22 September Preview
Rapid Science Synthesis*

Questions A, C, D, E – Emissions: P-3 data
- **Measured isoprene concentrations vs. biogenics inventory (Carsten Warneke)**

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- **NO_x point sources (Tom Ryerson)**

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- **Ship channel emissions (Johan Mellqvist)**

Questions G, H – Regional Background Aerosol: Satellite data
- **Regional and local biomass burning (Brad Pierce)**

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

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- **Measured isoprene concentrations vs. biogenics inventory (Carsten Warneke)**

Isoprene measurements on the NOAA WP-3 using PTR-MS

Carsten Warneke
Lori Del Negro
Joost de Gouw

PTR-MS

Proton-Transfer-Reaction Mass Spectrometry

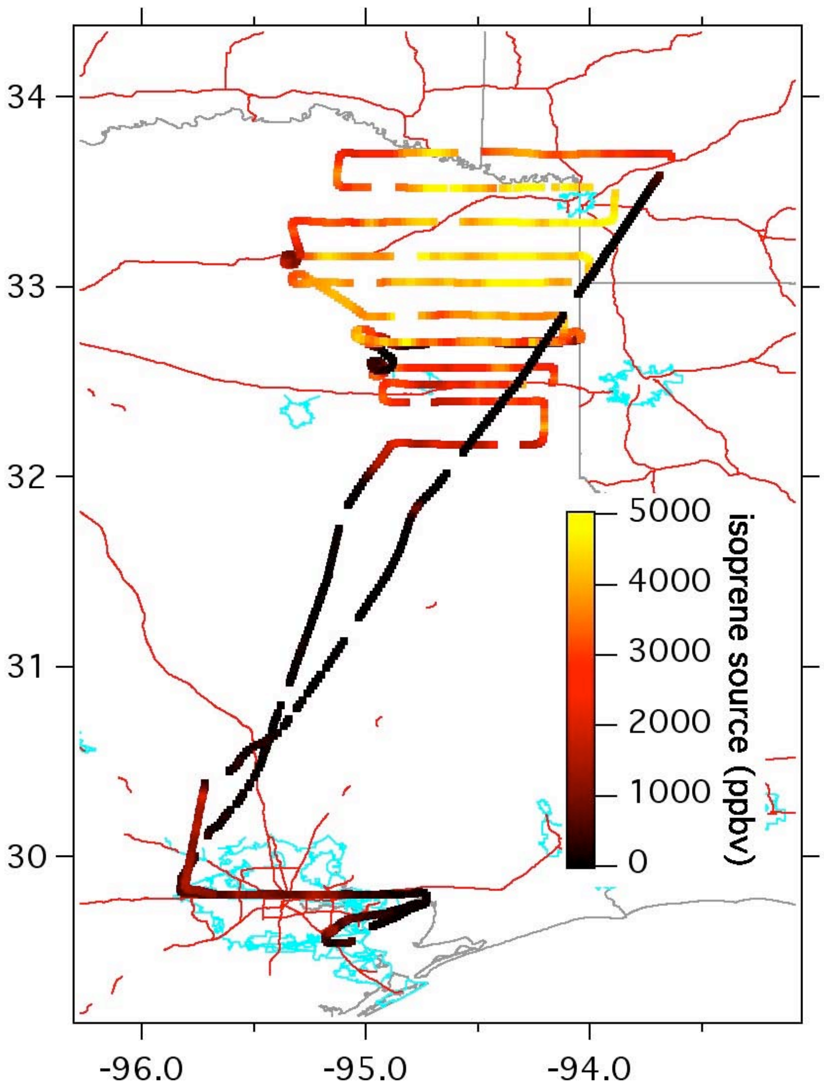
15 volatile organic compounds (VOCs) every 16 seconds

Aromatics: urban and industrial marker
Oxygenates: chemical transformation
Acetonitrile: biomass burning marker

Biogenics:
isoprene, methyl vinyl ketone+methacrolein
sum monoterpenes

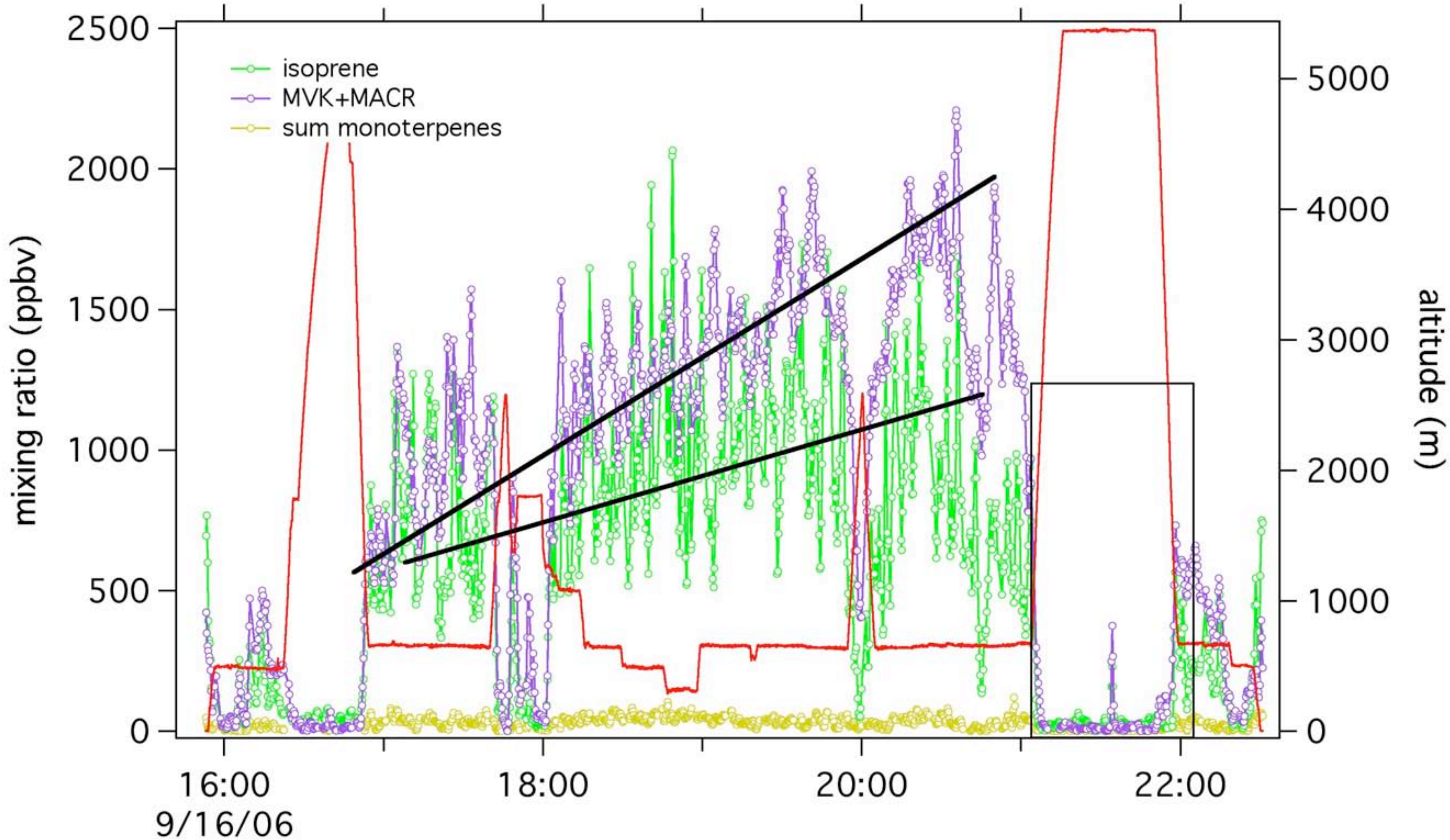
PTR-MS and LPAS in the NOAA WP-3

LPAS: fast ethylene measurements



Flight: 09/16/2006

NE Texas: Martin Lake PP plume over forest

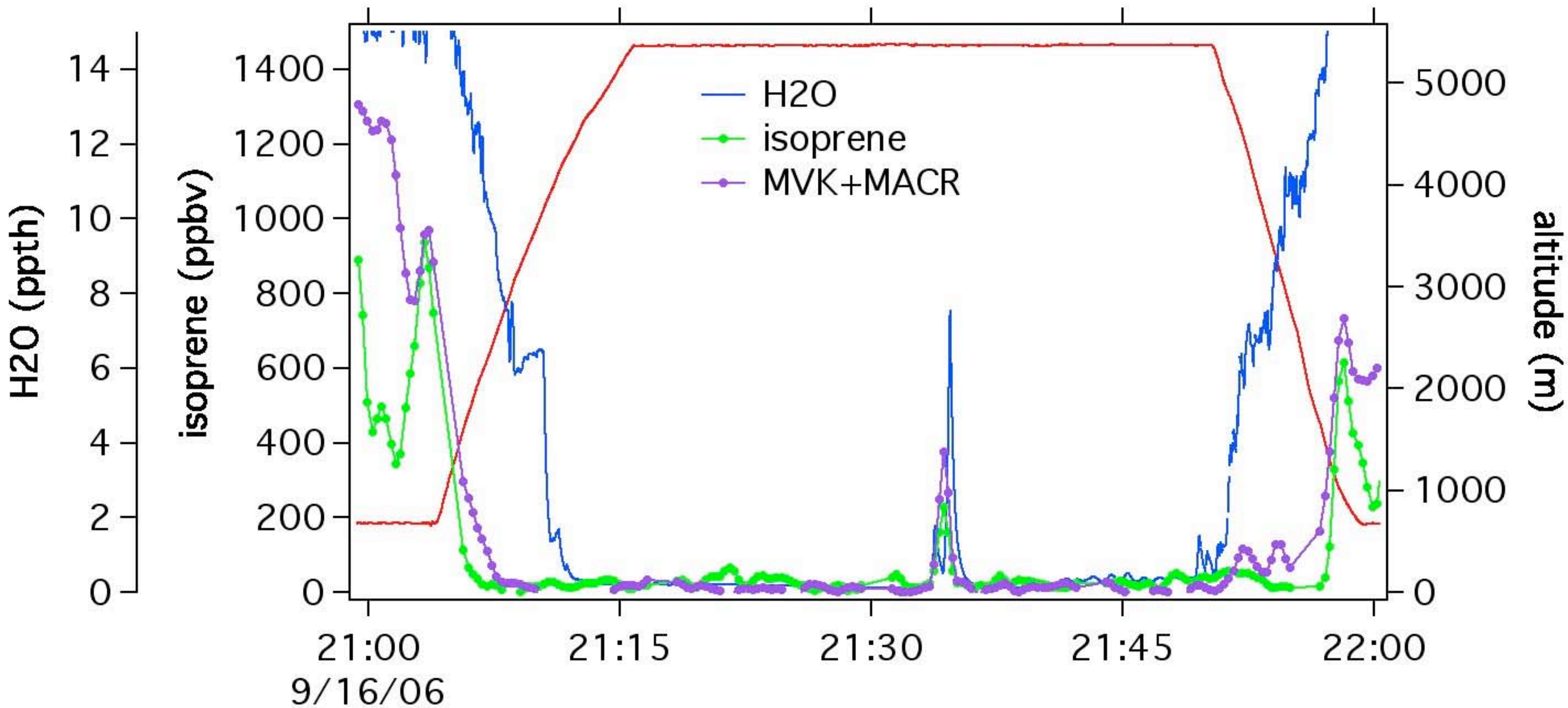


Variability from emissions (Instrument Precision is about 50 pptv)

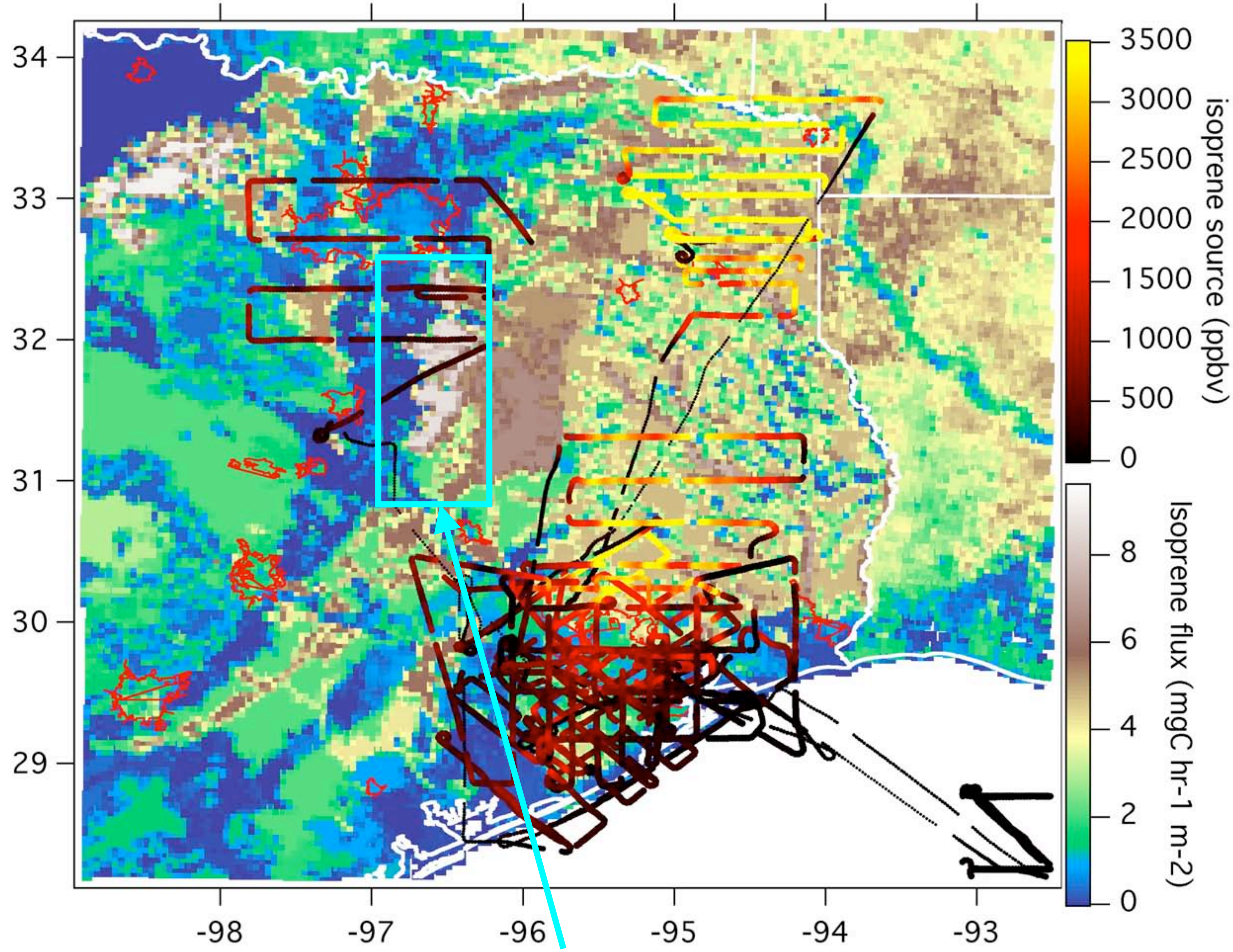
Increase during day: isoprene emissions increase (temperature and light dependence)

MVK+MACR: fast chemistry

Monoterpenes were very small



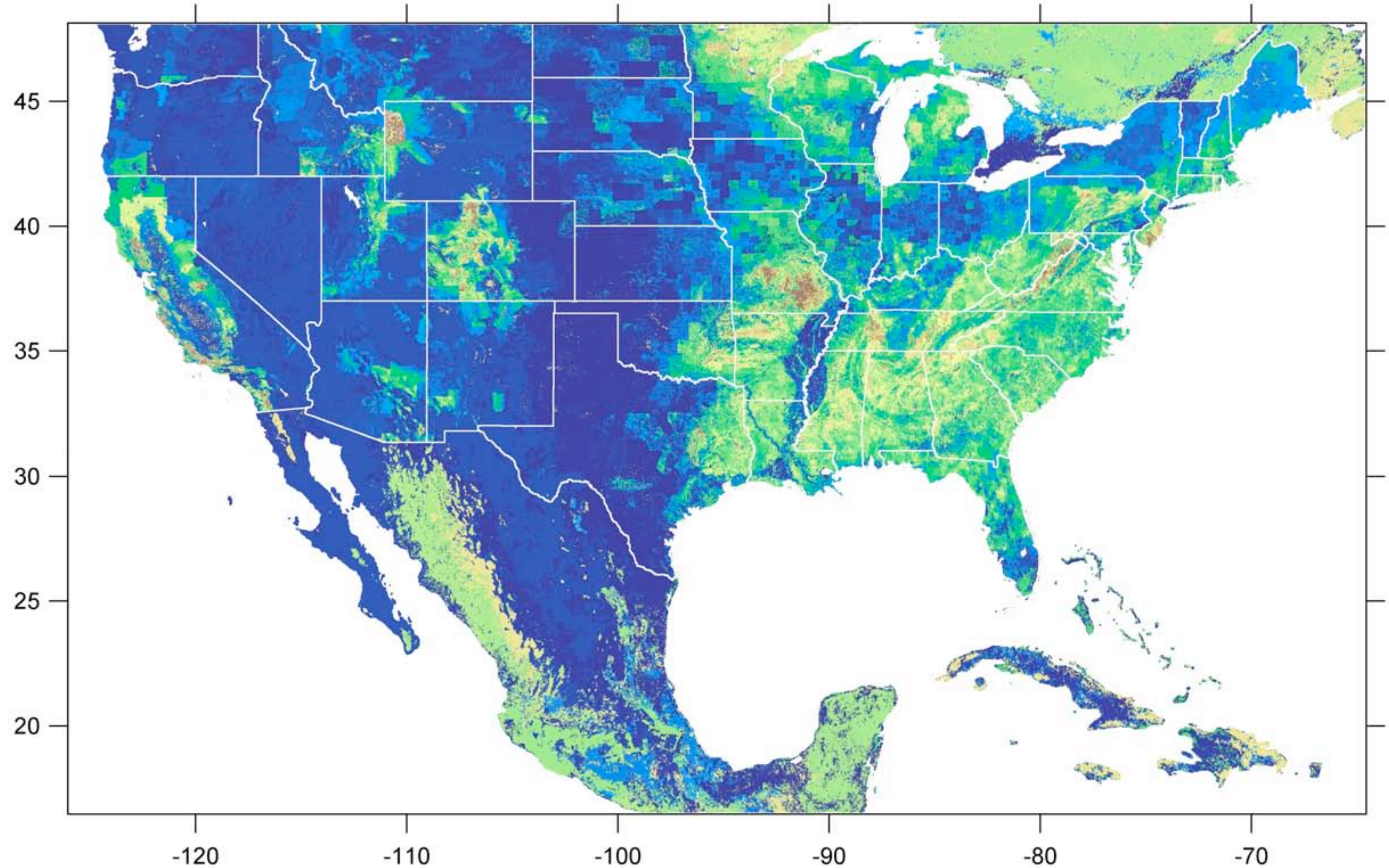
Evidence for rapid vertical transport



GLOBEIS emissions inventory: agrees well except

Isoprene source = isoprene + 2*(MVK+MACR)   to account for chemistry

Transport and changing boundary layer height influence mixing ratios



BEIS3 isoprene emissions potential

East Texas: high emissions and warm temperatures

Questions A, C, D, E – Emissions: P-3 data

- **NO_x point sources (Tom Ryerson)**

A quick look at P-3 data:

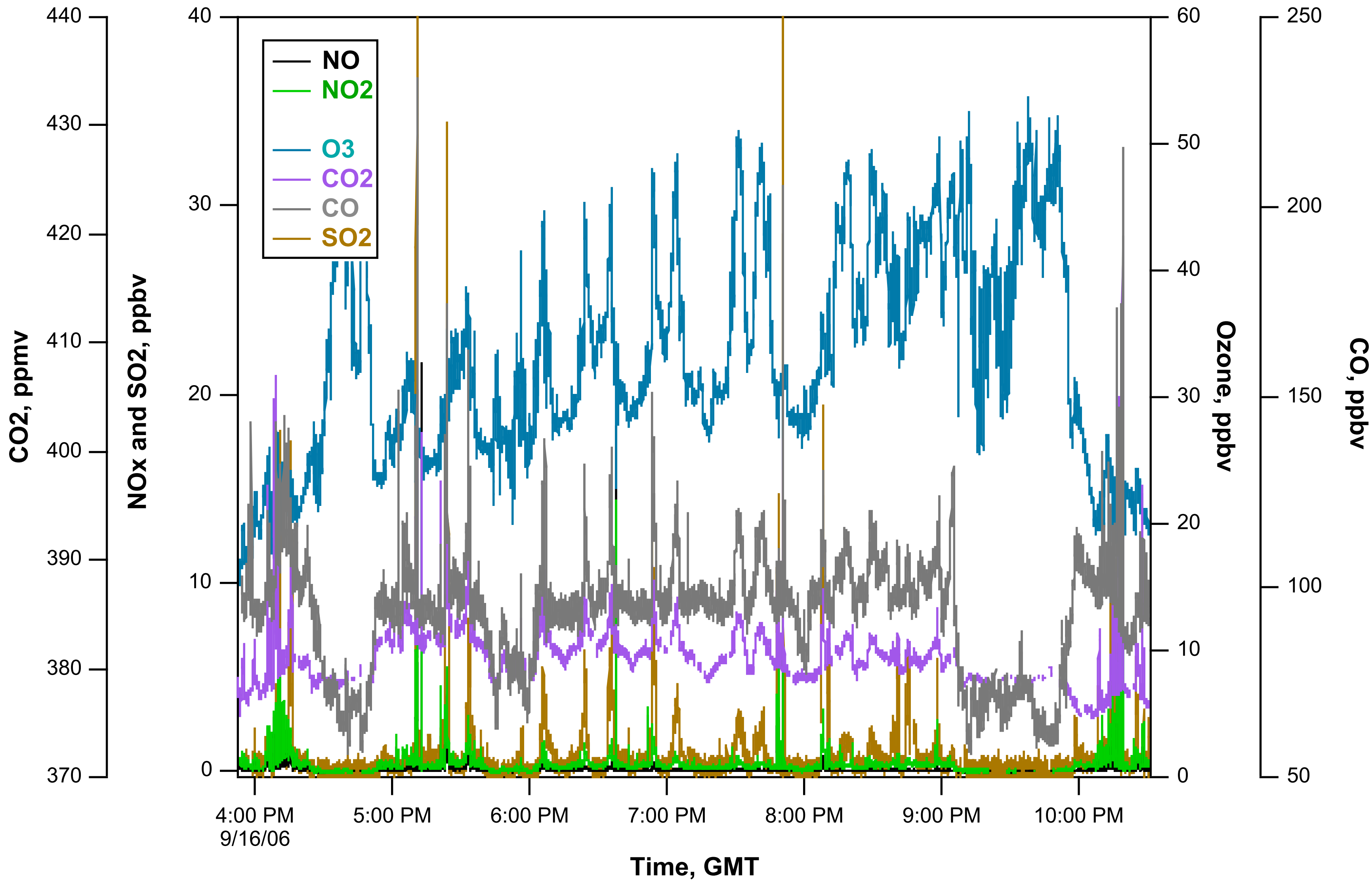
Point sources in NE Texas

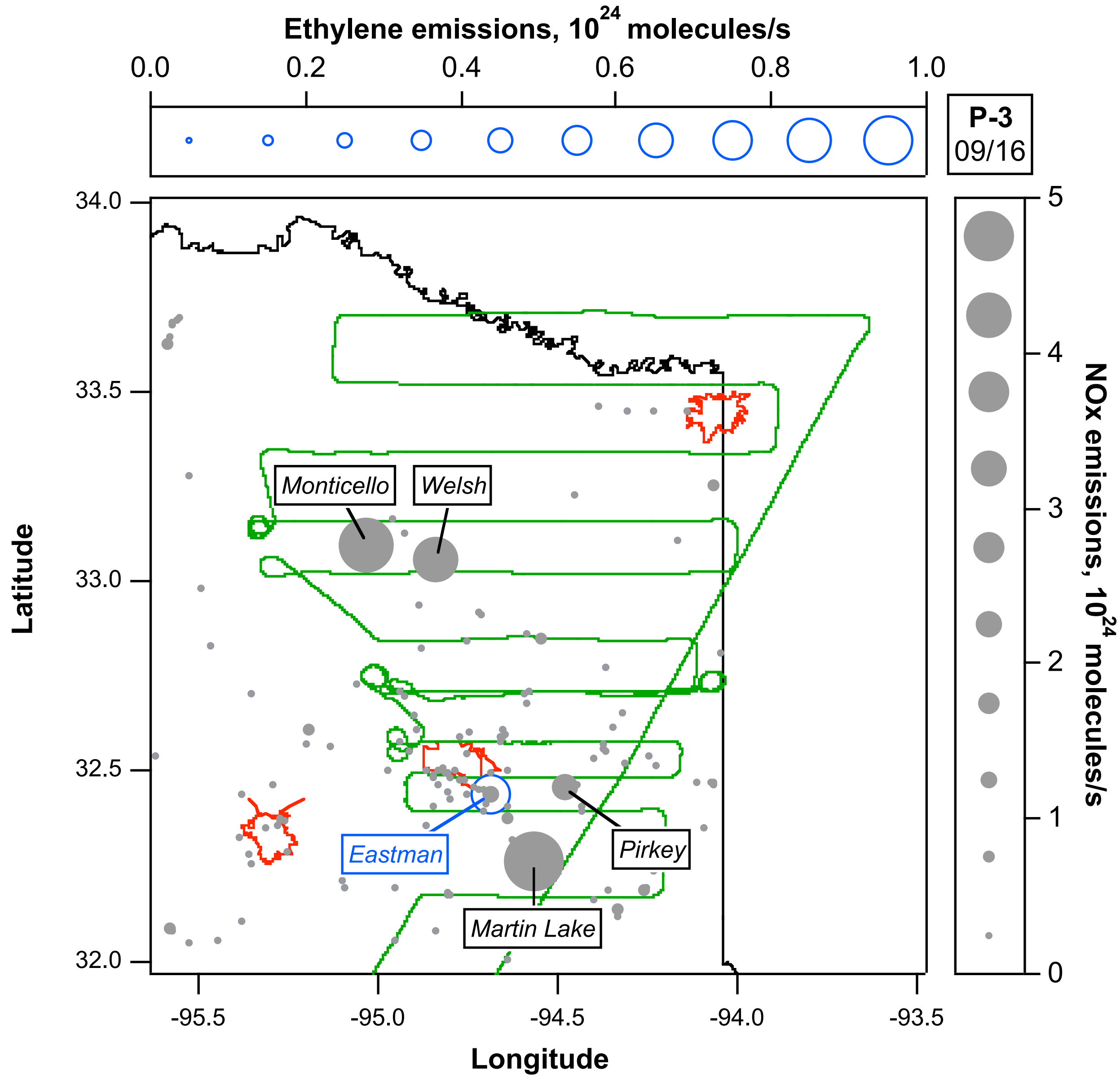
Flyby of an instrumented tower in Moody, TX

Changes in W.A. Parish emissions since 2000

Ga. Tech HO_x measurements in plumes

Point sources in NE Texas

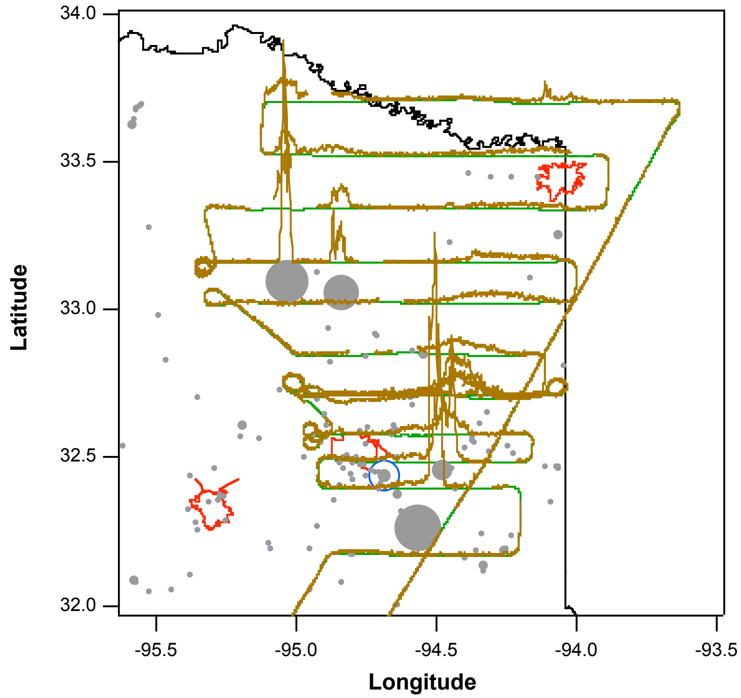




Ethylene emissions, 10^{24} molecules/s
0.0
0.2
0.4
0.6
0.8
1.0
P-3
09/16
34.0
33.5
33.0
32.5
32.0
Latitude
-95.5
-95.0
-94.5
-94.0
-93.5
Longitude
Monticello
Welsh
Eastman
Pirkey
Martin Lake
5
4
3
2
1
0
NOx emissions, 10^{24} molecules/s

NE Texas: power plant CO emissions

SO$_2$ plotted along flight track



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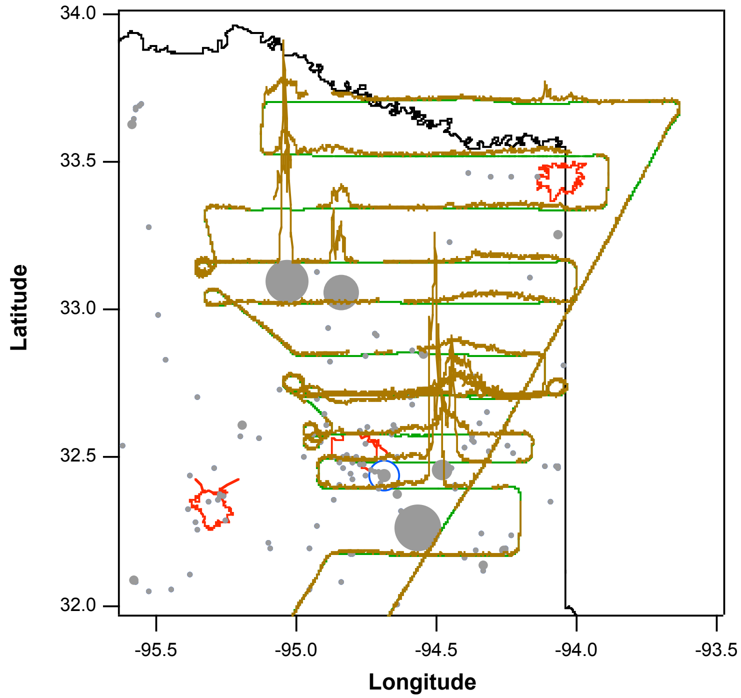
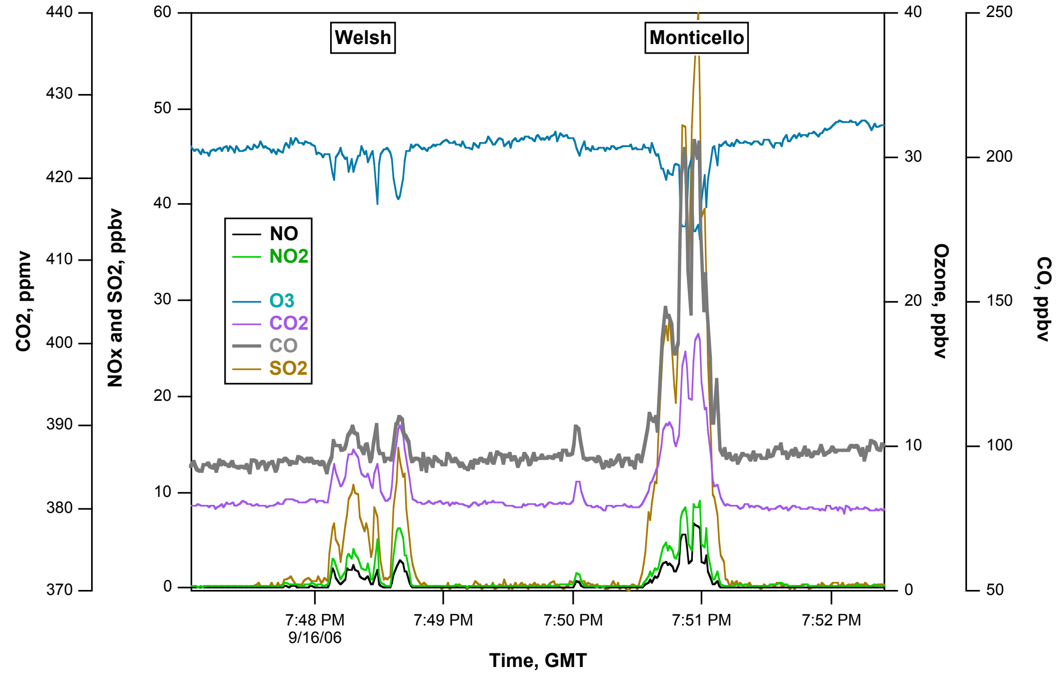
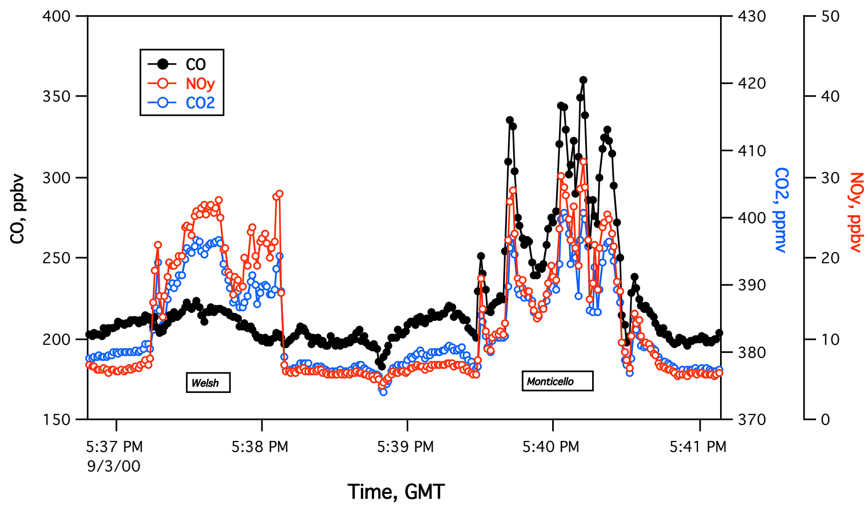
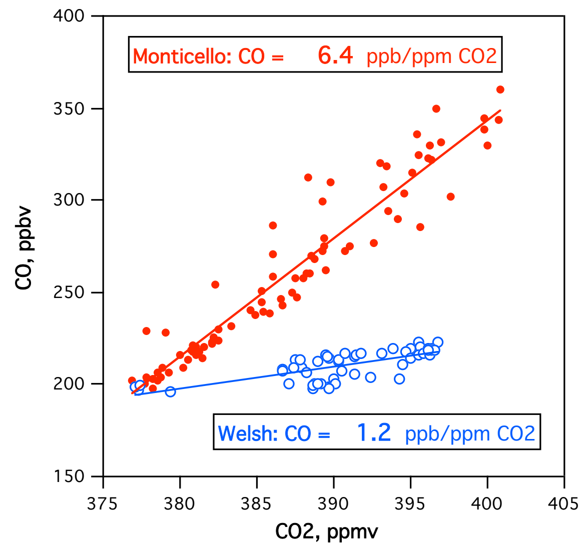




