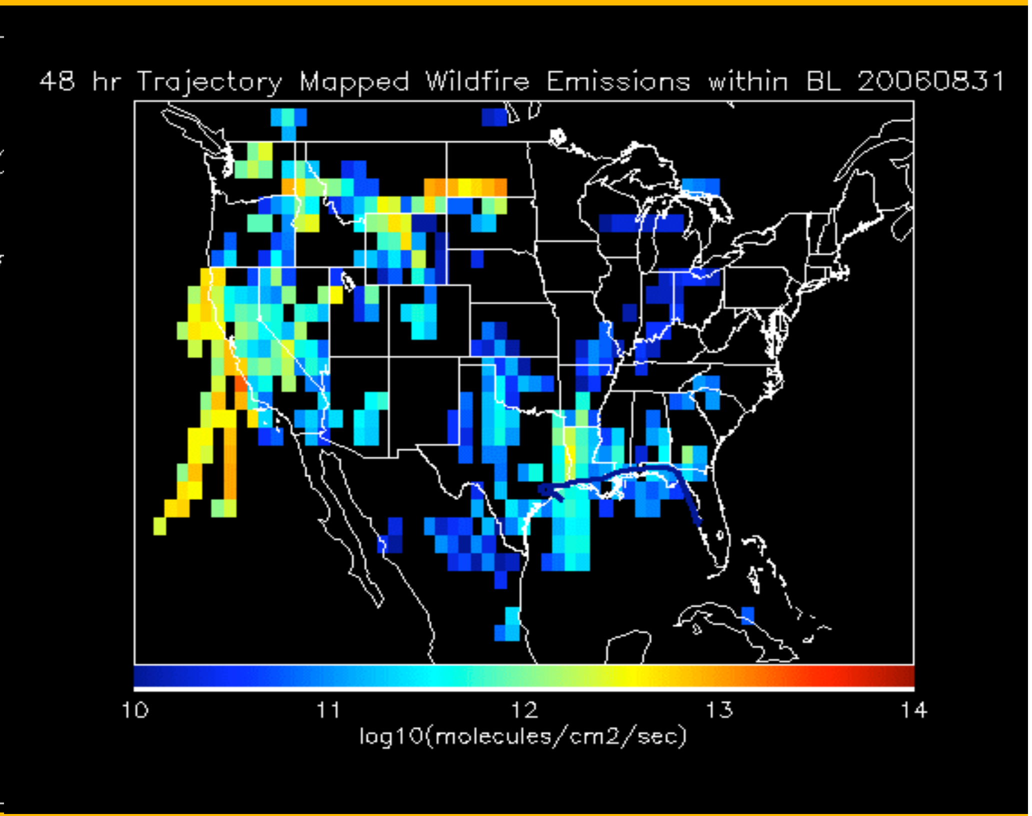


Predicted regional scale, boundary layer CO enhancements along P3 flight track are influenced by long-range transport of North Western wildfire emissions.

Near field Boundary Layer Wildfire Influences 20060831

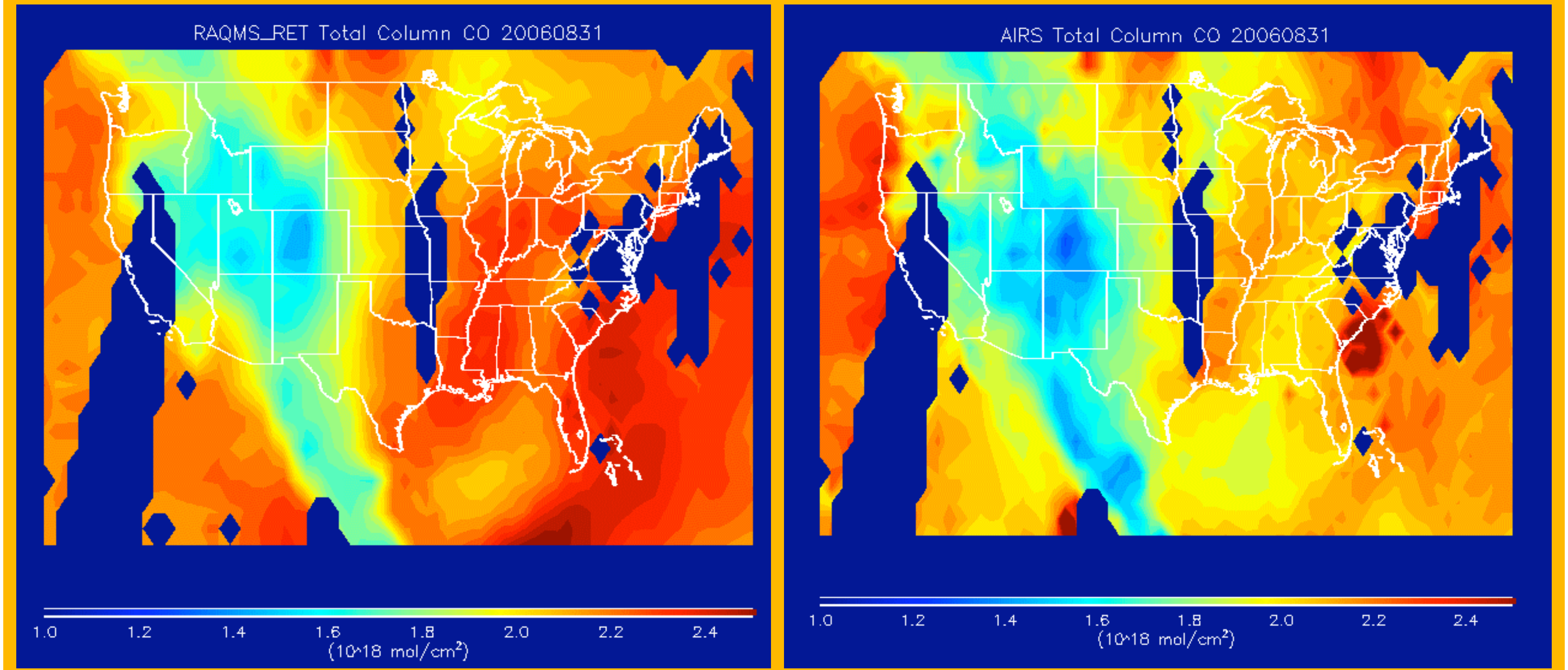
(Ensemble average emission rates computed from 0-48 hr wildfire trajectories found within boundary layer)





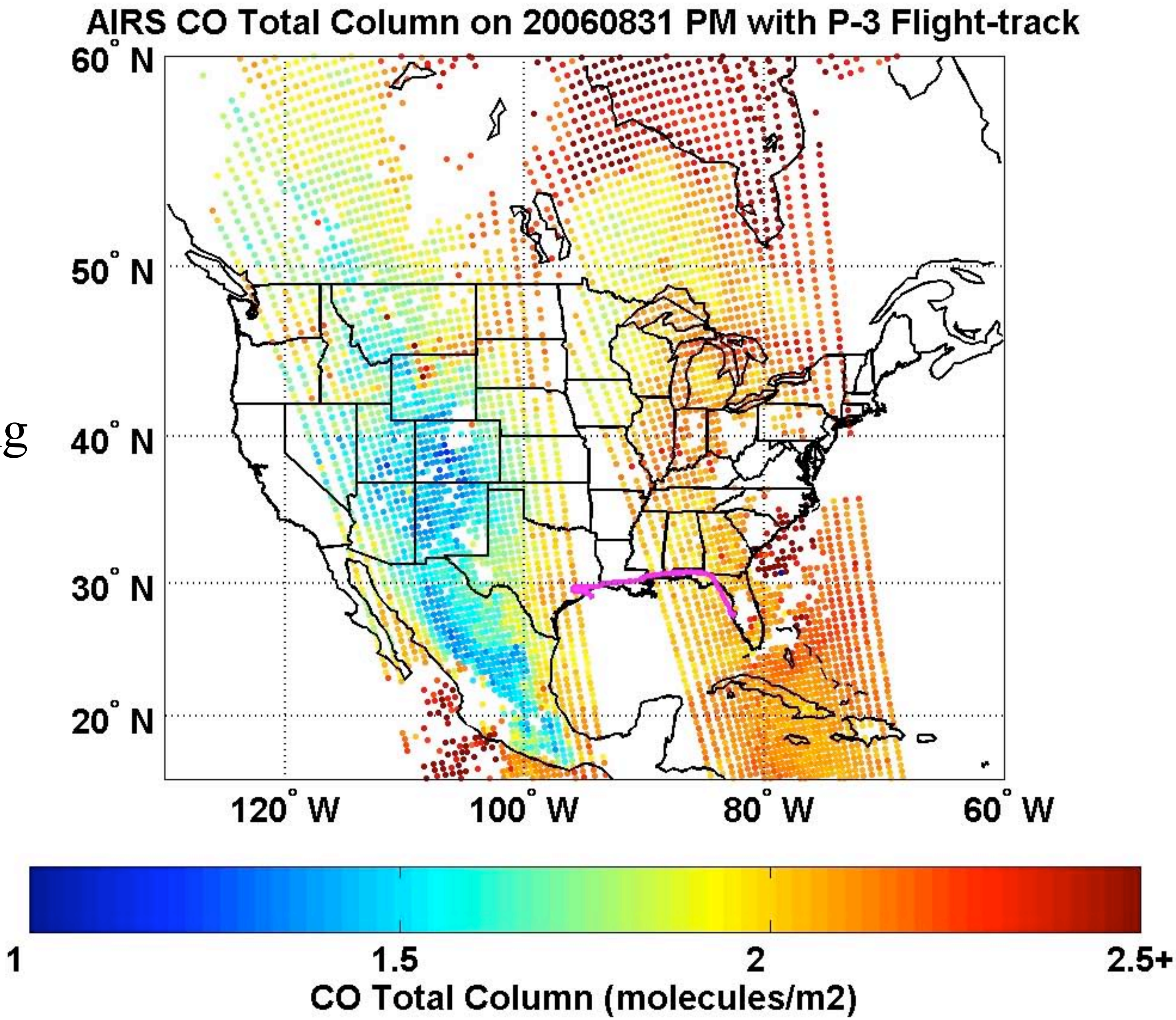
Observed, finescale boundary layer CO enhancements along P3 flight track are influenced by recent local biomass burning in Northern Louisiana.

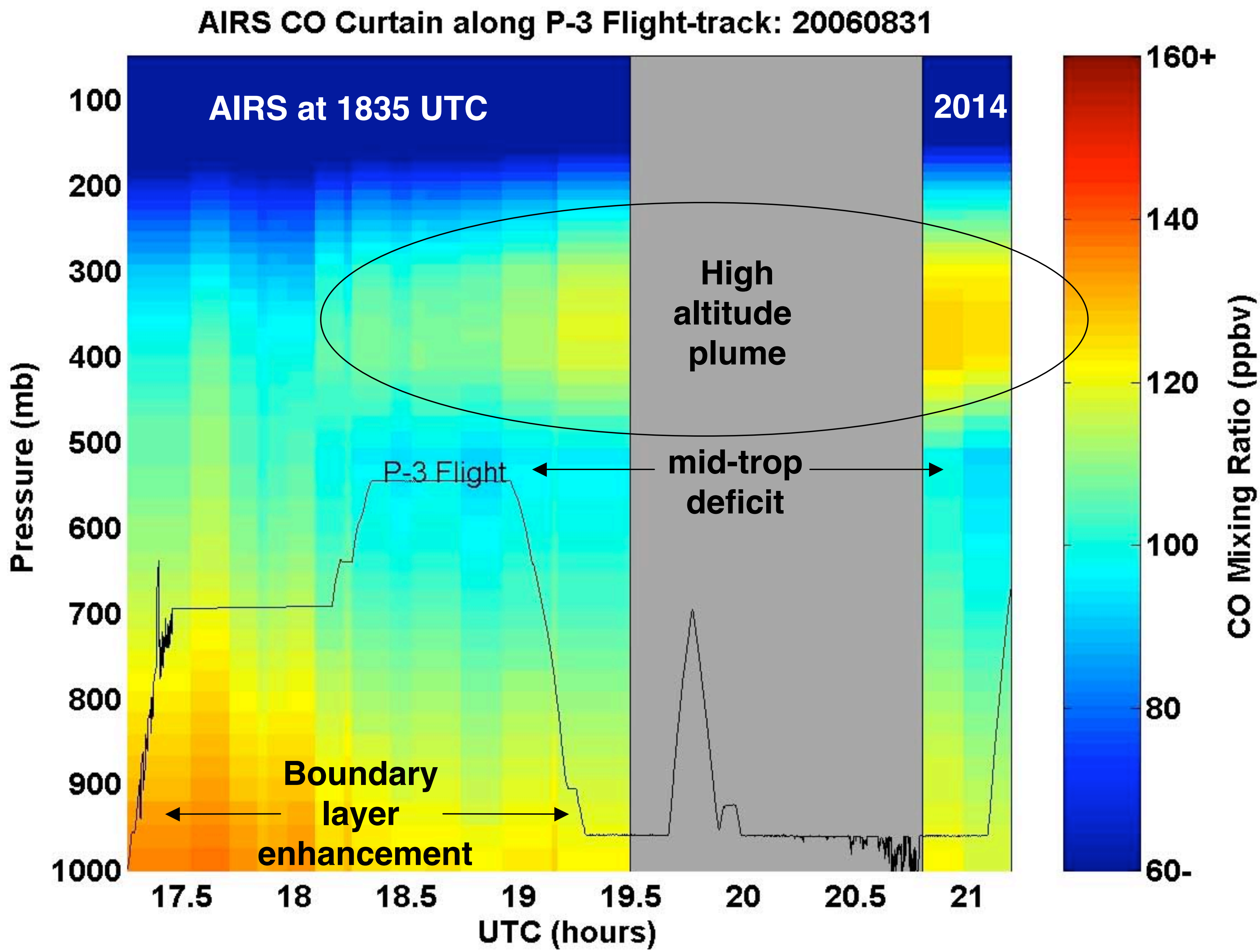
AIRS vs RAQMS Total Column CO 20060831
(AIRS observation operator applied to RAQMS)

