

**Top-down Emissions Verification (TDEV)
of HGA Petrochemical Sources
and
Quantitative Analysis of Their Downwind
Secondary Impact of Ozone, HCHO and NO_x
for 4 More Days (besides 13 Sep 2006)**

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**Collaborators:
Chalmers U. (SOF),
Baylor (Aztec),
NOAA (WP-3),
NOAA Twin Otter (LIDAR),
TCEQ/UH (Chem and Met data),
NOAA Smart Balloon,
TAMU (Wx forecast),
UAH (planning/coord'n)**

Top-down Emissions Verification (TDEV) of Industrial Sources

TexAQS I (2000)

- Not much upfront planning for TDEV
- Very sparse (spatial-temporal) data of primary VOC (e.g., ethene, propene)
- Mobile measurements from aircraft only
- Closest downwind measurements as much as 20 km from the source

TDEV based mainly on

- (a) VOC_i/NO_x based on sparse VOC canister data
- + (b) Diagnostic LRPM analyses to reconcile emissions with data of secondary products (e.g., O₃, HCHO)

TexAQS II (2006)

Upfront planning for TDEV

Some continuous data of primary VOC
(e.g., Surface SOF-FTIR, aircraft RAD, Ethylene, etc.)
(ethene, propene) (Aztec) (P3)

TDEV based mainly on
(a) Continuous data of VOC_i in the near-field, and diagnostic LESchem modeling to reconcile observations of primary species with emissions } TCEQ support

(b) Also based on diagnostic LRPM modeling to reconcile the primary emissions with observed data of primary species close-in and secondary products farther downwind } TERC support
(e.g., O₃, HCHO)

1 day
In progress
(LES and LRPM)

4 more days
proposed here
(LRPM)

Project Objectives

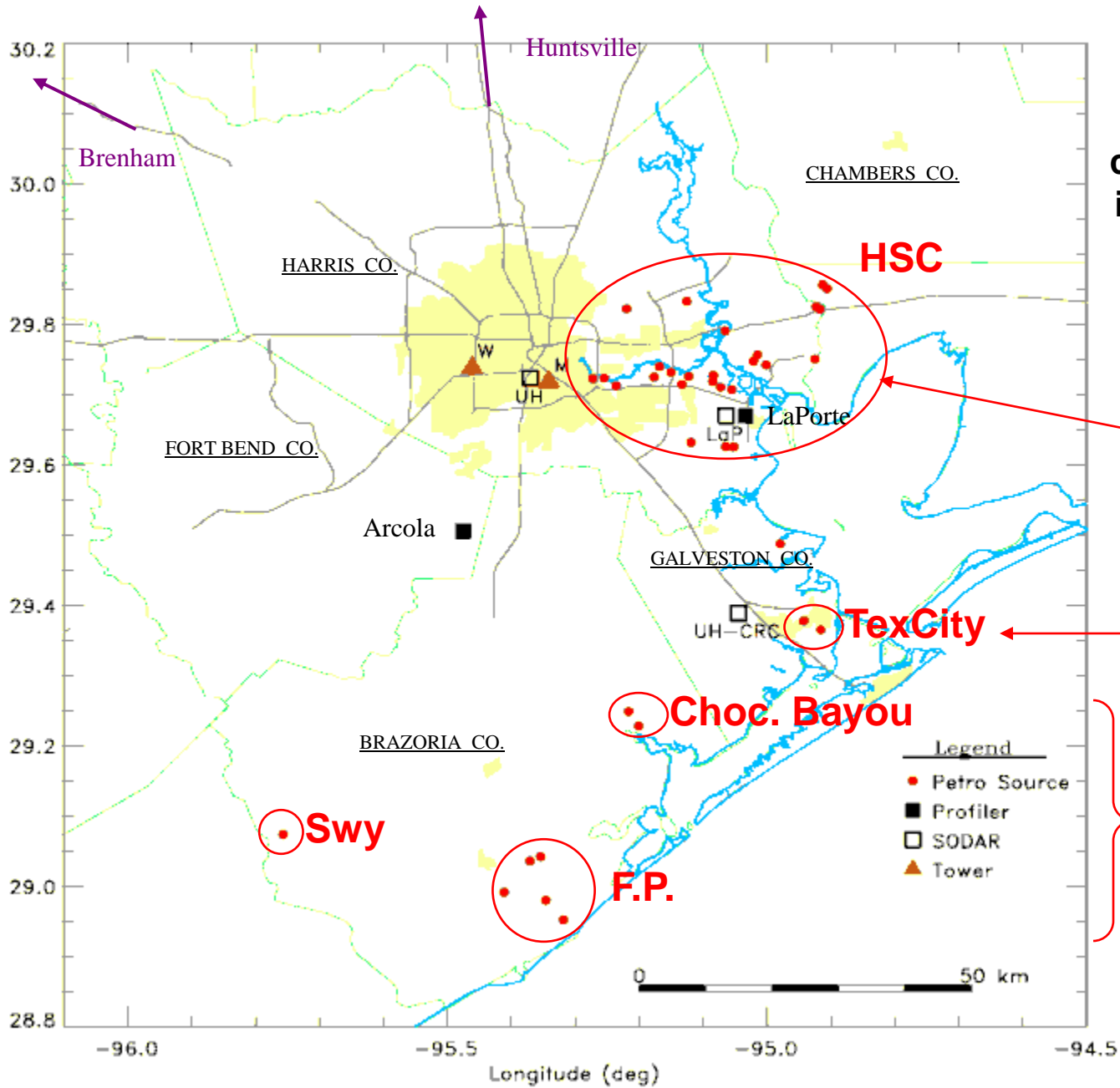
1. Perform TDEV of the petrochemical sources in HGA based on diagnostic LRPM modeling and TEXAQS II data of four days --- Aug. 30 (HSC and TC),
Aug. 31 (HSC and downtown),
Sep 20 (TC, CB and FP),
and Sep 27 (CB, FP and Sw);