NE Texas: power plant CO emissions

(Nicks et al., J. Env. Monitoring, 5, pp. 35-39 (2003)





TexAQS

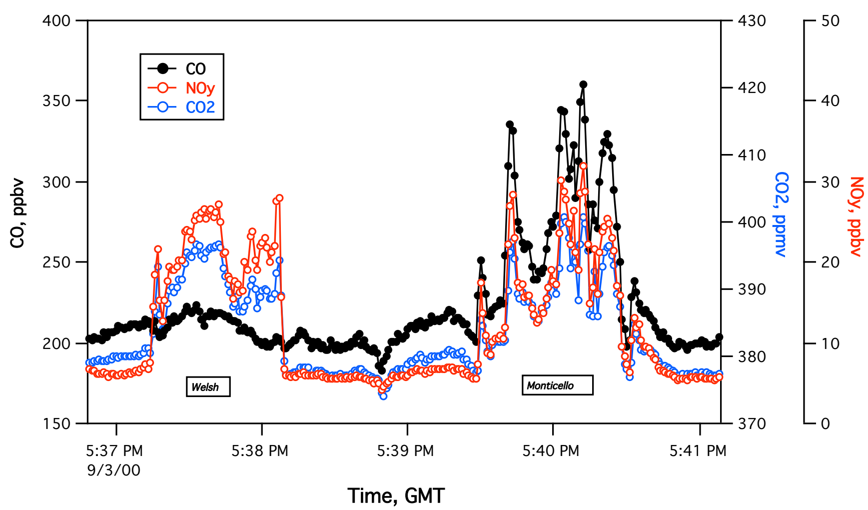
09/03/2000

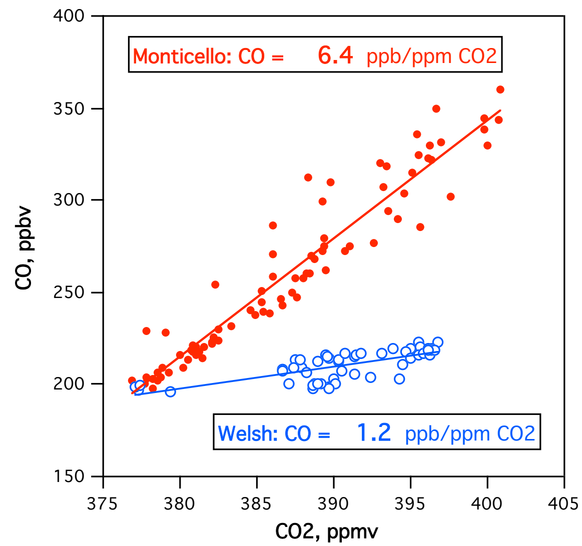
TexAQS II

09/16/2006

NE Texas: power plant CO emissions

(Nicks et al., J. Env. Monitoring, 5, pp. 35-39 (2003))





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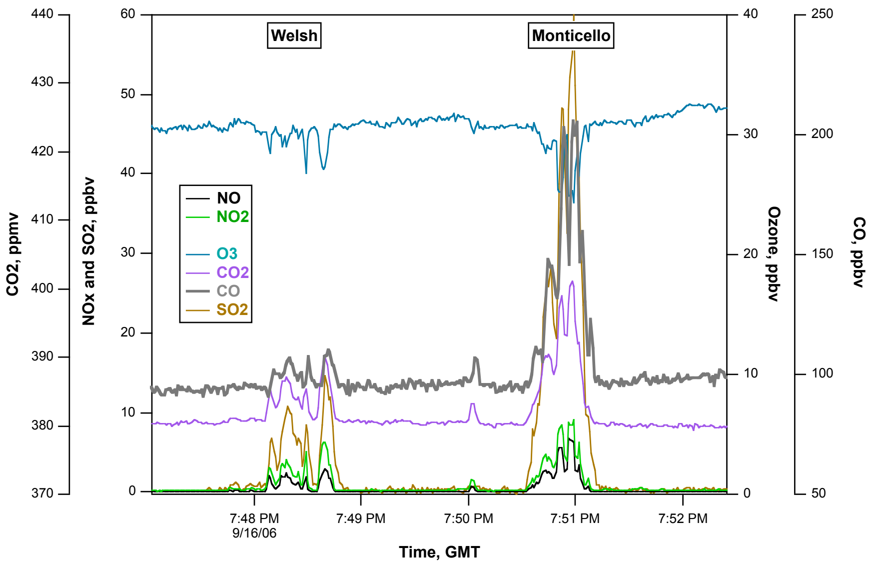
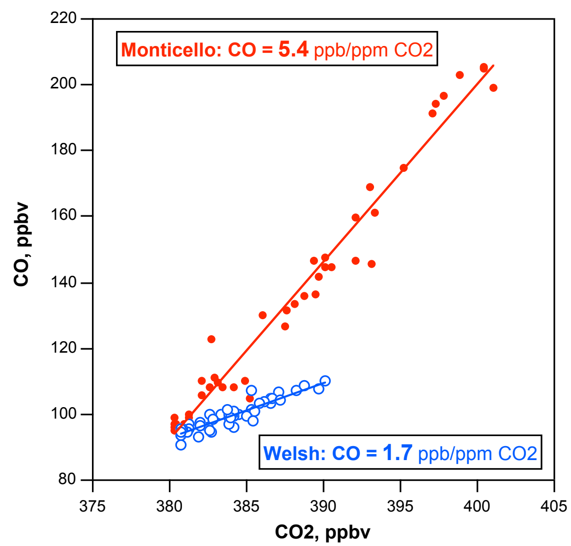
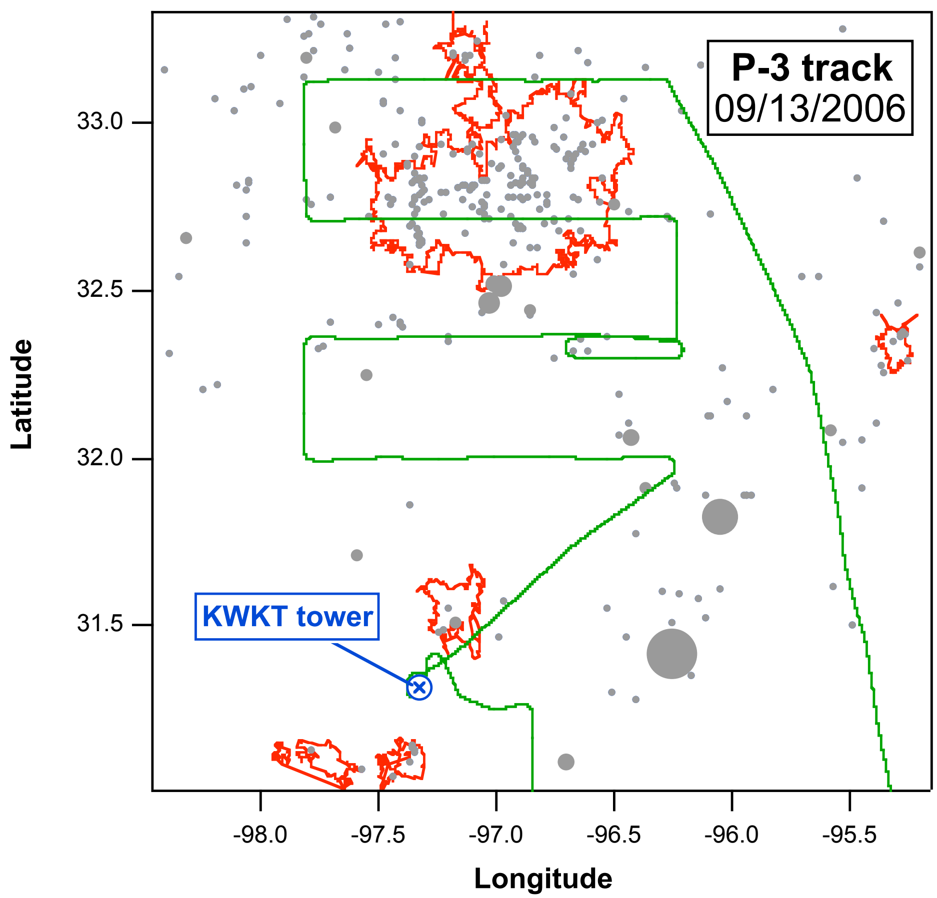




TexAQS II

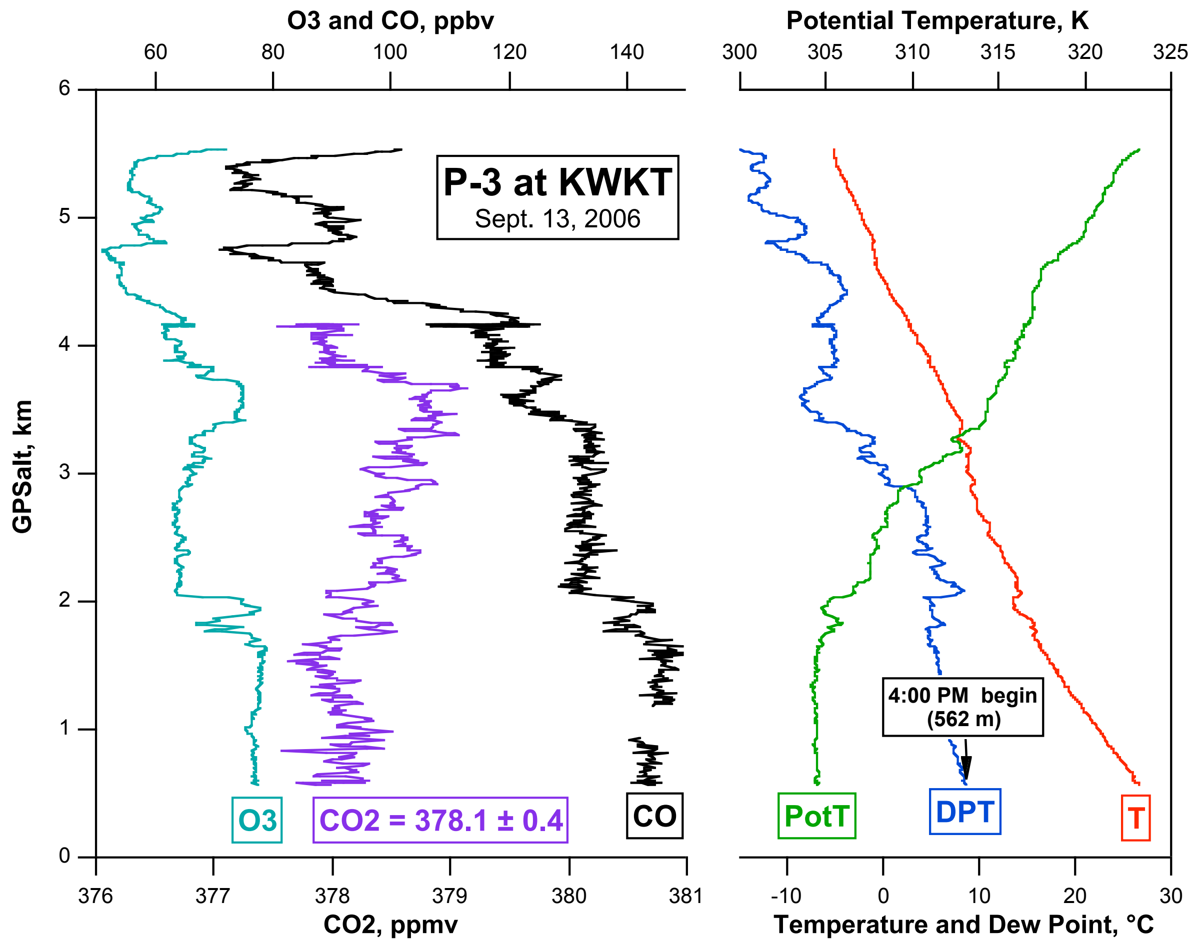
09/16/2006

NOAA Global Monitoring Division
instrumented tall tower - Moody, TX



CO_2, CO, O_3, and met. at 496 meters on the KWKT tower

NOAA Global Monitoring Division instrumented tall tower - Moody, TX



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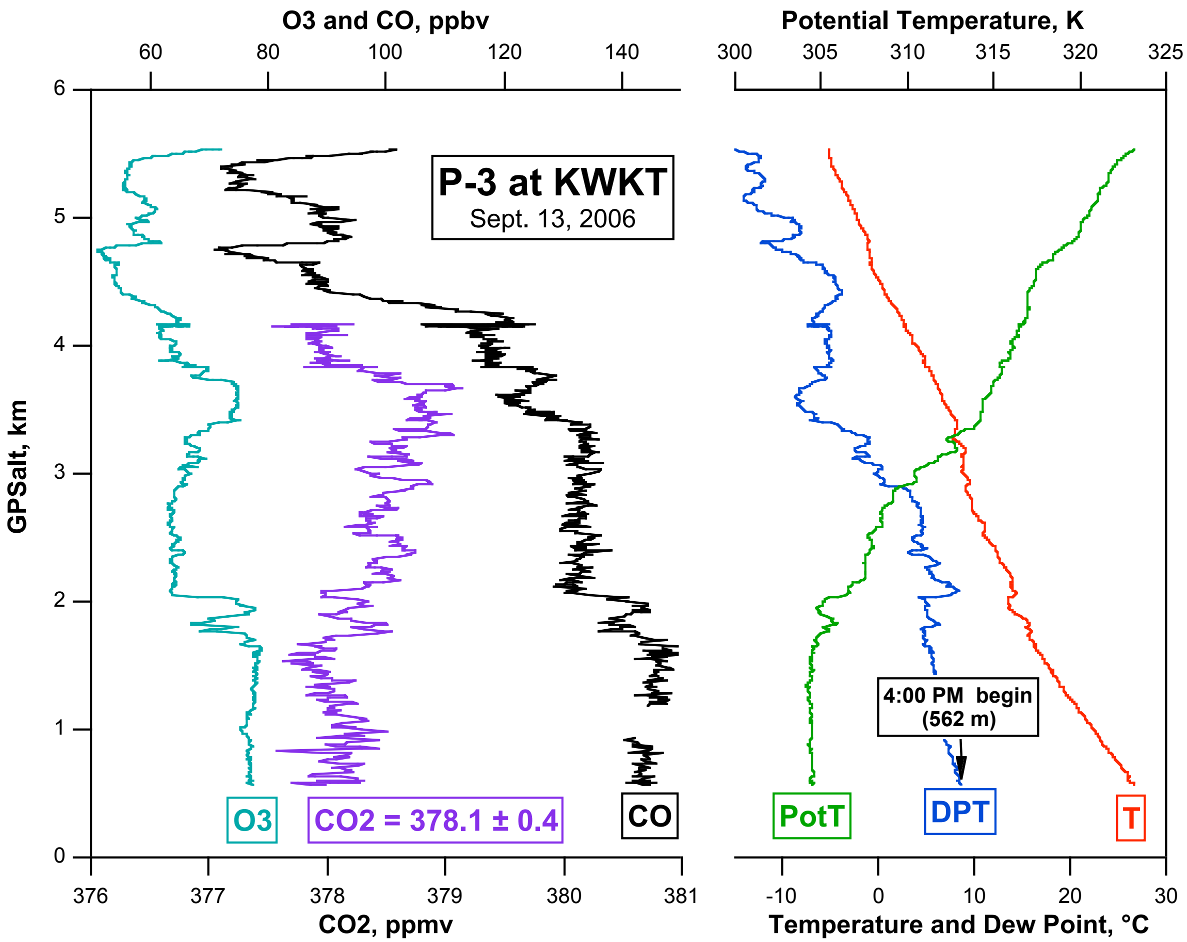
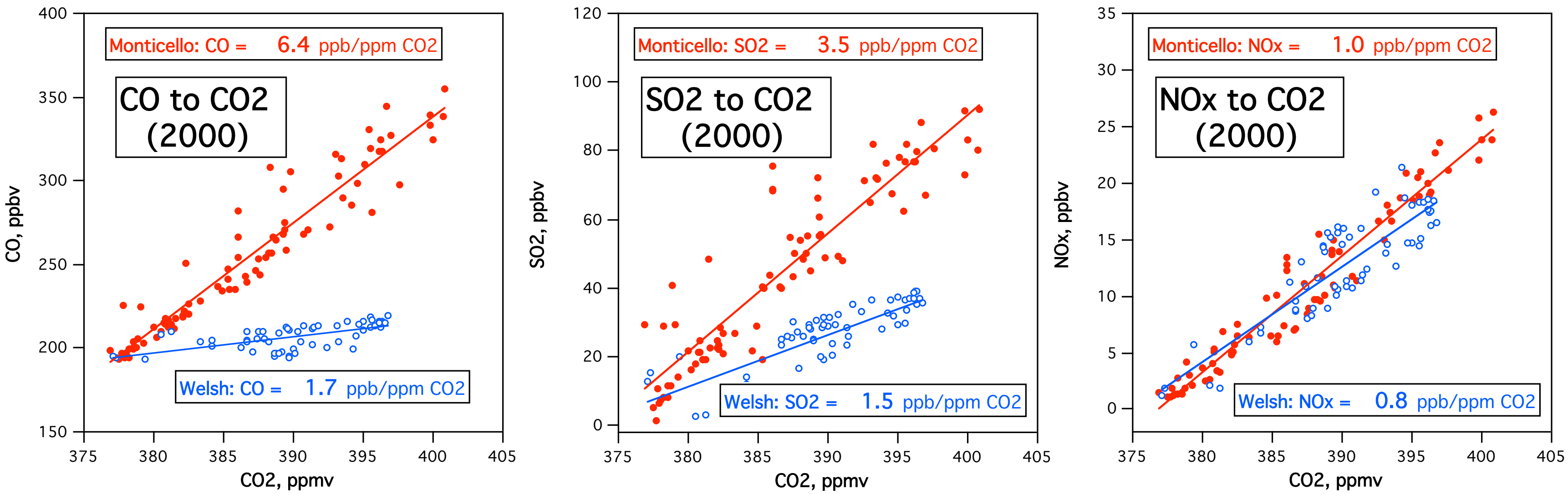


Tower: CO_2 378.3 ±0.1

NE Texas: NOx changes since 2000



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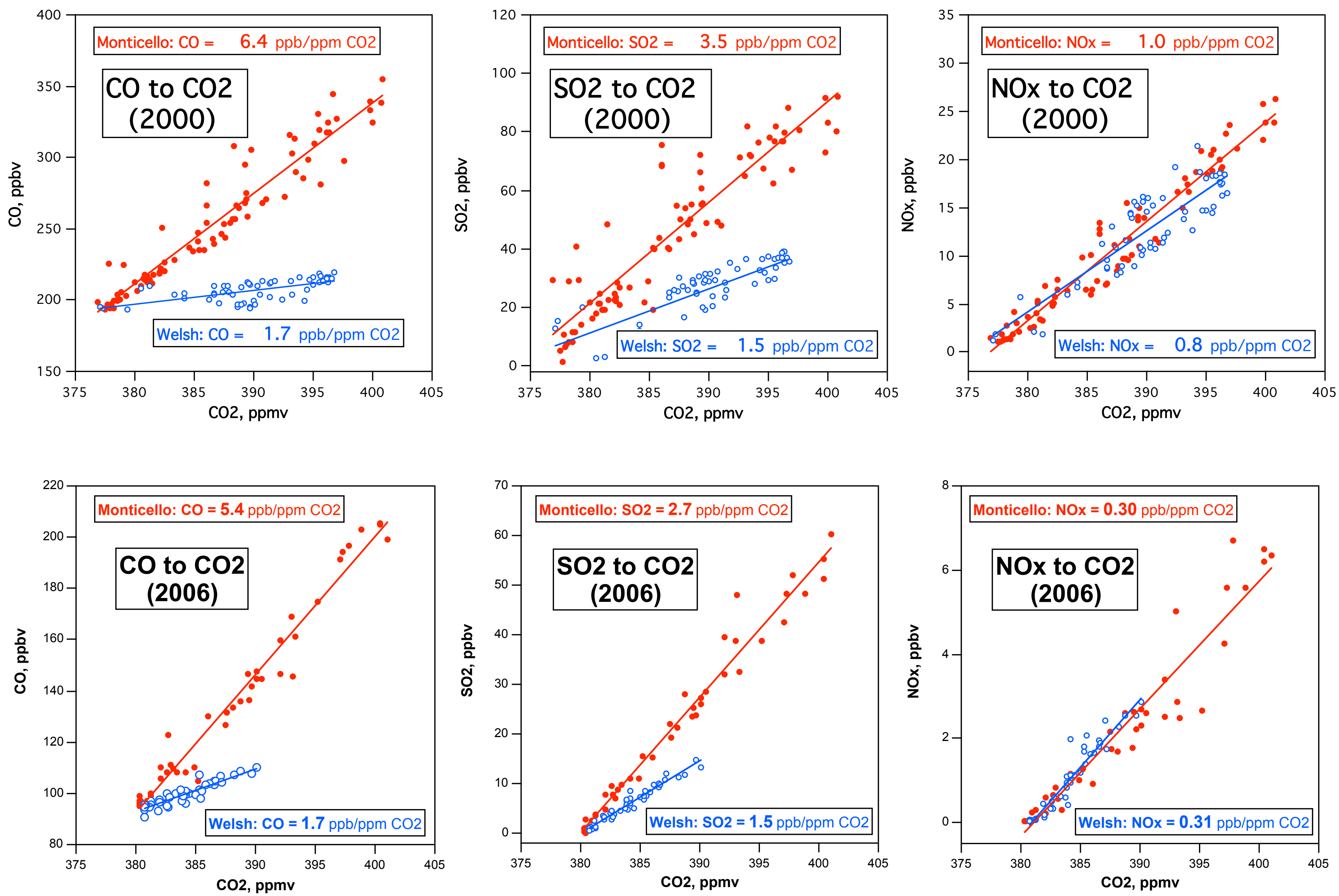
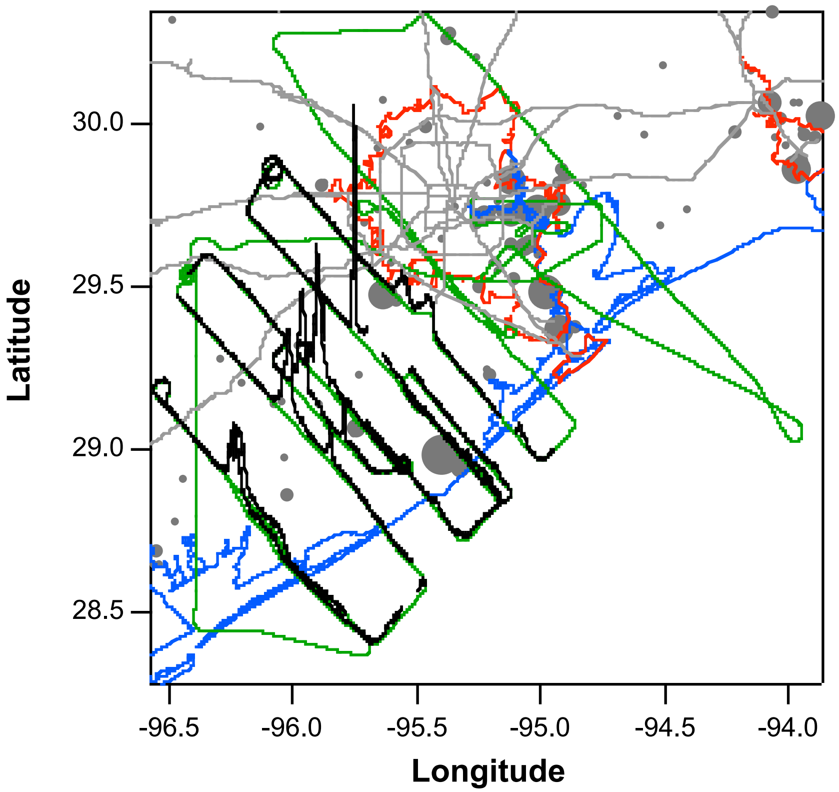
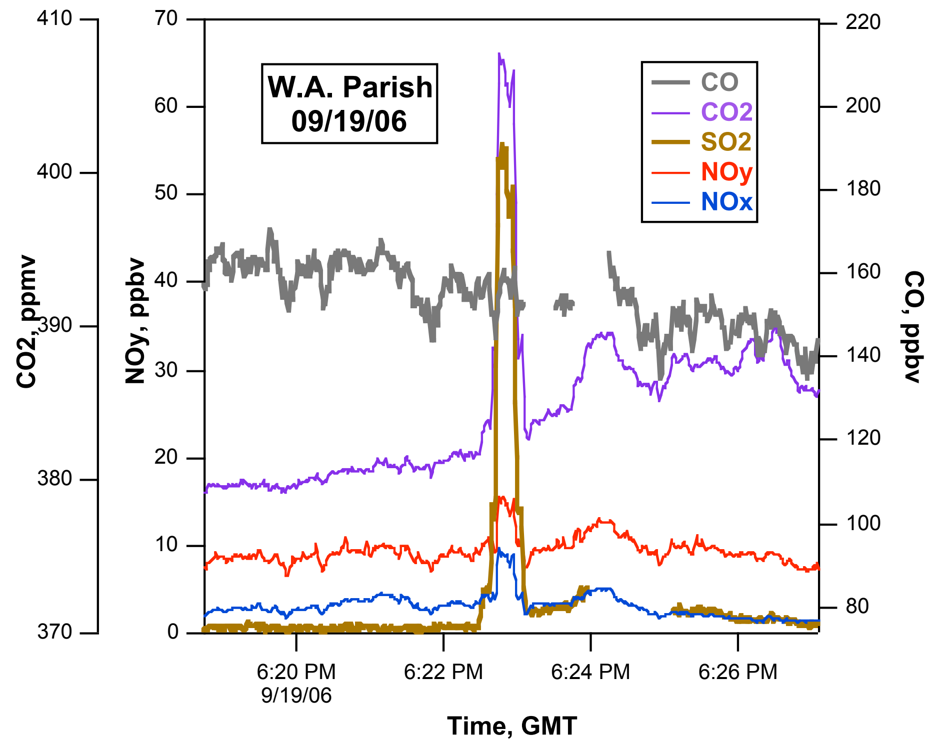


W.A. Parish: changes since 2000





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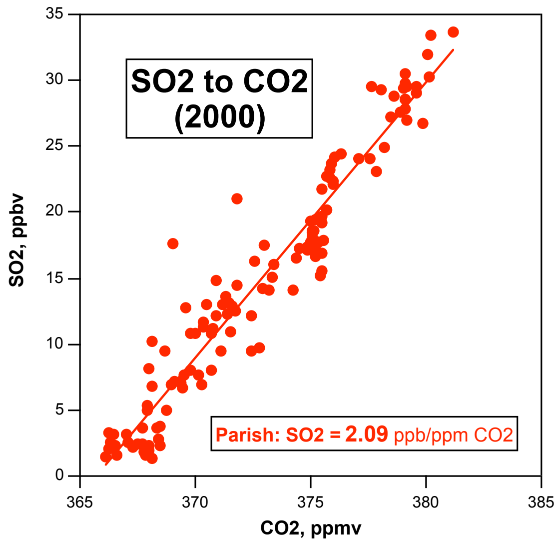

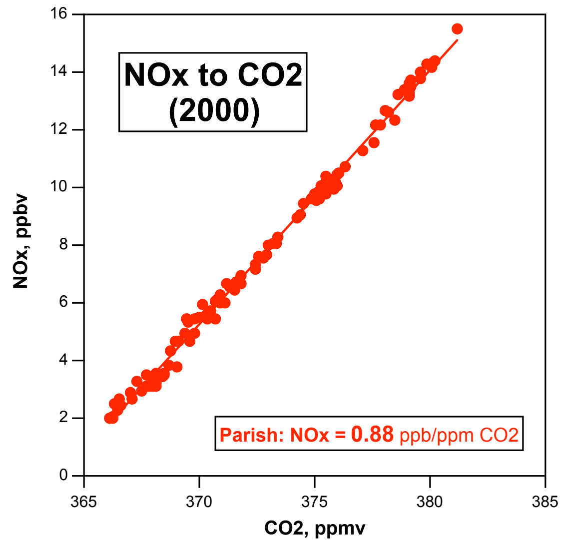

TexAQS
08/28/2000

TexAQS II
09/19/2006

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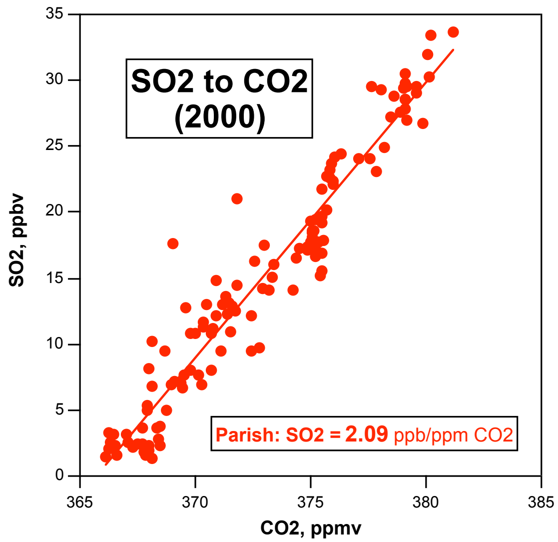

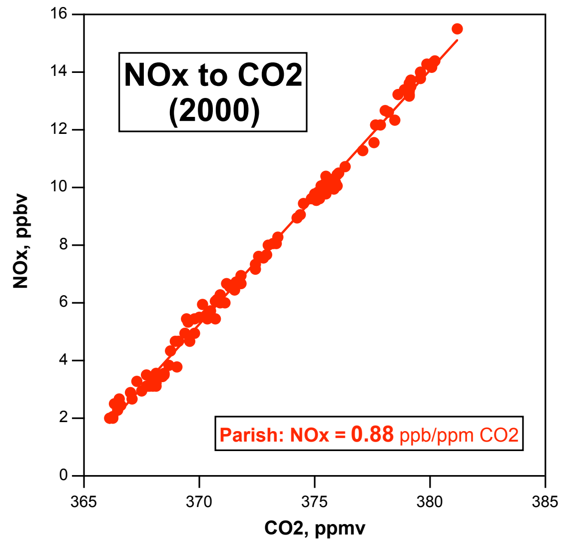

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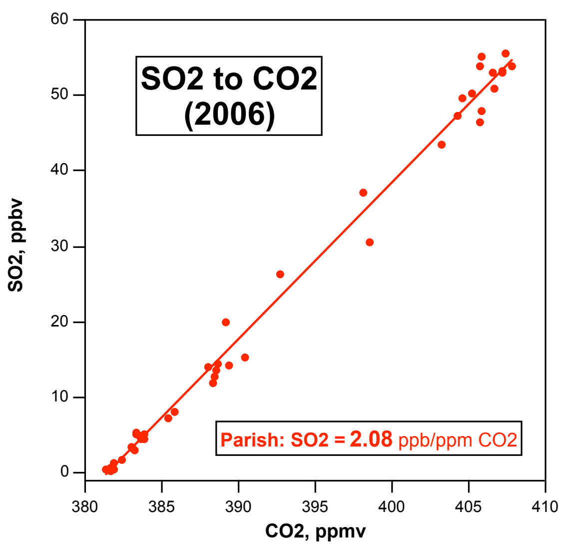

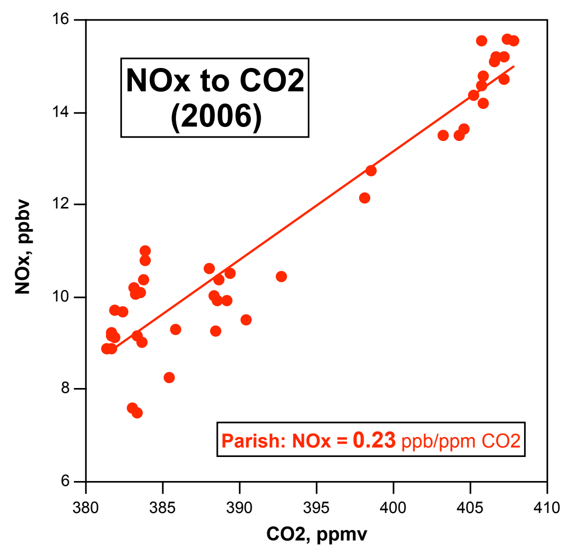

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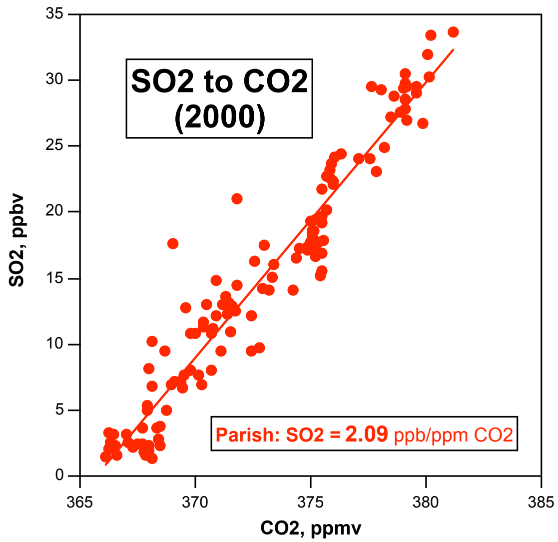