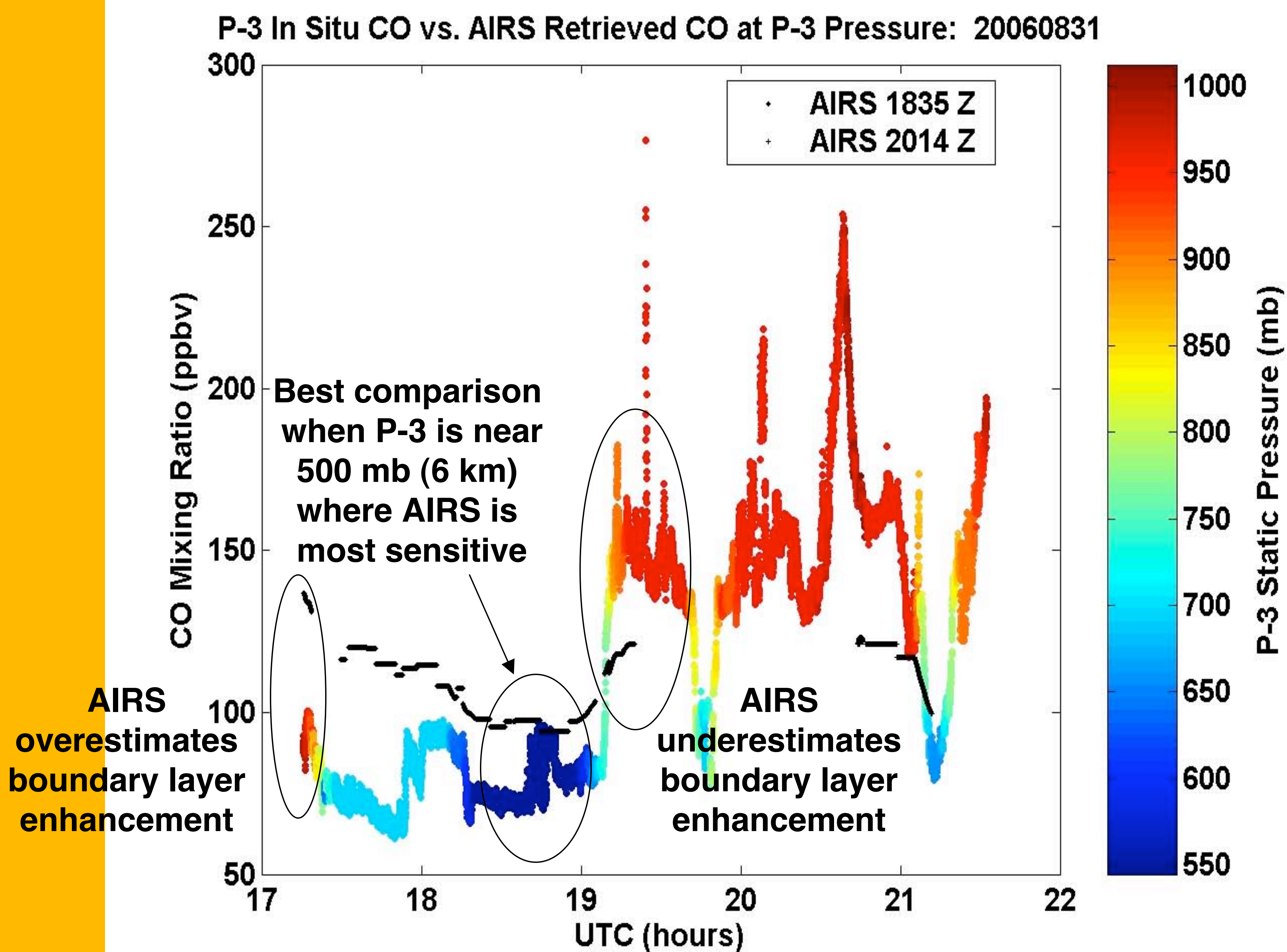


AIRS provides verification of model predictions and a regional context for P3 measurements: CO, O_3, H_2O, Temperature

AIRS CONUS coverage during the NOAA P3 flight




AIRS CO Curtain along P-3 Flight-track: 20060831
AIRS at 1835 UTC
2014
High altitude plume
P-3 Flight
mid-trop deficit
Boundary layer enhancement
Pressure (mb)
100
200
300
400
500
600
700
800
900
1000
17.5
18
18.5
19
19.5
20
20.5
21
UTC (hours)
160+
140
120
100
80
60-
CO Mixing Ratio (ppbv)

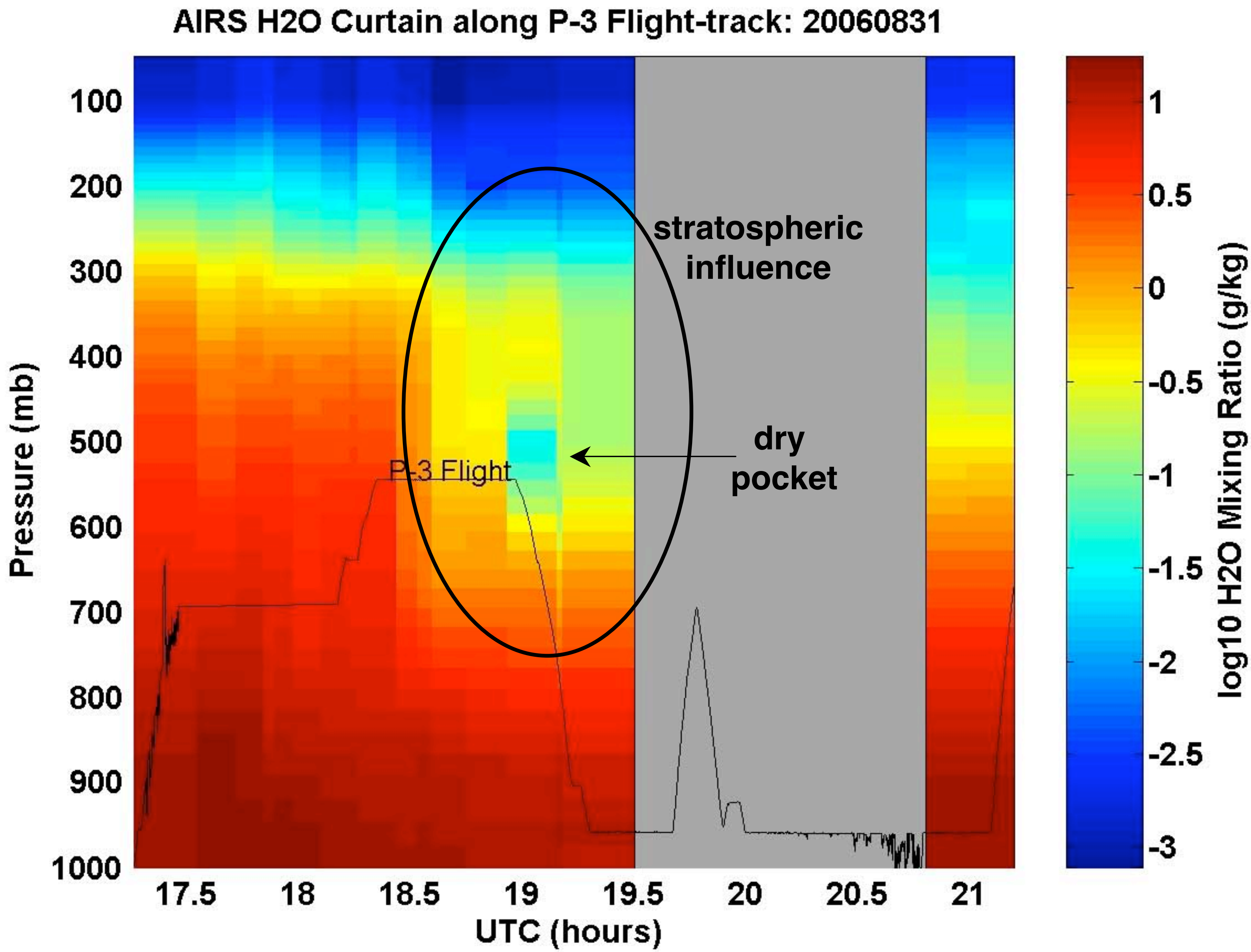

P-3 In Situ CO vs. AIRS Retrieved CO at P-3 Pressure: 20060831
AIRS 1835 Z
AIRS 2014 Z
CO Mixing Ratio (ppbv)
300
250
200
150
100
50
17
18
19
20
21
22
UTC (hours)
P-3 Static Pressure (mb)
1000
950
900
850
800
750
700
650
600
550
Best comparison when P-3 is near 500 mb (6 km) where AIRS is most sensitive
AIRS overestimates boundary layer enhancement
AIRS underestimates boundary layer enhancement

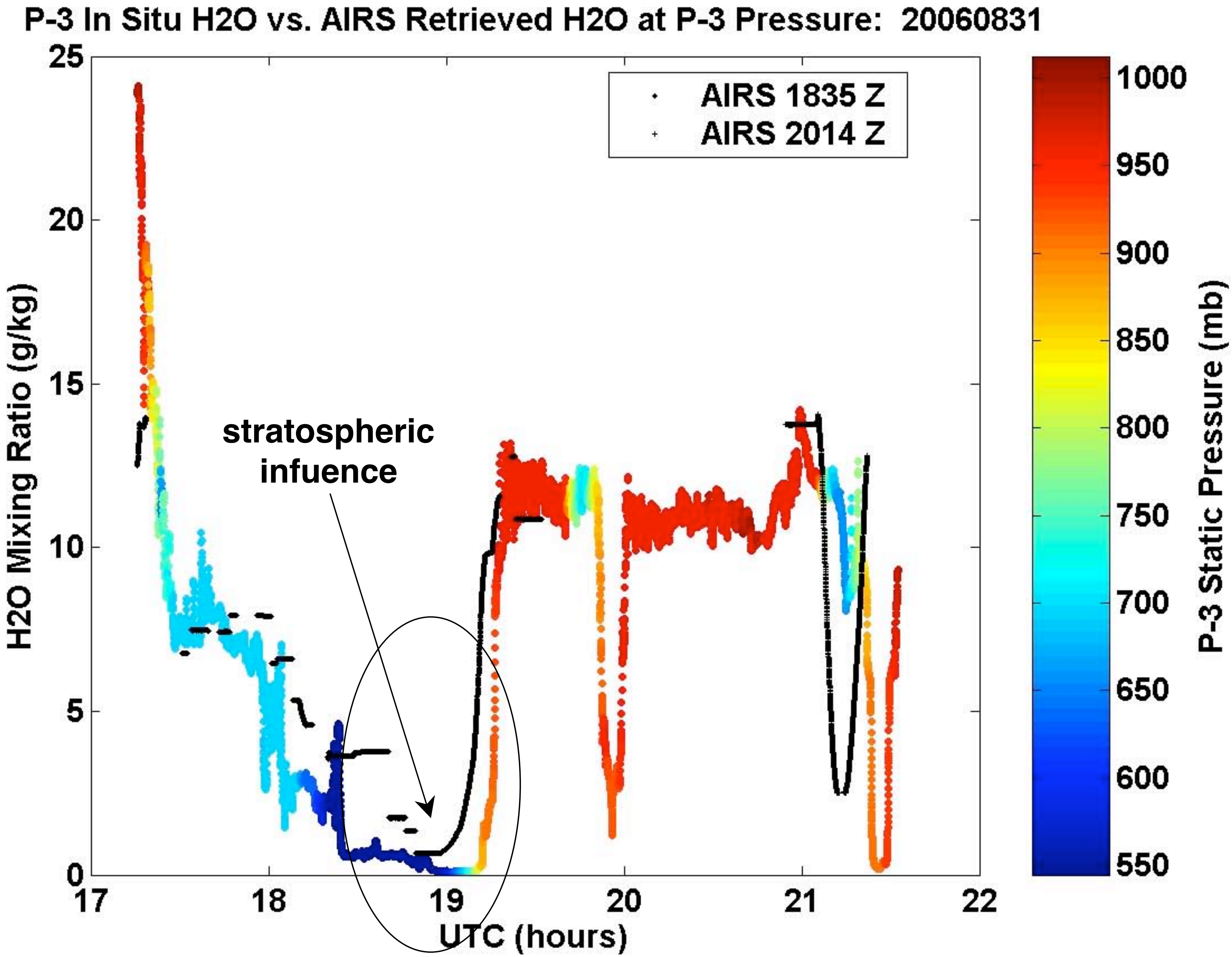
Summary

- Synthesis of Houston AIRNOW, NOAA P3, NASA AIRS measurements, and RAQMS predictions:
  - AIRS provides regional context for interpretation of ground and airborne measurements.
  - Model and trajectory analysis provides link between local air quality and regional observations.
  - Comparisons to P3 guide interpretation of model predictions and AIRS retrieved boundary layer CO enhancements.

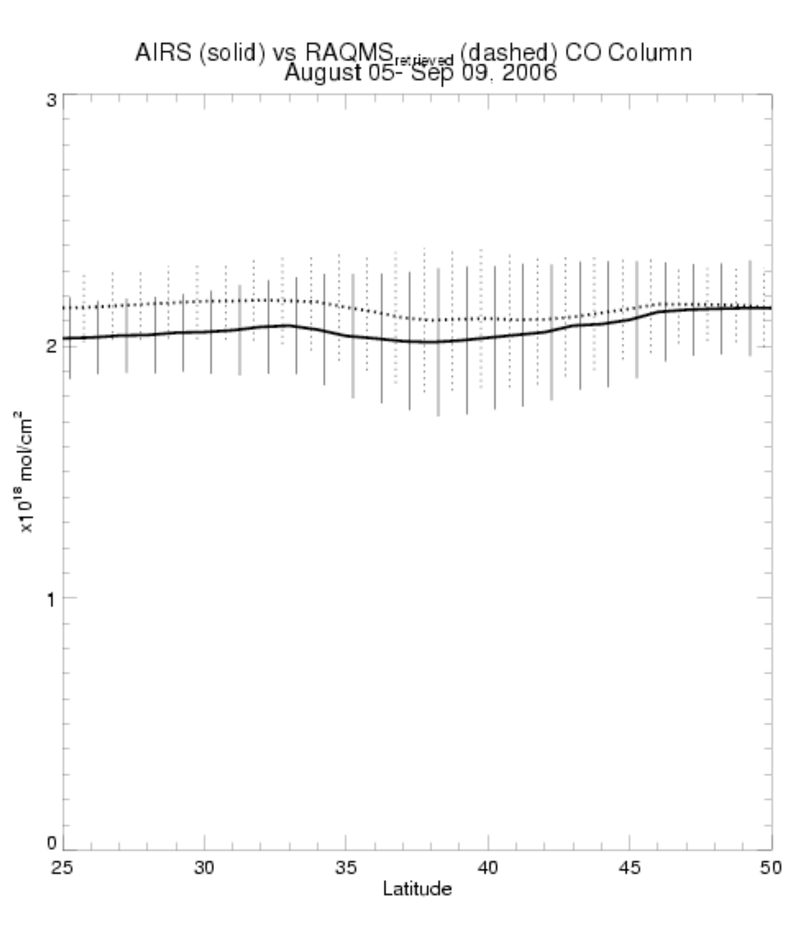
- Results suggest:
  - Up to 30 ppbv regional scale O_3 enhancement contributed to Houston air quality August 30-September 2, 2006.
  - Near-field (Louisiana) and remote (Pacific Northwest) biomass burning contributed to the regional scale enhancement.