Sep 13 data (HSC + TC)
analysis in progress now
(H-85)

Focus on ... primary species in the near-field and
... secondary species farther downwind.

2. Use the data and the model to explore the downwind impact of secondary products --- O₃, NO_x, and HCHO
3. Use the data and model to quantitatively explore the role of
--- primary v. secondary HCHO, and
--- HONO production
in the context of radical chemistry

The Target Sources



Houston-Galveston petrochemical source complexes aggregated into 37 sources in this map.

**Sep 13 (HSC + TC)
Aug 30 (HSC + TC)
Aug 31 (HSC + dntr)**

Sep 20 (TC + CB + FP)

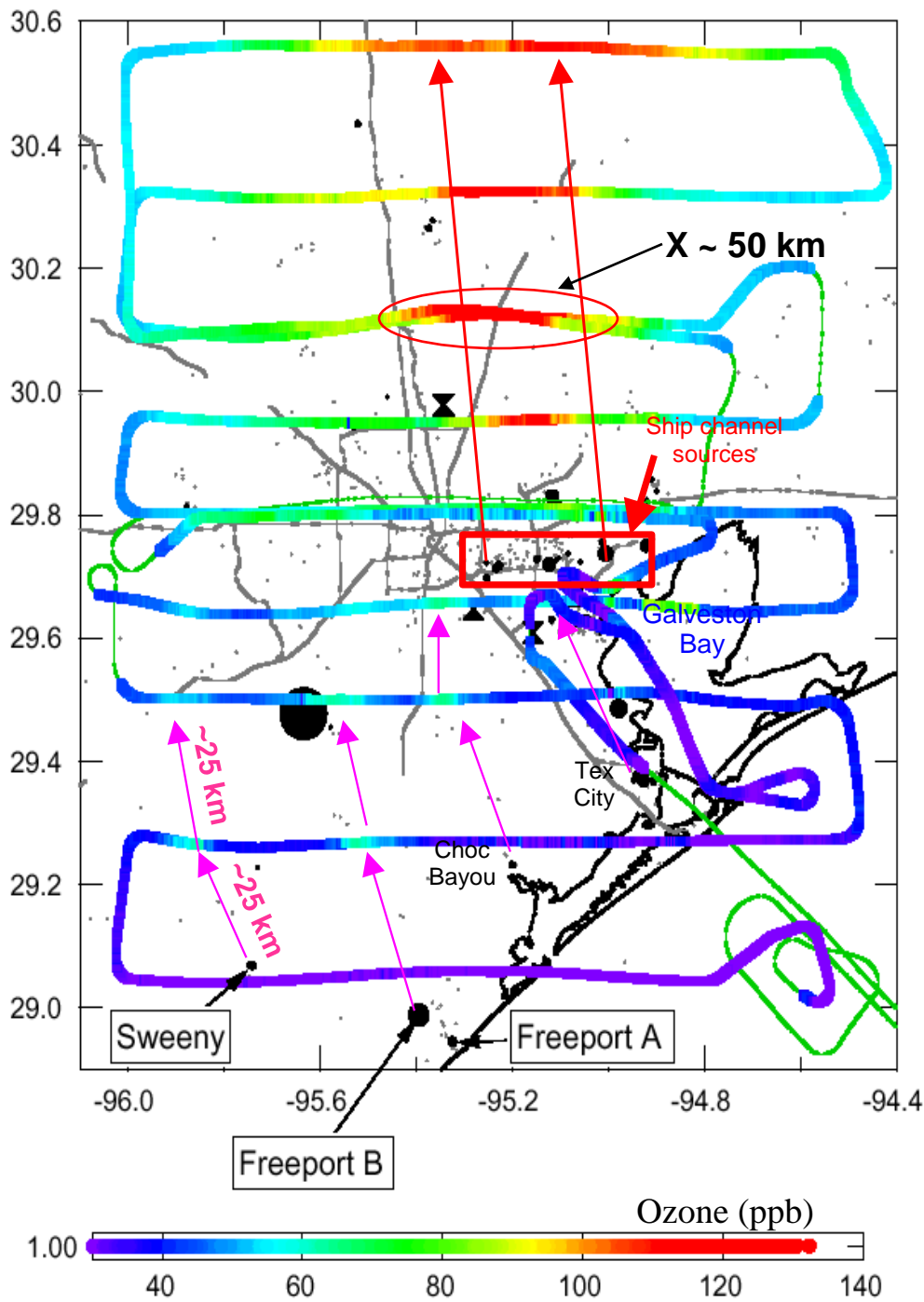
Sep 27 (CB + FP + Sw)

TexAQS I (2000) Scenario

A “Good”
measurement Scenario

(28 Aug 2000,
NCAR Electra Mission)