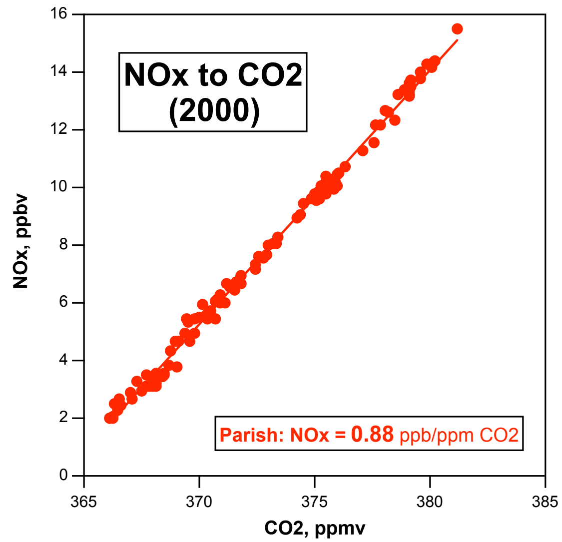

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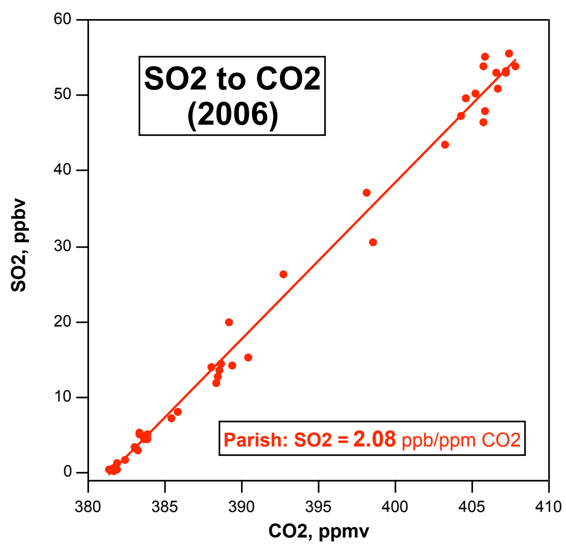
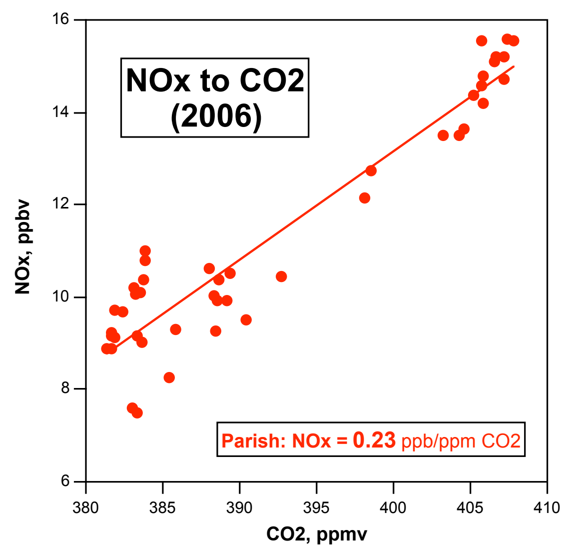


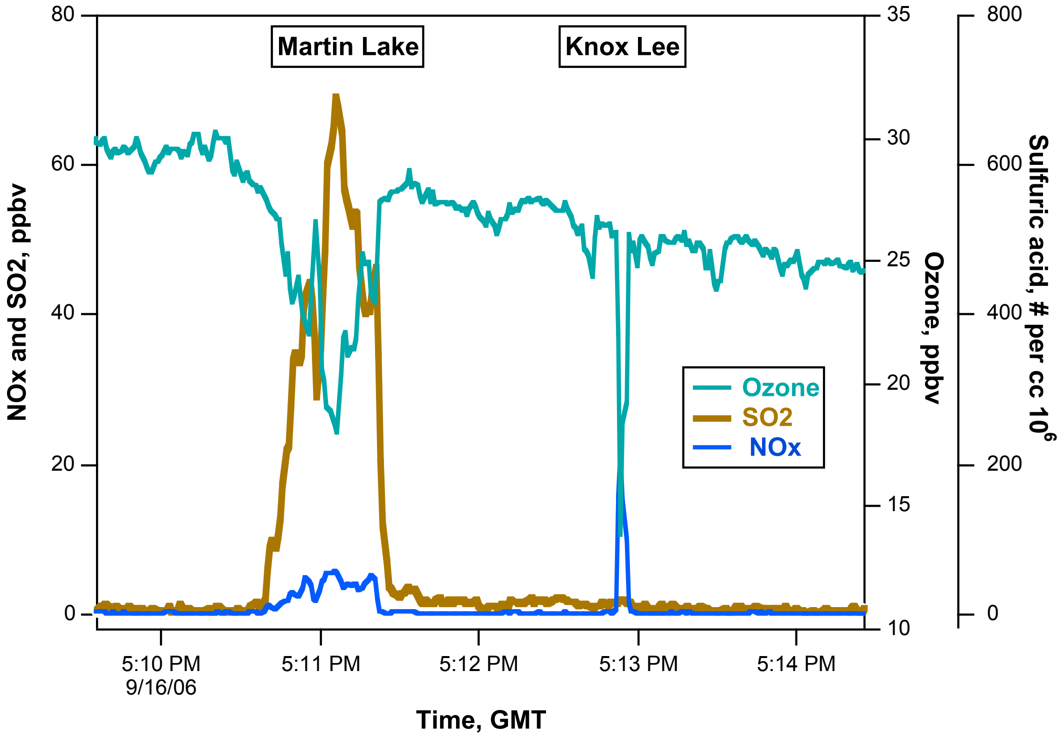


TexAQS II
09/19/2006

SO_2/NOy ratio
2004 (CEMS): 8.8
2006 (P-3): 7.8

Peroxy radicals and ozone formation

Greg Huey/David Tanner (Georgia Tech)
H_2SO_4 and HO_x measurements on the NOAA P-3



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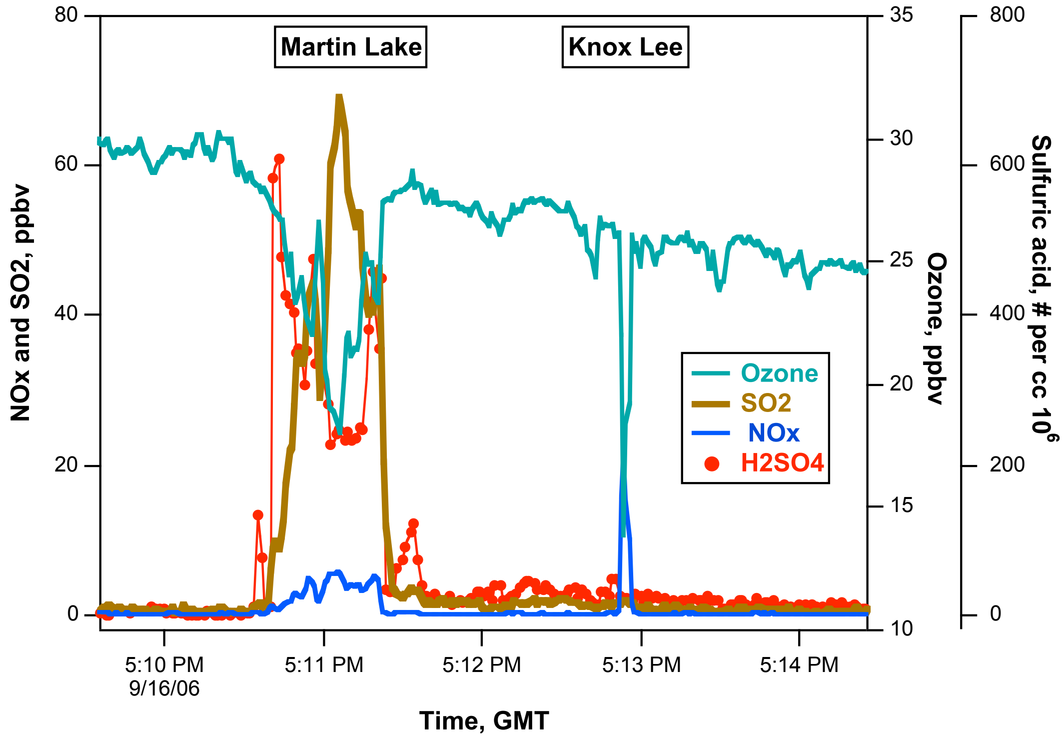

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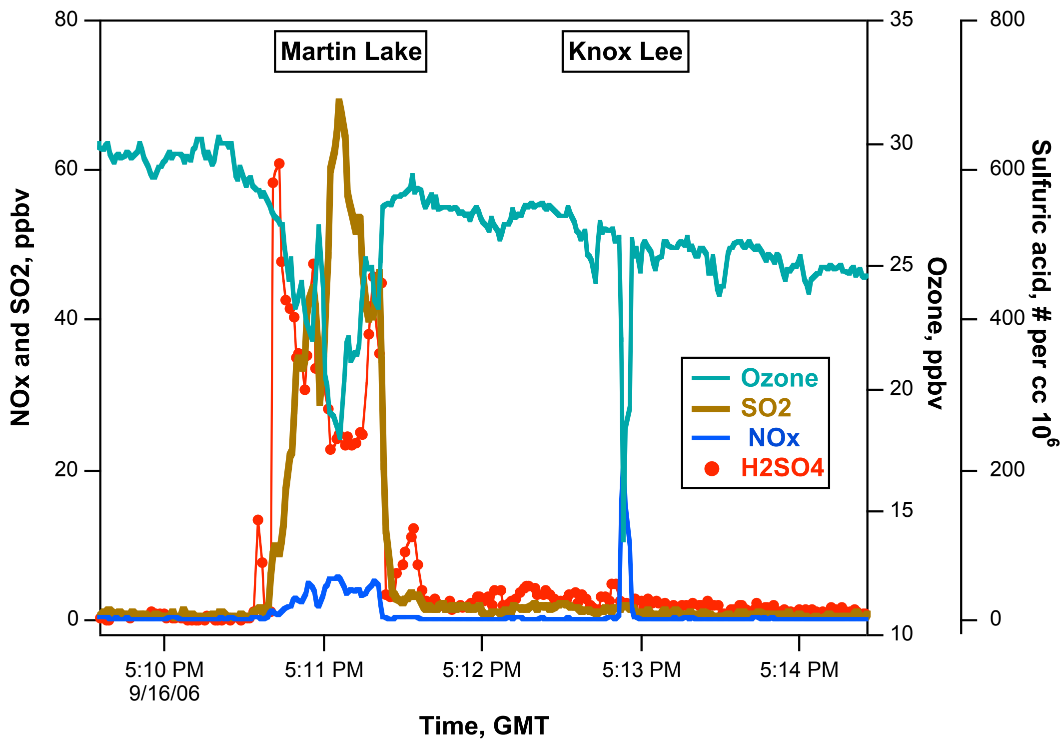


- New particle formation rates
- Aerosol acidity
- Ozone production dependence on [NOx]
- Direct estimates of ozone production rates

Questions A, C, D, E – Emissions: SOF data

- **Ship channel emissions (Johan Mellqvist)**

Solar Occultation Flux (SOF) measurements around the Houston Ship Channel and other source areas,

Johan Mellqvist, Jerker Samuelsson and Claudia Rivera
Radio and Space
Chalmers University of Technology
Göteborg, Sweden
jome@chalmers.se

Barry Lefer/Monica Patel
Institute of Multi-Dimensional Air Quality Study
University of Houston

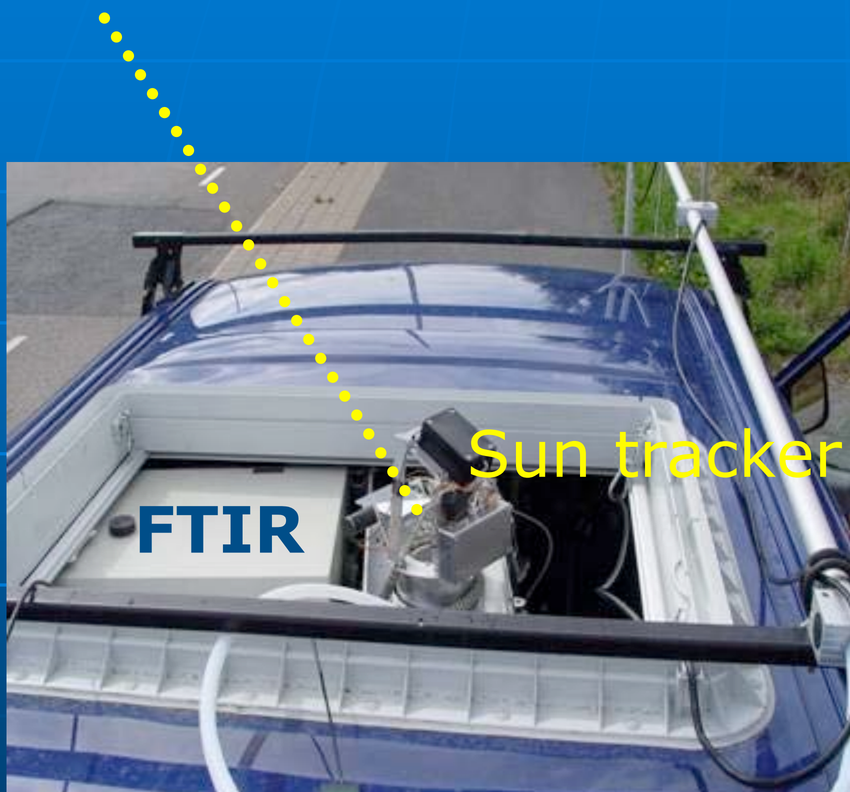
Funded by HARC/TCEQ

Aim

- Estimate of total emissions (tons/day) of various species (alkanes, ethylene, propylene, butadiene, NO2 and SO2) emitted from the Houston Ship Channel and other source areas, using the Solar Occultation Flux method (SOF) and mobile zenith sky measurements (DOAS)

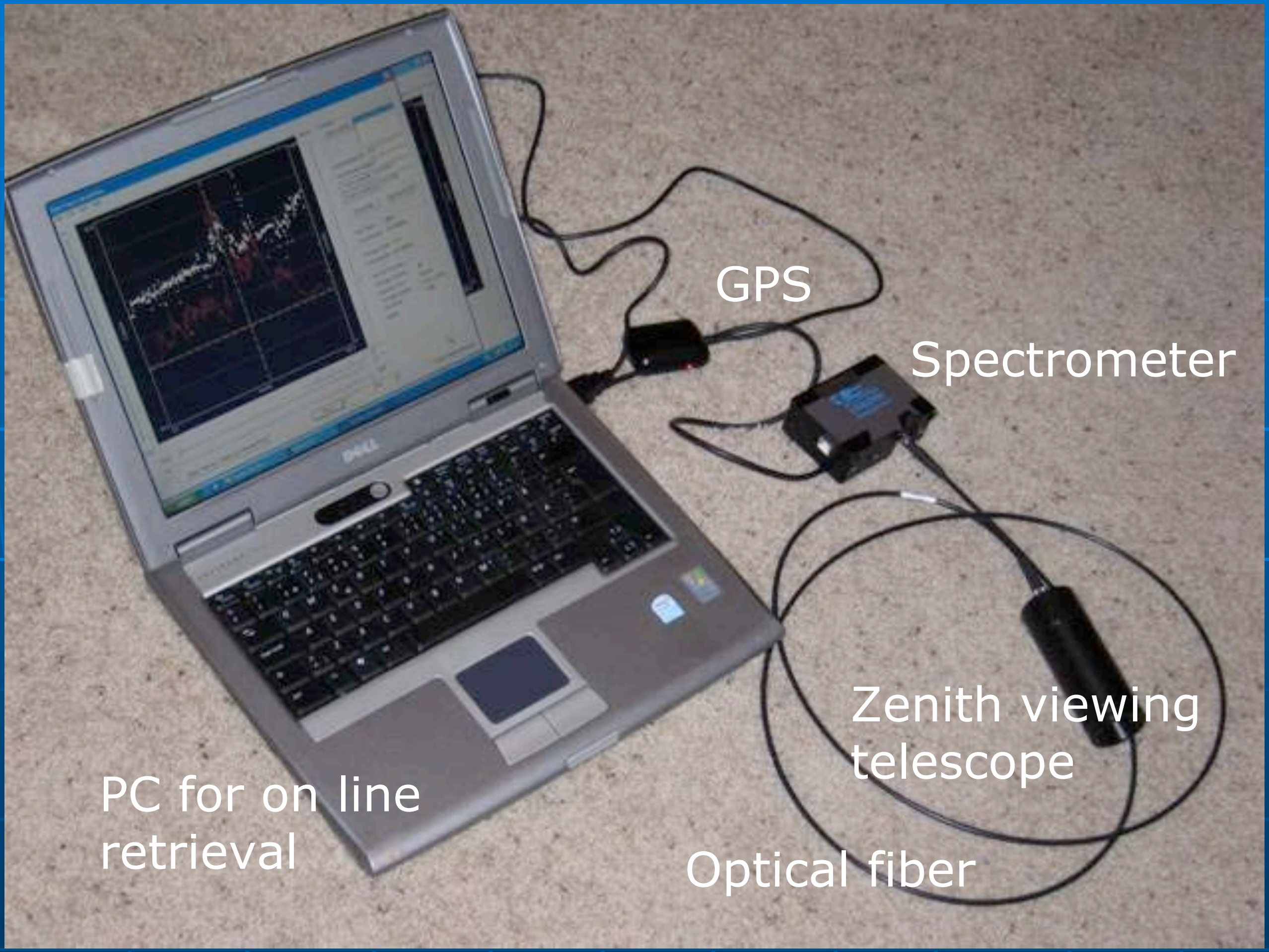
- Comparison and use of additional information (concentration height profiles, chemical composition) from airborne measurements by the Baylor Aztec (TDEV project, Gillani) and NOAA P3

The Solar Occultation Flux method (SOF) (alkenes & alkanes)

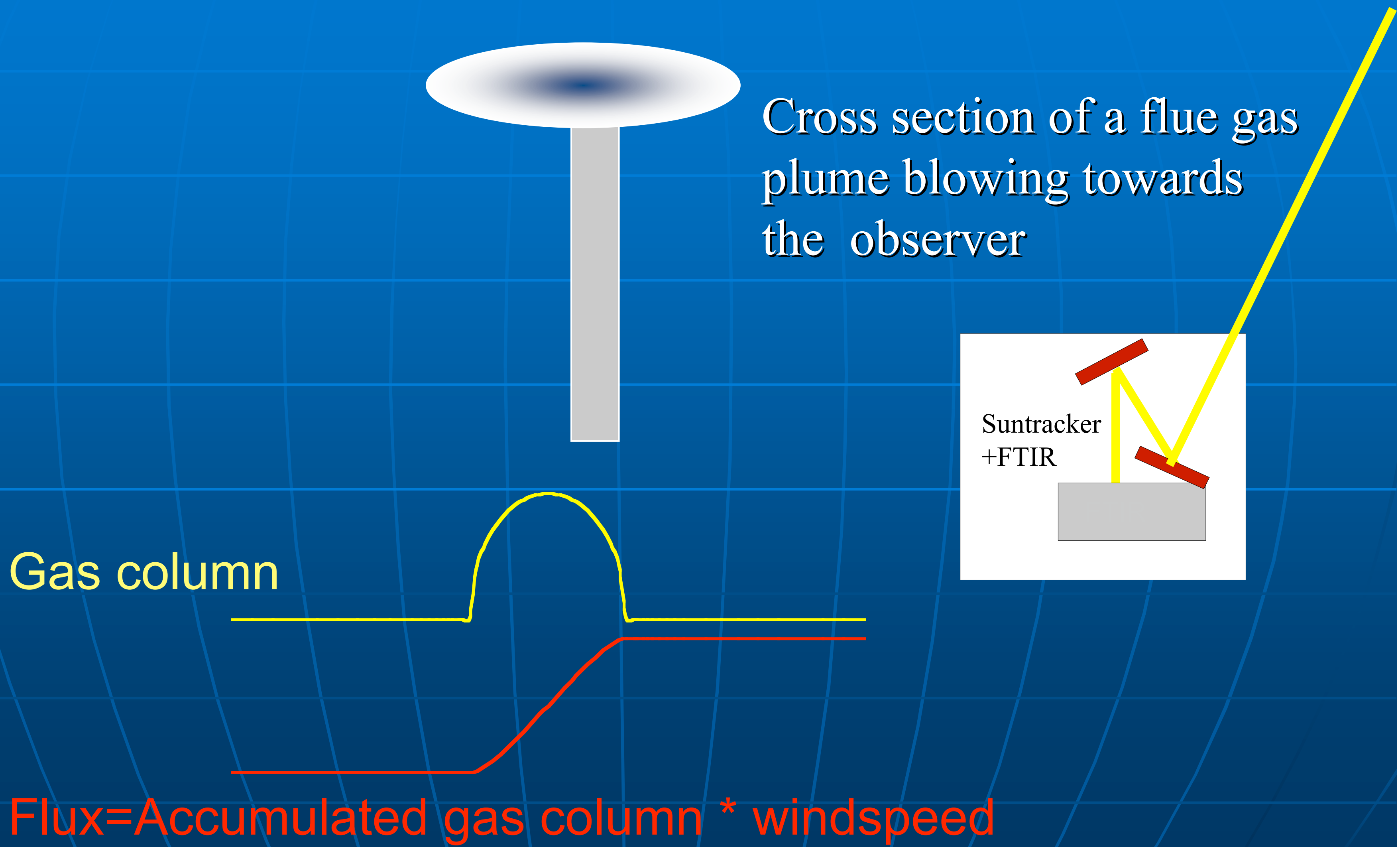


UV/visible zenith sky (NO2, SO2)

System developed for volcanic meaurements (Galle, Johansson et al., Radio and Space, Chalmers)



SOF (Solar Occultation Flux) method



Windprofile measurements with GPS sondes (UH)

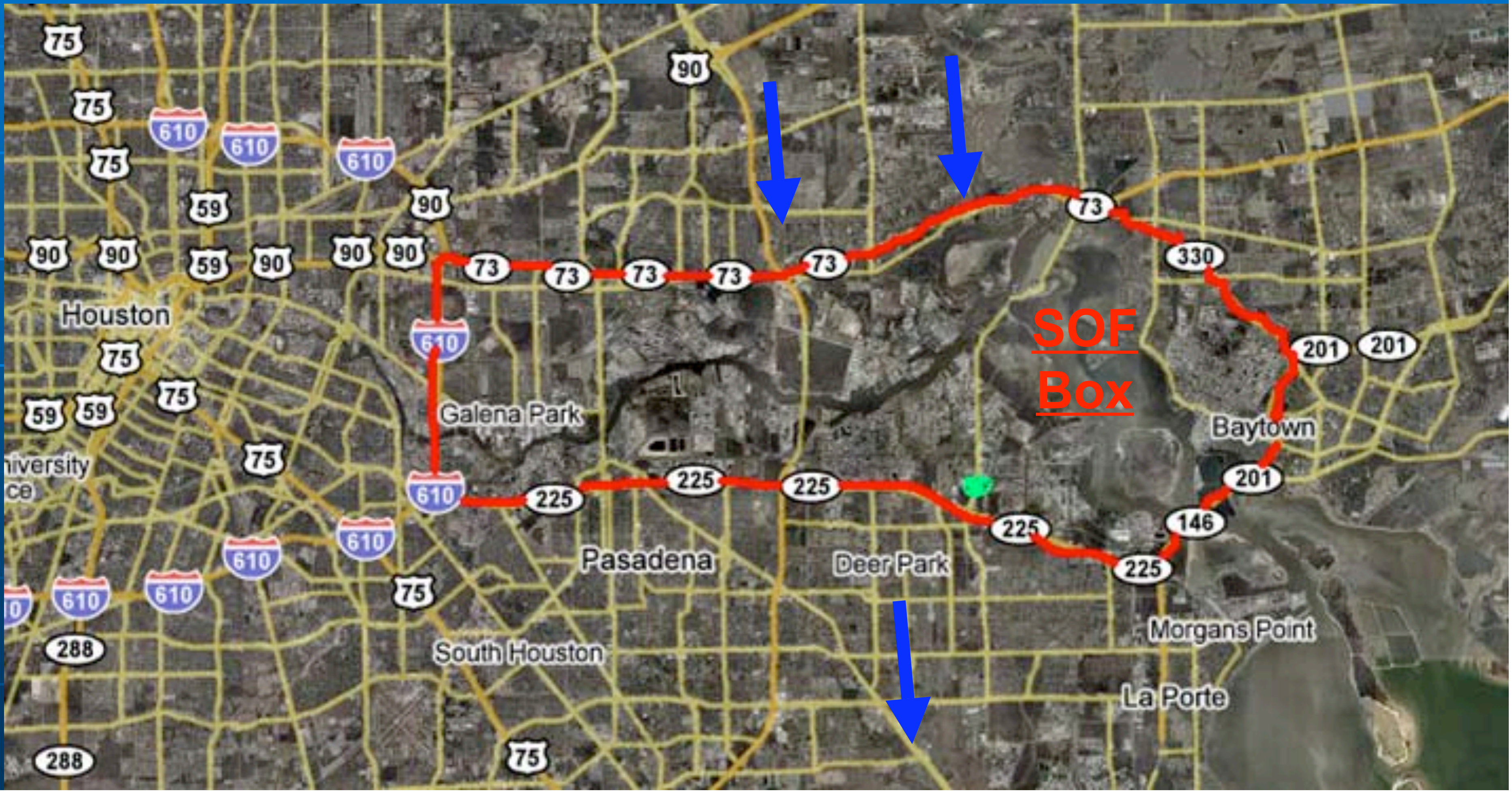
Barry Lefer,
Monica Patel &
Craig Clements

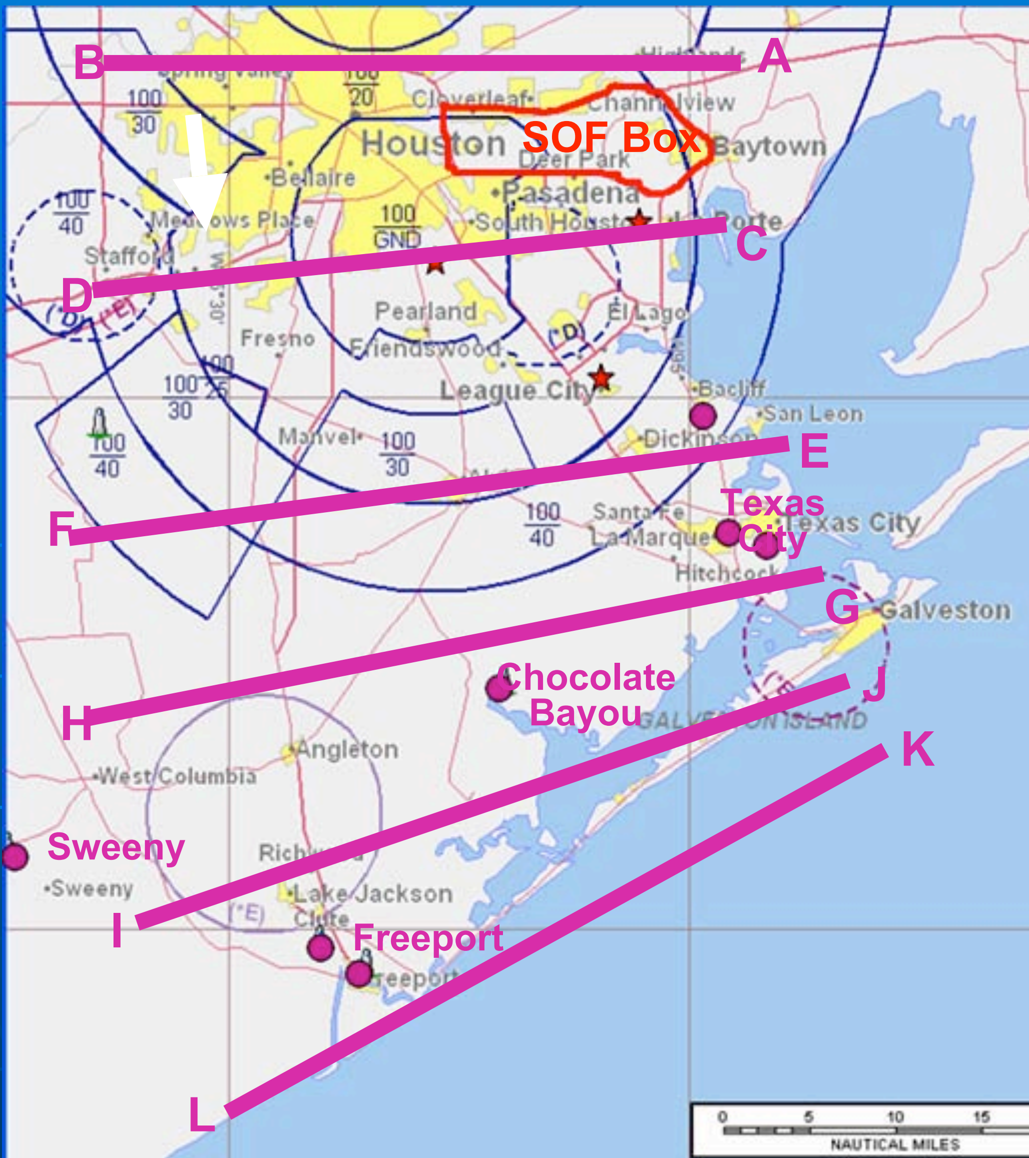
Error budget*

- Retrieval method: 5-10%
- Lineparameters 5-10%
- Optical artifacts/interference 5-15%
- Wind field 15-25%
- Sum= 20-35%

** This budget is consistent with validation experiments*

Objective : Enclosure of emissions by "box measurements"





In conjunction with the SOF box, airborne measurements have been conducted (TDEV, Gillani et al.)

Date	SOF O : Olefines A : Alkanes	UV NO_2 SO_2	Related activities	Wind
30 Aug	HSC box: O	HSC box	Aztec	N
31 Aug	HSC-Battleground Rd: O+A	HSC box Battleground Rd Baytown	Aztec	E
1 Sep	HSC-Battleground Rd: O Channelview: O+A	HSC-Battleground Rd Channelview		NE
2 Sep	Texas City: O+A	Texas City		NE
3 Sep	Sweeny (E half of plant) : O+A	Sweeny (total)		E
4 Sep	Baytown : O	HSC box Baytown		NE

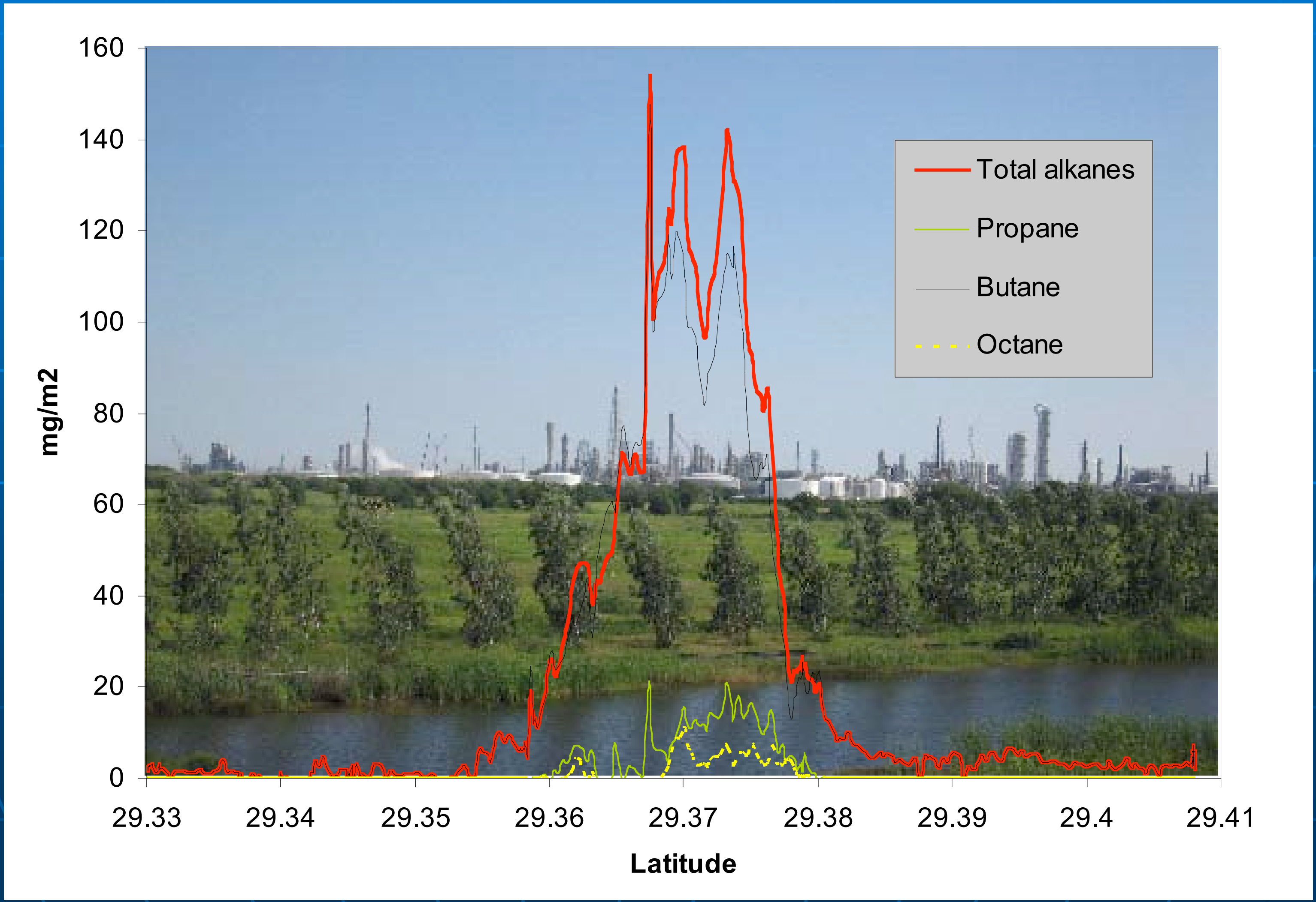
Date	**SOF** **O : Olefines** **A : Alkanes**	**UV** **NO_2** **SO_2**	**Related activities**	**Wind**
7 Sep	Baytown : O+A	Baytown	Ron Brown on HSC	NE
10 Sep		HSC box		N
11 Sep		HSC box		N
13 Sep	HSC box: O+A Baytown: A	HSC box: O+A Baytown: A		N
14 Sep	Texas City: A HSC-Battleground Rd: O+A	Texas City HSC-Battleground Rd		NE
16 Sep		Freeport		S
17 Sep		HSC box		S

Date	SOF O : Olefines A : Alkanes	UV NO_2 SO_2	Related activities	Wind
18 Sep		HSC box		NE
19 Sep	HSC box : O+A Belview: O Baytown: O	HSC box Belview	NOAA-P3	N
20 Sep	Texas City: O+A	Texas City	Aztec, NOAA-P3	E
21 Sep	Sweeny: O+A	Sweeny	NOAA-P3	SW

Some preliminary results

- *The following values should only be considered in a qualitative manner at this stage*

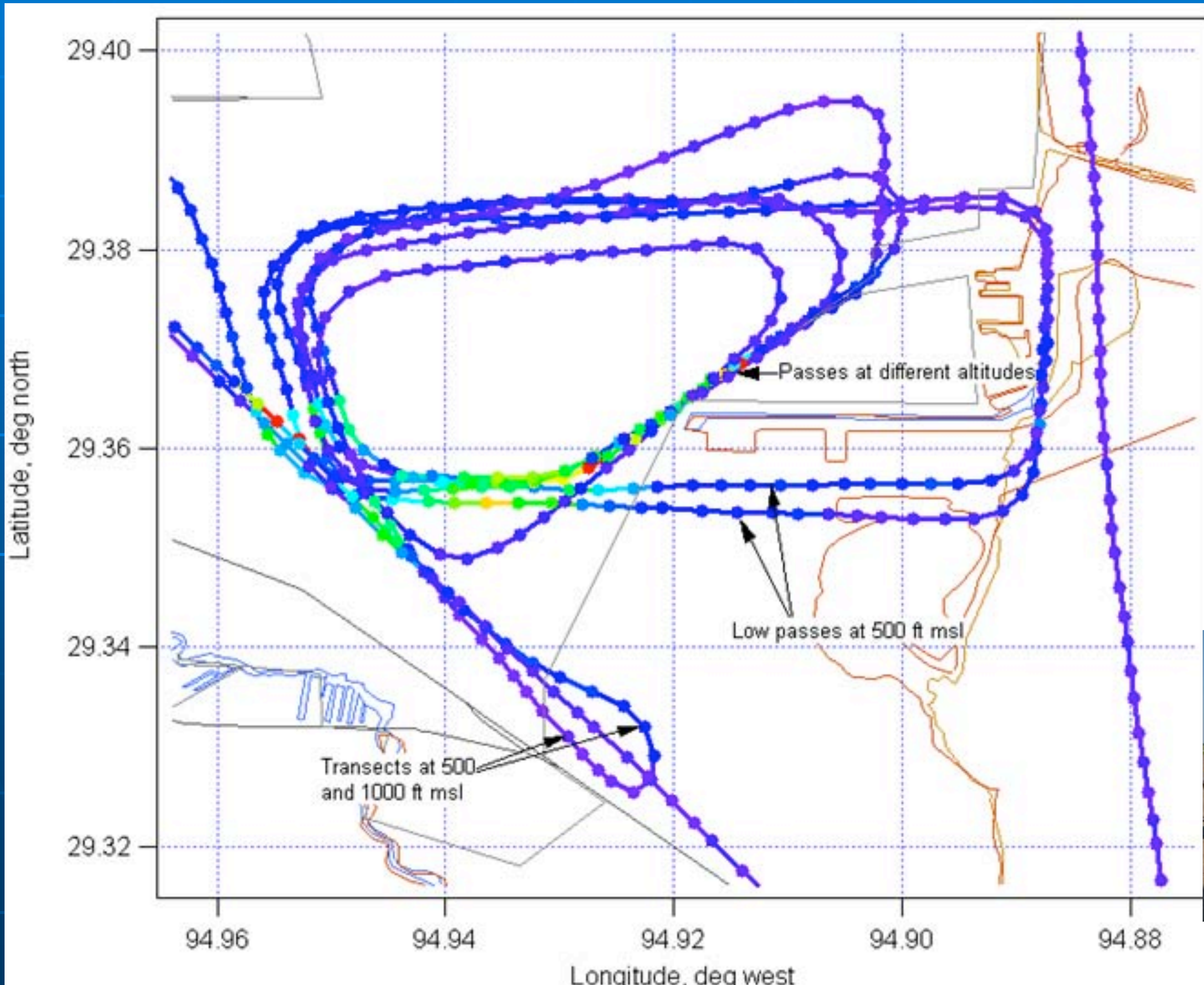
Alkane mass downwind of Texas city measured by SOF on september 20 (Measurements in conjunction with airborne measurements (Aztec and P3)



The alkane channel is sensitive to all VOCs? Knowledge of speciation therefore important (Canisters done by Rappengluck et al. UH)

Compound	**Cross sensitivity as mass of Butane**
Propane	0.98
n-Butane	1.00
Ethane	0.26
Iso-Butane	1.60
n-Pentane	1.01
Iso-Pentane	1.29
Decane	0.74
Hexane	0.94
2-Methylpentane	1.05
3-Methylpentane	1.02
Cyclohexane	0.21
n-Heptane	0.76
Octane	0.55
Nonane	0.42
Toluene	*0.04*
Benzene	*0.00*
Ethylbenzene	*0.27*
1,2,4-TMB	*0.00*
1,3,5-TMB	*0.00*
m+p-xylene	*0.03*
o-xylene	*0.10*
Etene	0.02

Airborne measurements (Aztec) at Texas city by Baylor university (Alvarez et al.)