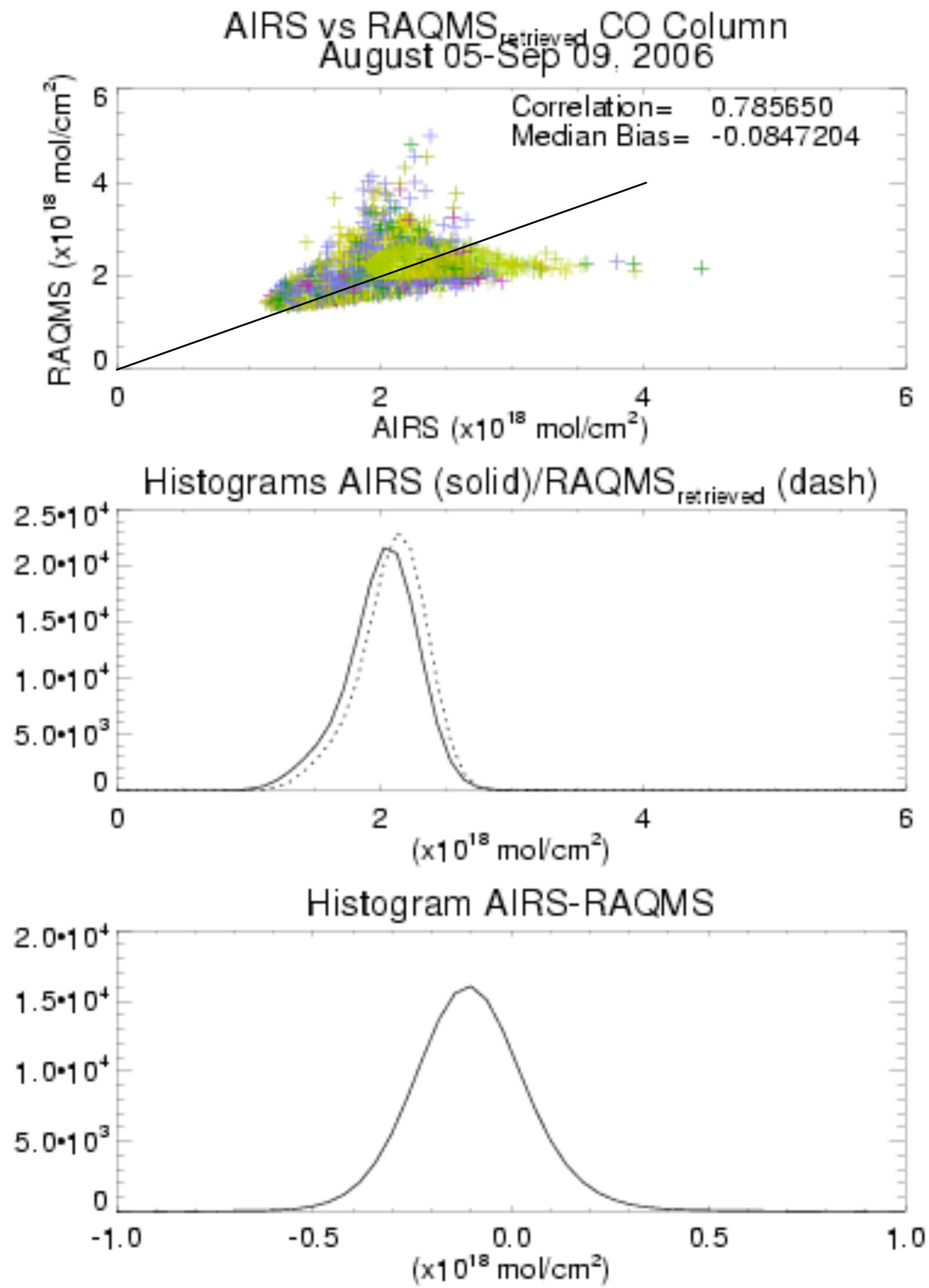
Extra slides


AIRS H2O Curtain along P-3 Flight-track: 20060831
Pressure (mb)
100
200
300
400
500
600
700
800
900
1000
17.5
18
18.5
19
19.5
20
20.5
21
UTC (hours)
stratospheric
influence
dry
pocket
P-3 Flight
log10 H2O Mixing Ratio (g/kg)
1
0.5
0
-0.5
-1
-1.5
-2
-2.5
-3



P-3 In Situ H2O vs. AIRS Retrieved H2O at P-3 Pressure: 20060831
AIRS 1835 Z
AIRS 2014 Z
stratospheric
infuence
H2O Mixing Ratio (g/kg)
UTC (hours)
P-3 Static Pressure (mb)
0
5
10
15
20
25
17
18
19
20
21
22
550
600
650
700
750
800
850
900
950
1000





RAQMS$_{retrieved}$ CO column is highly correlated (r=0.78) with AIRS CO column over CONUS but has a slight (0.08×10^{18} mol/cm^2) high bias, particularly south of 35^{o}N

Questions A, C, D, E – Emissions

- **Modeled isoprene concentrations vs. 2000 observations (Elena McDonald-Buller)**

Comparisons Of Modeled and Observed Isoprene Concentrations In Southeast Texas

The University of Texas at Austin
Center for Energy and Environmental Resources
and
ENVIRON International Corporation

Objective

- Compare isoprene concentrations recorded using ground and aircraft measurements collected during the Texas Air Quality Study 2000 to model predictions; this provides the starting point for the science synthesis questions dealing with biogenic emission inventories
- Comparisons of predictions of eulerian models (CAMx) with ground and aloft (Electra and G-1) measurements

Modeling Methodology

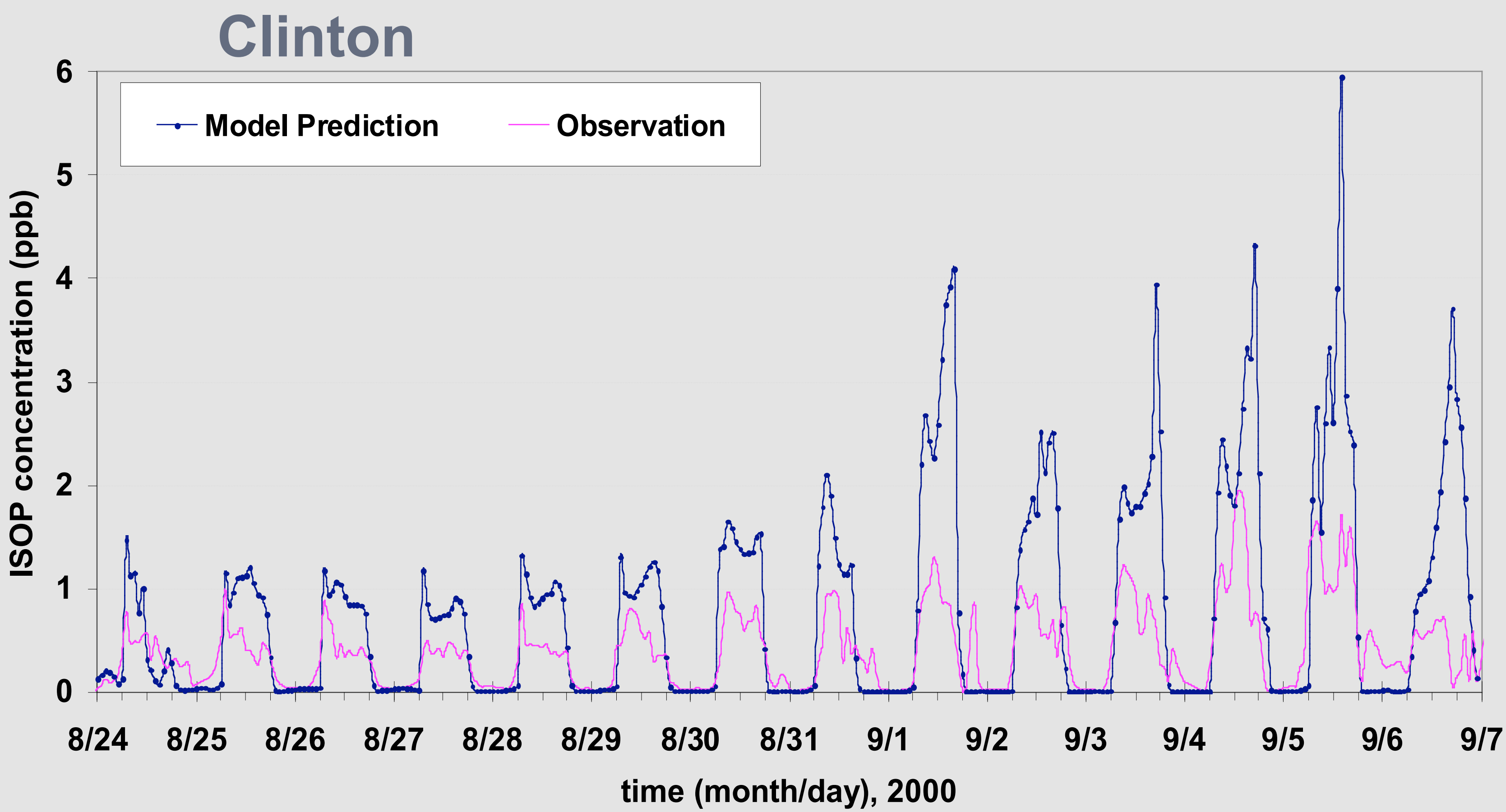
- Biogenic Emissions Modeling:
  - GloBEIS v. 3.1
  - Land cover/land use data from Wiedinmyer et al. (2001) for Texas
  - Surface temperature from interpolation of NWS and other data
  - PAR fluxes from University of Maryland and NOAA for the GEWEX GCIP
  - Wind speed and humidity from MM5.

- Air Quality Modeling:
  - CAMx v. 4.03
  - August 22-September 6, 2000 episode with nested regional/urban grid
  - Base 5b emission inventories from TCEQ SIP modeling
  - CB-IV chemical mechanism

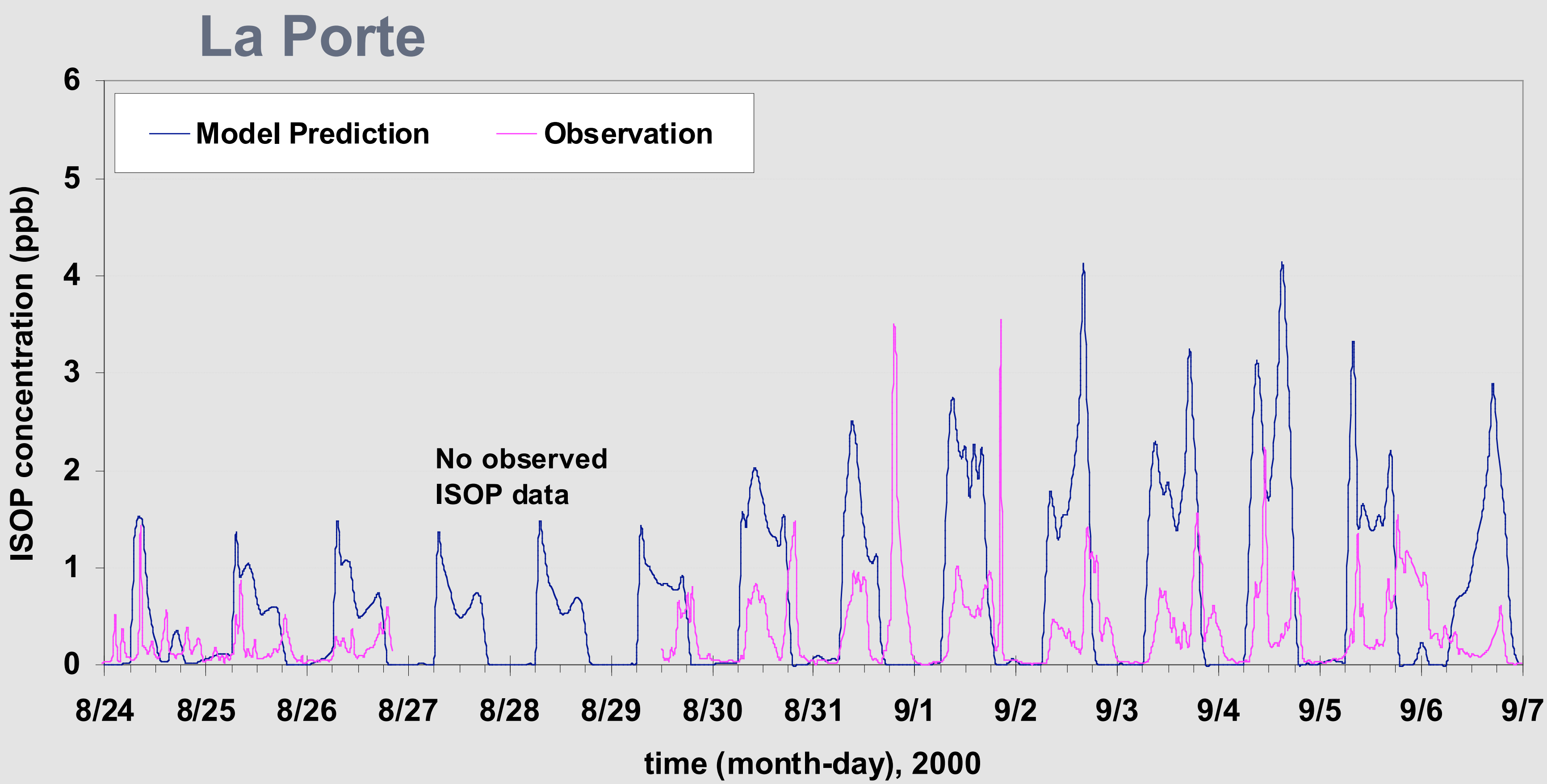
Aircraft and Ground Data

- NCAR Electra aircraft operated by NOAA
  - Canister samples collected at 600-700 m AGL in the late morning to early afternoon. Isoprene concentrations measured using FID and MS
  - Continuous measurements with a PTR-MS operated by the University of Innsbruck
- BNL G-1 aircraft
  - Canister samples at 400 and 600 m AGL during the daytime. Samples analyzed by GC.
- Auto-GC and other measurements at five surface monitoring stations: La Porte, Clinton, Deer Park, Bayland Park, and Aldine.
  - One-hour average concentrations

Modeled Isoprene vs. Surface Data



Modeled Isoprene vs. Surface Data



Modeled Isoprene vs. Aloft Canister Samples

NOAA

Date of sample collection	Number of pairs	Mean (ppb)		$Mean_{pred}$ /$Mean_{obs}$	MNB (%)	MNGE (%)
		Observed	**Predicted**			
8/25	14	**0.37**	**0.38**	**1.0**	37.	101.
8/27	17	**0.38**	**0.28**	**0.7**	3.	77.
8/28	18	**0.36**	**0.30**	**0.9**	-37.	58.
8/30	10	**0.27**	**0.13**	**0.5**	-15.	84.
Total	59	**0.35**	**0.29**	**0.8**	-4.	78.

BNL

Date of sample collection	Number of pairs	Mean (ppb)		$Mean_{pred}$ /$Mean_{obs}$	MNB (%)	MNGE (%)
		Observed	**Predicted**			
8/26	25	**0.39**	**0.36**	**0.9**	53.	129.
8/29	27	**0.23**	**0.23**	**1.0**	83.	141.
Total	52	**0.30**	**0.29**	**1.0**	68.	135.

Summary

- Results present a complex and ambiguous picture of modeled isoprene concentrations
- Modeled ground-level isoprene concentrations are a factor of 2-3 higher than observed values at all sites.
- Mean predicted isoprene concentrations and NOAA aircraft canister observations are reasonably consistent, although the model tends to under predict observed concentrations. Agreement between mean predicted isoprene concentrations with BNL G-1 aircraft canister concentrations is quite good.
- Agreement between mean modeled and PTR-MS observations aloft in Waller and Montgomery Counties is good, but model under predicts mean observed concentrations over Harris County urban area and aloft of surface monitoring sites, with some differences between sites and episode days.
- Process Analysis indicates that dominant processes (emissions, chemical loss, and vertical transport) are similar between episode days and between urban and rural sites, but relative rates of processes and importance of horizontal transport exhibit variability between days.