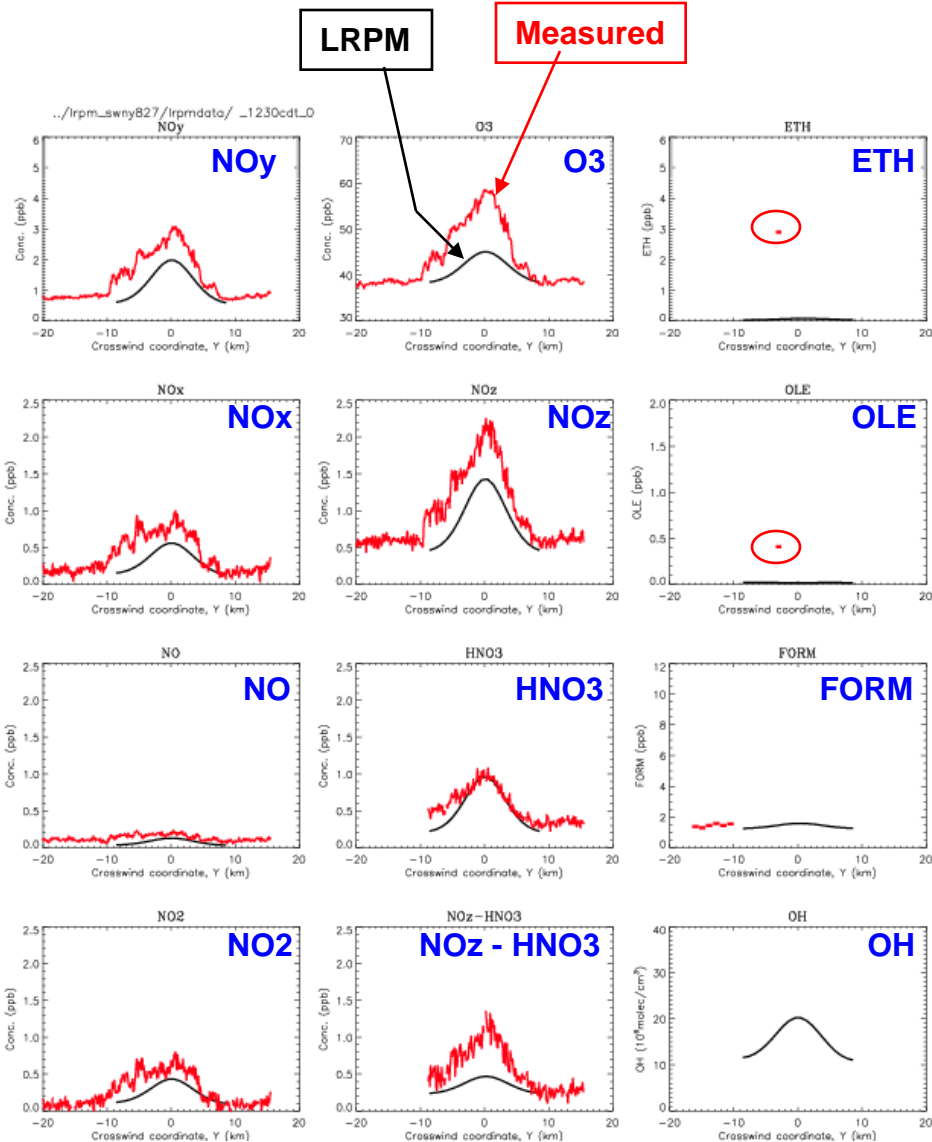
was simulated by LRPM
for TDEV



--- Sweeny plume at ~25 km downwind on 8/28/2000 ---

Comparison of observed data and LRPM simulation