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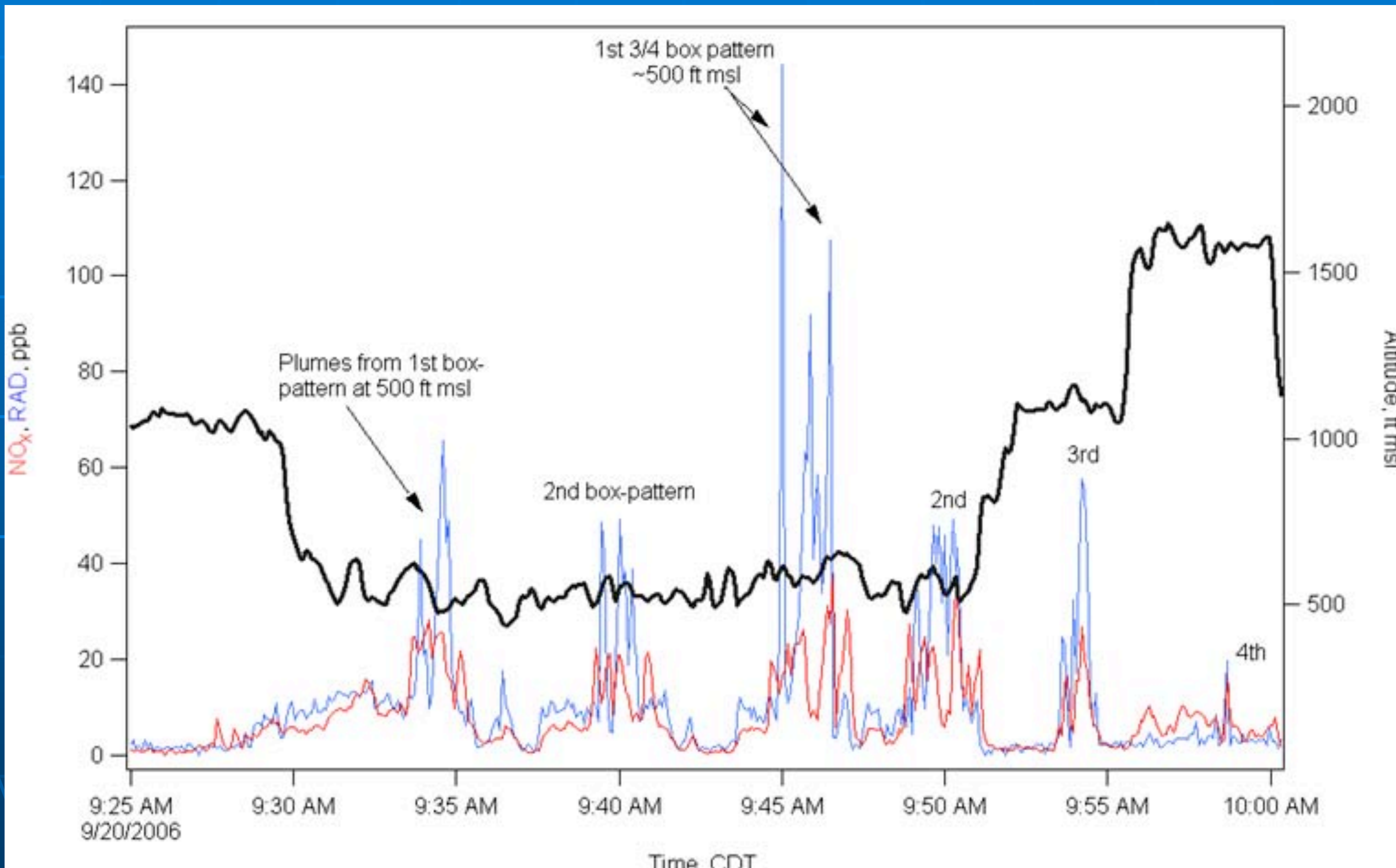
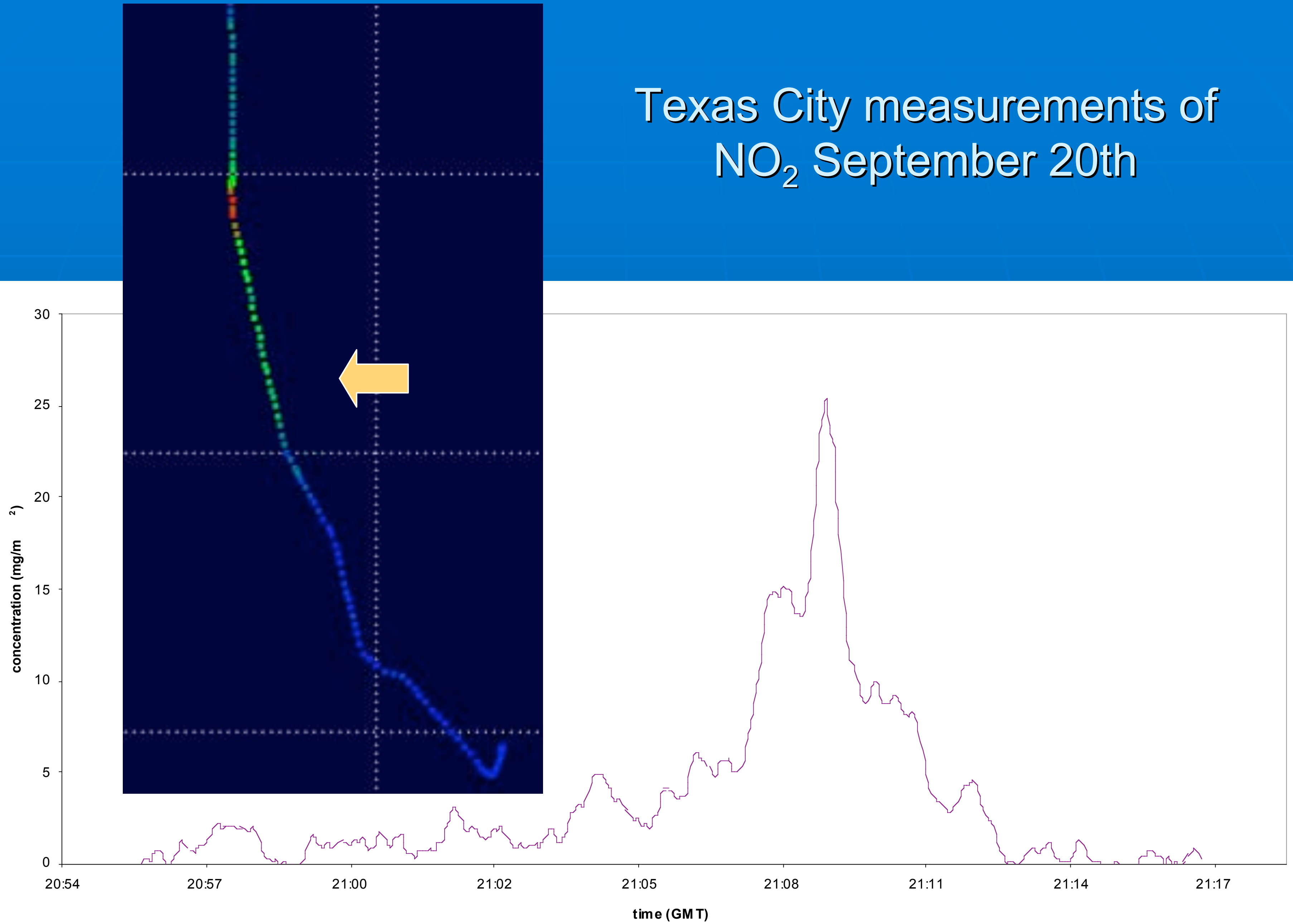
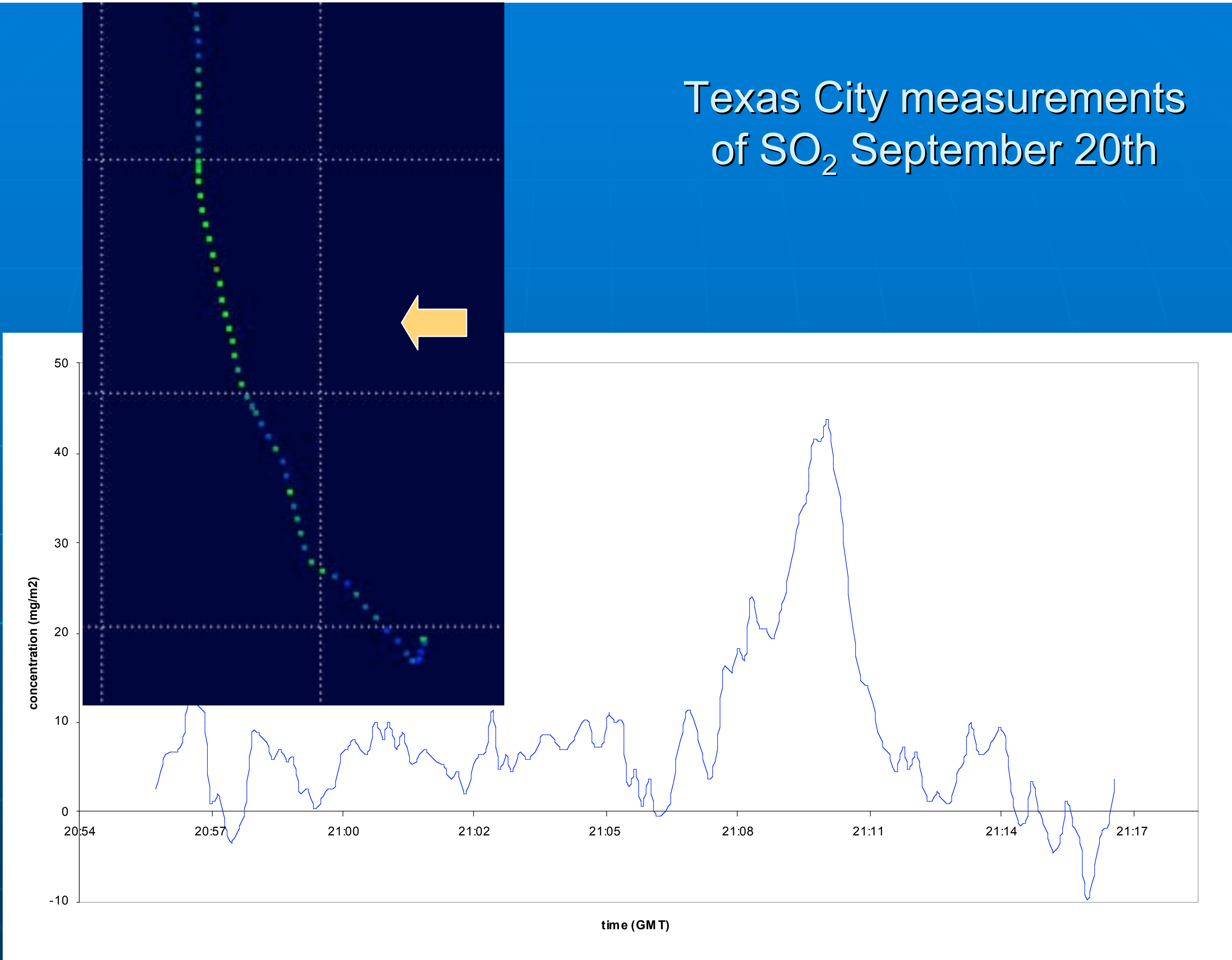


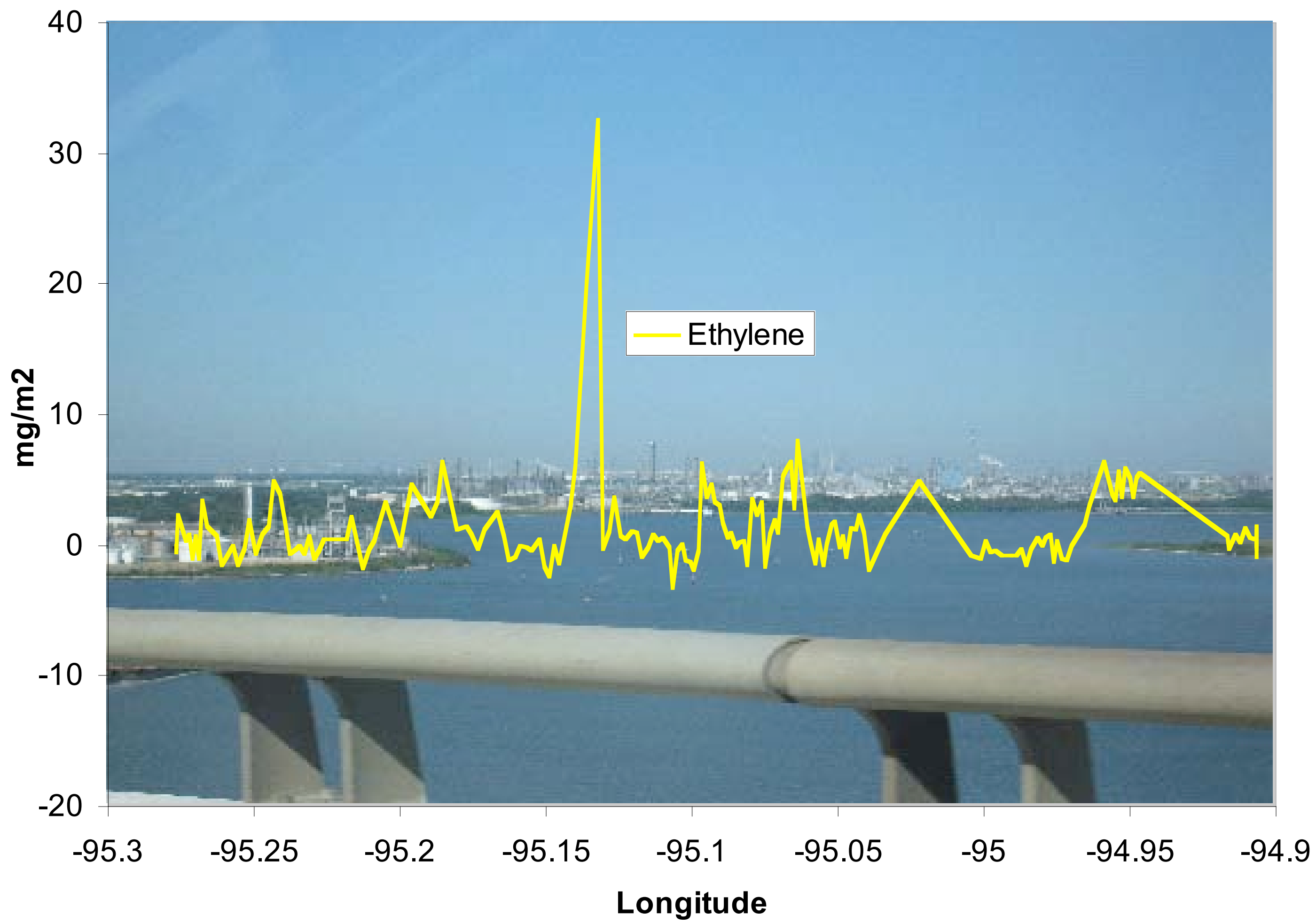
Texas City measurements of NO_2 September 20th



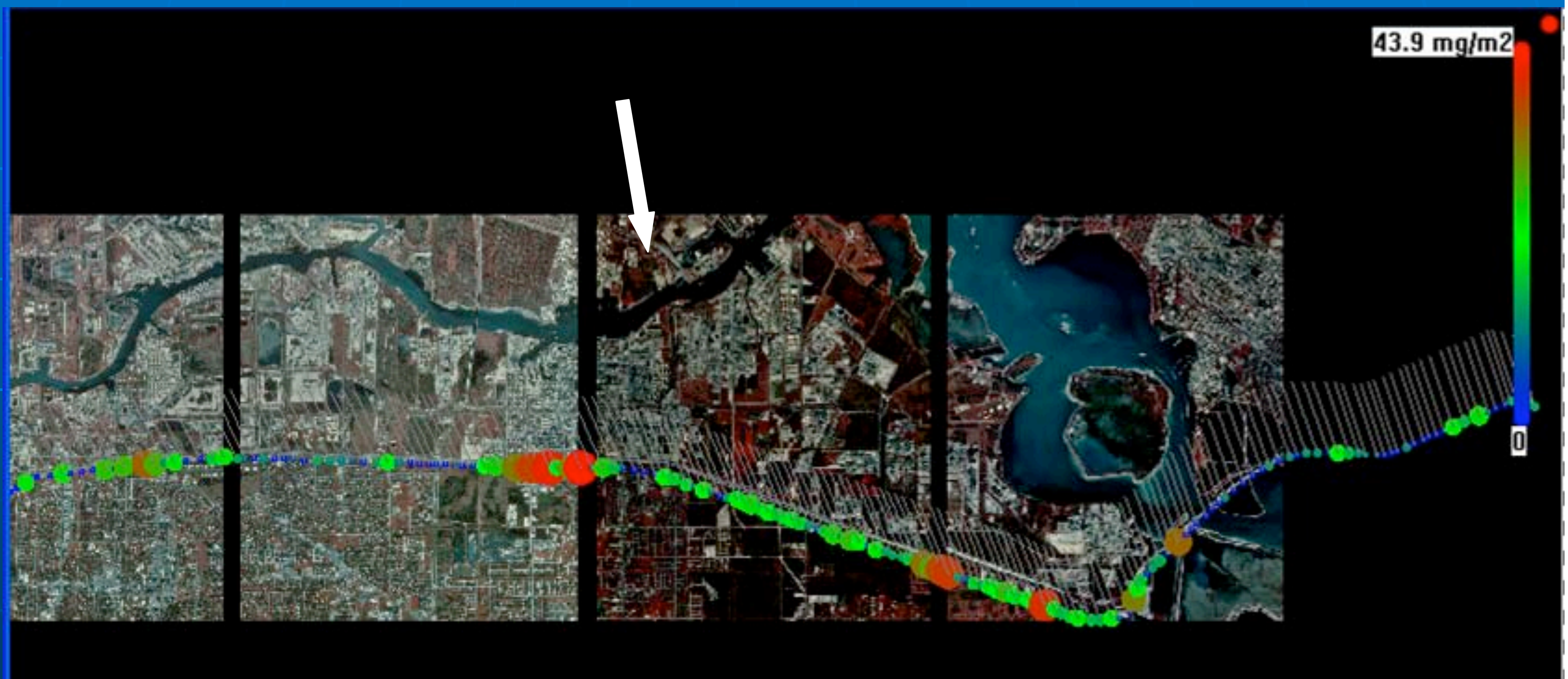
Texas City measurements of SO_2 September 20th



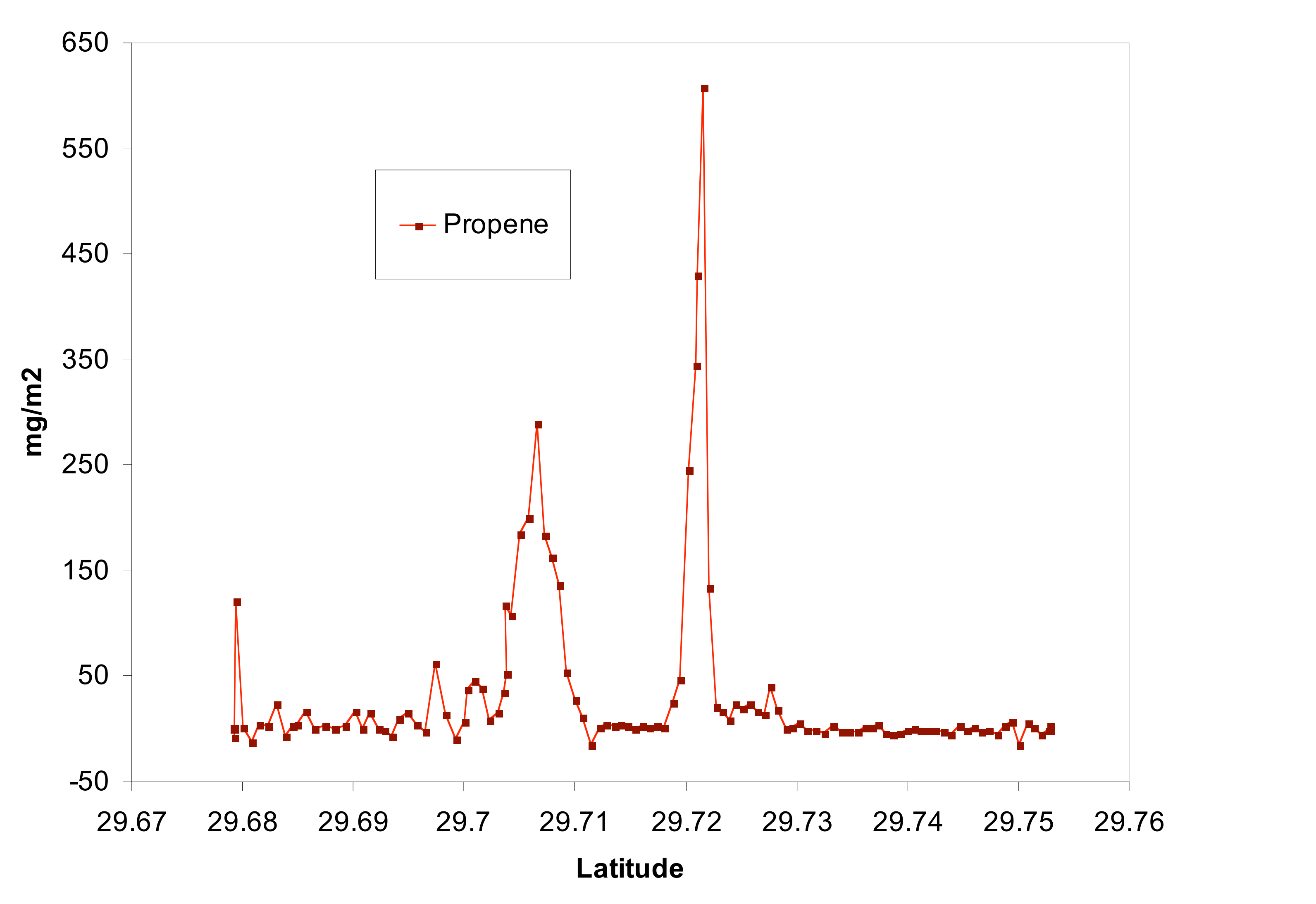
Ethylene mass downwind of HSC measured by SOF on Aug 30 (Measurements in conjunction with Aztec)

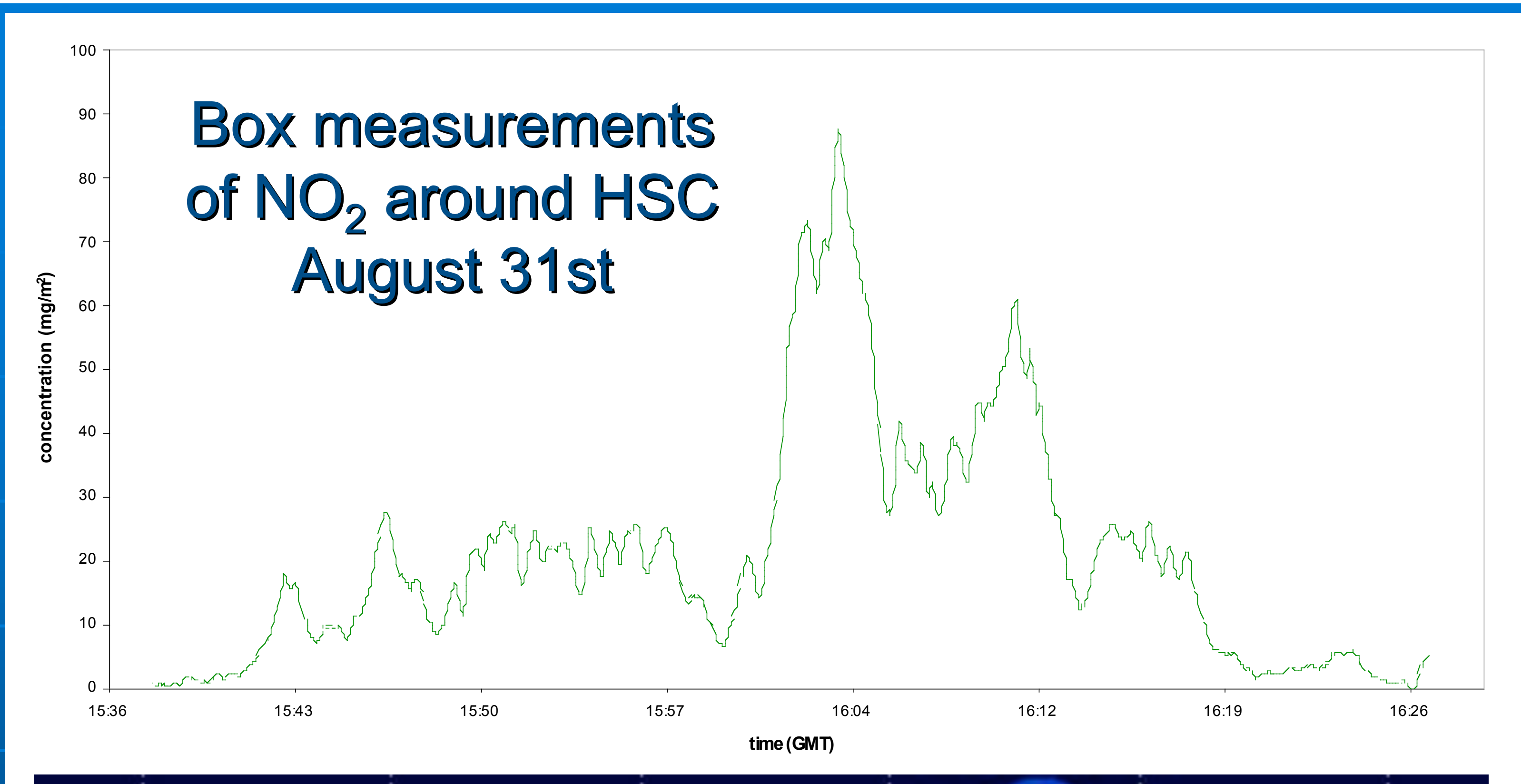


Ethylene mass downwind of HSC measured by SOF on Aug 30 (Measurements in conjunction with Aztec) Log scale

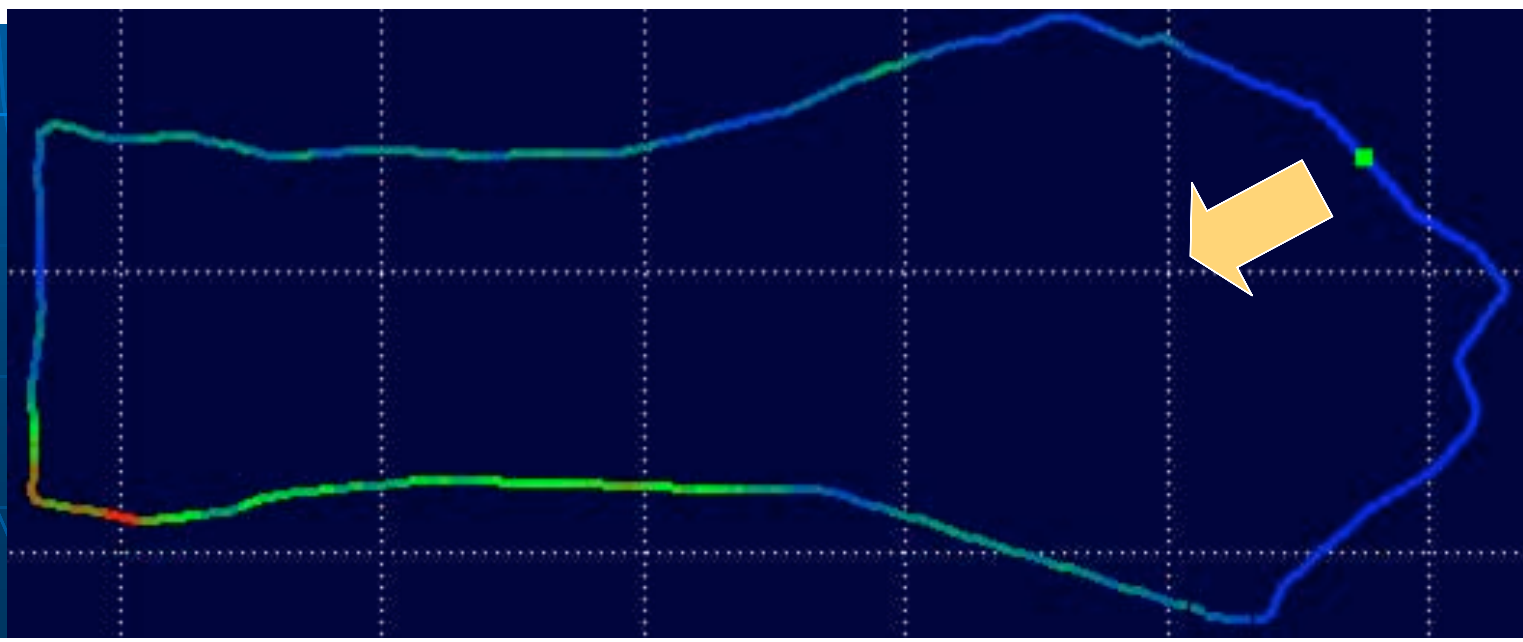


Propene measured by SOF for a N-S traverse from Lynchbury ferry crossing to Laporte airfield (NE wind) Aug 31