Model sensitivity studies

- Model systematically predicts larger ground concentrations compared to observations
- Modeled mean concentrations are in good agreement with aircraft measurements
- Sensitivity studies performed examining both uncertainties in the inventory and other model uncertainties:
  - Change vertical mixing
  - Systematic siting bias for ground stations
  - Effect of underprediction of free radical concentrations
  - Possible land cover changes and drought effects
  - All are potentially important; TexAQS 2000 data do not allow us to distinguish between these causes

Implications for TexAQS II

- Need for better characterization of vertical mixing and spatial gradients of isoprene, as well as chemical loss processes.
  - Radical related measurements at Moody Tower and from NOAA P-3
  - Vertical mixing structure from LIDAR measurements
  - Updating of landcovers
  - Measurements of isoprene reaction products

Question B – Mixed Layer Height: Moody Tower data
(Ryan Perna, James Flynn)

Question I – Chemical mechanisms: Moody Tower data
- **Ozone and radical production**

(Xinrong Ren, Jingqiu Mao, Bernhard Rappenglueck, Barry Lefer)

Questions A, C, D, E – Emissions: Moody Tower data
- **Aerosol production**

(Casey Anderson, Luke Ziemba, Dean Atkinson, Olga Pikelnaya)

Some Results from the UH Moody Tower

- **Meteorology Overview of September 6-7**

  Ryan Perna, James Flynn

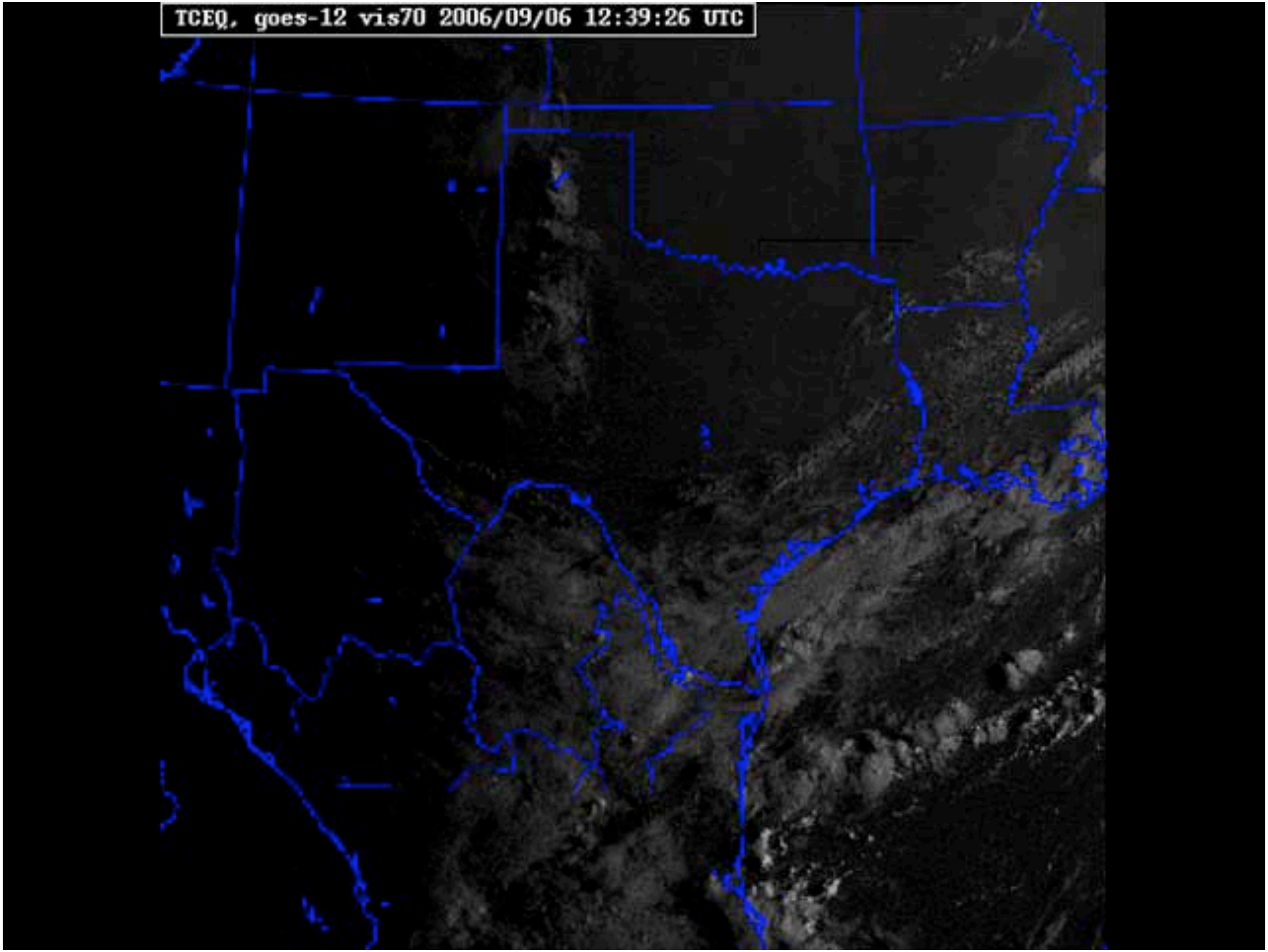
- **Photochemical Processes**

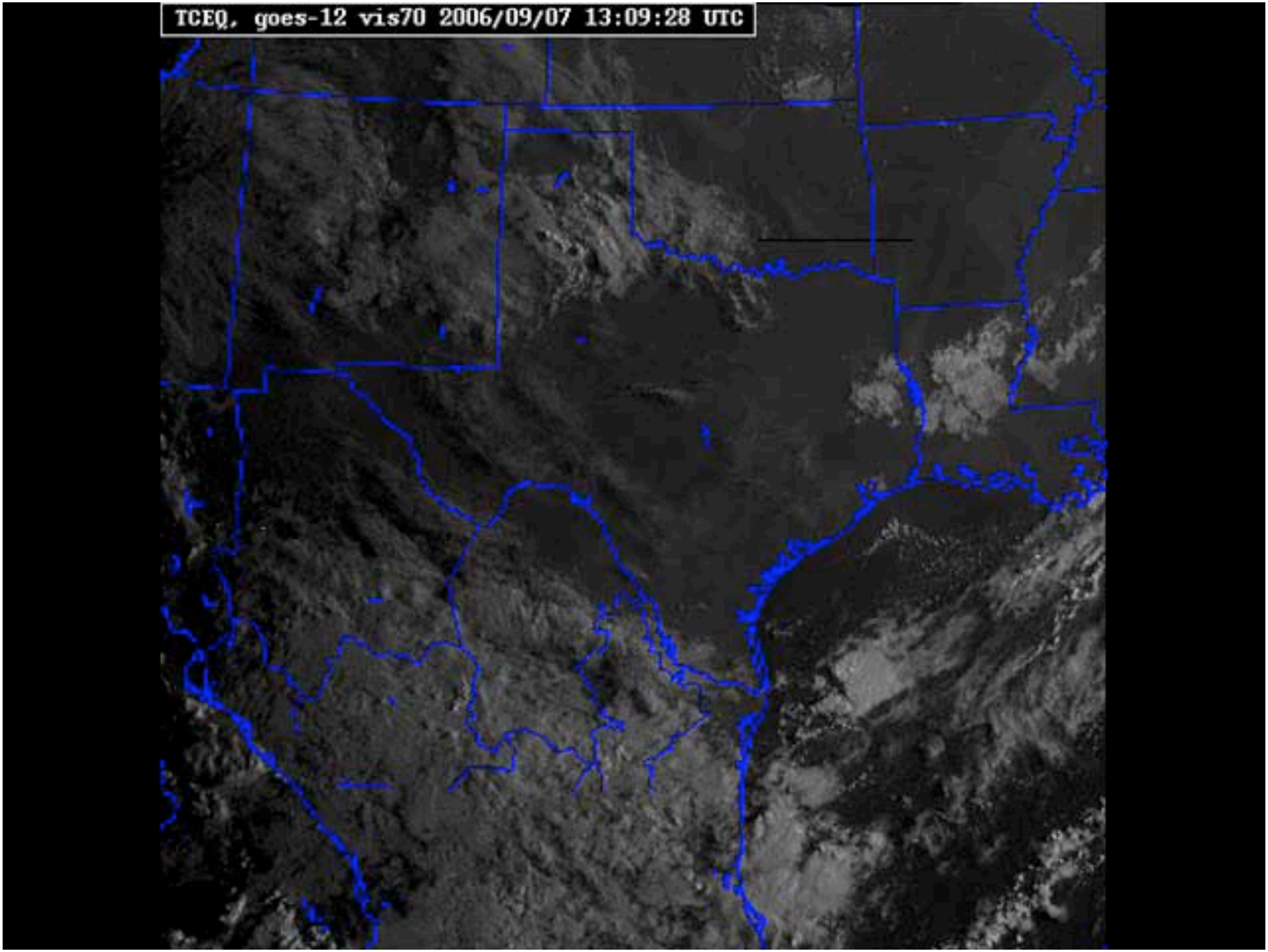
  Xinrong Ren, Jingqiu Mao, Bernhard Rappenglueck, Barry Lefer, Jochen Stutz, Michael Leuchner