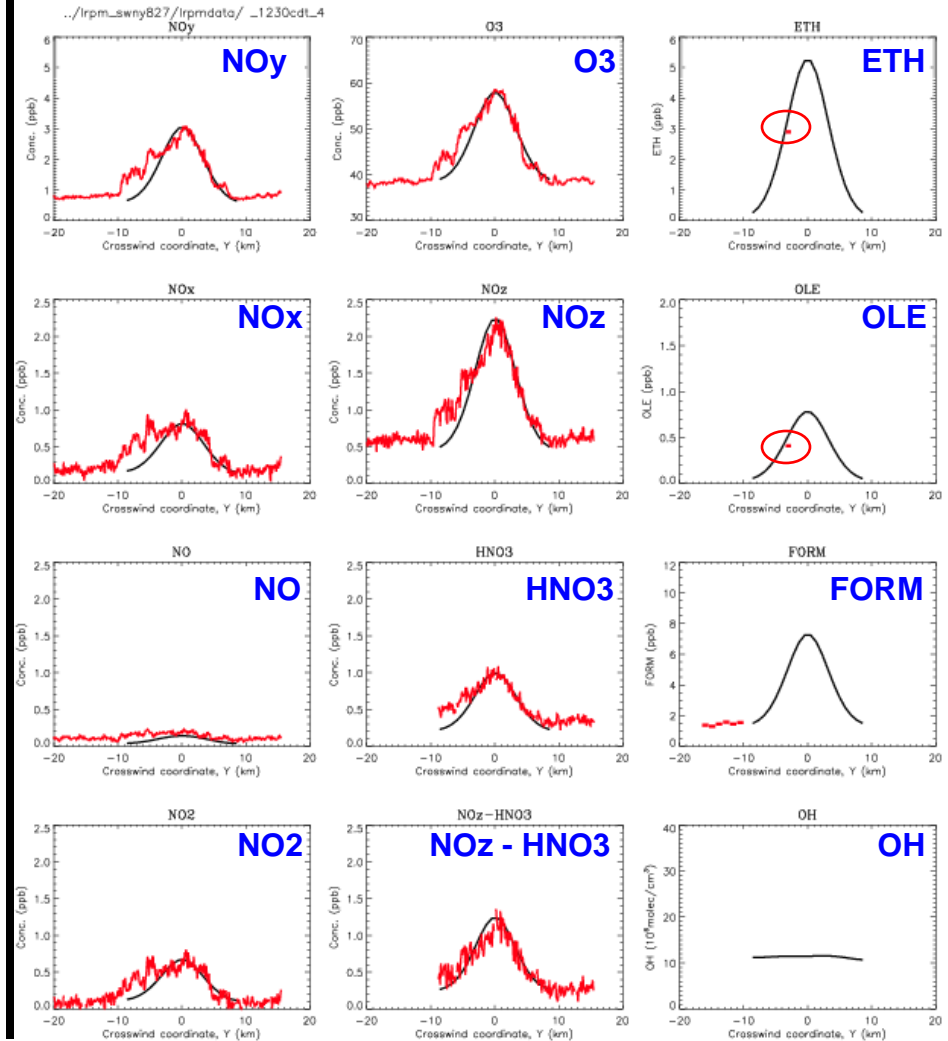
NOx, ETH, OLE emissions --- EI



NOx, ETH, OLE emissions --- "corrected"

$$Q_{\text{NOx}}(\text{corr}) \sim 1.8 Q_{\text{NOx}}(\text{EI})$$