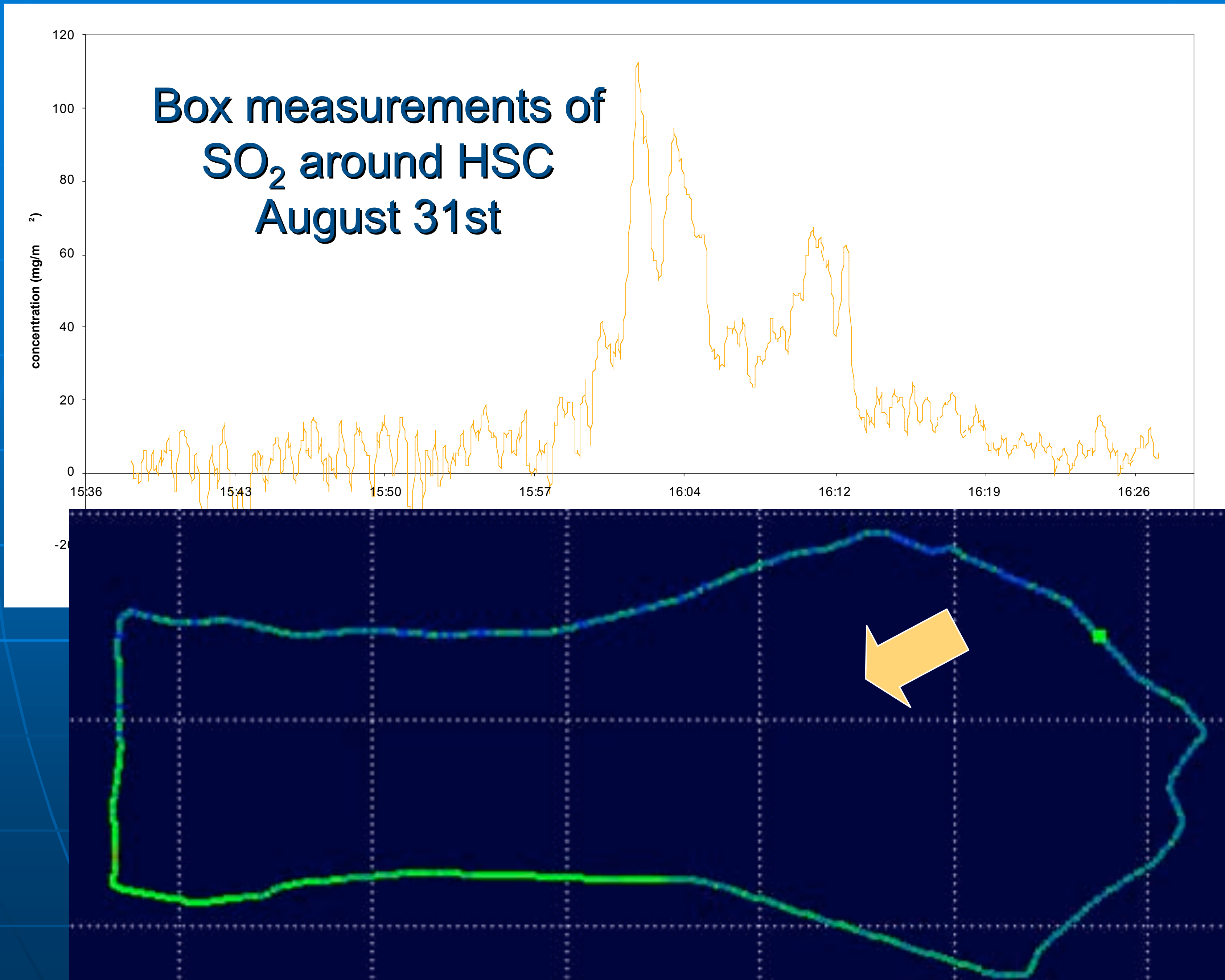




Box measurements of NO_2 around HSC August 31st
100
90
80
70
60
50
40
30
20
10
0
concentration (mg/m²)
15:36
15:43
15:50
15:57
16:04
16:12
16:19
16:26
time (GMT)



Box measurements of SO_2 around HSC August 31st



Plan

- Measurements continue until Oct 2
  - Freeport
  - Choc Bayou
  - HSC-total
  - Joint measurements Aztec (1 flight)+P3
  - Other, possible on site meas
- During the next months spectroscopic retrievals will be conducted of eten, propene, butadiene, NH3, alkanes and formaldehyde

Questions G, H – Regional Background Aerosol: Satellite data

- **Regional and local biomass burning (Brad Pierce)**

North and South American Influences During September 17, 2006 HSRL CALIPSO Validation/Biomass burning Survey

Synthesis of NASA HSRL, MODIS, CALIPSO, AIRS, and NOAA P3 measurements Using Ensemble trajectories, RAQMS and STEM chemical/aerosol analyses

Brad Pierce, Chris Hostetler, Rich Ferrare, John Hair,
Chieko Kittaka, Jassim Al-Saadi
(NASA LaRC)
Youhua Tang and Greg Carmichael
(University of IOWA)
Arlindo da Silva
(NASA GSFC/GMAO)
Chris Schmidt
(CIMSS)

With thanks to
David Winker (NASA LaRC), Wallace McMillan (UMBC), John Holloway (NOAA)
Dirk Richter, Jim Walega, Petter Weibring and Alan Fried (UCAR)
Liam Gumley and Allen Huang (CIMSS), and Lorraine Remer (NASA GSFC)

for providing satellite and insitu data sets used in this analysis

Addressing RSS Science Questions G, H
"Background ozone and aerosol concentrations and the role of regional transport"

Philosophy :

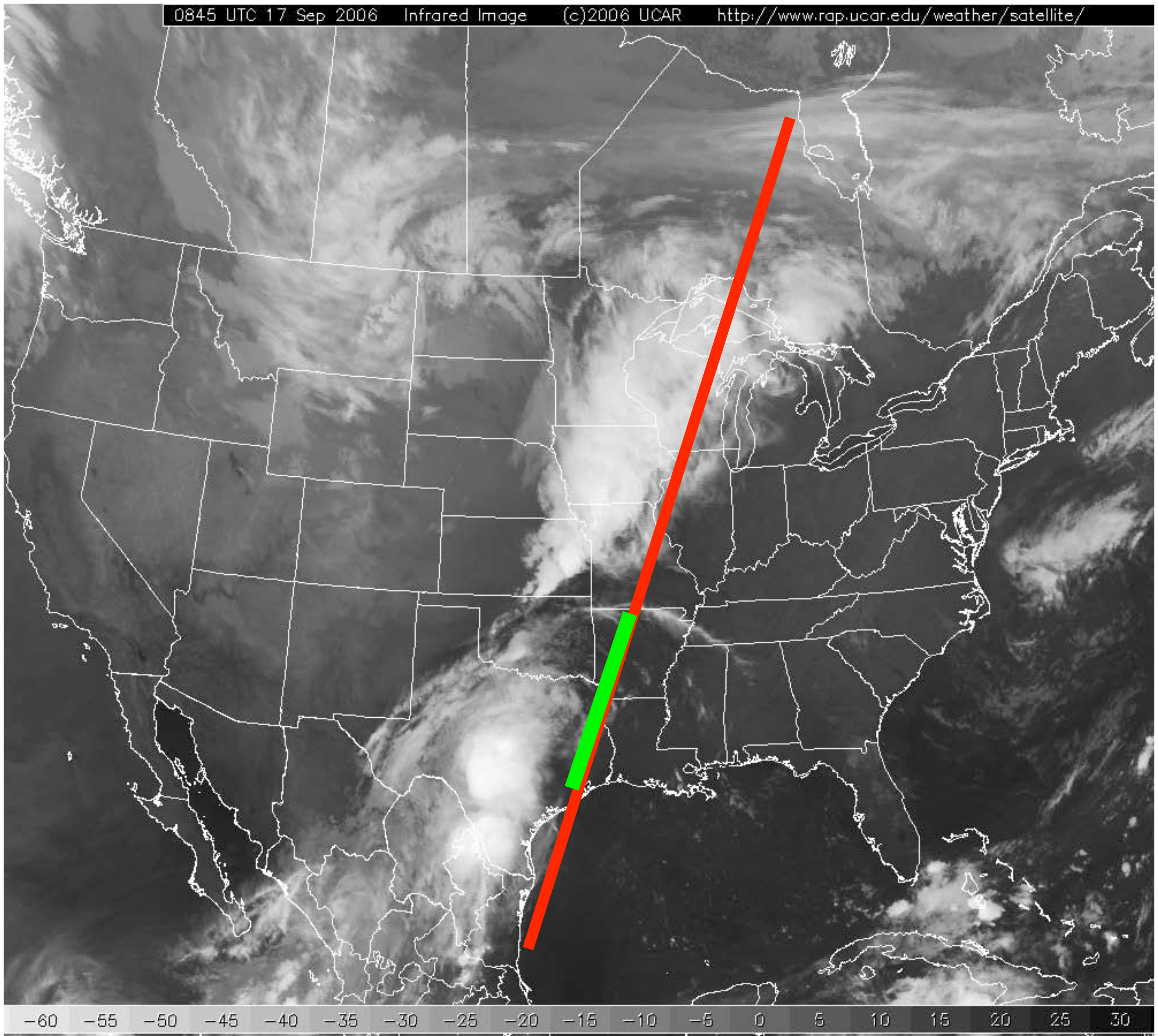
Use chemical/aerosol forecast models and Lagrangian trajectory analysis to link local airborne lidar and insitu observations within receptor regions (Texas) to satellite observations in source regions (CONUS, S. America, etc..)

Approach:

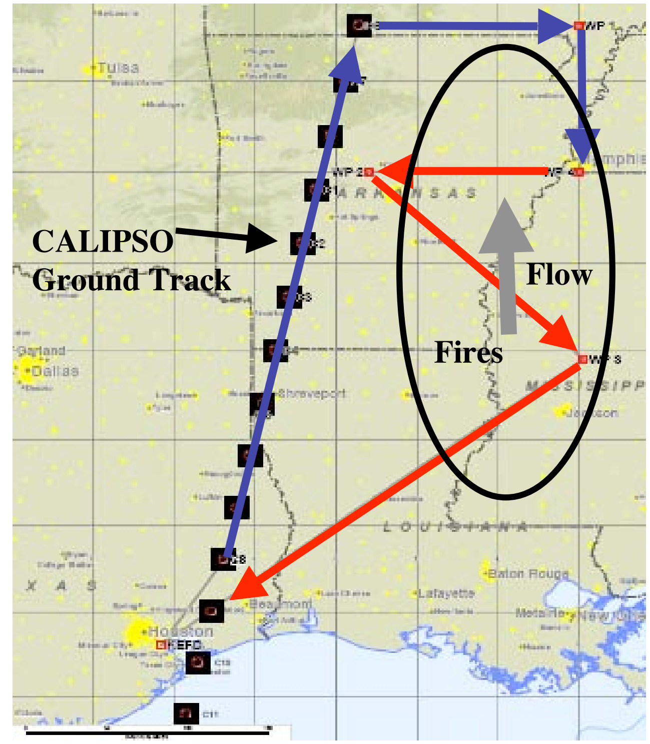
•**<u>Surface and airborne measurements</u>** are used to characterize receptor region and verify model forecasts on local scale
•**<u>Nested (global-to-regional) chemical and aerosol forecast models</u>** are used to provide estimates of background composition
•**<u>Ensemble Lagrangian trajectories</u>** are used to identify remote source regions. Trajectories sample forecasted chemical and aerosol fields to understand chemical transformation during transport.
•**<u>Satellite measurements</u>** are used to quantify source strengths and verify model forecasts on a regional to global scale.

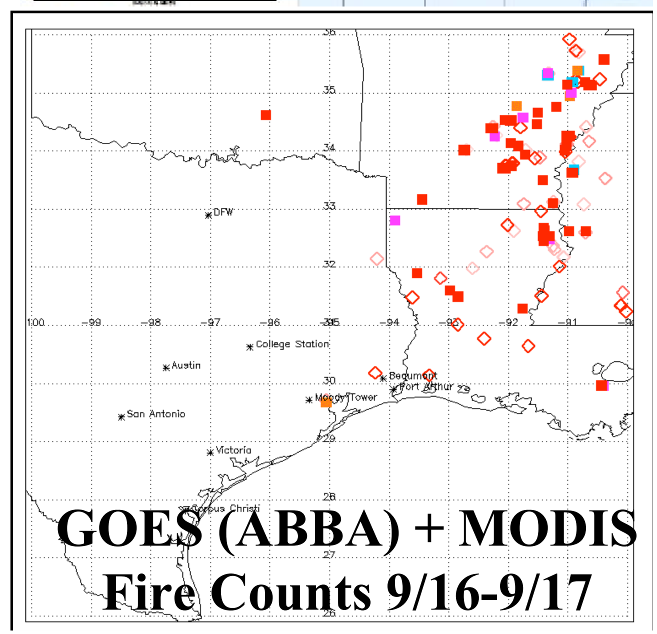
NASA King Air 09/17/06 Objectives:

- CALIPSO validation under-flight
- Raster pattern to sample smoke from fires



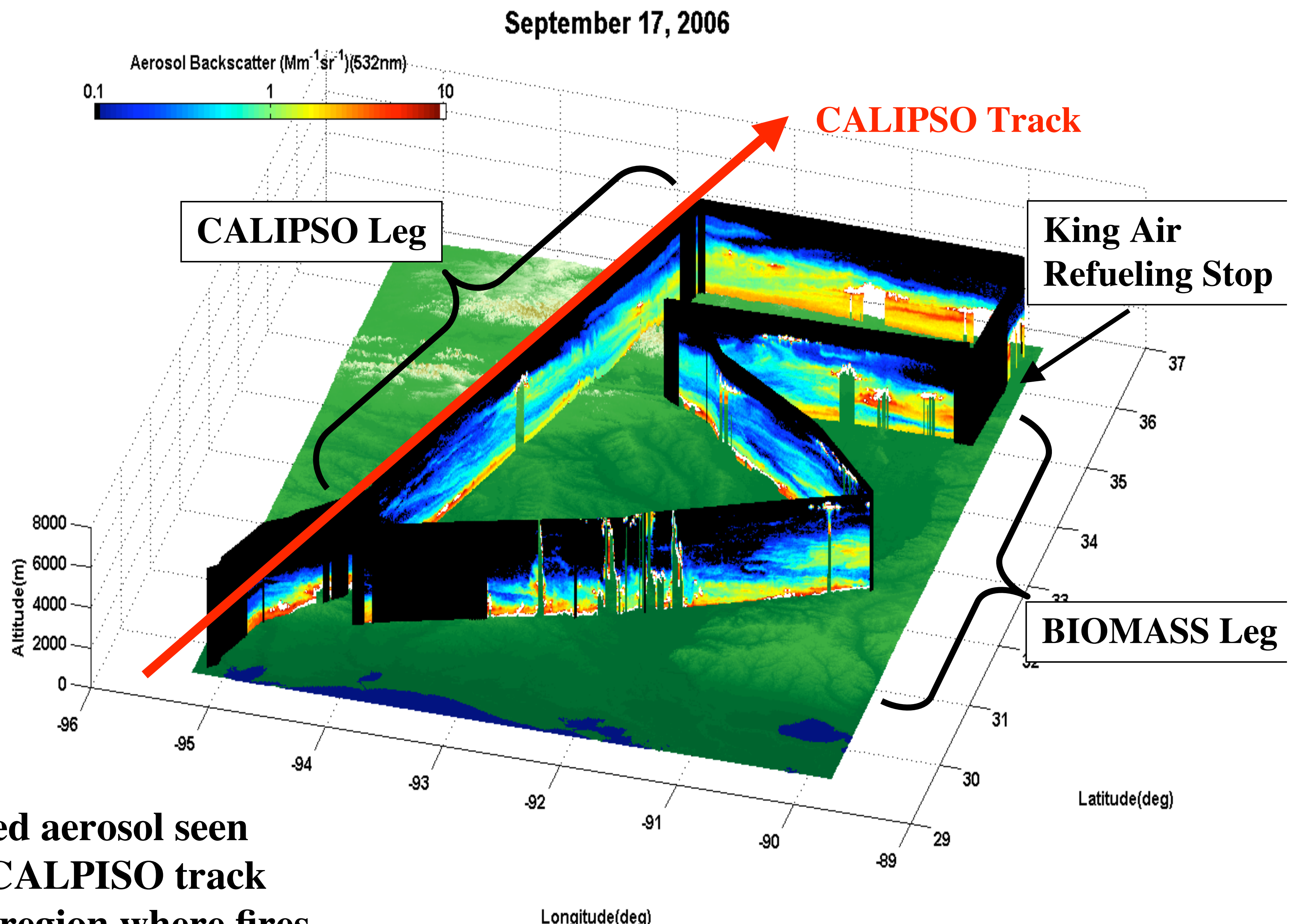
NASA King Air Flight Plan





GOES (ABBA) + MODIS Fire Counts 9/16-9/17

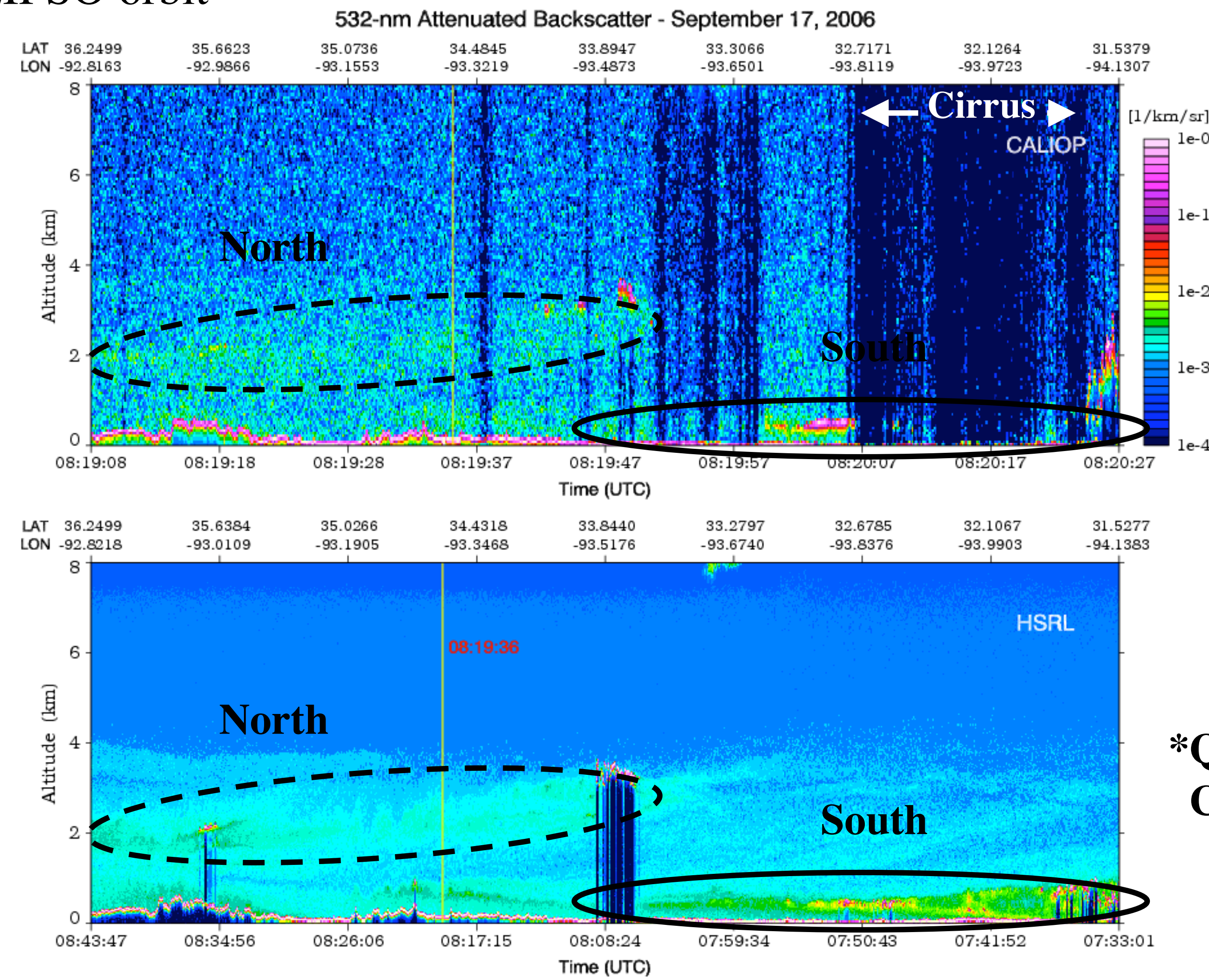
NASA LaRC High Spectral Resolution Lidar (HSRL) Backscatter



Elevated aerosol seen along CALPISO track and in region where fires have been detected.

CALIPSO* validation Leg:

- Both attenuated backscatter measurements show elevated layer of enhanced aerosol on northern portion of CALIPSO leg (dash).
- Aerosol observed by HSRL on southern portion (solid) is obscured by high cirrus along CALIPSO orbit

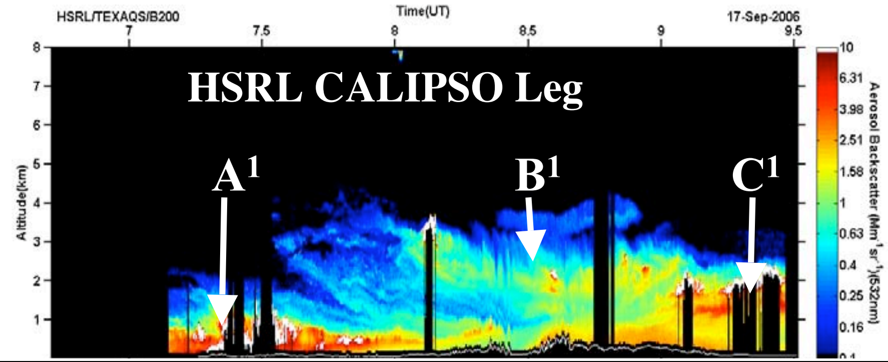


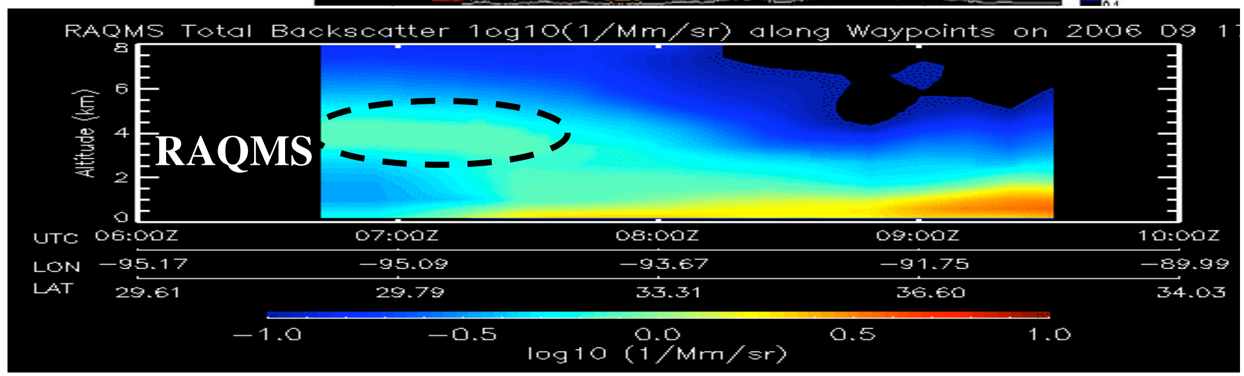
*Quick look CALIPSO data

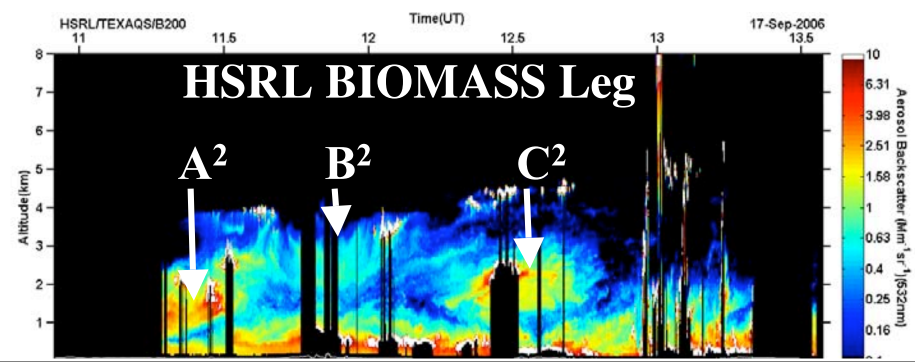
HSRL Model Verification: aerosol backscatter RAQMS$_{regional}$ (80km)

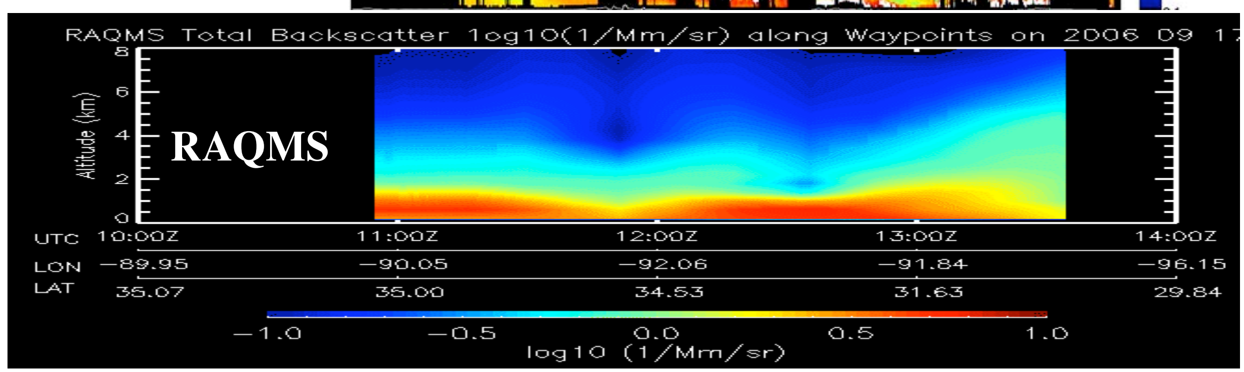
RAQMS provides a good prediction of the magnitude of BL aerosol backscatter, but:

1) misses elevated aerosol suspected of being smoke (B^1, C^1, A^2, B^2, C^2) and BL enhancement near Houston (A^1)
1) predicts elevated aerosol layer at beginning of CALIPSO underflight that is not observed (dash)







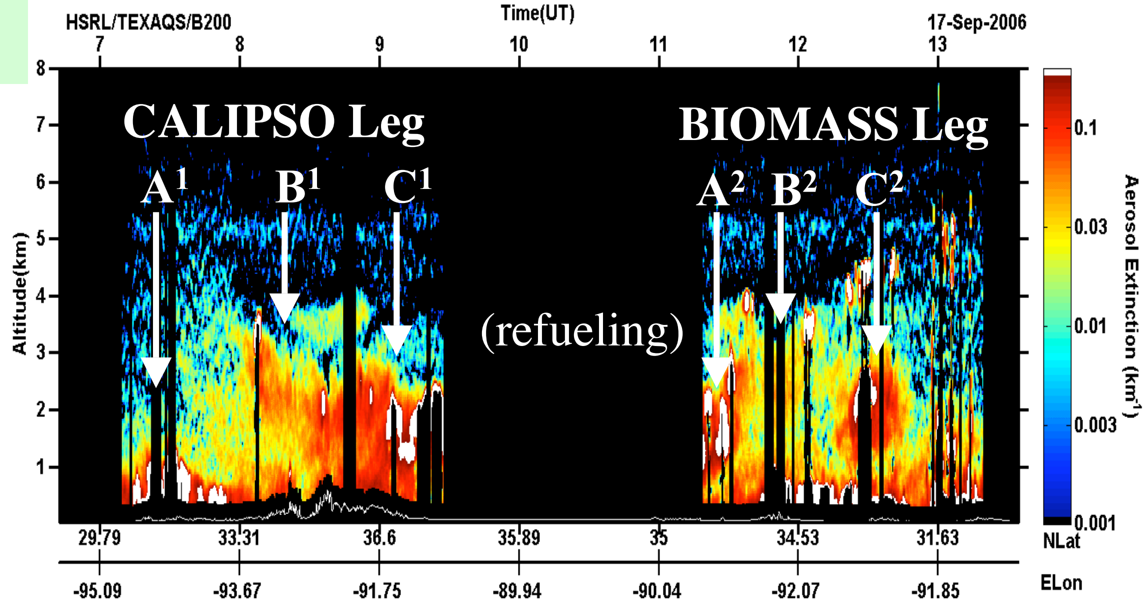


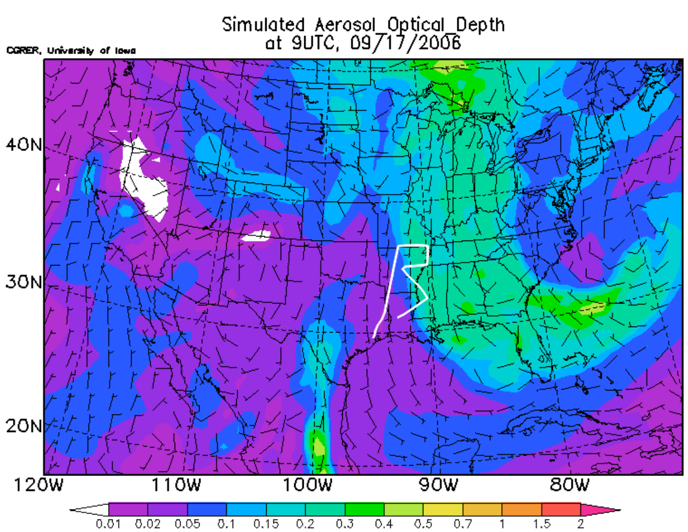
HSRL Model Verification: aerosol extinction STEM (60km)

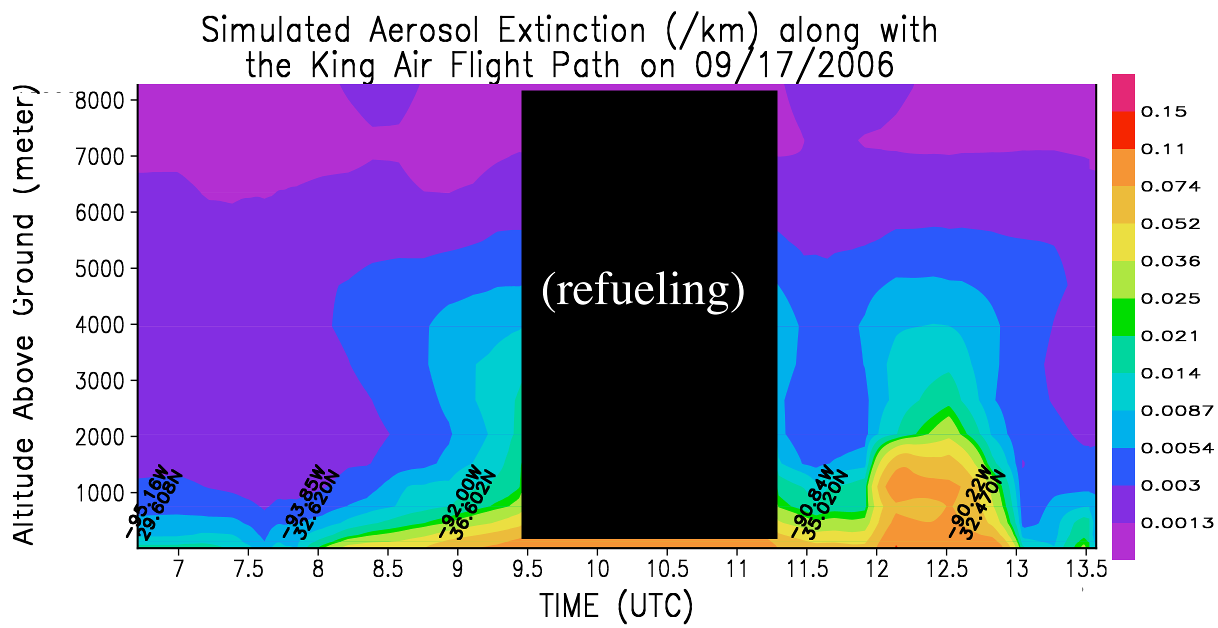
STEM provides a better prediction of elevated aerosols (C^1,A^2,C^2) but:

1) also misses elevated lower backscatter features (B^1,B^2) and aerosol loading near Houston (A^1)
2) underestimates aerosol extinction, particularly above 2 km.