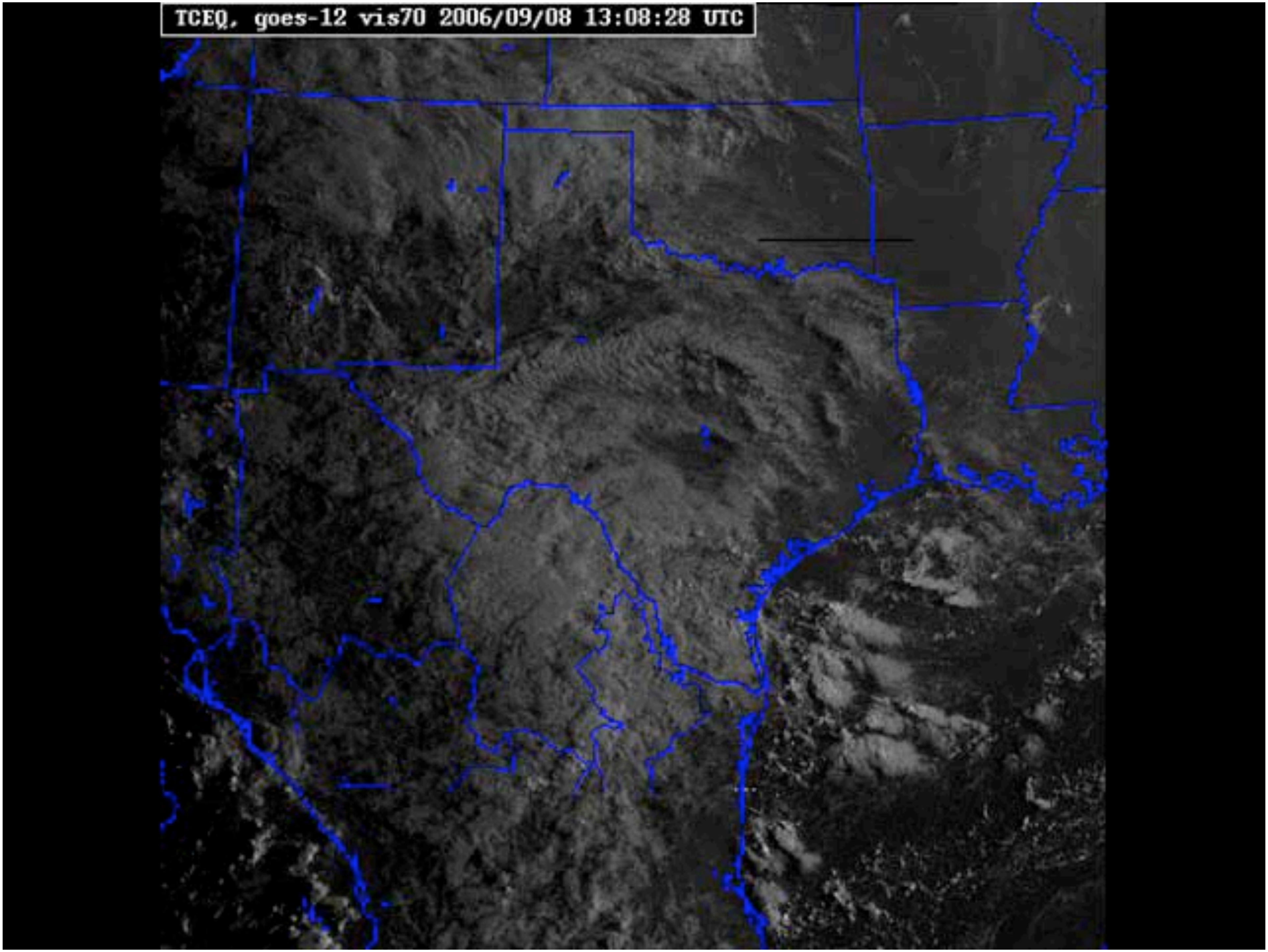
- **Aerosol Formation**

  Casey Anderson, Luke Ziemba, Dean Atkinson, Olga Pikelnaya

NOTE: All data preliminary

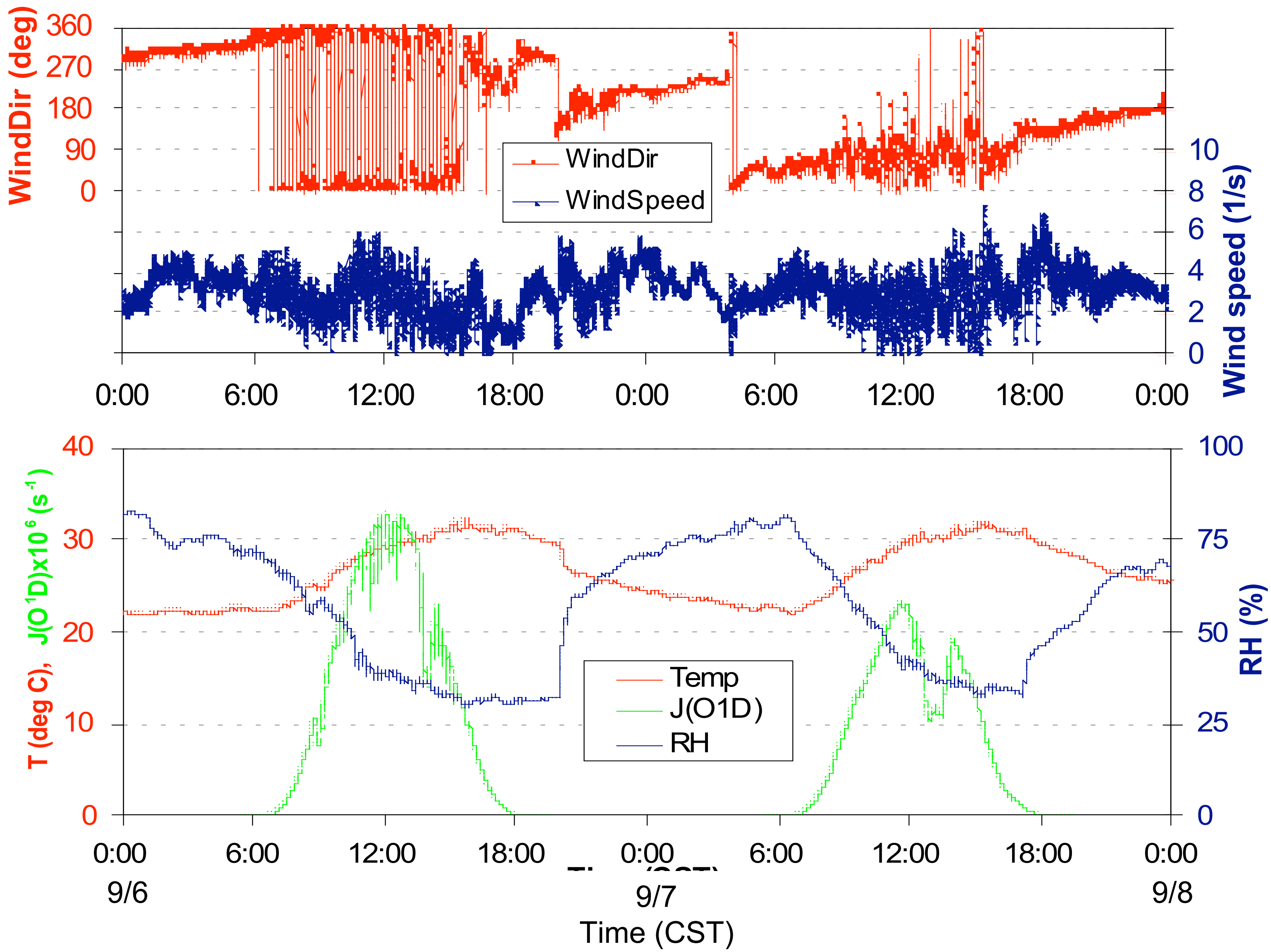

TCEQ, goes-12 vis70 2006/09/06 12:39:26 UTC

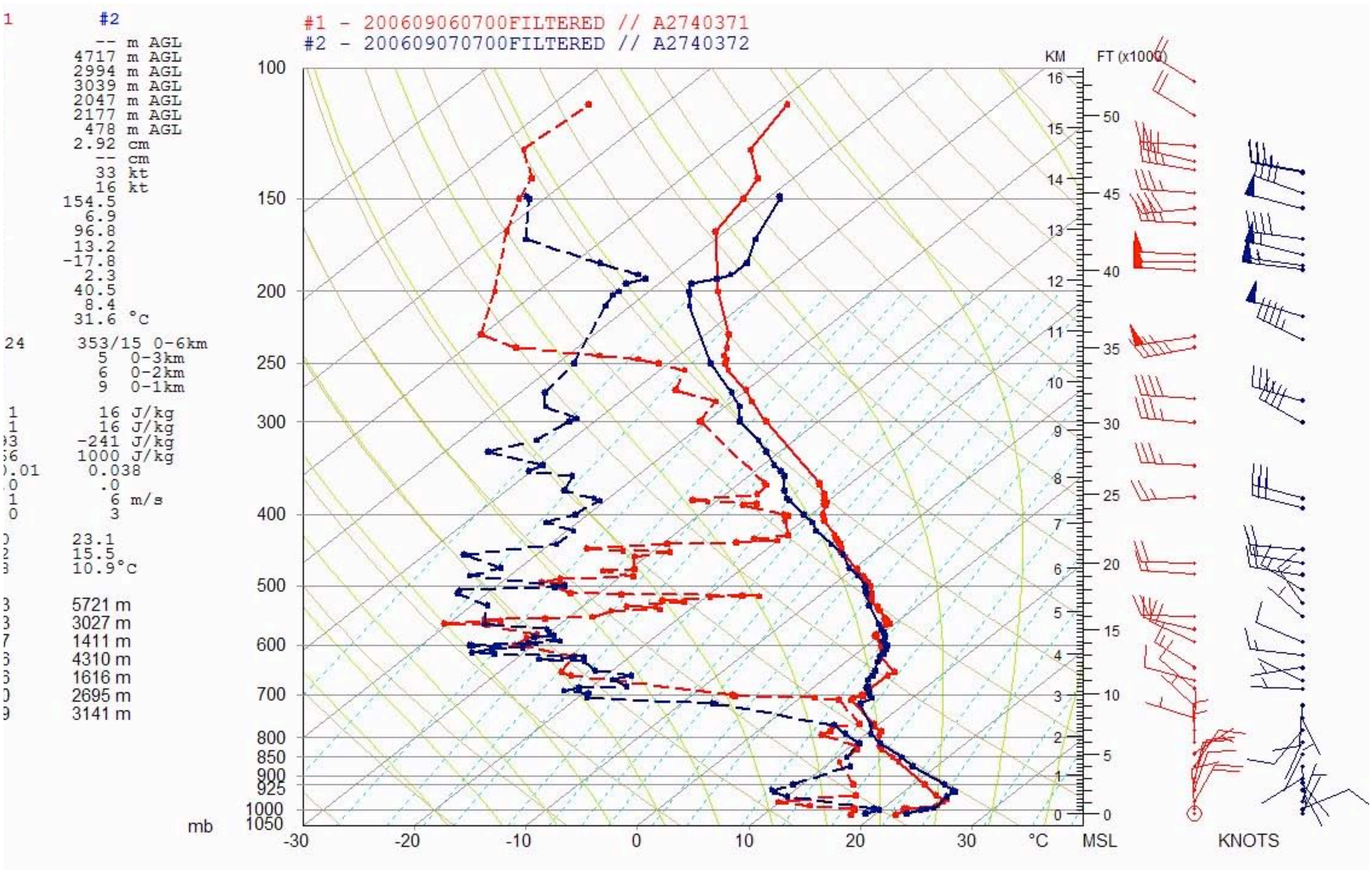

TCEQ, goes-12 vis70 2006/09/07 13:09:28 UTC


TCEQ, goes-12 vis70 2006/09/08 13:08:28 UTC

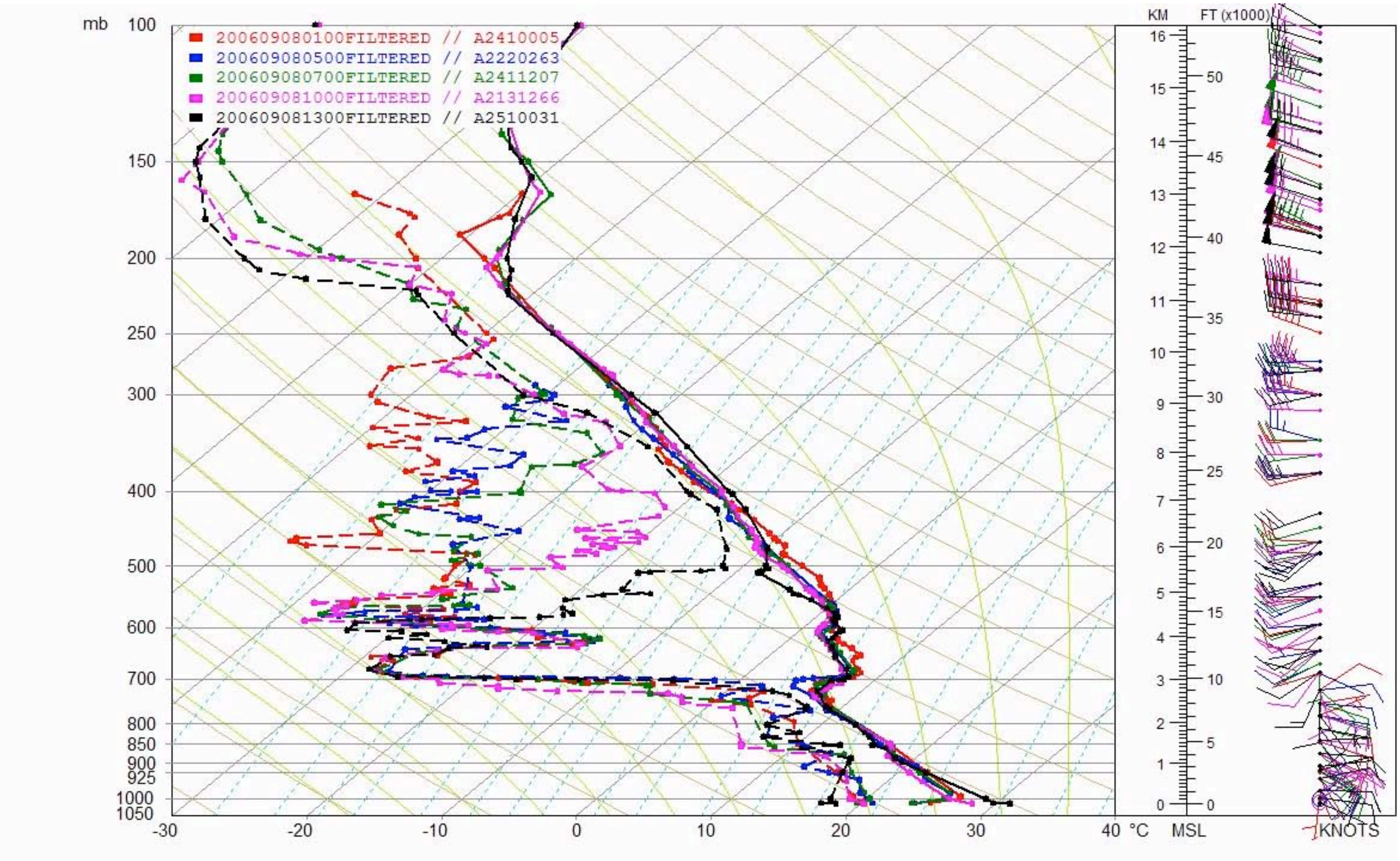
Preliminary Observed Data at Moody Tower (Sep. 6 – Sep. 7)

Meteorological Conditions





#1 - 200609060700FILTERED // A2740371
#2 - 200609070700FILTERED // A2740372
#2
-- m AGL
4717 m AGL
2994 m AGL
3039 m AGL
2047 m AGL
2177 m AGL
478 m AGL
2.92 cm
-- cm
33 kt
16 kt
154.5
6.9
96.8
13.2
-17.8
2.3
40.5
8.4
31.6 °C
353/15 0-6km
5 0-3km
6 0-2km
9 0-1km
16 J/kg
16 J/kg
-241 J/kg
1000 J/kg
0.038
.0
6 m/s
3
23.1
15.5
10.9°C
5721 m
3027 m
1411 m
4310 m
1616 m
2695 m
3141 m
mb
KM
FT (x1000)
MSL
KNOTS
°C



mb
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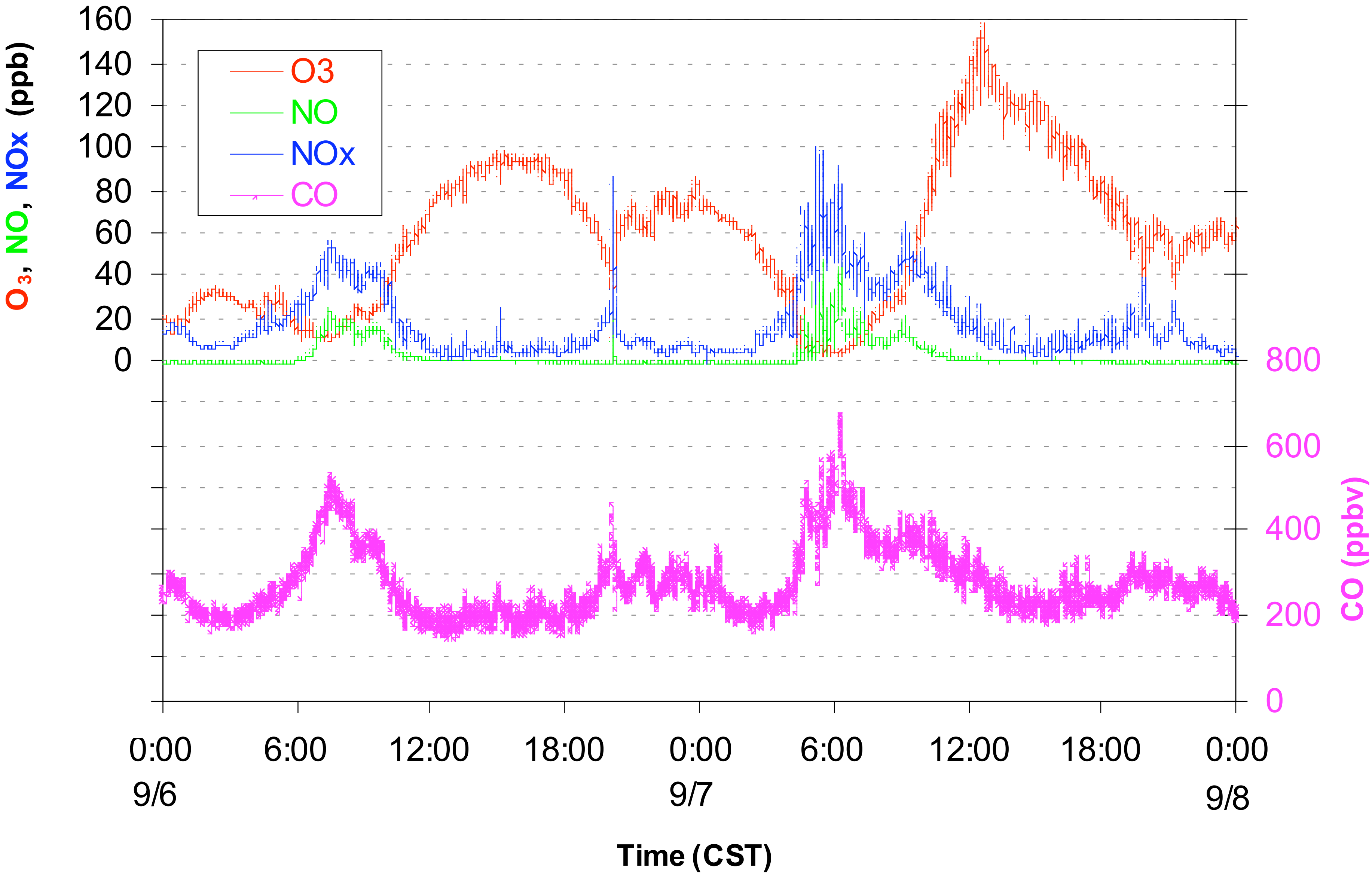
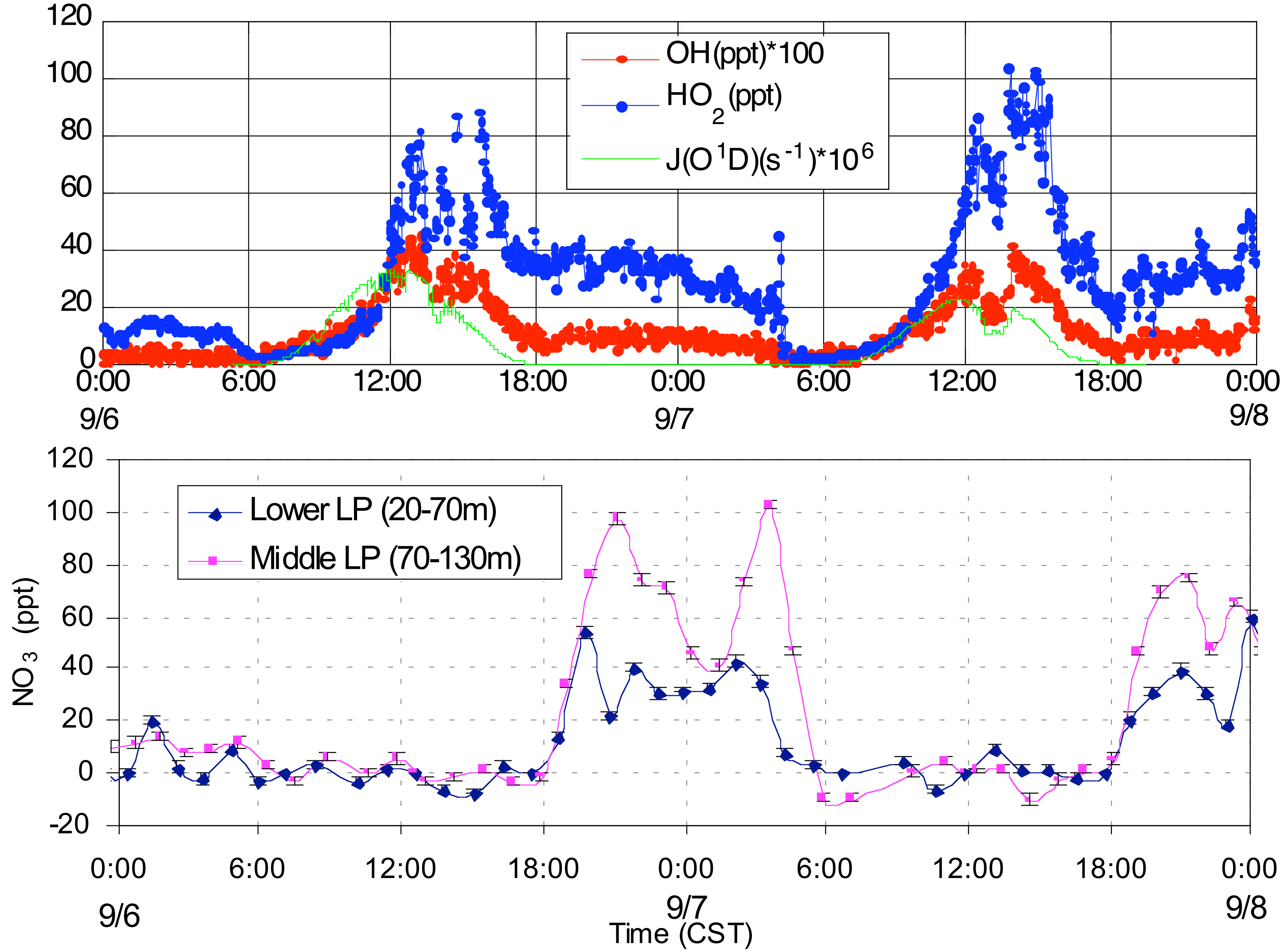
KM
FT (x1000)
°C
MSL
KNOTS