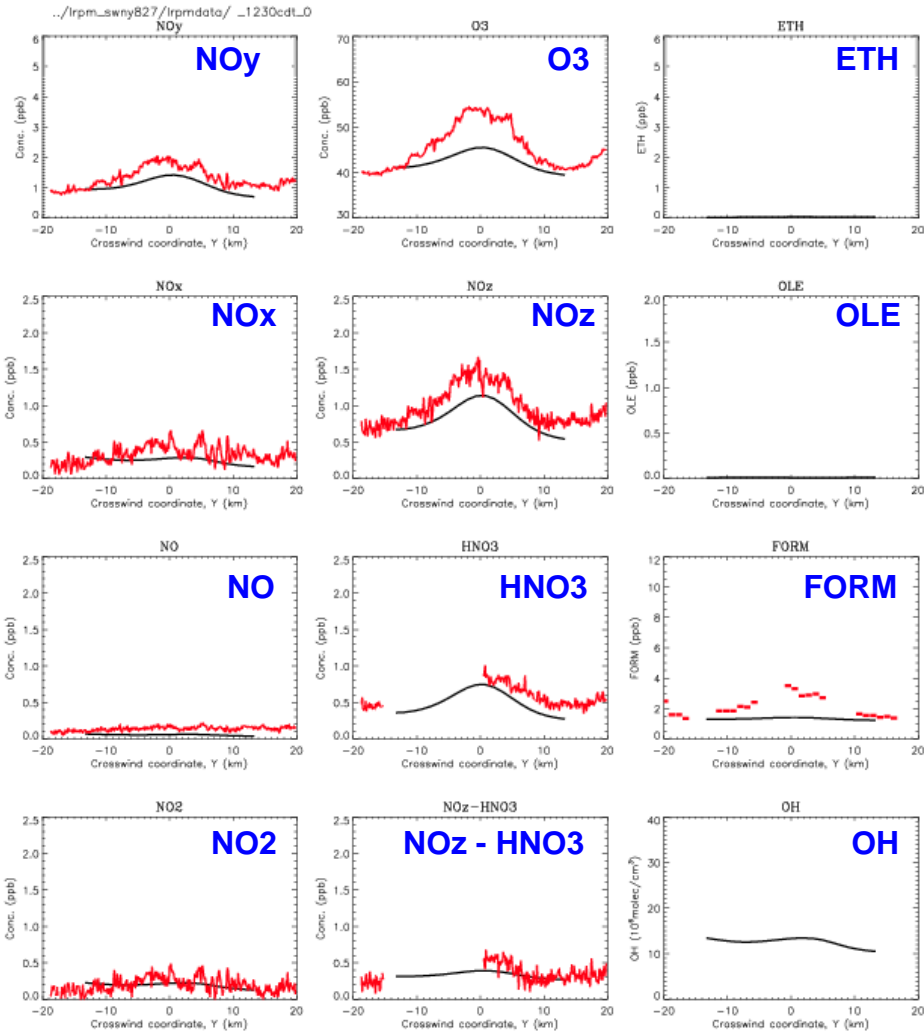
$$Q_{\text{ETH}}(\text{c}) \sim 67 Q_{\text{ETH}}(\text{EI}); Q_{\text{OLE}}(\text{c}) \sim 35 Q_{\text{OLE}}(\text{EI})$$