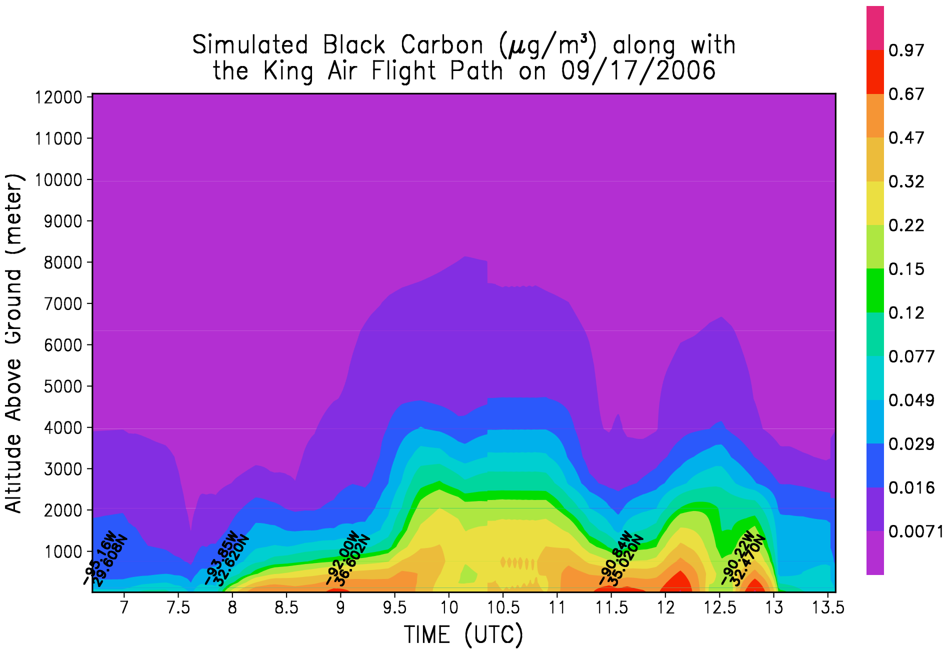
HSRL 532nm Extinction

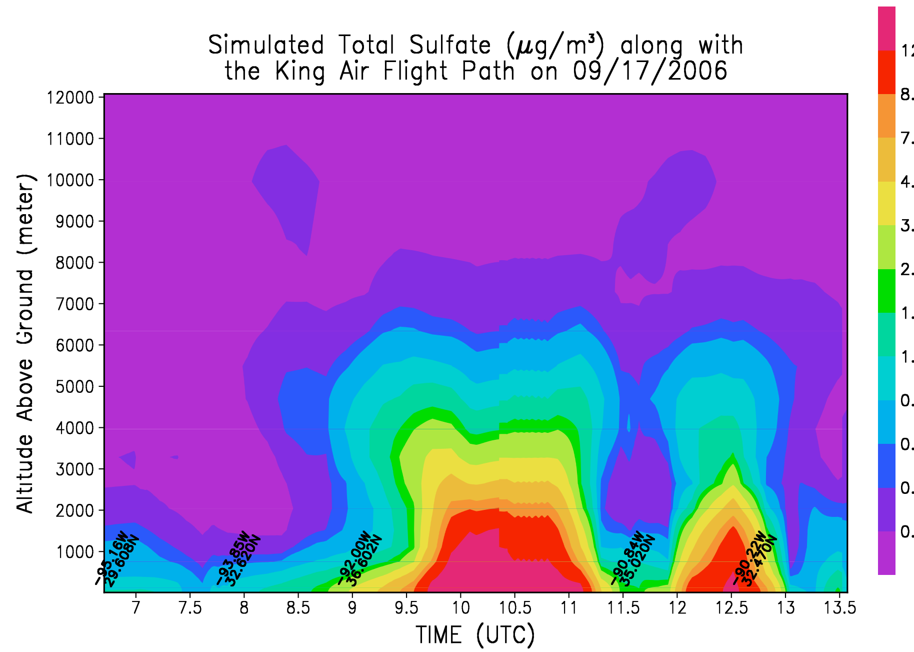




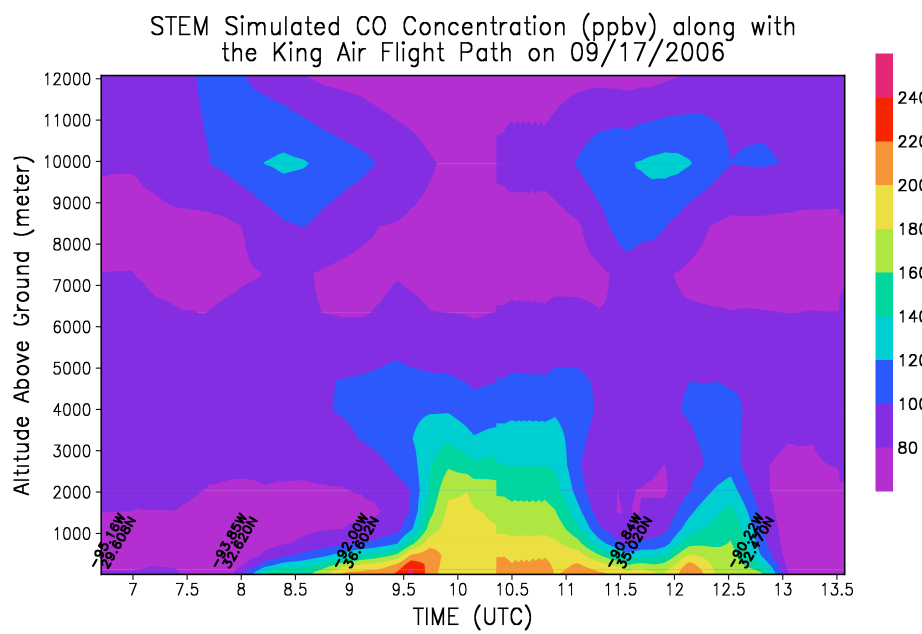


Model predictions provide insight into aerosol composition

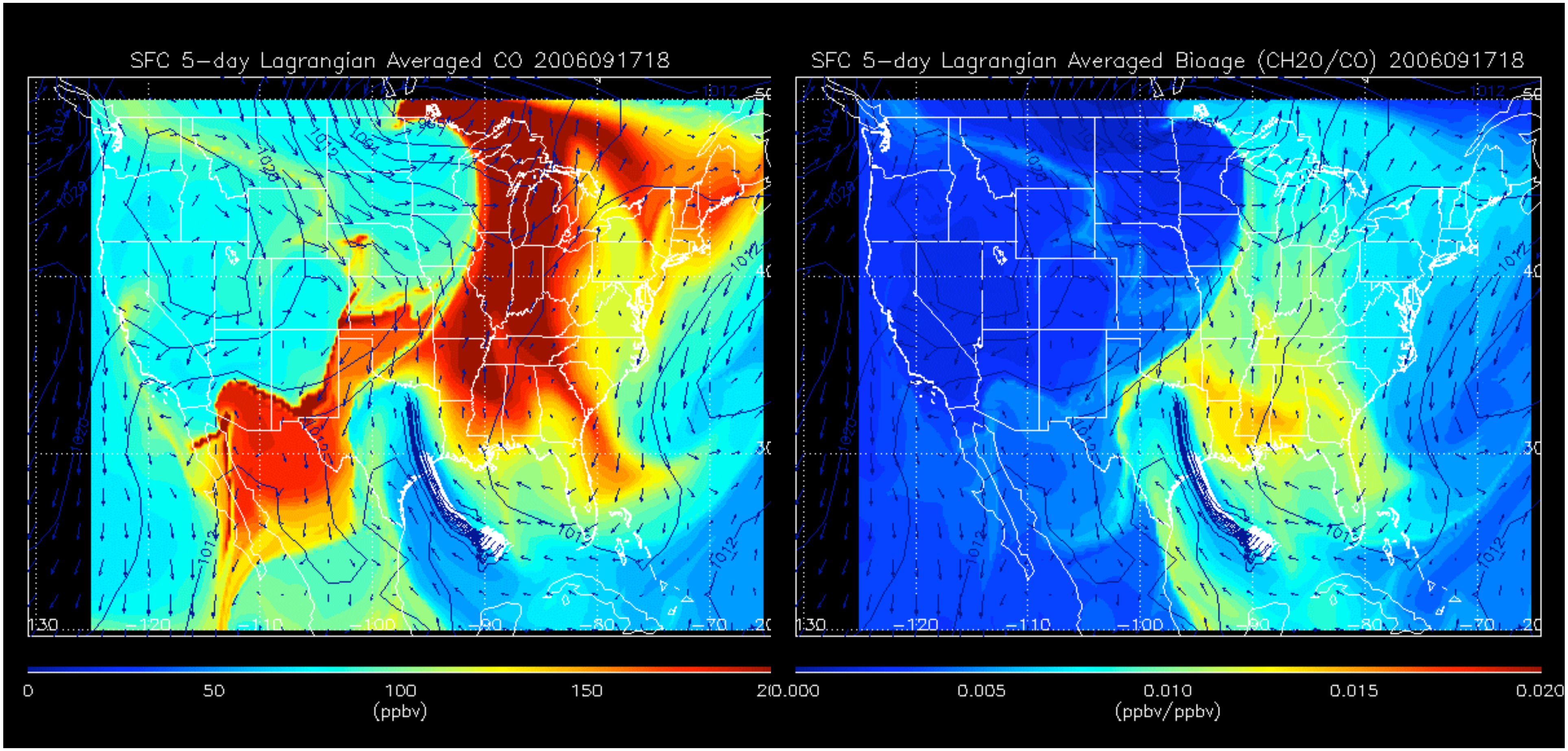




STEM predicts Sulfate/BC aerosol composition with BC component most strongly correlated with CO

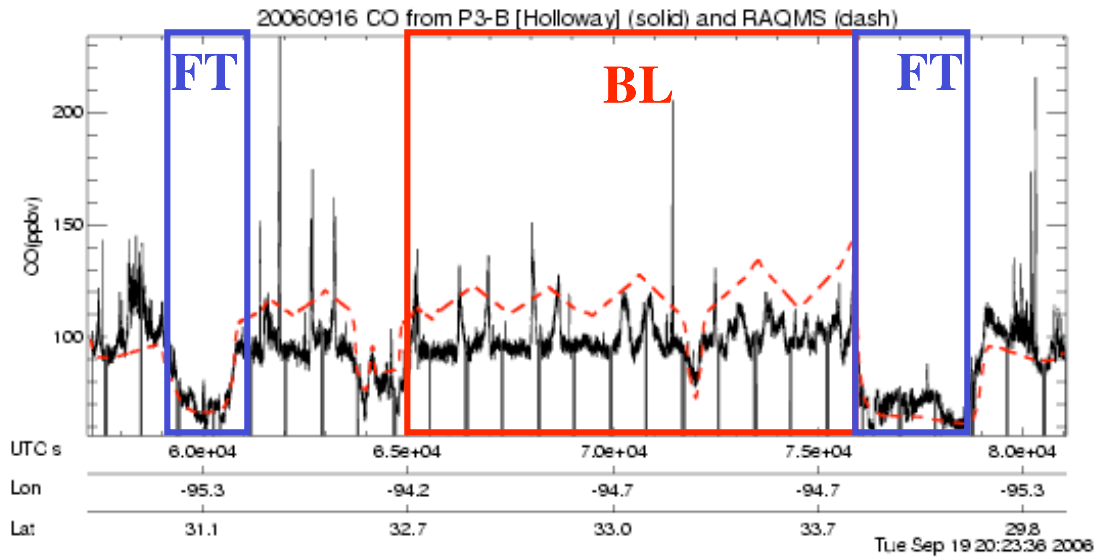


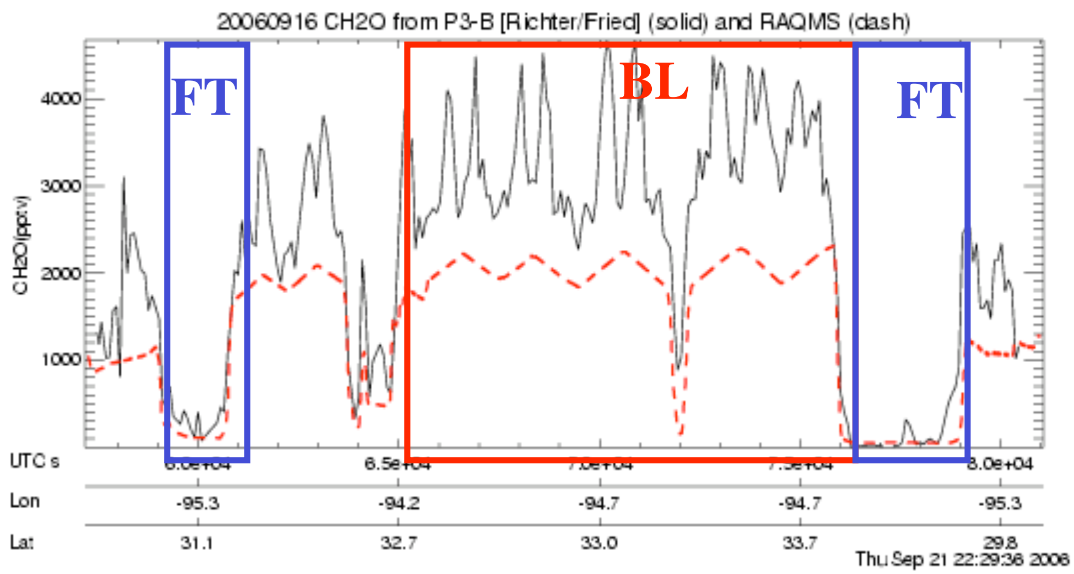
Reverse Domain Filling (RDF) back-trajectories provide insight into time/location of aerosol source region



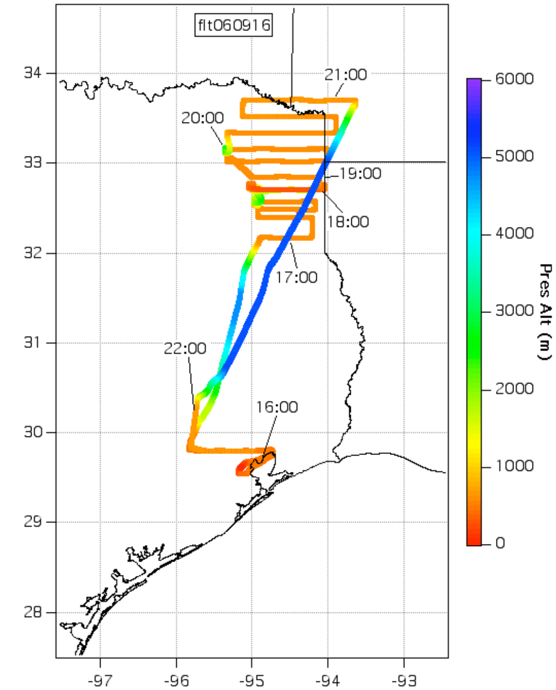
RAQMS$_{global}$ RDF trajectories allow Lagrangian sampling of airmass chemical history (CO emissions, Biogenic age) prior to HSRL observation

P3 Model Verification: CO & CH2O RAQMS$_{global}$ (2^ox2^o)



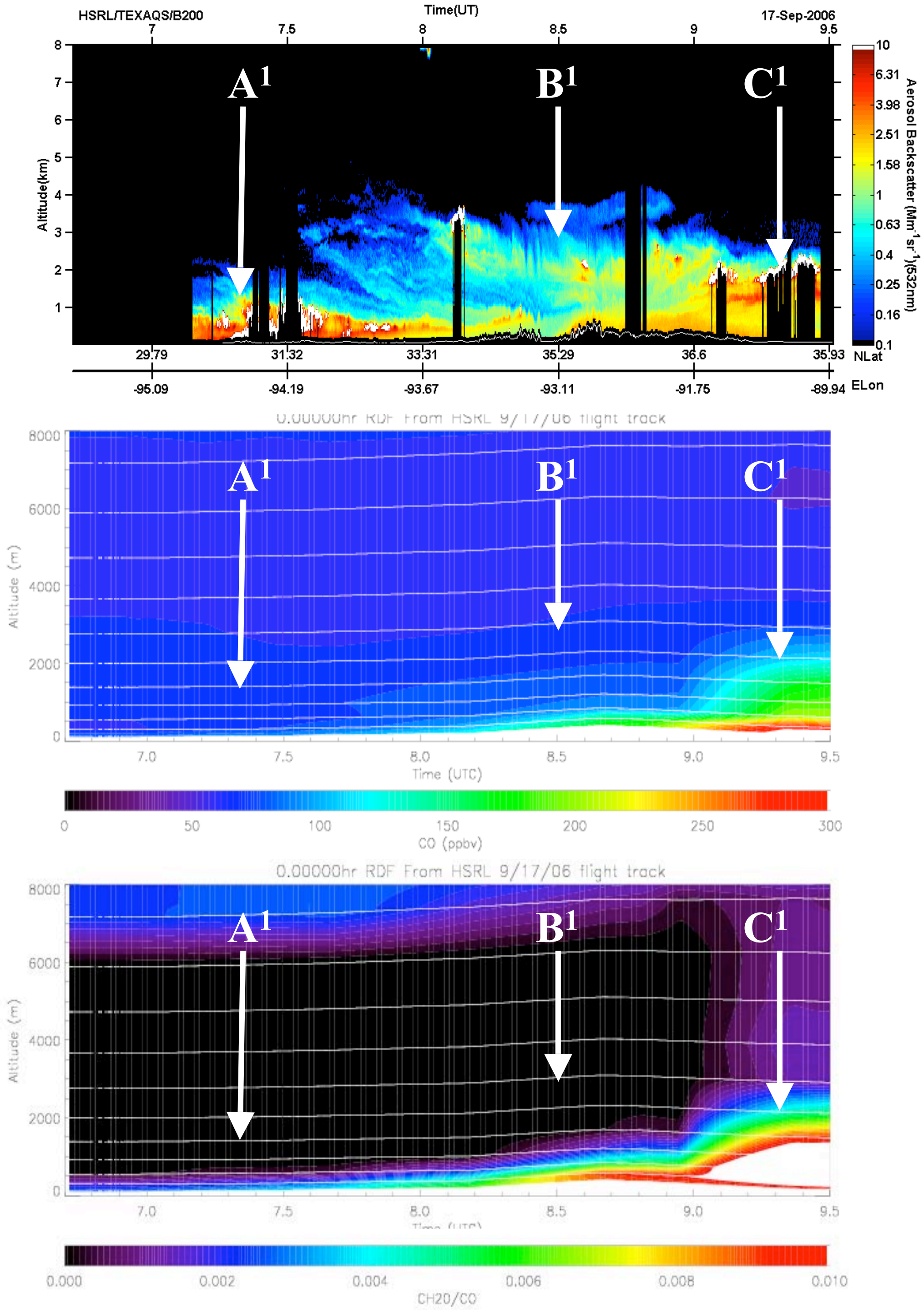


P3 Flight on 9/16



1. point sources not explicitly represented in model
2. free tropospheric (FT) CO and CH2O predictions are in good agreement with P3
3. overestimates (underestimates) CO (CH2O) in boundary layer (BL) => "old" bias in biogenic age (CH2O/CO)

HSRL CALIPSO Leg



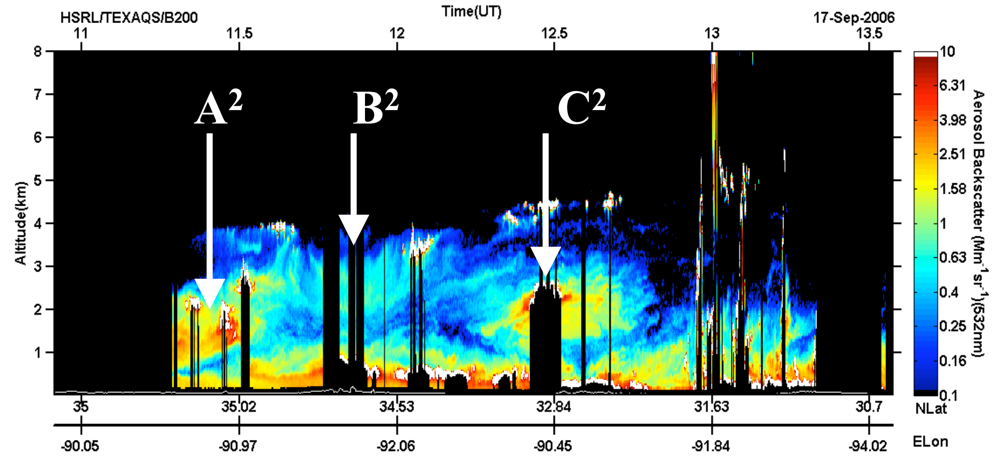
Model CO and CH2O/CO provide information on "age" of aerosols

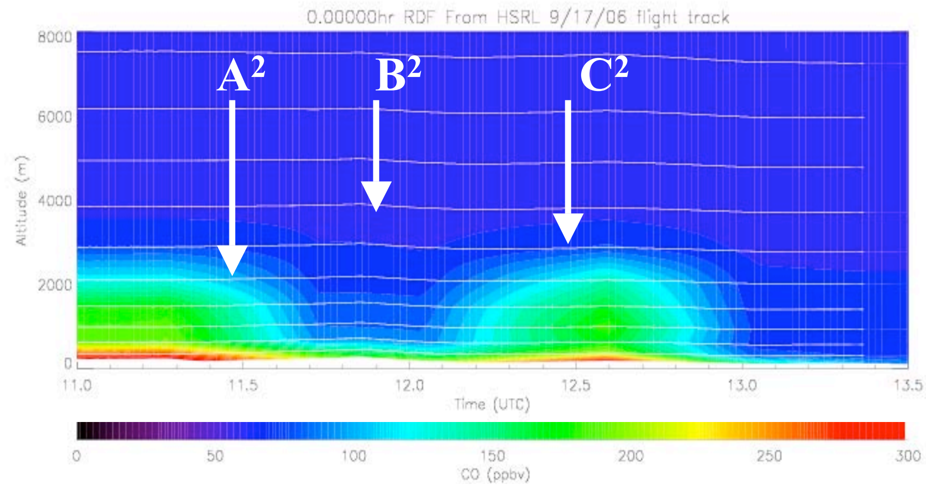
$\mathrm{RAQMS}_{\mathrm{global}}$ indicates fresh (high CH2O/CO) emissions at C^1 and background CO within aged aerosol (low CH2O/CO) at A^1 and B^1

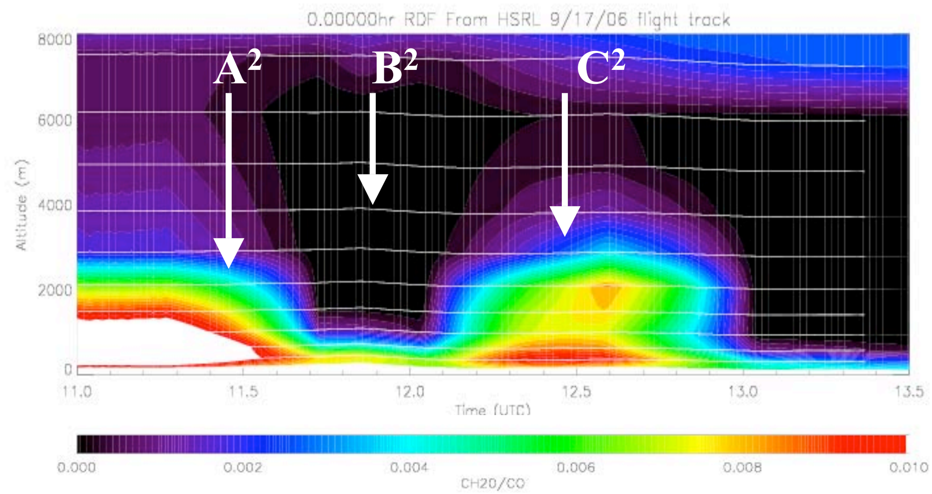
HSRL BIOMASS Leg

Model CO and CH2O/CO provide information on “age” of aerosols

RAQMS$_{global}$ indicates fresh (high CH2O/CO) emissions at A^2 and C^2 with background CO within aged aerosol (low CH2O/CO) at B^2



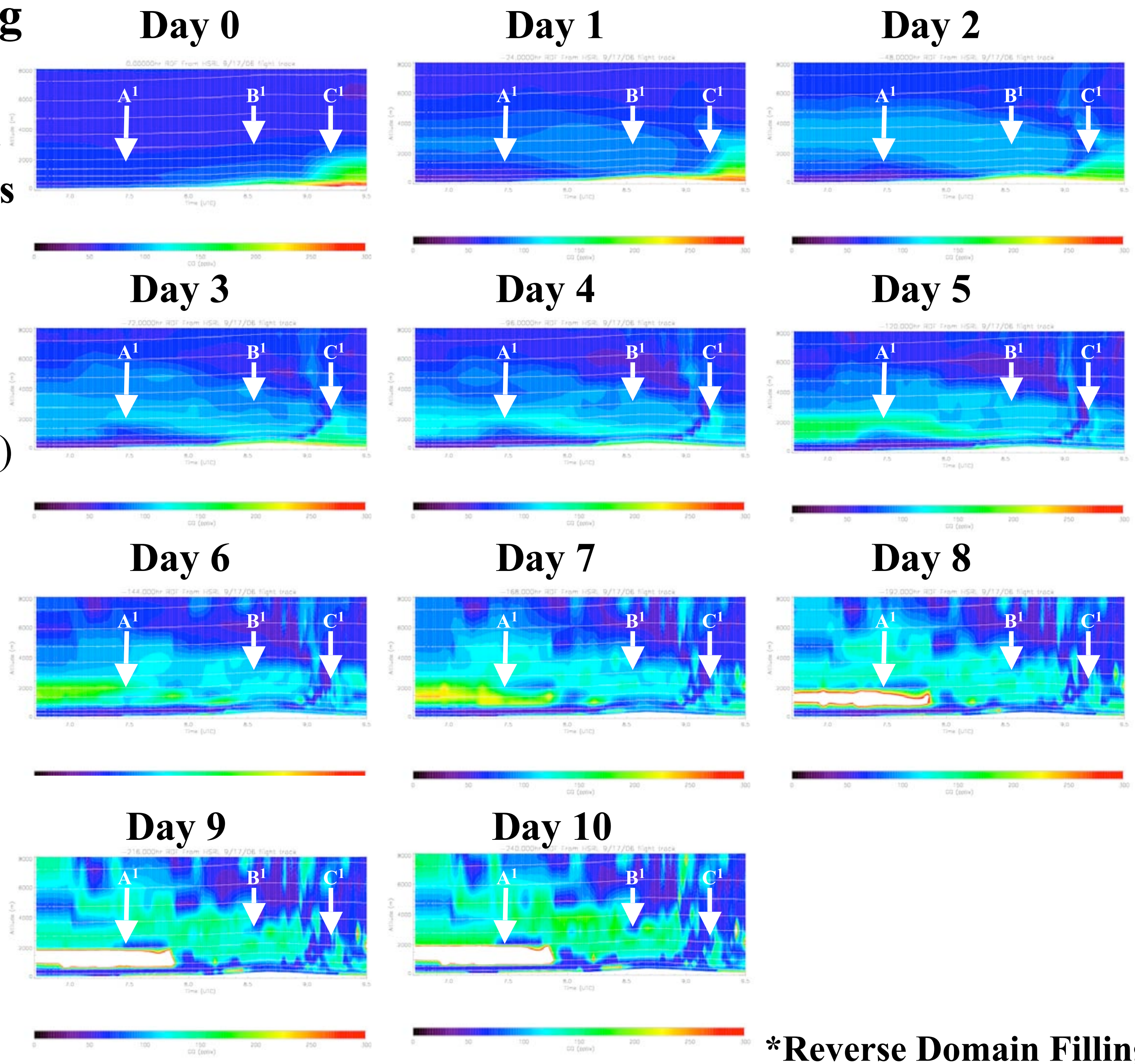




CALIPSO Leg

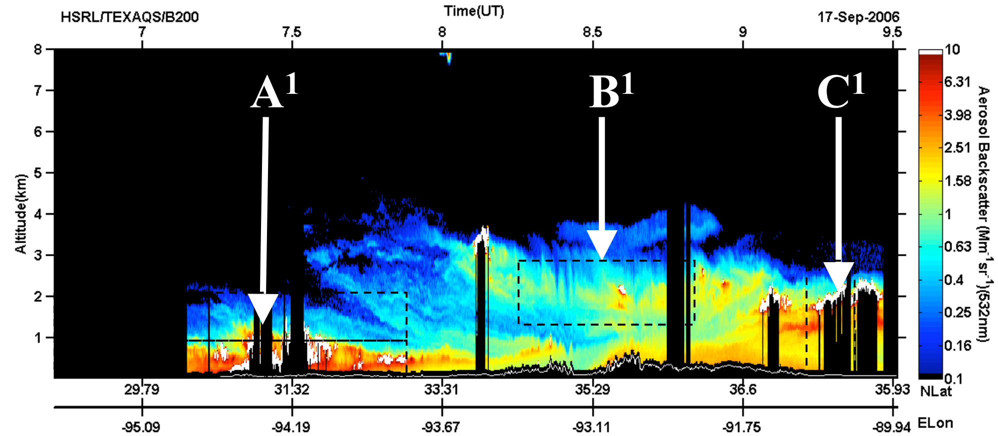
RAQMS RDF*
CO along HSRL
Back-trajectories

Significant CO enhancement near Houston (A[1]) and aloft (B[1]) at 09/07/06 (10 days back)

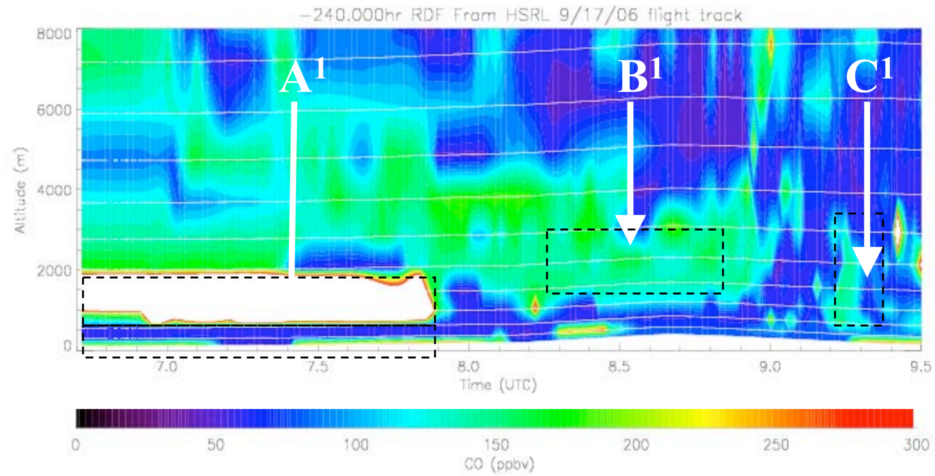


***Reverse Domain Filling**

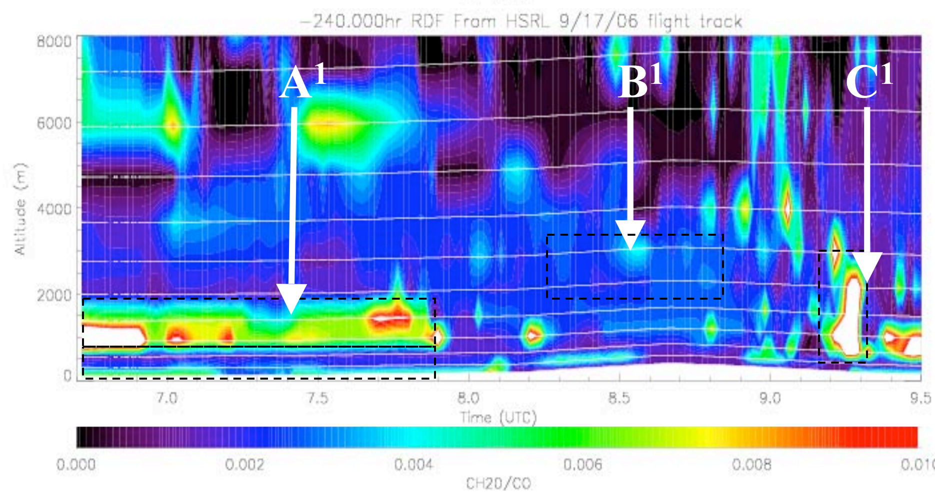
CALIPSO Leg



RAQMS$_{global}$ 10-day RDF Back-trajectory:



RDF analysis shows 10-day old source of fresh emissions (high CO, high CH2O/CO) at points A[1] (1-2km and 0-0.5km) and C[1].



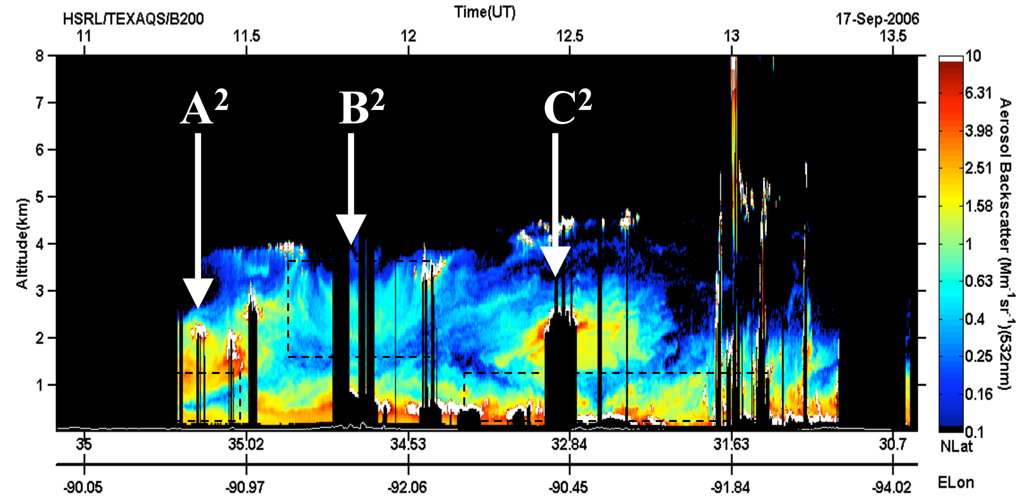
RDF analysis shows 10-day old pollution (elevated CO, moderate CH2O/CO) at point B[1].

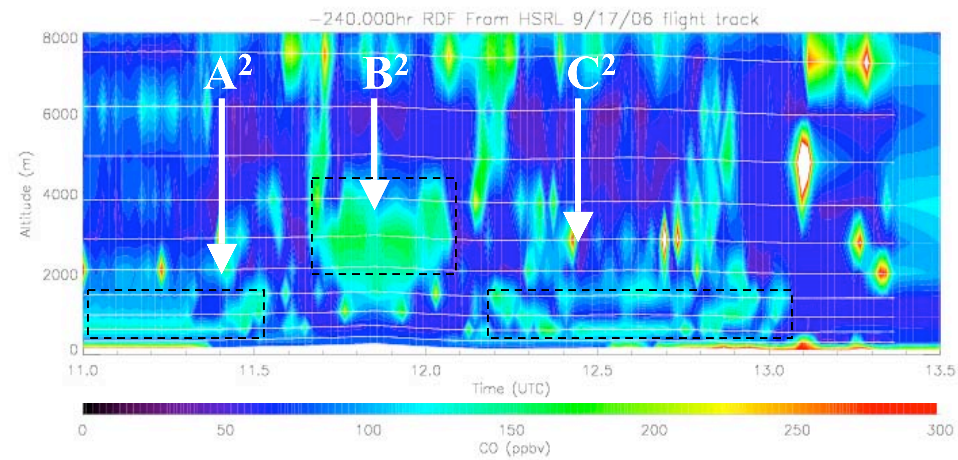
HSRL BIOMASS Leg

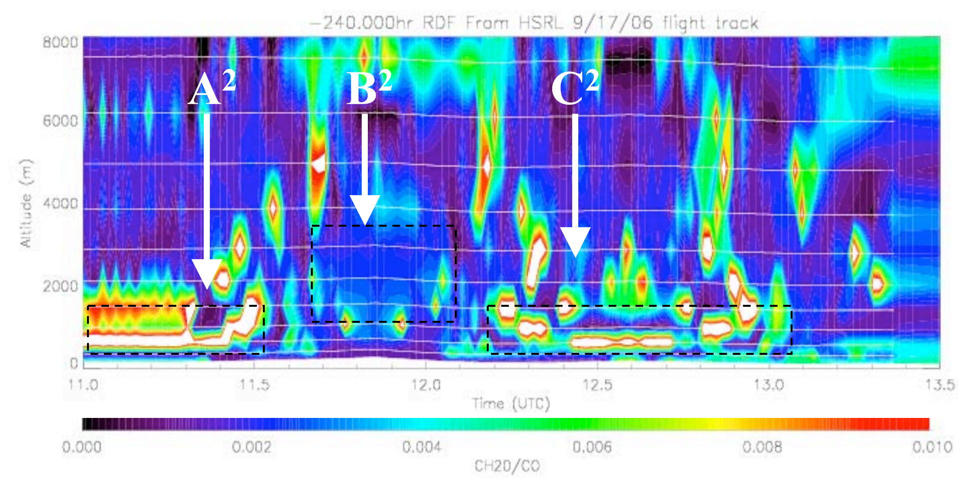
RAQMS$_{global}$ 10-day RDF Back-trajectory:

RDF analysis shows 10-day old source of fresh emissions (elevated CO, high CH2O/CO) in boundary layer at points A^2 and C^2.