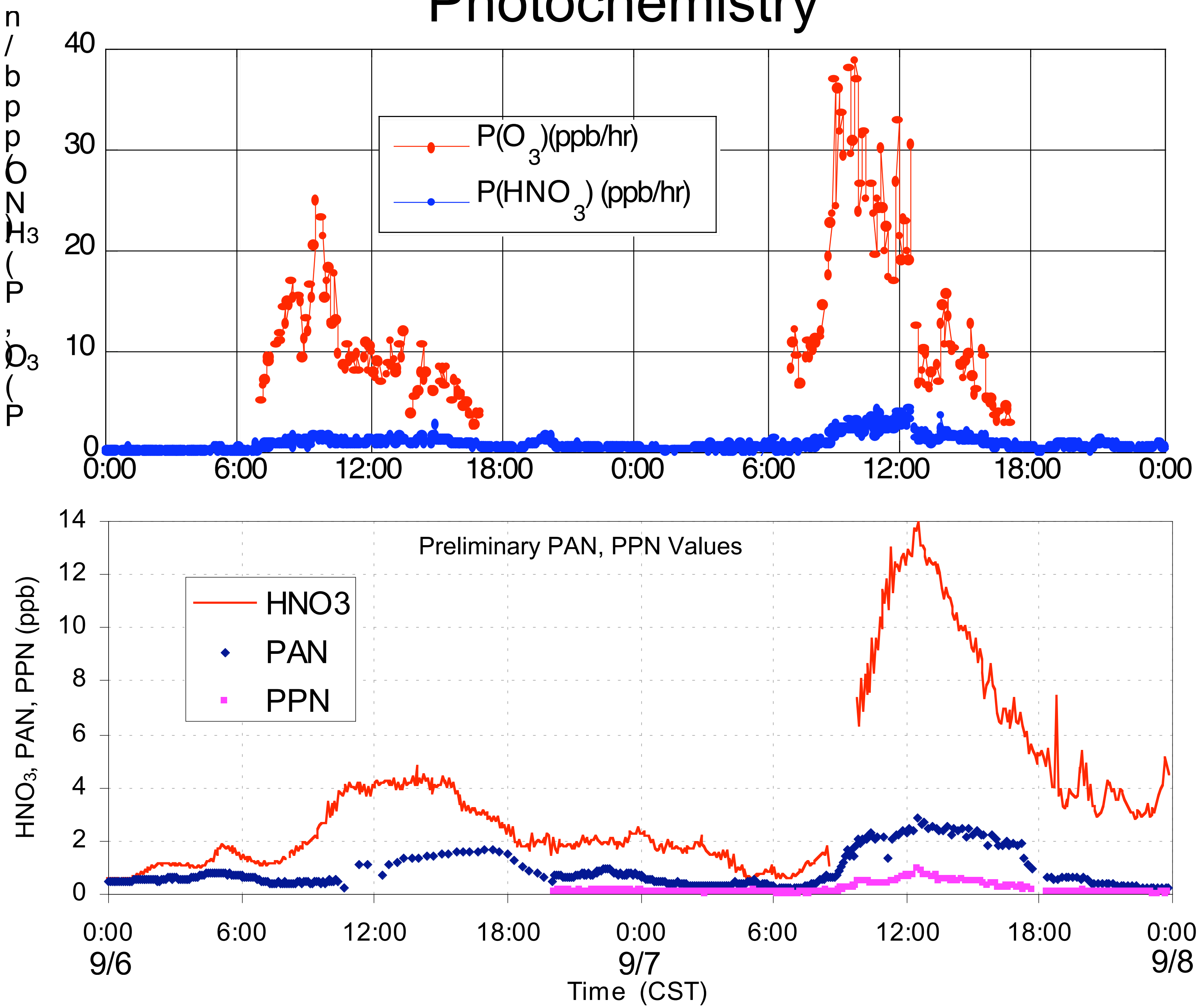


O3
NO
NOx
CO
O_3, NO, NOx (ppb)
CO (ppbv)
160
140
120
100
80
60
40
20
0
800
600
400
200
0
0:00
6:00
12:00
18:00
0:00
6:00
12:00
18:00
0:00
9/6
9/7
9/8
Time (CST)

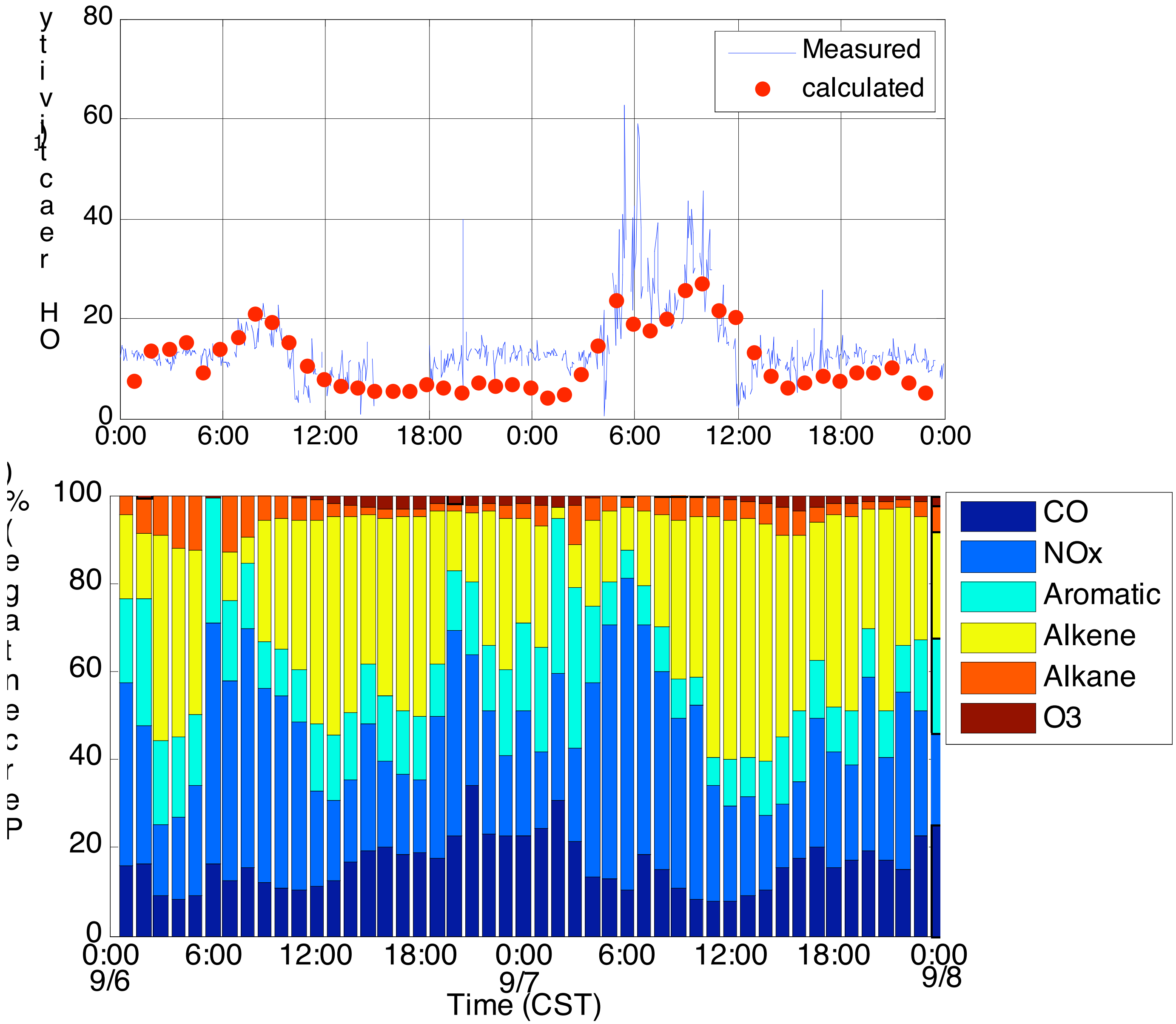
OH, HO_2, and NO_3 observations

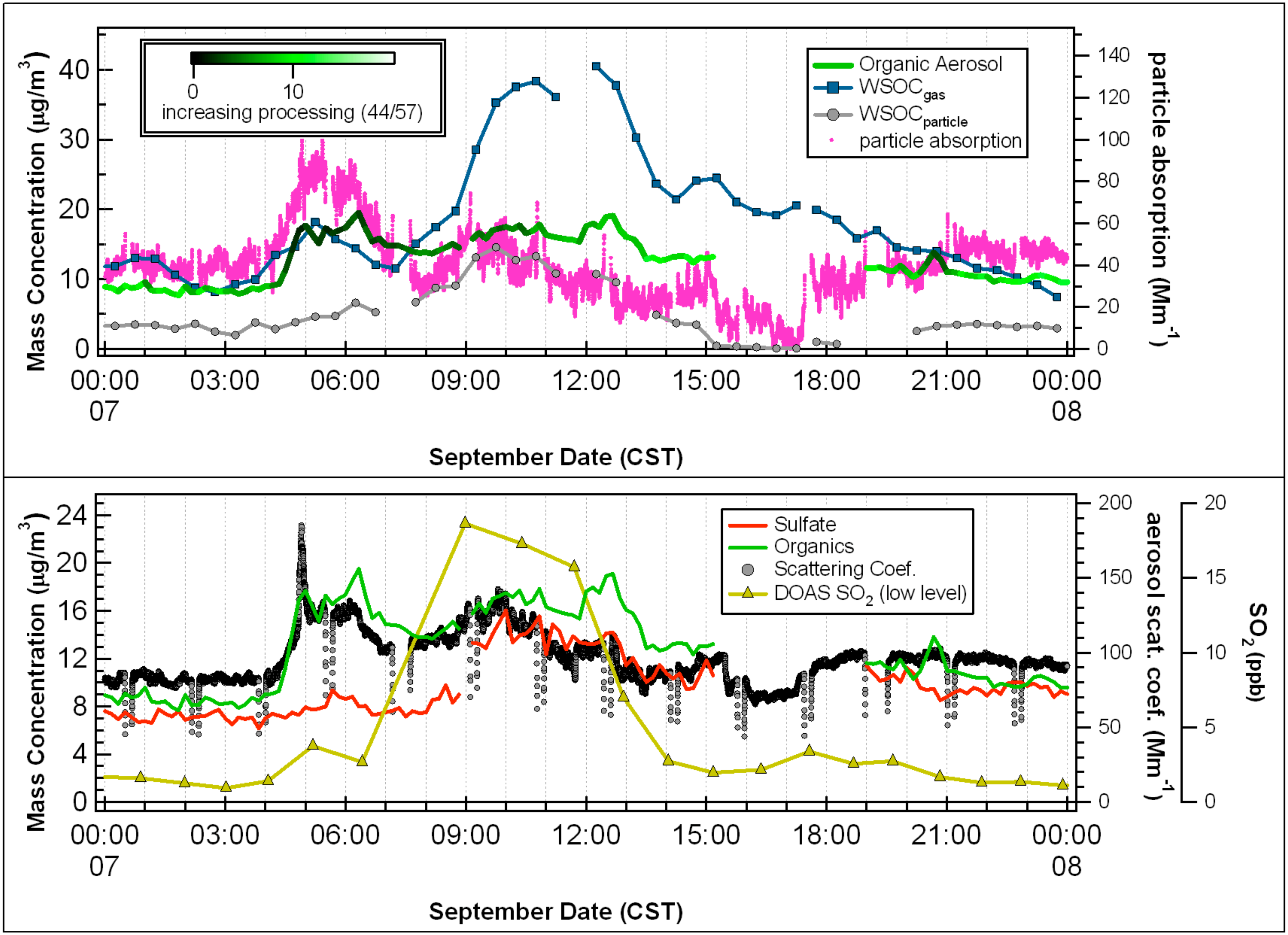


Photochemistry

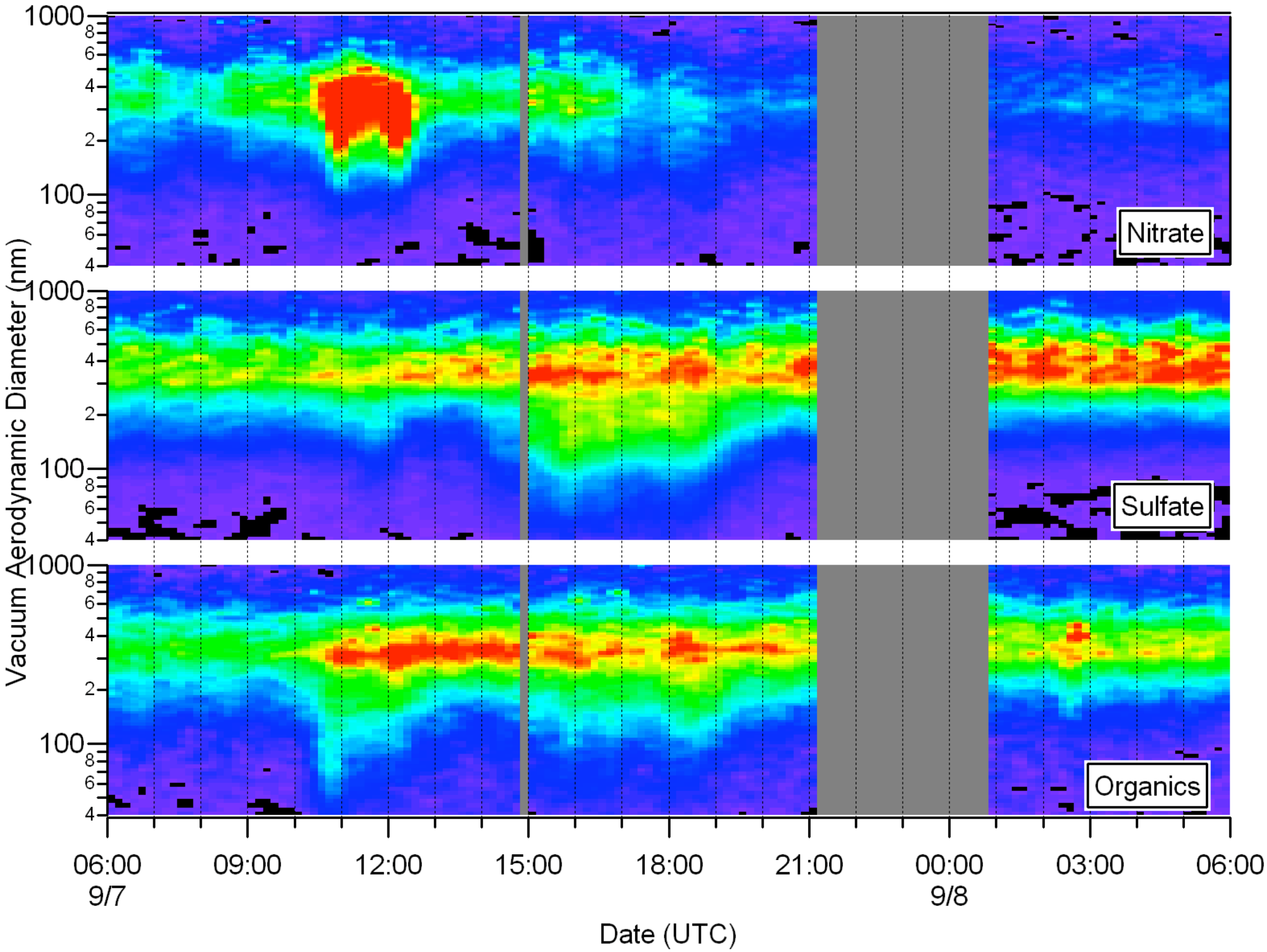


OH reactivity and comparison with observations





0
10
increasing processing (44/57)
Organic Aerosol
WSOC$_{gas}$
WSOC$_{particle}$
particle absorption
Mass Concentration (µg/m^3)
particle absorption (Mm^{-1})
September Date (CST)
Sulfate
Organics
Scattering Coef.
DOAS SO$_2$ (low level)
aerosol scat. coef. (Mm^{-1})
SO$_2$ (ppb)