--- Sweeny plume at ~50 km downwind on 8/28/2000 ---

Comparison of observed data and LRPM simulation

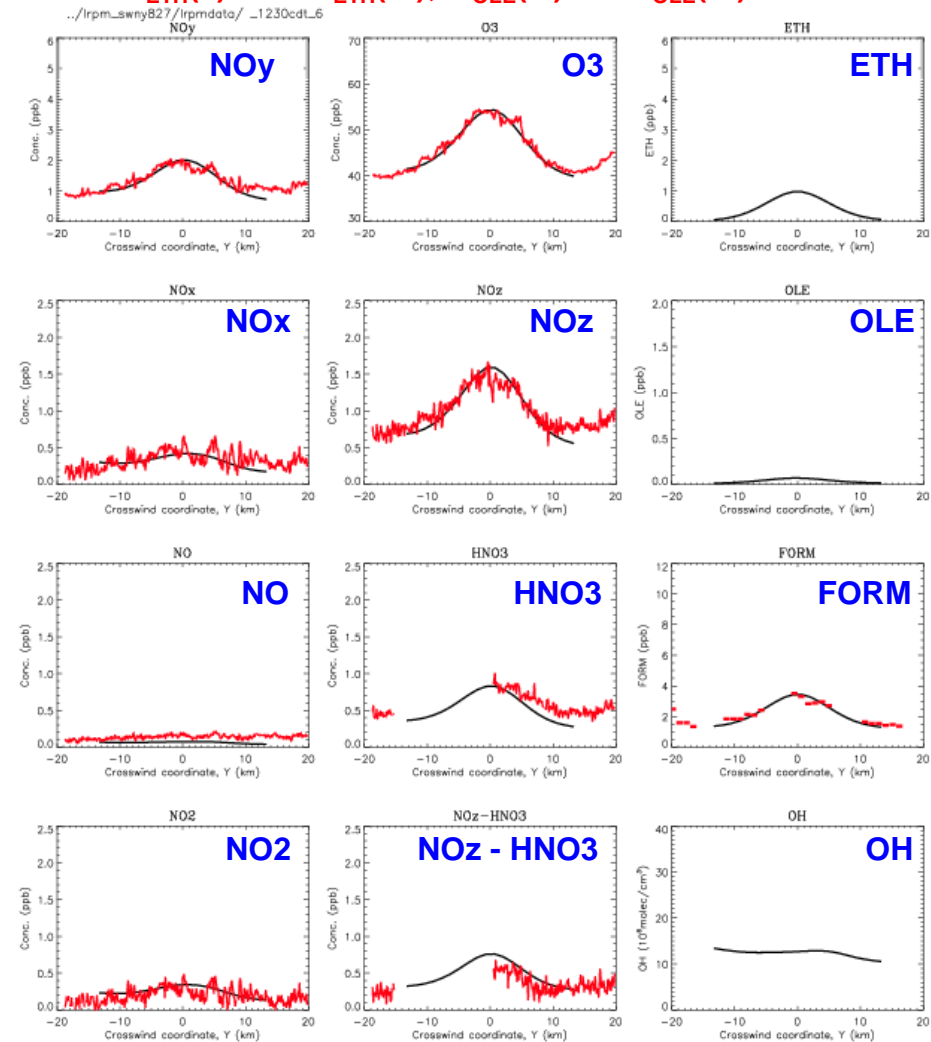
NOx, ETH, OLE emissions uncorrected



NOx, ETH, OLE emissions "corrected"

$$Q_{\text{NOx}}(\text{corr}) \sim 1.8 Q_{\text{NOx}}(\text{EI})$$

$$Q_{\text{ETH}}(\text{c}) \sim 67 Q_{\text{ETH}}(\text{EI}); Q_{\text{OLE}}(\text{c}) \sim 35 Q_{\text{OLE}}(\text{EI})$$