RDF analysis shows 10-day old pollution (elevated CO, moderate CH2O/CO) at point B^2.

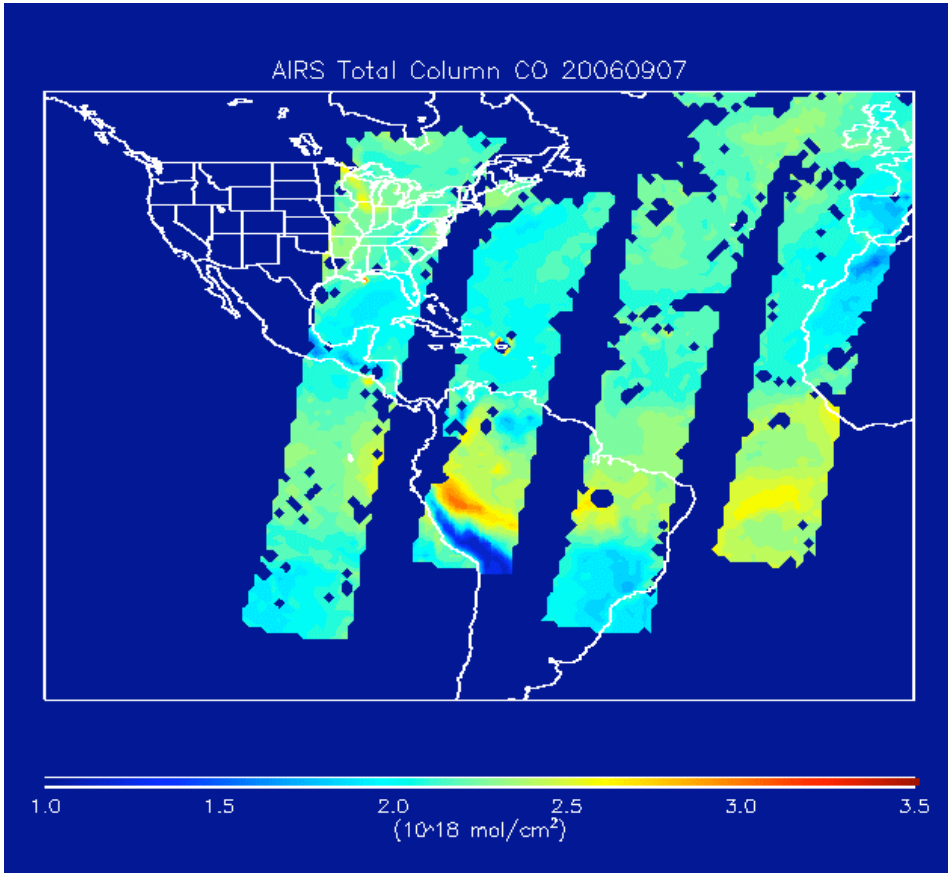


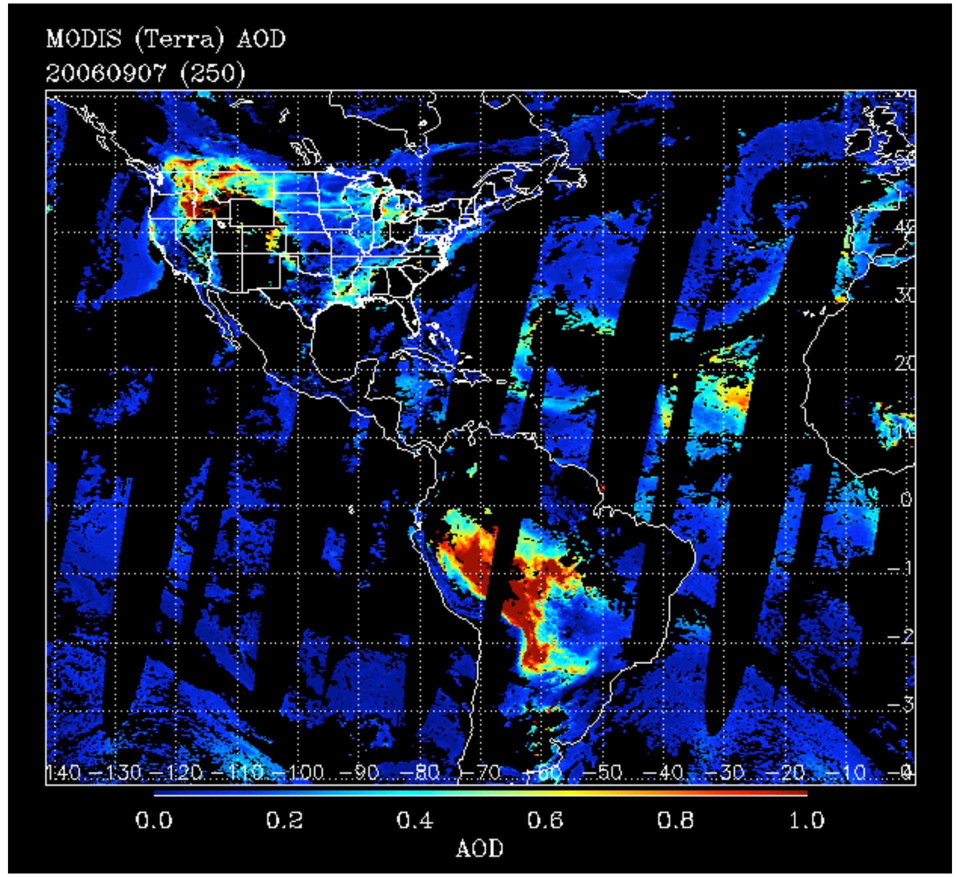




AIRS Column CO and MODIS AOD on 09/07/06

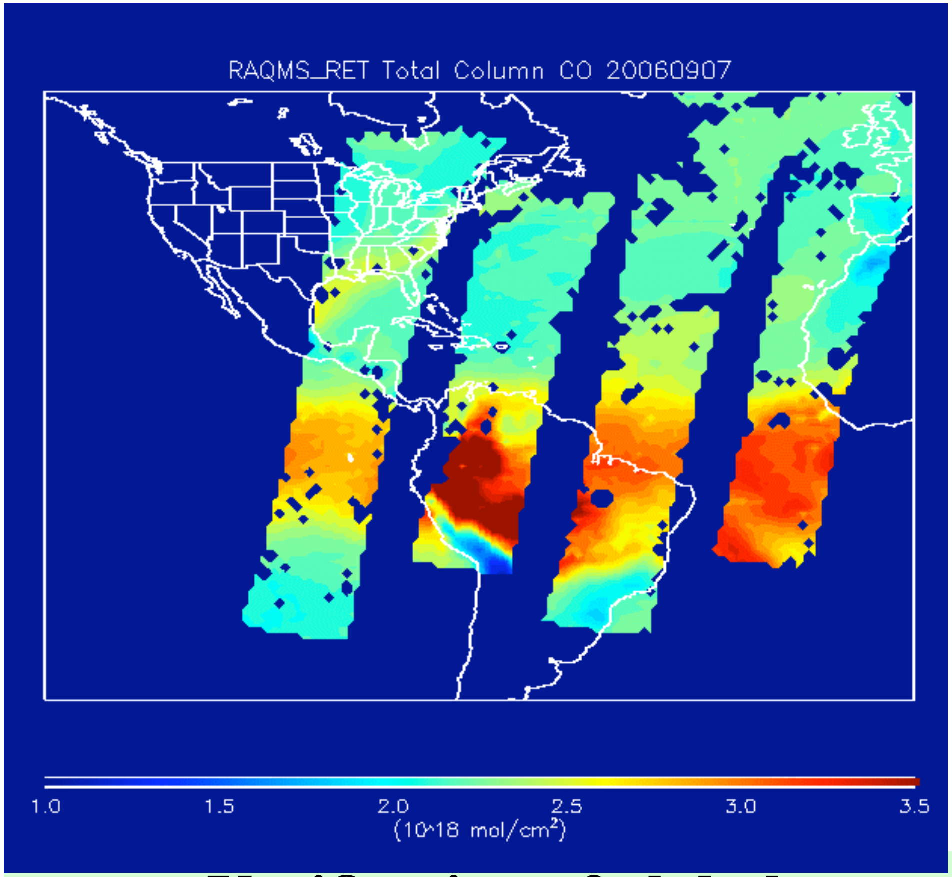
(10-days prior to local HSRL observations)

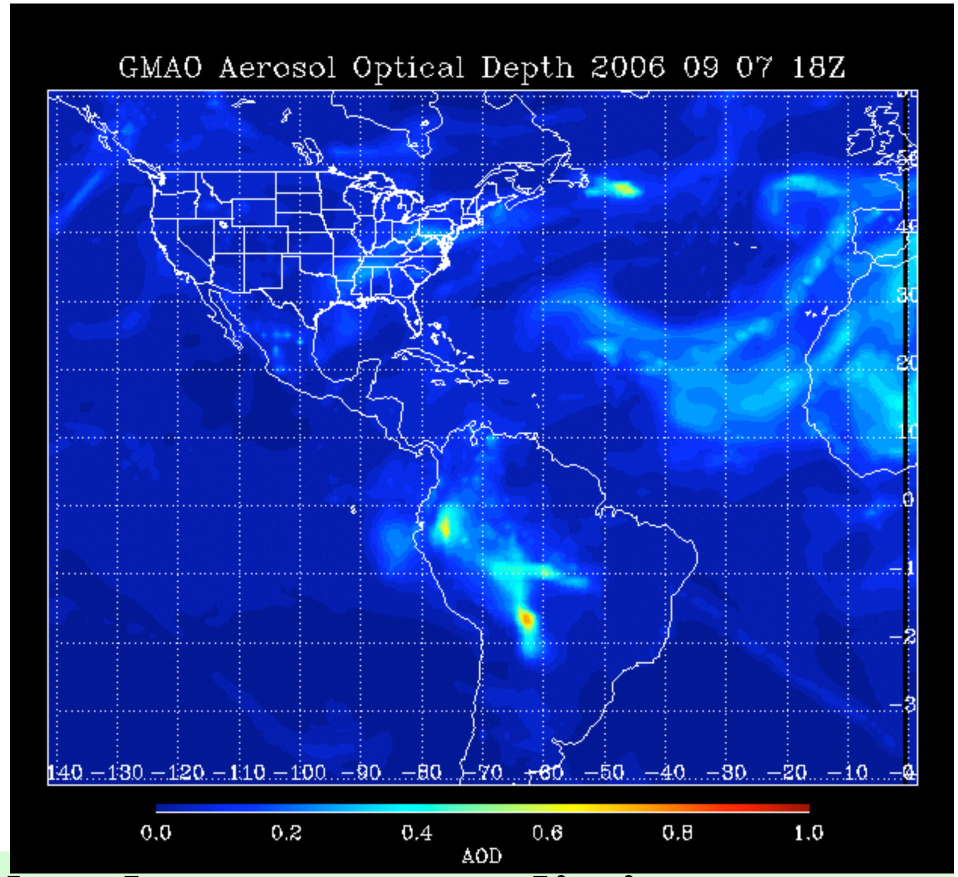




Satellite data provides constraints on aerosol and trace-gas composition in remote source regions.

RAQMS$_{retrieved}$ Column CO and GMAO AOD on 09/07/06
(10-days prior to local HSRL observations)

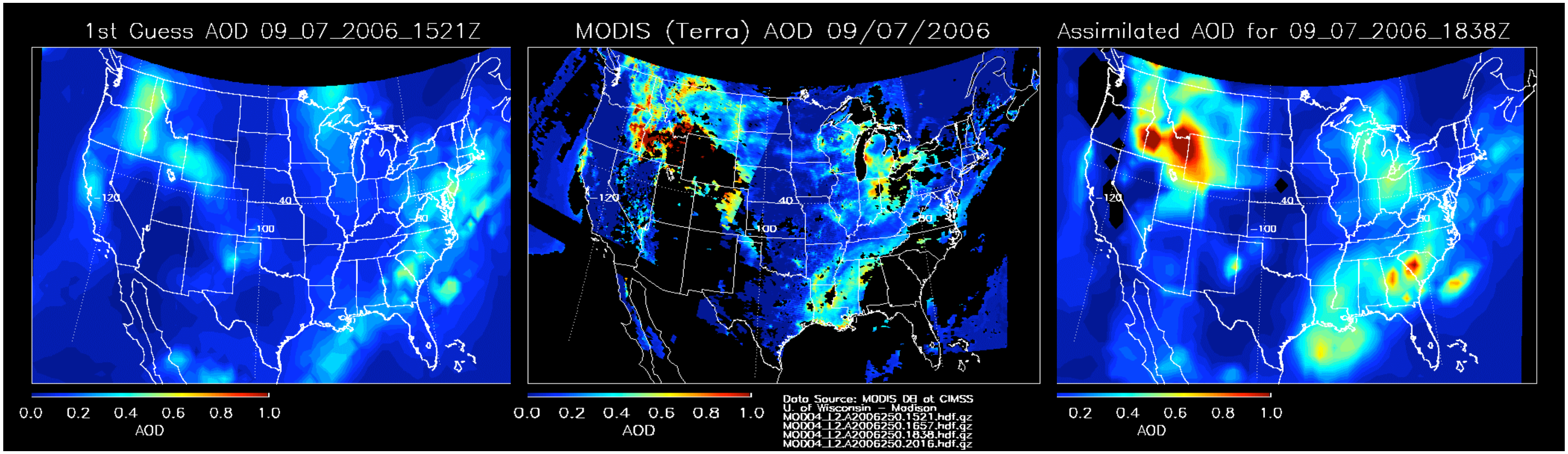




Verification of global aerosol and trace-gas predictions:

- RAQMS overestimates CO column over S. America and Gulf Coast
- GMAO underestimates AOD over S. America and Pacific NW
- Models utilize NRT biomass burning emissions that are under development and have large uncertainties

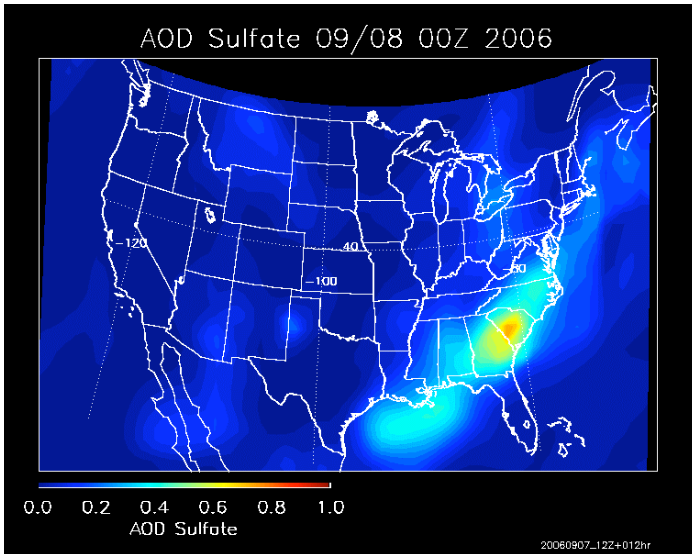
RAQMS$_{regional}$ MODIS AOD Assimilation cycle 09/07/06

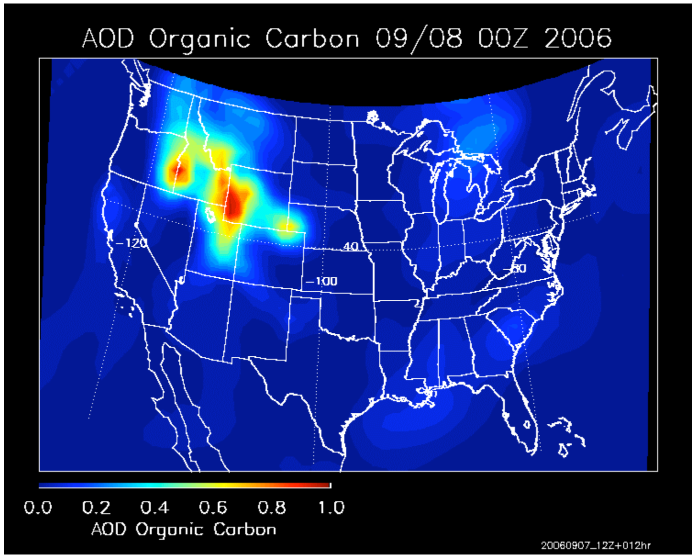


MODIS AOD assimilation constrains total AOD

RAQMS$_{regional}$ First Guess determines composition

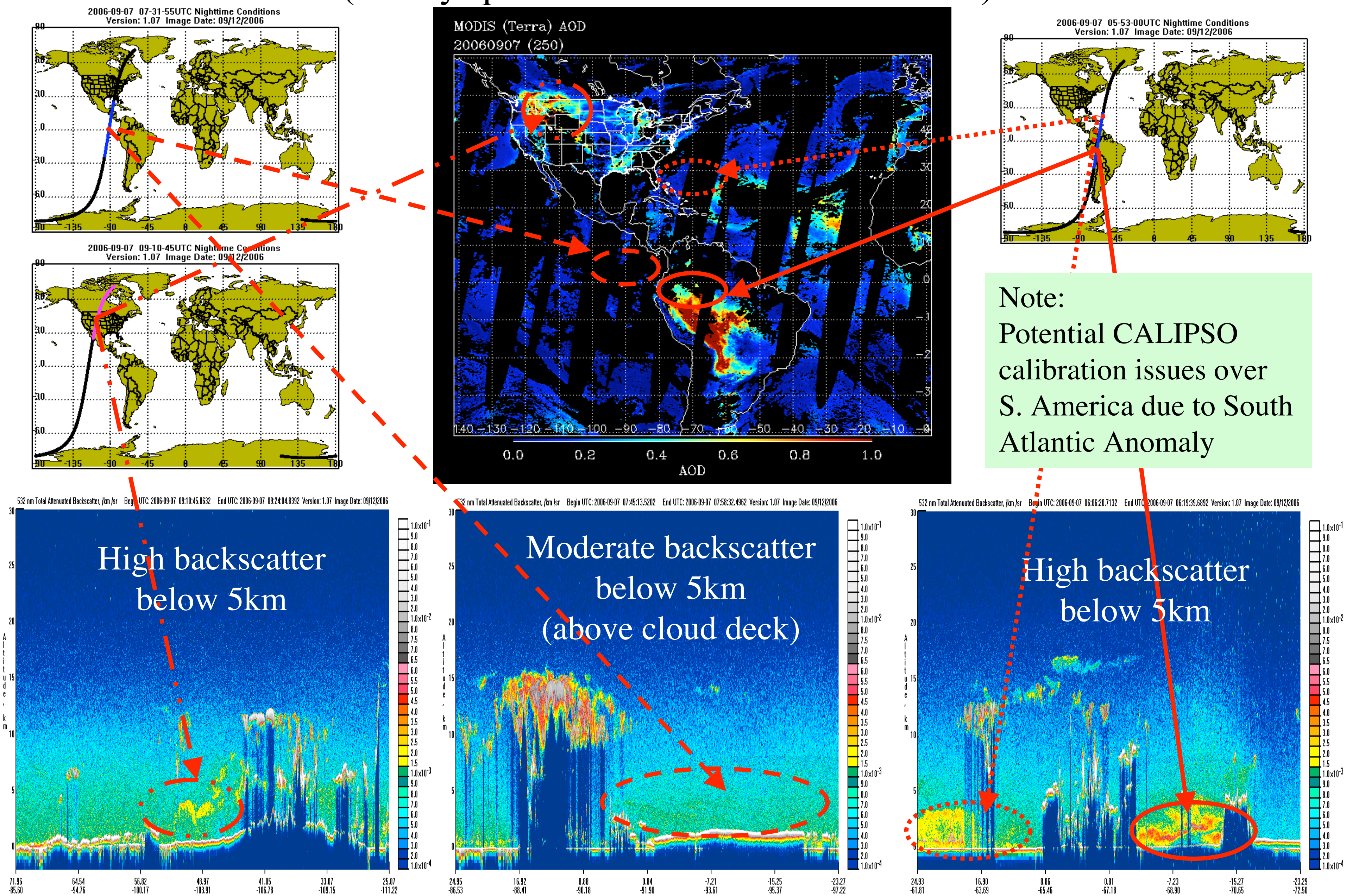
Results in improved estimate of NW biomass and SE sulfate aerosol distributions



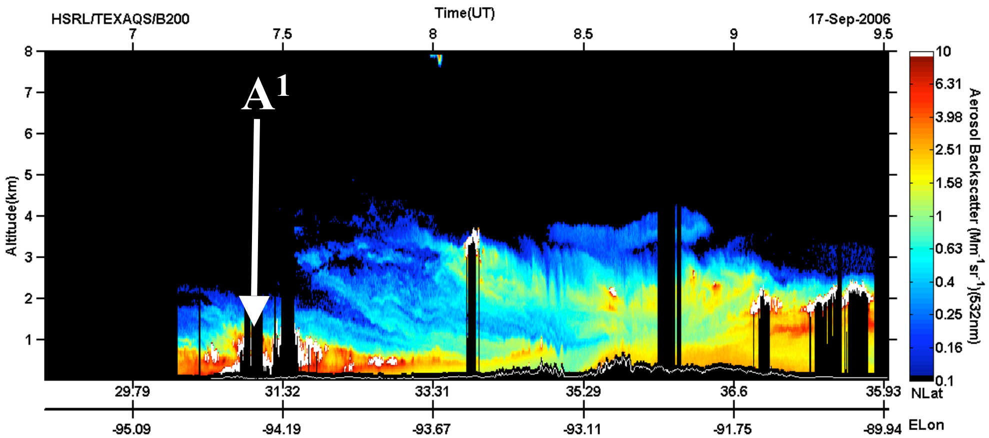


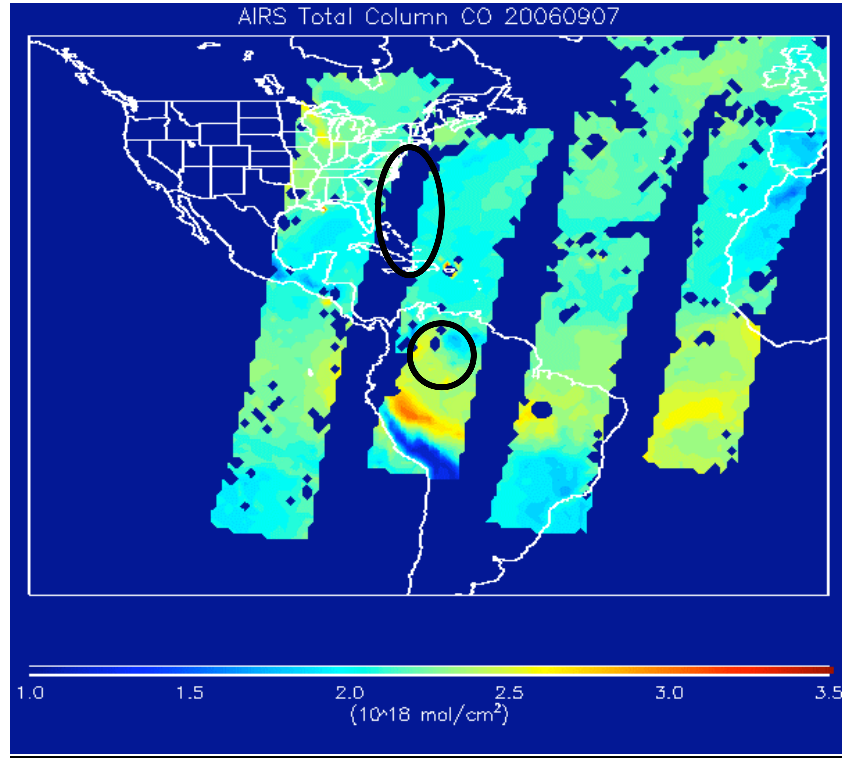
CALIPSO Attenuated Backscatter measurements on 09/07/06

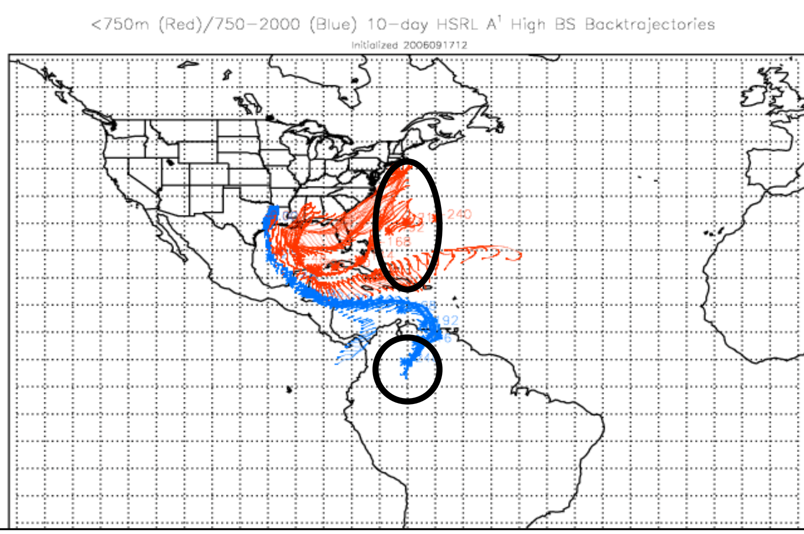
(10-days prior to local HSRL observations)

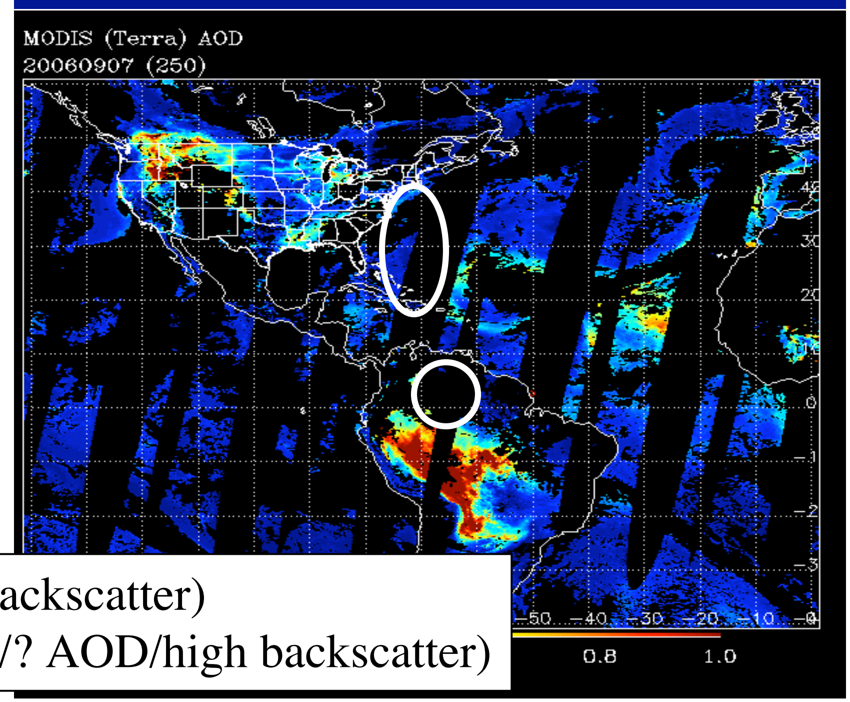


RDF back-trajectories link HSRL CALIPSO Leg to AIRS, MODIS, and CALIPSO measurements



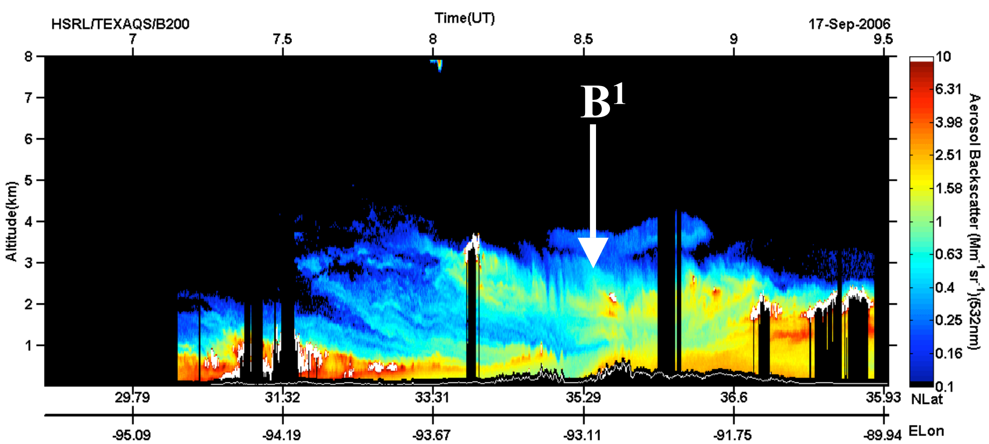


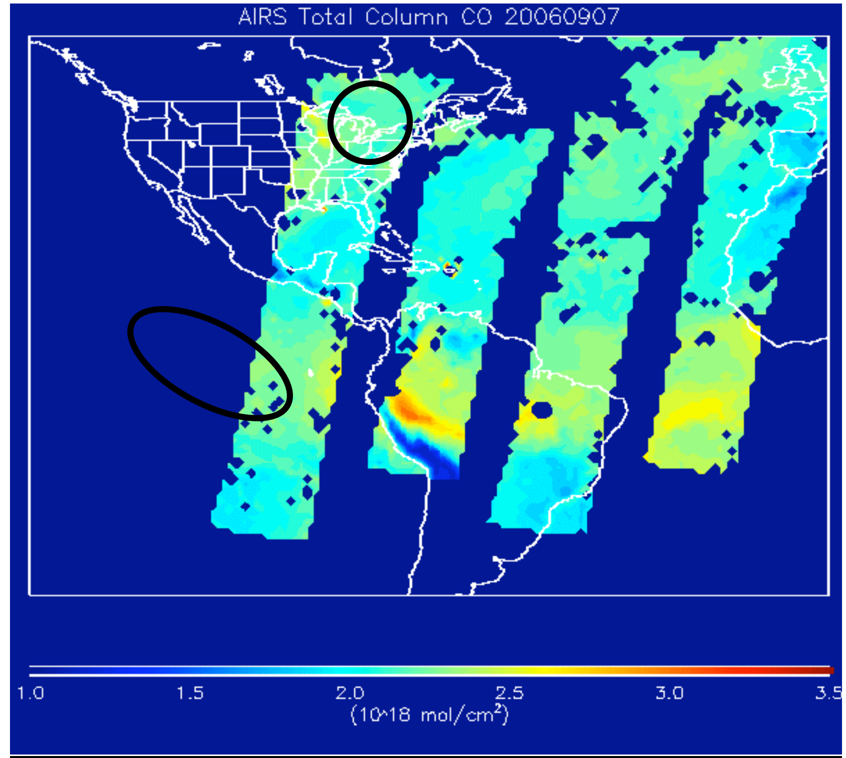


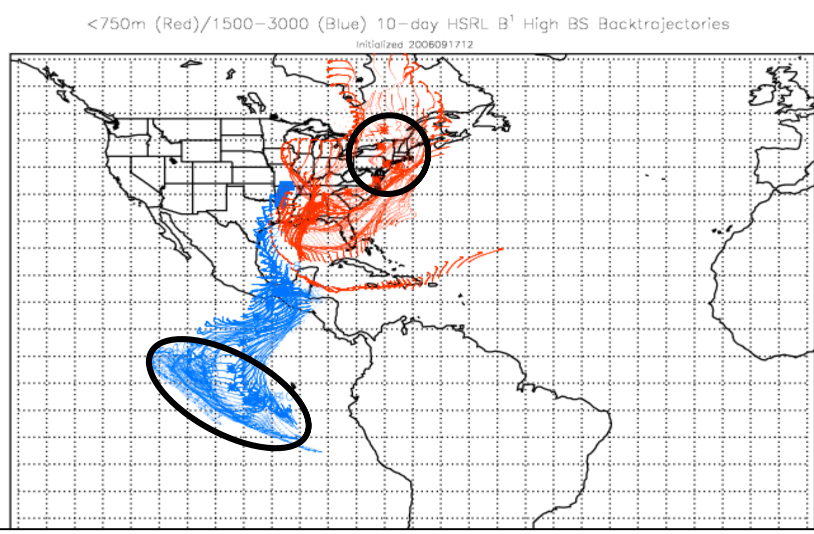


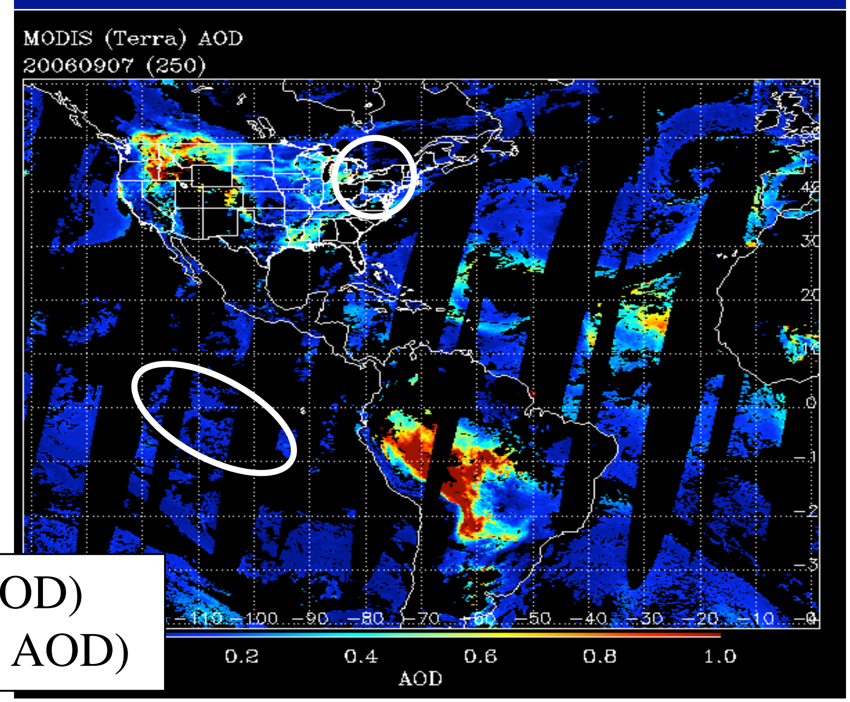
Red = (z°<750m) Atlantic source (? CO/? AOD/high backscatter)
Blue = (750<z°<2000m) S. American source (high CO/? AOD/high backscatter)