Nitrate
Sulfate
Organics
Vacuum Aerodynamic Diameter (nm)
1000
100
06:00
9/7
09:00
12:00
15:00
18:00
21:00
00:00
9/8
03:00
06:00
Date (UTC)

Questions A, C, D, E – Emissions: RH Brown data

- VOC measurements vs. inventory (Lori Del Negro)

Preliminary attempts to identify plume VOC sources in the Houston Ship Channel

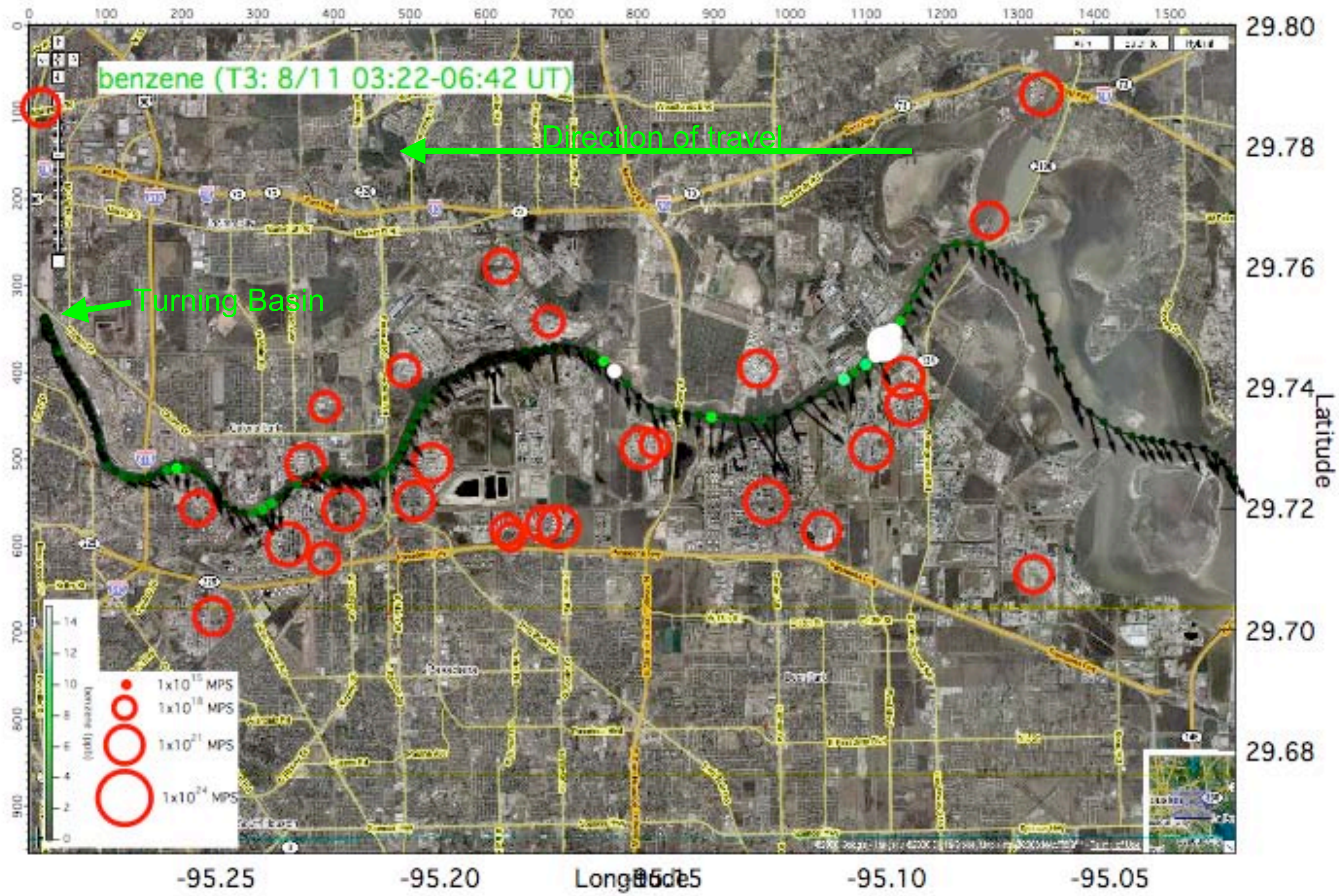
PITMS data from the *Ronald H. Brown*

Investigators: Joost de Gouw

Carsten Warneke

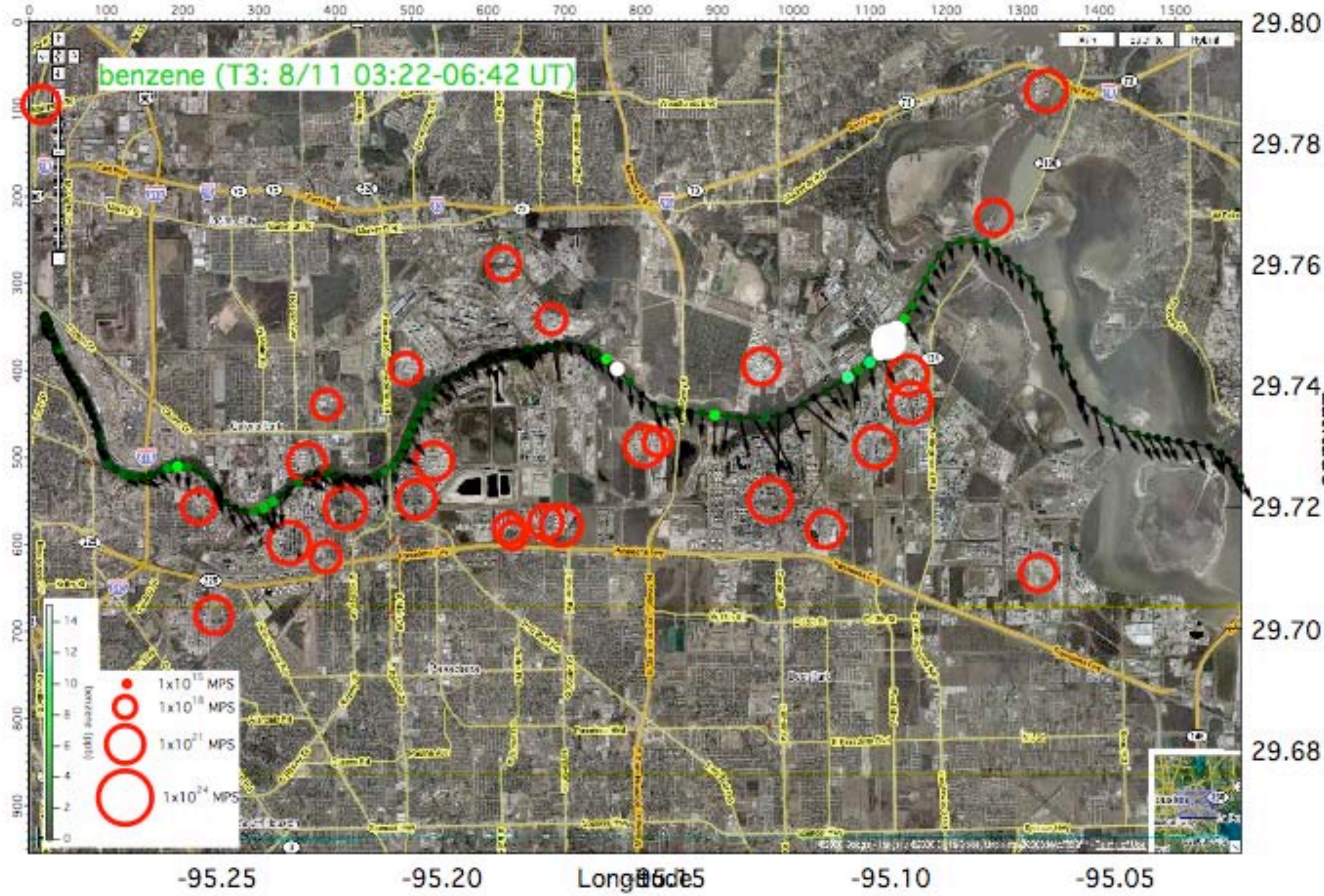
Dan Welsh-Bon

Lori Del Negro

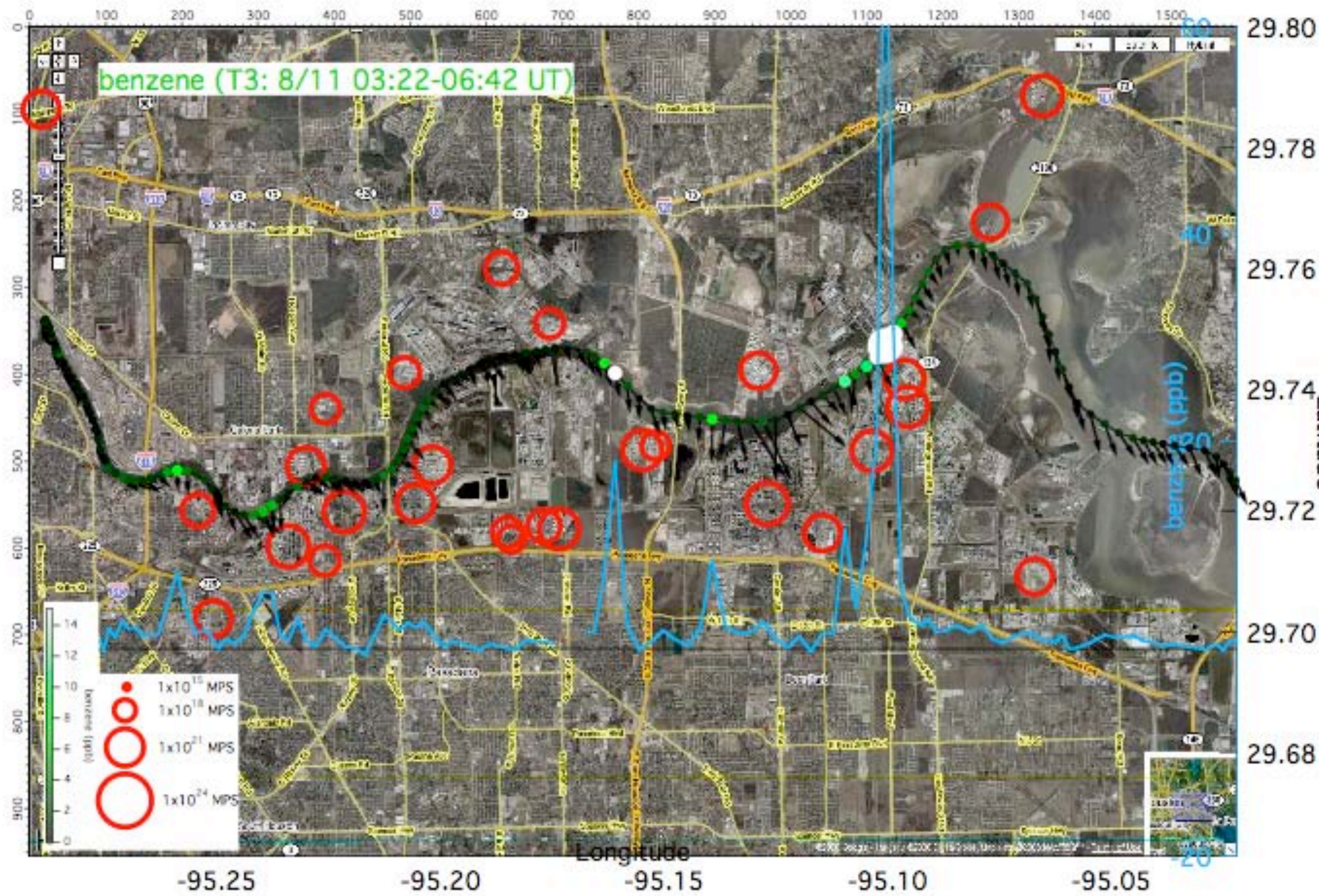

benzene (T3: 8/11 03:22-06:42 UT)
Direction of travel
Turning Basin
1x10^15 MPS
1x10^18 MPS
1x10^21 MPS
1x10^24 MPS
benzene (ppb)
29.80
29.78
29.76
29.74
29.72
29.70
29.68
Latitude
-95.25
-95.20
-95.15
-95.10
-95.05
Longitude