Houston Ship Channel Mega-plume, 8/28/2000, at X = 50 km downwind Comparison of observed data and LRPM simulation

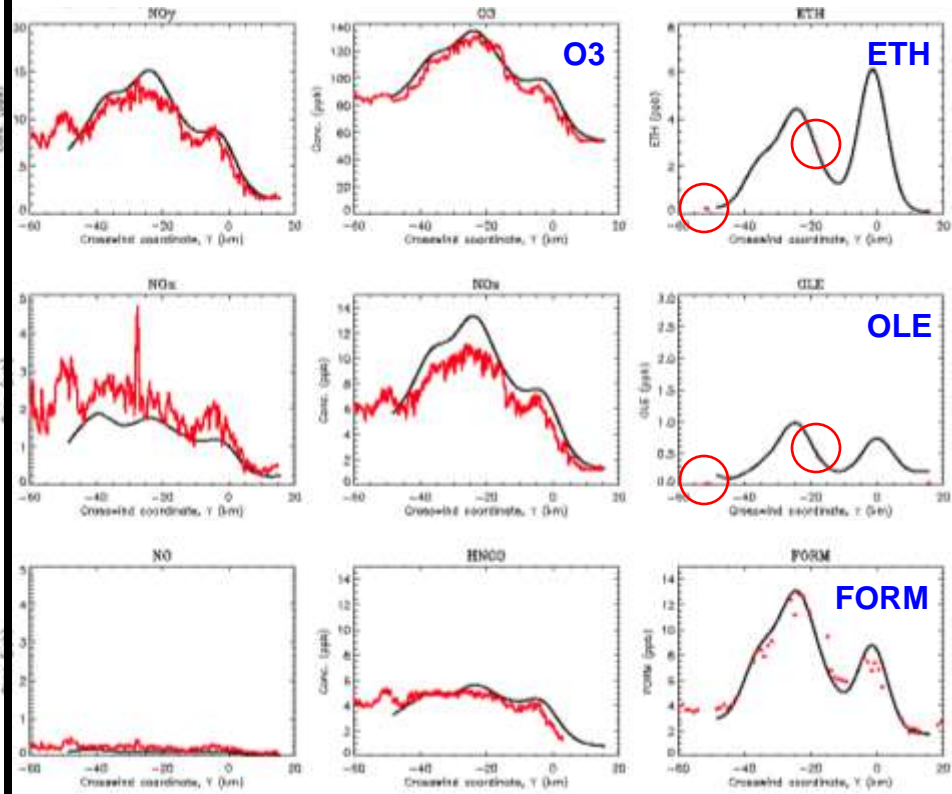
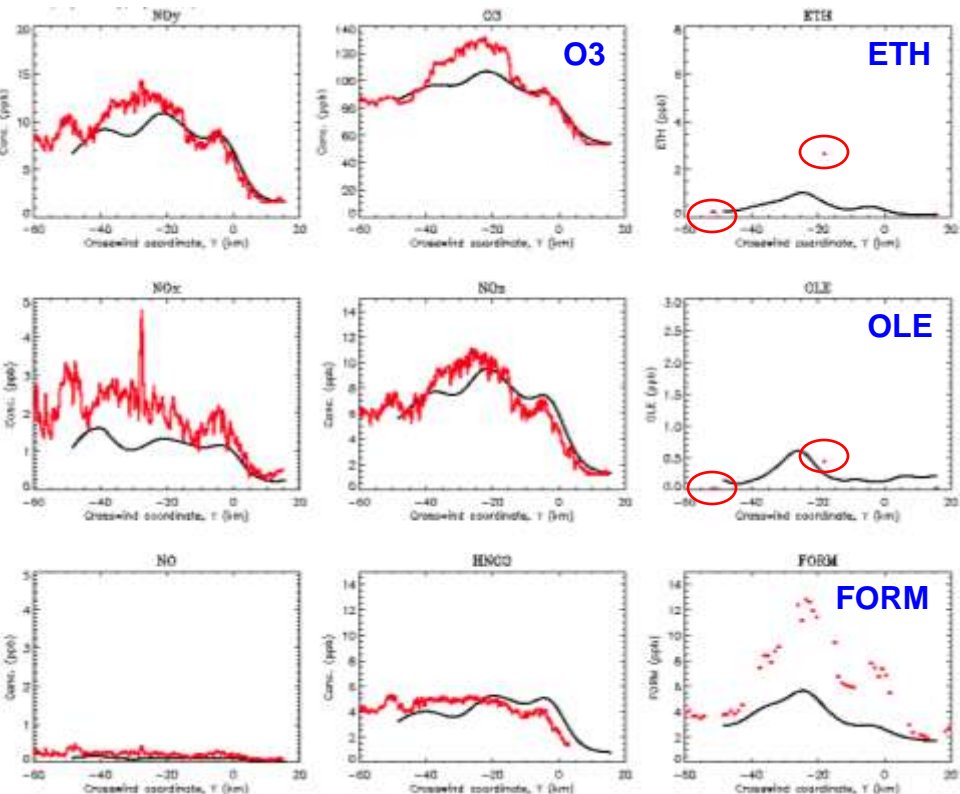
NO_x, ETH, OLE emissions --- EI