RDF back-trajectories link HSRL CALIPSO Leg to AIRS, MODIS, and CALIPSO measurements



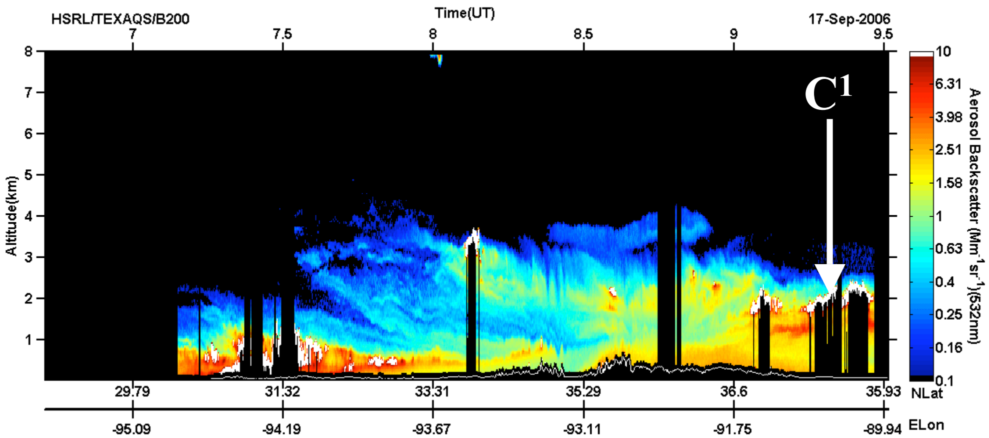


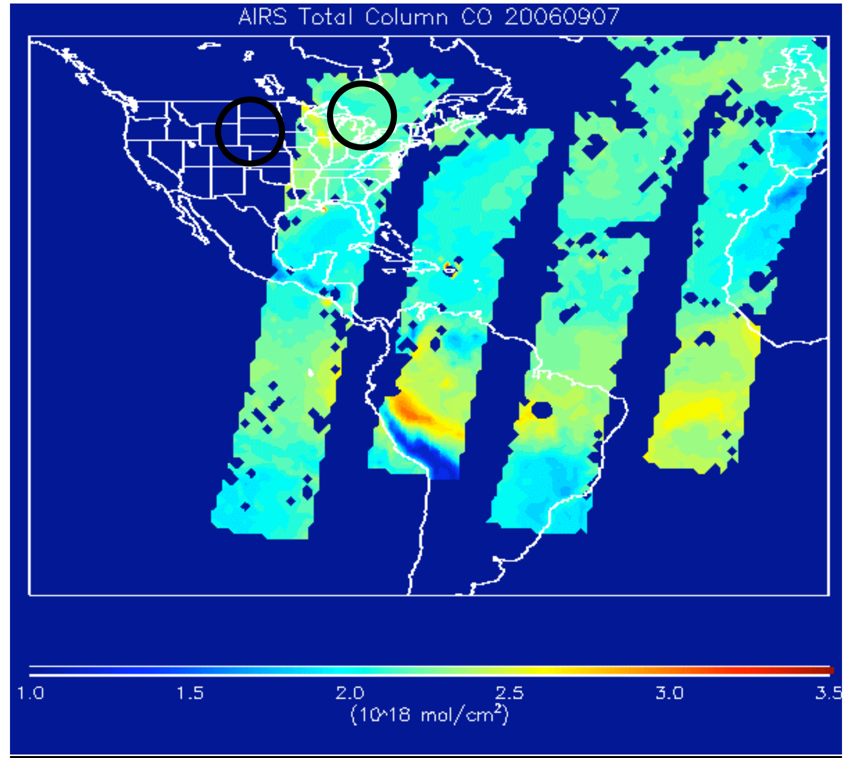


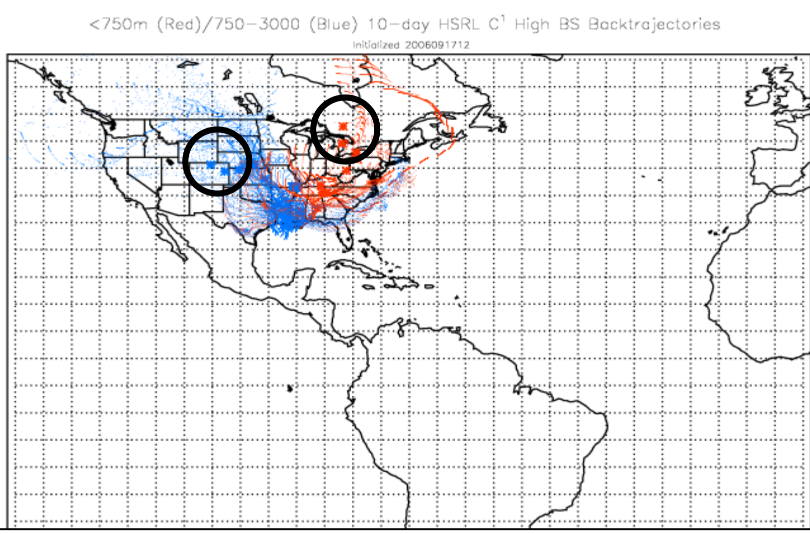


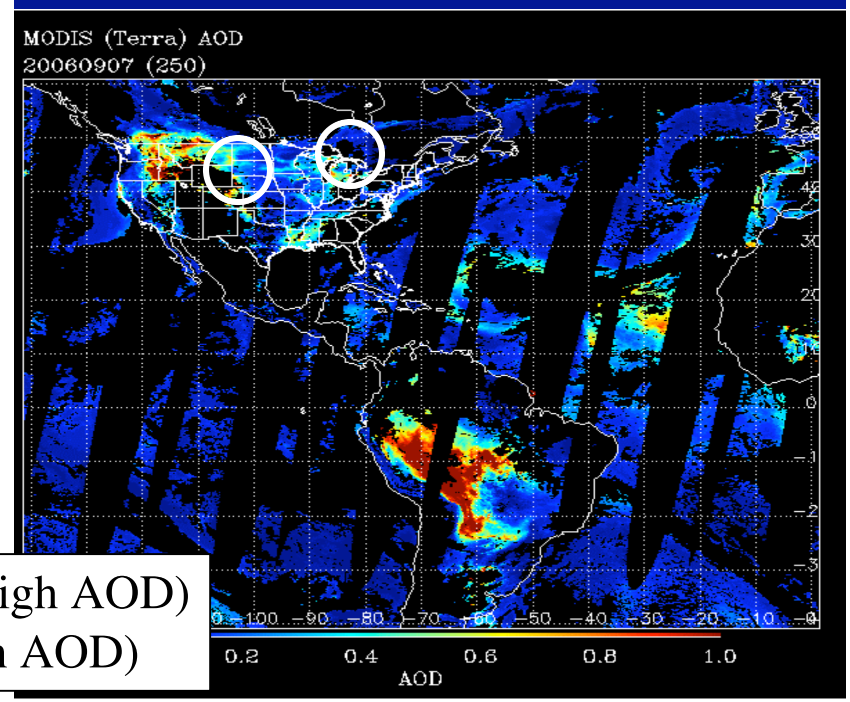
Red = ($z^o<750$m) NE US source (moderate CO/high AOD)
Blue = ($1500<z^o<3000$m) Pacific source (high CO/low AOD)

RDF back-trajectories link HSRL CALIPSO Leg to AIRS & MODIS measurements



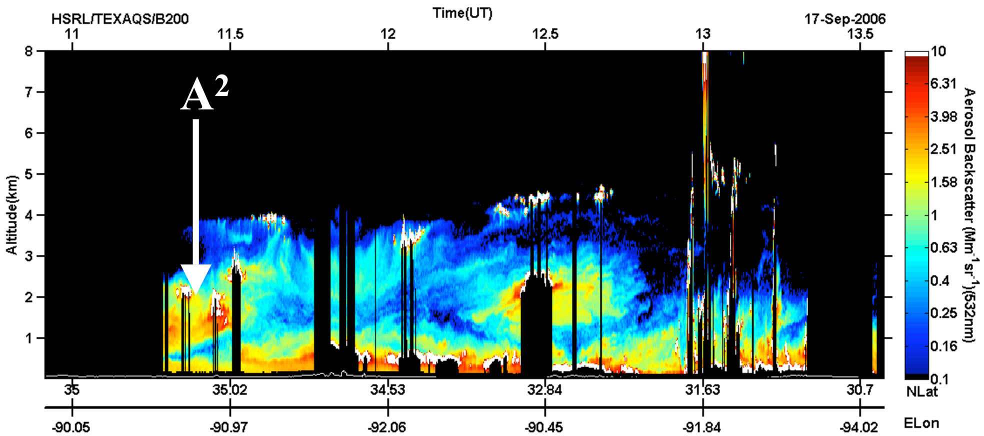


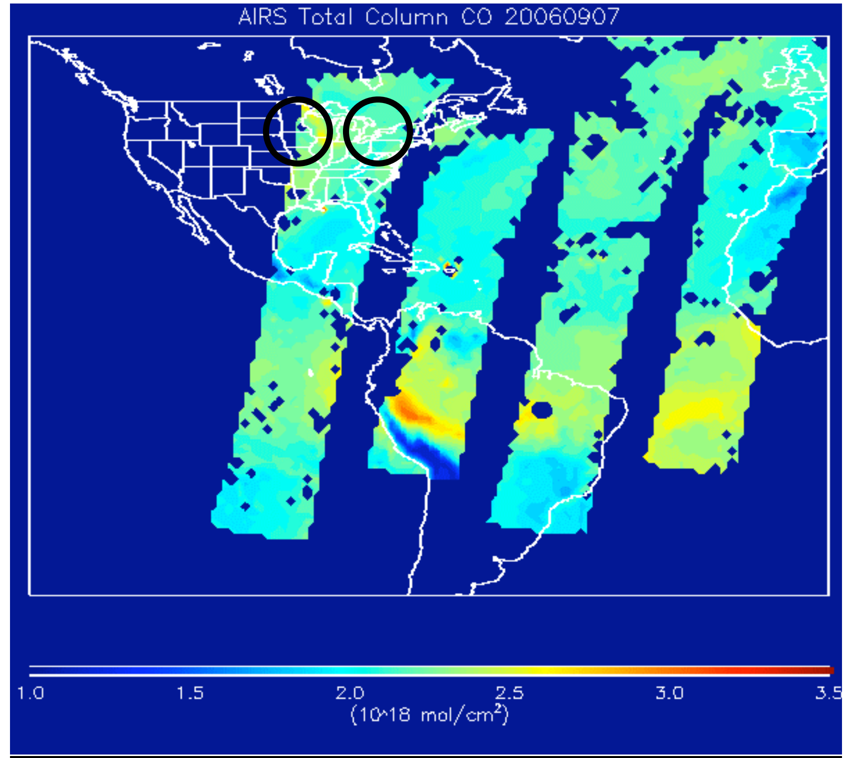


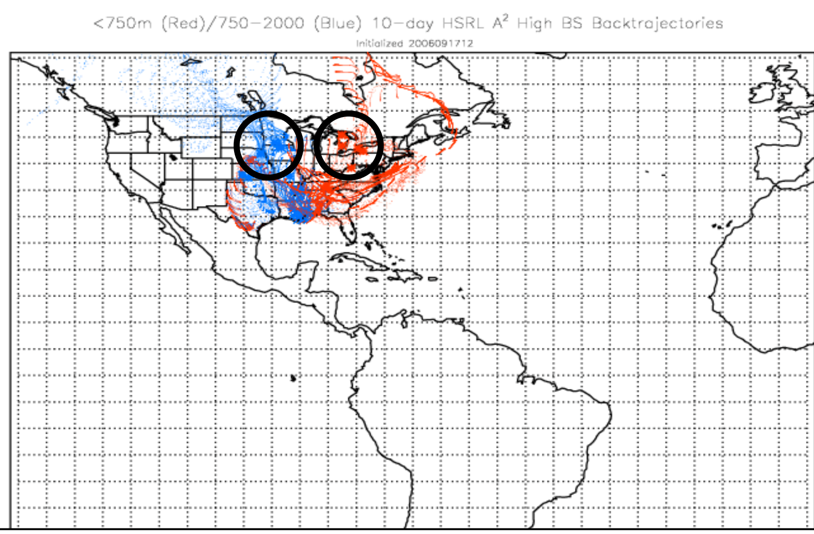


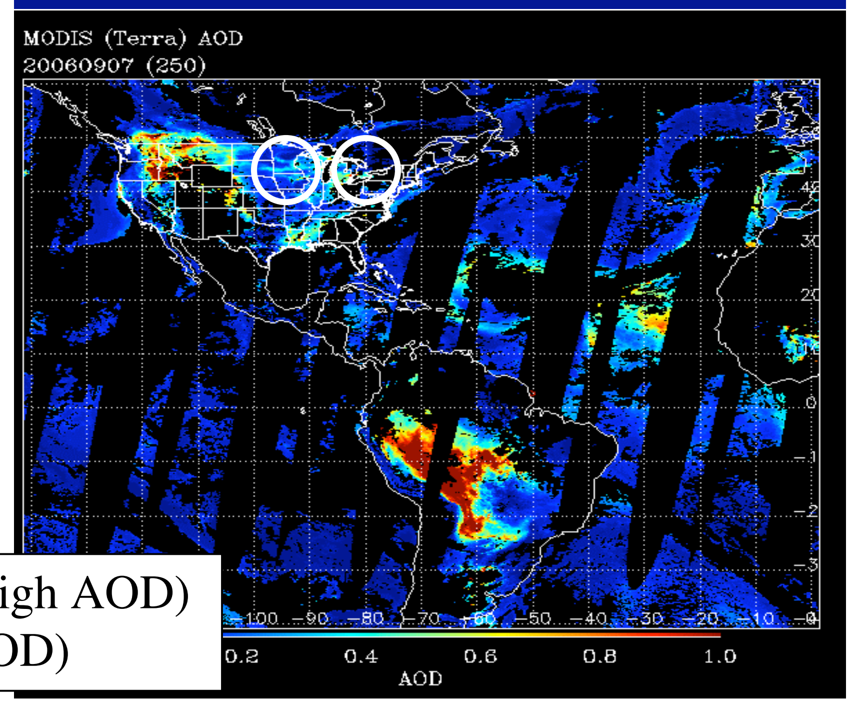
Red = (z^o<750m) Great Lakes source (moderate CO/High AOD)
Blue = (750<z^o<3000m) Central US source (? CO/high AOD)

RDF back-trajectories link HSRL BIOMASS Leg to AIRS & MODIS measurements



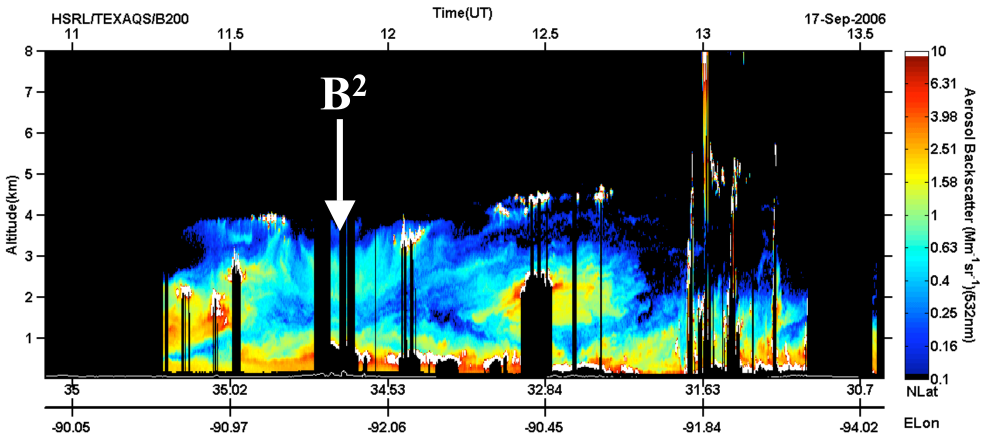


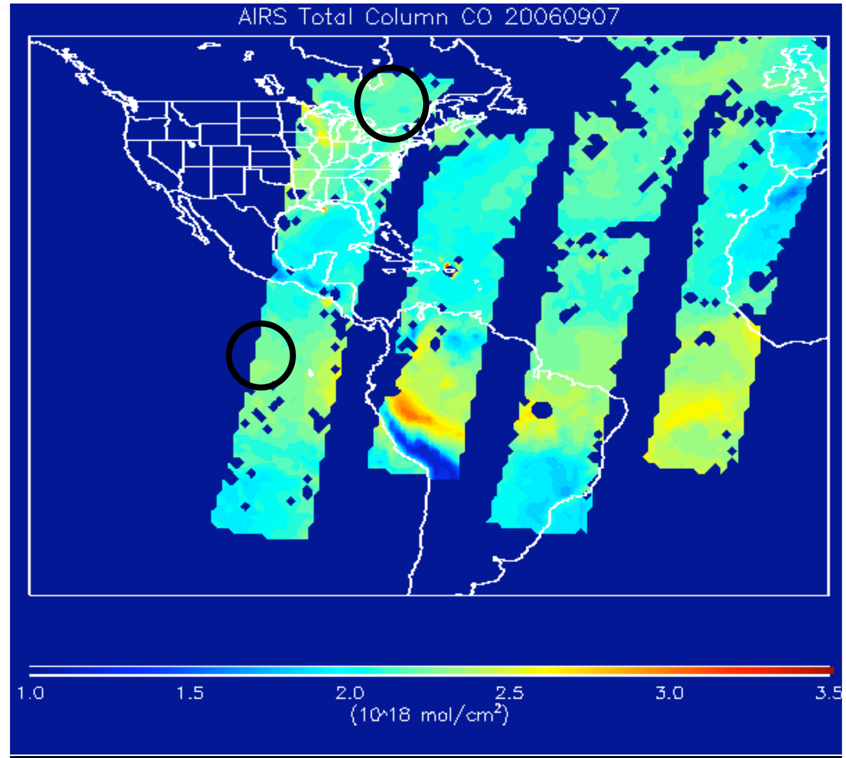


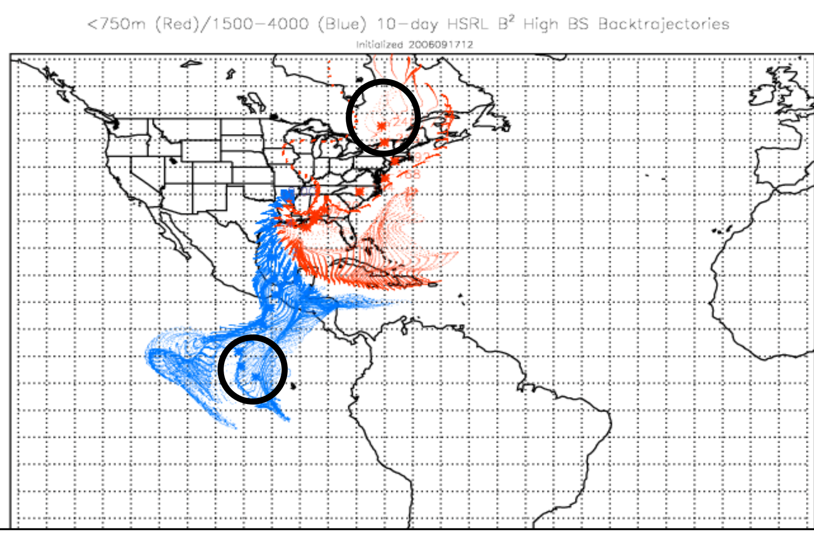


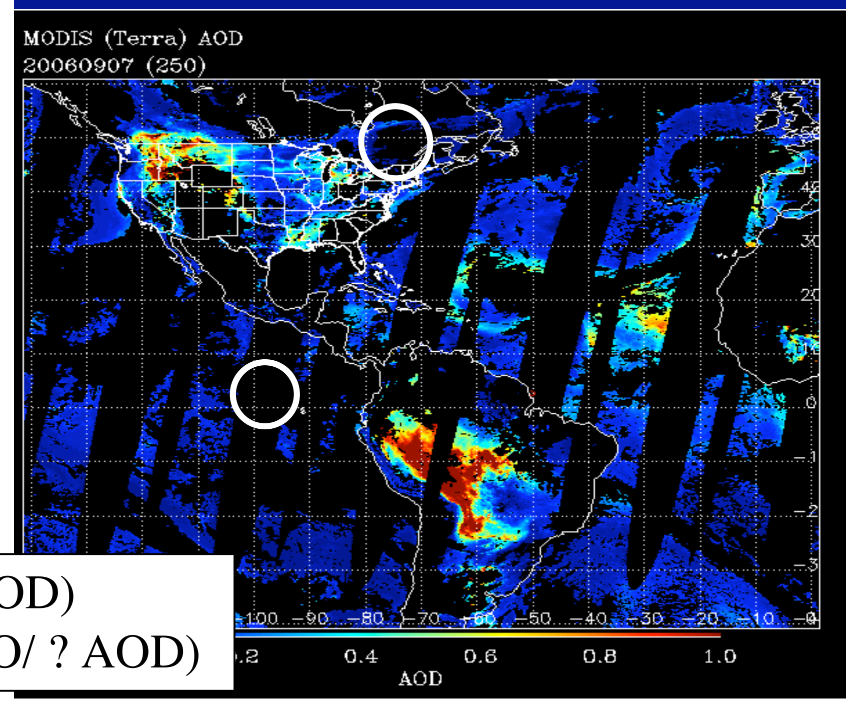
Red = (z°<750m) Great Lakes source (moderate CO/High AOD)
Blue = (750<z°<2000m) Midwest source (High CO/AOD)

RDF back-trajectories link HSRL BIOMASS Leg to AIRS & MODIS measurements









Red = (z°<750m) Canadian source (moderate CO/ ? AOD)

Blue = (1500<z°<4000m) S. American source (high CO/ ? AOD)

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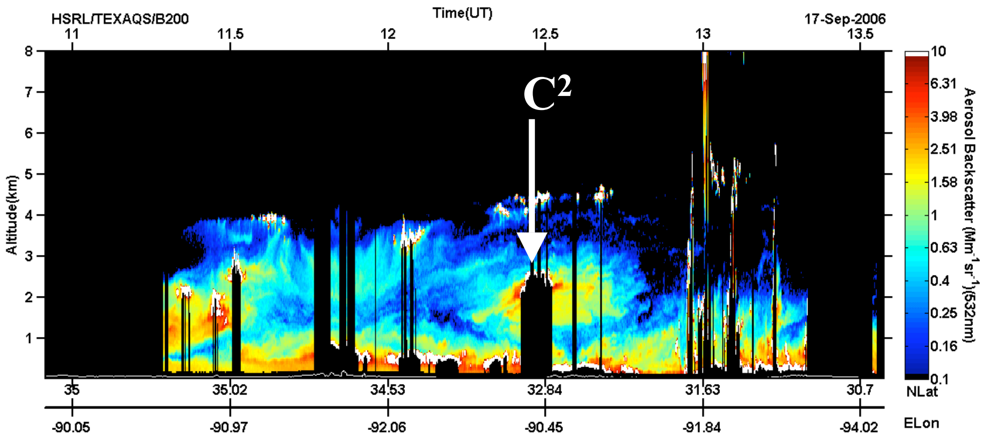
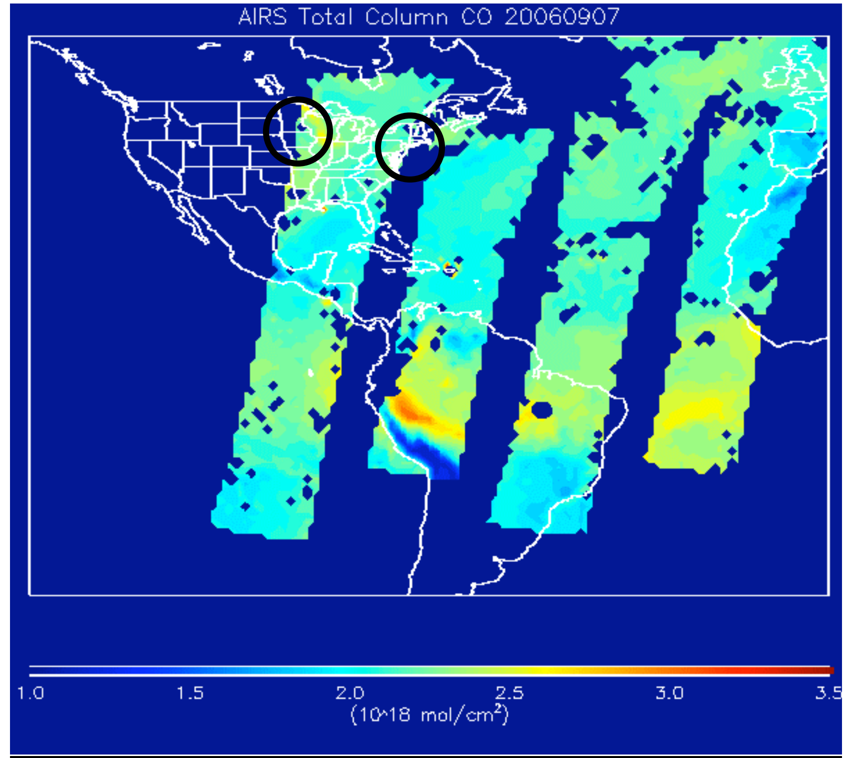
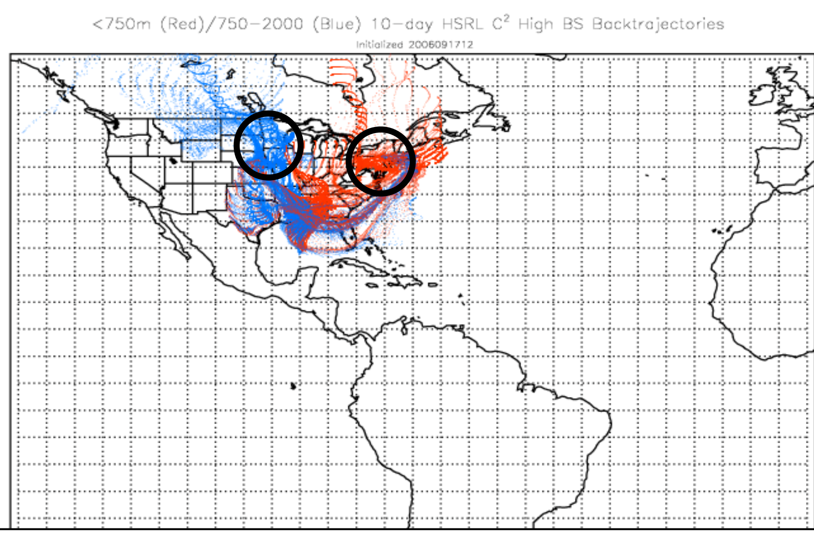
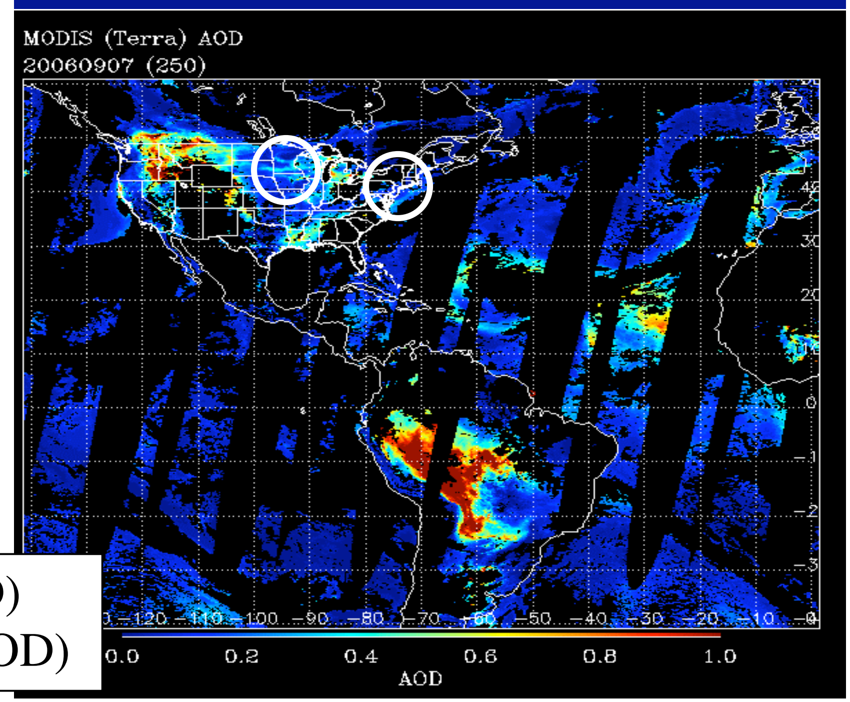


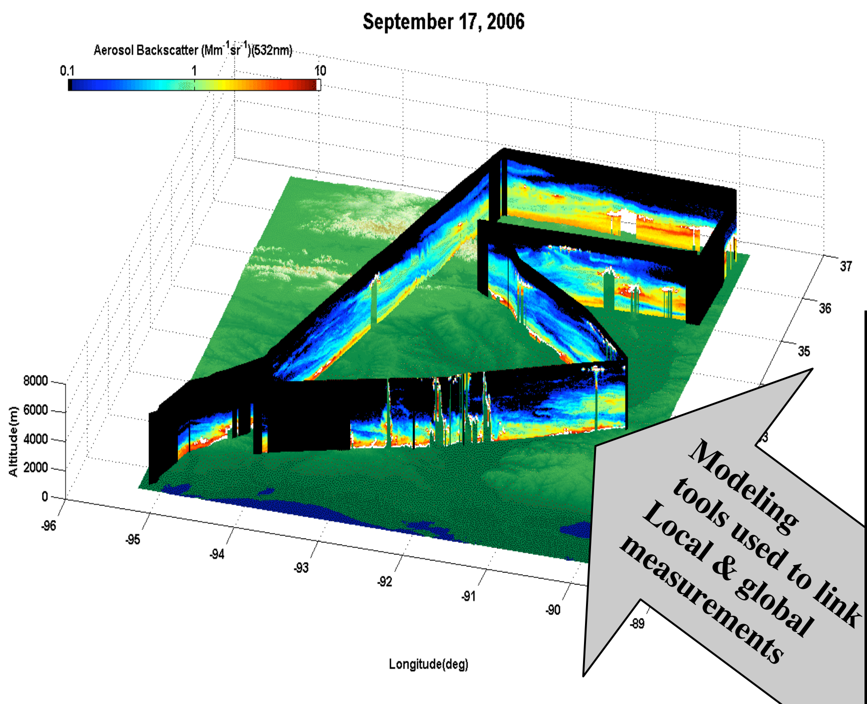


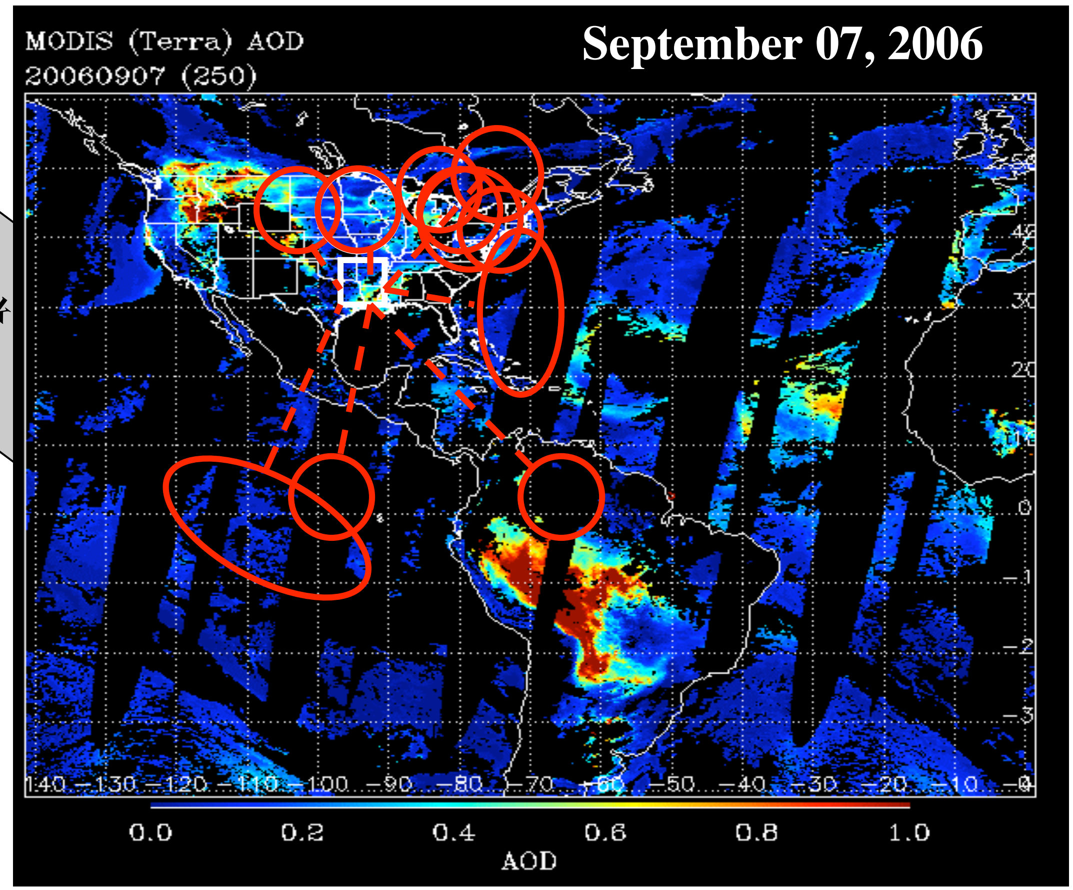




Red = (z° < 750m) NE source (moderate CO/High AOD)
Blue = (750 < z° < 2000m) Midwest source (High CO/AOD)

Summary: Ensemble Lagrangian trajectory analysis and Eulerian chemical/aerosol predictions are used to link HSRL aerosol lidar measurements of the Texas regional background to large-scale observations from CALIPSO, MODIS, and AIRS





Conclusions: CALIPSO and HSRL lidar measurements over E. TX/LA/AR show that the regional aerosol distribution on 09/17/06 was strongly influenced by fresh emissions associated with local biomass burning in LA/AR.

Model/Satellite synthesis studies indicate that:

•long range transport of biomass burning emissions from the Pacific NW and S. America was the most likely source of enhanced lofted aerosol backscatter.

•sulfate production during transport over the SE US contributed to high backscatter observed in the boundary layer throughout the flight