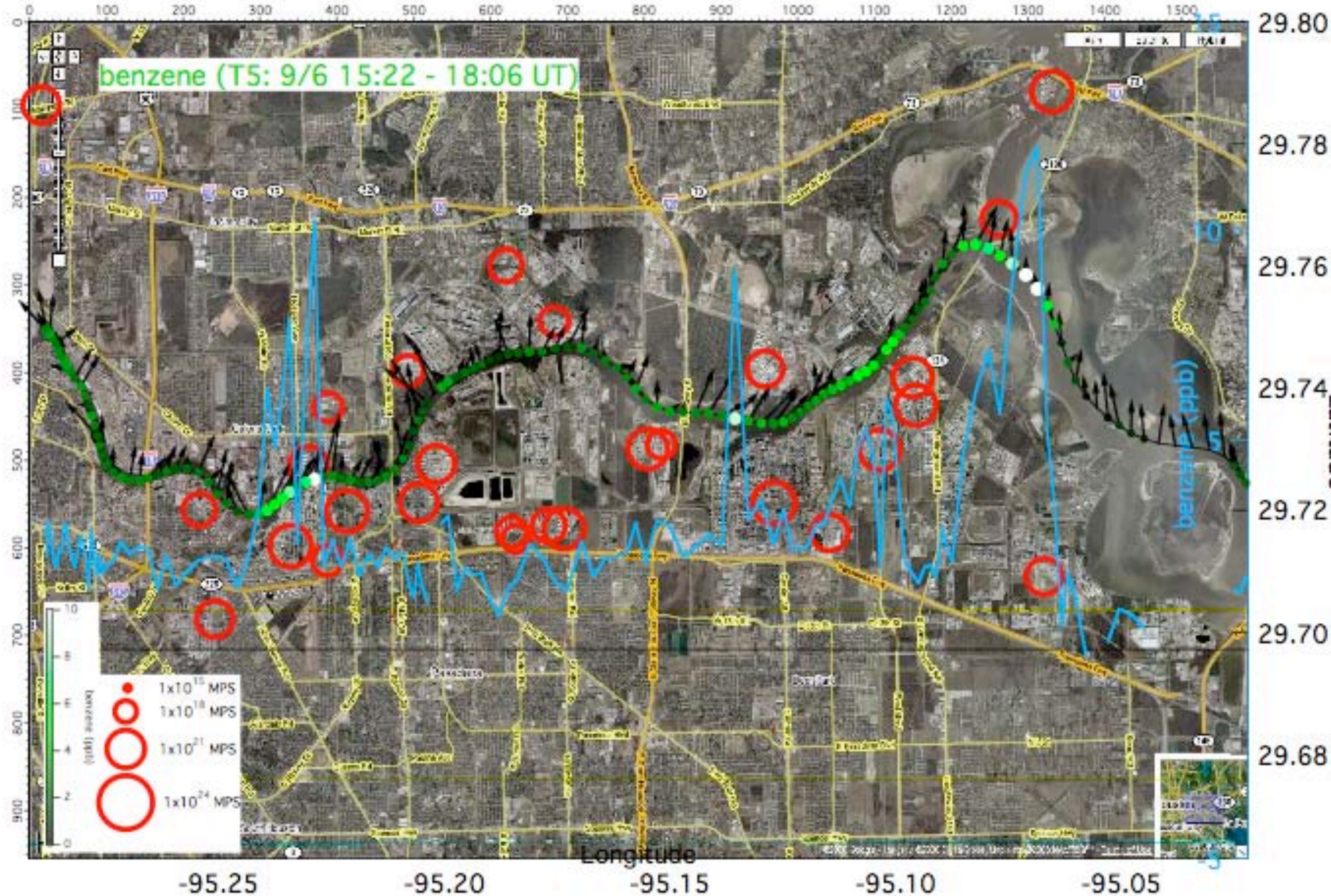
Key Features of the Plot

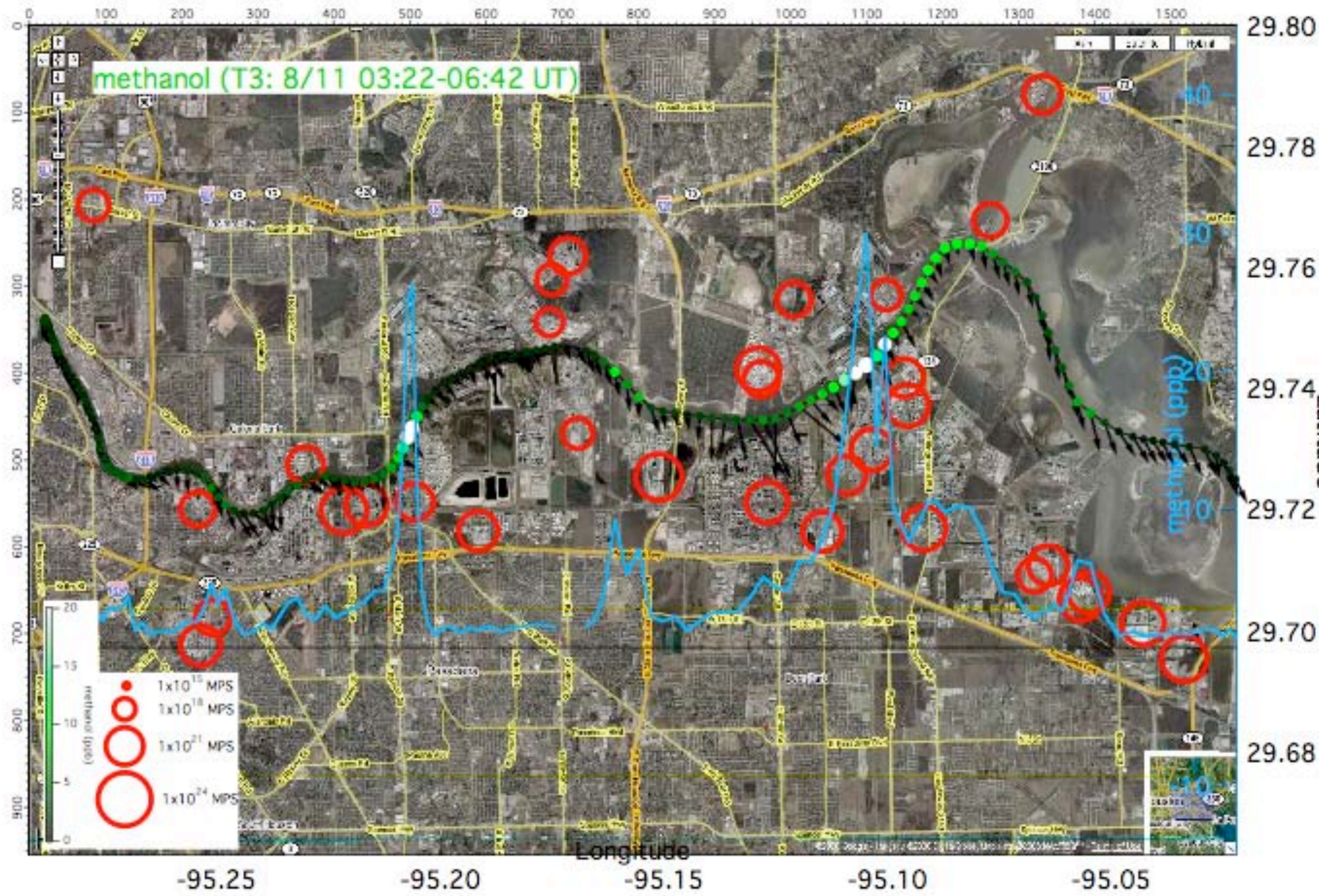
- Arrows point upwind at the time of measurement, “toward” the source
- Solid marker size and color based on magnitude of VOC measurement
- Inventory markers sized by the log of emission rate in molecules per second



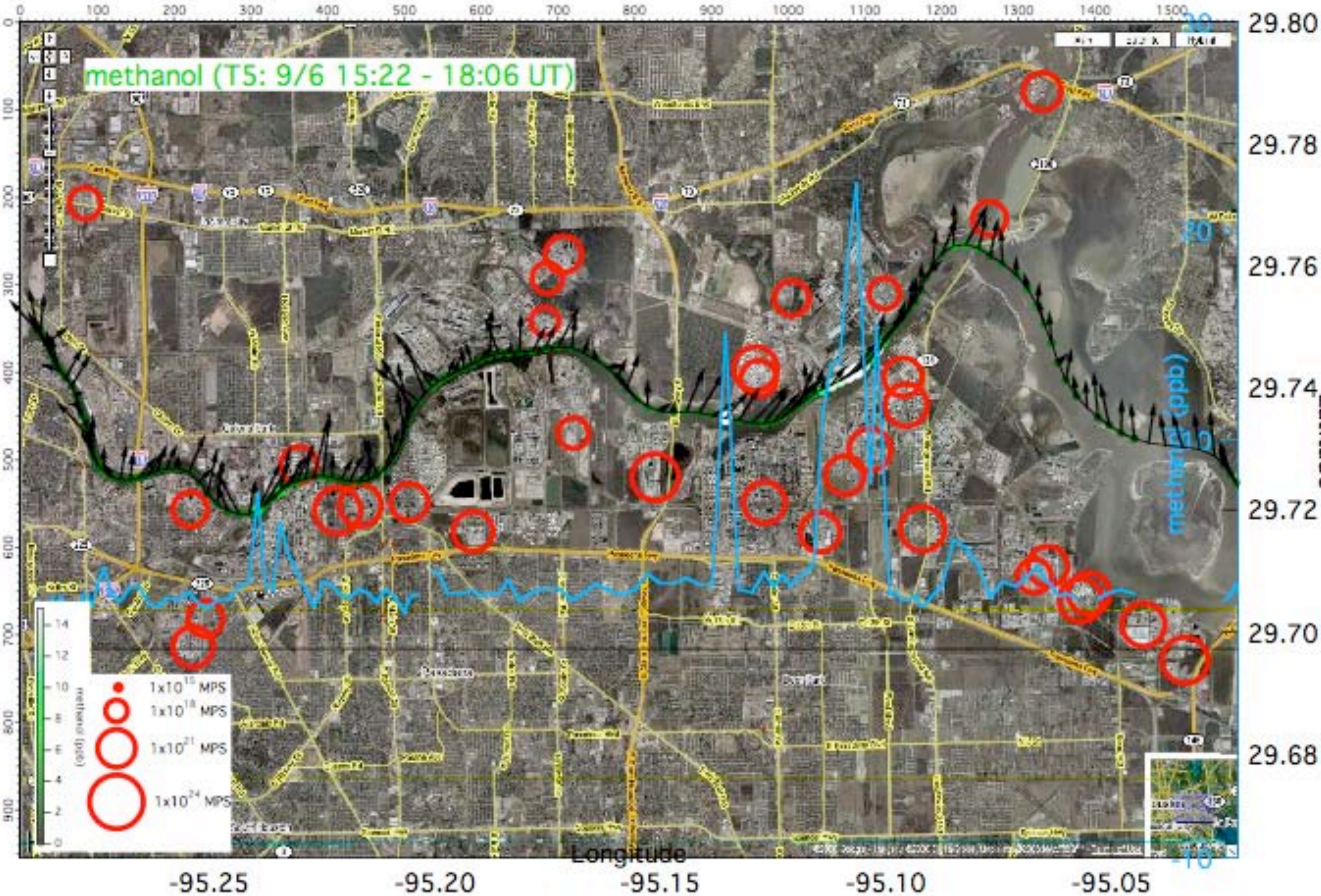
benzene (T3: 8/11 03:22-06:42 UT)
1x10^15 MPS
1x10^18 MPS
1x10^21 MPS
1x10^24 MPS
benzene (ppb)
29.80
29.78
29.76
29.74
29.72
29.70
29.68
Latitude
-95.25
-95.20
-95.15
-95.10
-95.05
Longitude


benzene (T3: 8/11 03:22-06:42 UT)
Longitude
Latitude
benzene (ppb)
1x10^15 MPS
1x10^18 MPS
1x10^21 MPS
1x10^24 MPS
-95.25
-95.20
-95.15
-95.10
-95.05
29.80
29.78
29.76
29.74
29.72
29.70
29.68

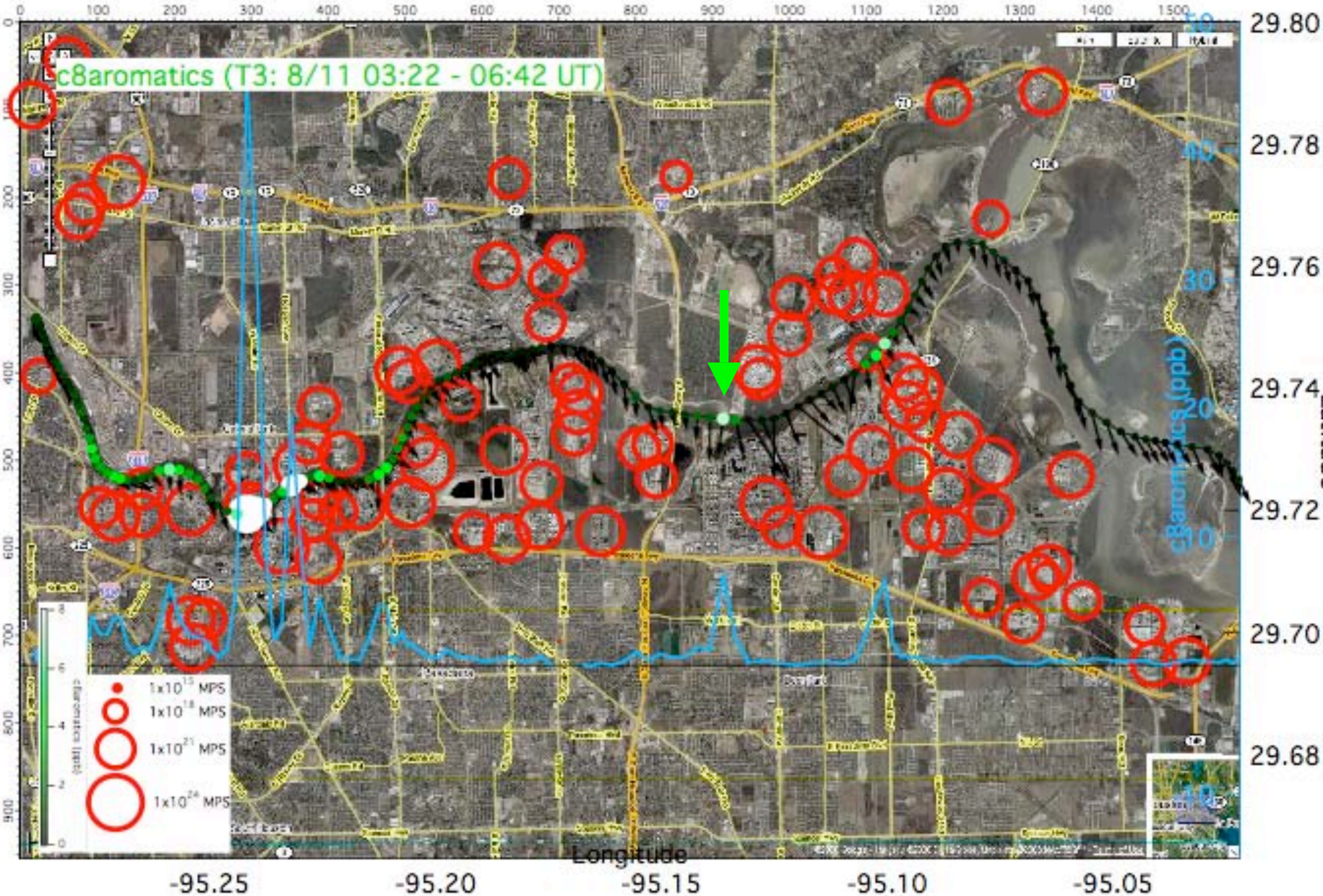

benzene (T5: 9/6 15:22 - 18:06 UT)
1x10^15 MPS
1x10^18 MPS
1x10^21 MPS
1x10^24 MPS
benzene (ppb)
Longitude
Latitude
29.80
29.78
29.76
29.74
29.72
29.70
29.68
-95.25
-95.20
-95.15
-95.10
-95.05



methanol (T3: 8/11 03:22-06:42 UT)
29.80
29.78
29.76
29.74
29.72
29.70
29.68
Latitude
methanol (ppb)
1x10^15 MPS
1x10^18 MPS
1x10^21 MPS
1x10^24 MPS
Longitude
-95.25
-95.20
-95.15
-95.10
-95.05



methanol (T5: 9/6 15:22 - 18:06 UT)
1x10^15 MPS
1x10^18 MPS
1x10^21 MPS
1x10^24 MPS
methanol (ppb)
Longitude
Latitude
-95.25
-95.20
-95.15
-95.10
-95.05
29.80
29.78
29.76
29.74
29.72
29.70
29.68



c8aromatics (T3: 8/11 03:22 - 06:42 UT)
1x10^15 MPS
1x10^18 MPS
1x10^21 MPS
1x10^24 MPS
c8aromatics (ppb)
Longitude
Latitude
-95.25
-95.20
-95.15
-95.10
-95.05
29.80
29.78
29.76
29.74
29.72
29.70
29.68