NO_x, ETH, OLE emissions --- "corrected"

$Q_{NOx}(corr) \sim 1-2 Q_{NOx}(EI)$

$Q_{ETH}(c) \sim 7-275 Q_{ETH}(EI); Q_{OLE}(c) \sim 4-395 Q_{OLE}(EI)$

(Ship channel represented here by ~30 composited sources)



**In the proposed analyses for 2006,
LRPM diagnostic analyses will compare
near-field and farther downwind model-data results for**

(a) Emissions based on TCEQ EI

(b) Emissions based on SOF

**(c) Emissions further corrected based on LRPM
primary and secondary reconciliations**

TDEV Data Base Overview

Emissions

Area source modeling emissions in CB05 at 2 km

--- 2005 STARS

Point-source modeling emissions in CB05

--- 2005 PEI & 2006 SHEI and ARD

Source

TCEQ

MET

Profilers (LaPorte, Arcola etc)

TCEQ

SODARs in the Houston area

TCEQ

Radiosonde

UH

Tethersonde

No data on 9/13/07

UH

Moody Tower

UH

SOF - minisonde

Chalmers U.

LS/LU data (NLCD)

LANDSAT 30m resolution data, 2001

USGS/USEPA

Surface Chem (auto-GC +)

8 auto-GCs in HSC area

TCEQ

SOF

Ethene, propene

Chalmers U.

Baylor Aztec

NO/NO₂/NO_y, SO₂, CO, RAD, O₃, HCHO, Nephelometer, can VOC

Baylor

NOAA P-3

NO/NO₂/NO_y, HNO₃, PANs, CO, CO₂, ethene, PTRMS VOC, can VOC, O₃, HCHO etc

NOAA-AL

NOAA-Twin Otter (Lidar)

Vertical profiles of O₃, aerosol backscatter

NOAA-ETL

NOAA-Smart Balloon

8/30, 9/13/06

NOAA

Ozonesonde

Valparaiso U.

Solar Radiation

GOES visible imagery

NASA_

MM5, CMAQ

UH

CB05 mechanism code

CB05 conversion file (measurements – mechanism)

EPA/CMAS

TCEQ

The Aztec Missions

	<u>DATE</u>	<u>TDEV TARGETS</u>	<u>TIME(S)</u>	<u>WD</u>
1.	8/30/06	Hou. Ship Chan (HSC) Texas City (TC)	am: 085843 – 110615 (2h 8min) pm: 141203 – 162024 (2h 8min)	↓
2.	8/31/06	HSC	am: 074552 – 103154 (2h 46min) pm: 141851 – 161818 (2h 00min)	↙
Currently in progress:				
3.	9/13/06	HSC, TC	am: 074953 – 123539 (4h 46min) pm: 144641 – 191745 (4h 31min)	↓
TCEQ – LES study TERC – LRPM study				
4.	9/20/06	TC, Choc. Bayou (CB), Freeport (FP), Sweeny (Sw)	081416 – 134414 (5h 30min)	↙
5.	9/27/06	CB + FP + Sw	<u>121327 – 173422 (5h 21min)</u>	↑
			<u>TOTAL = (29h 10min)</u>	

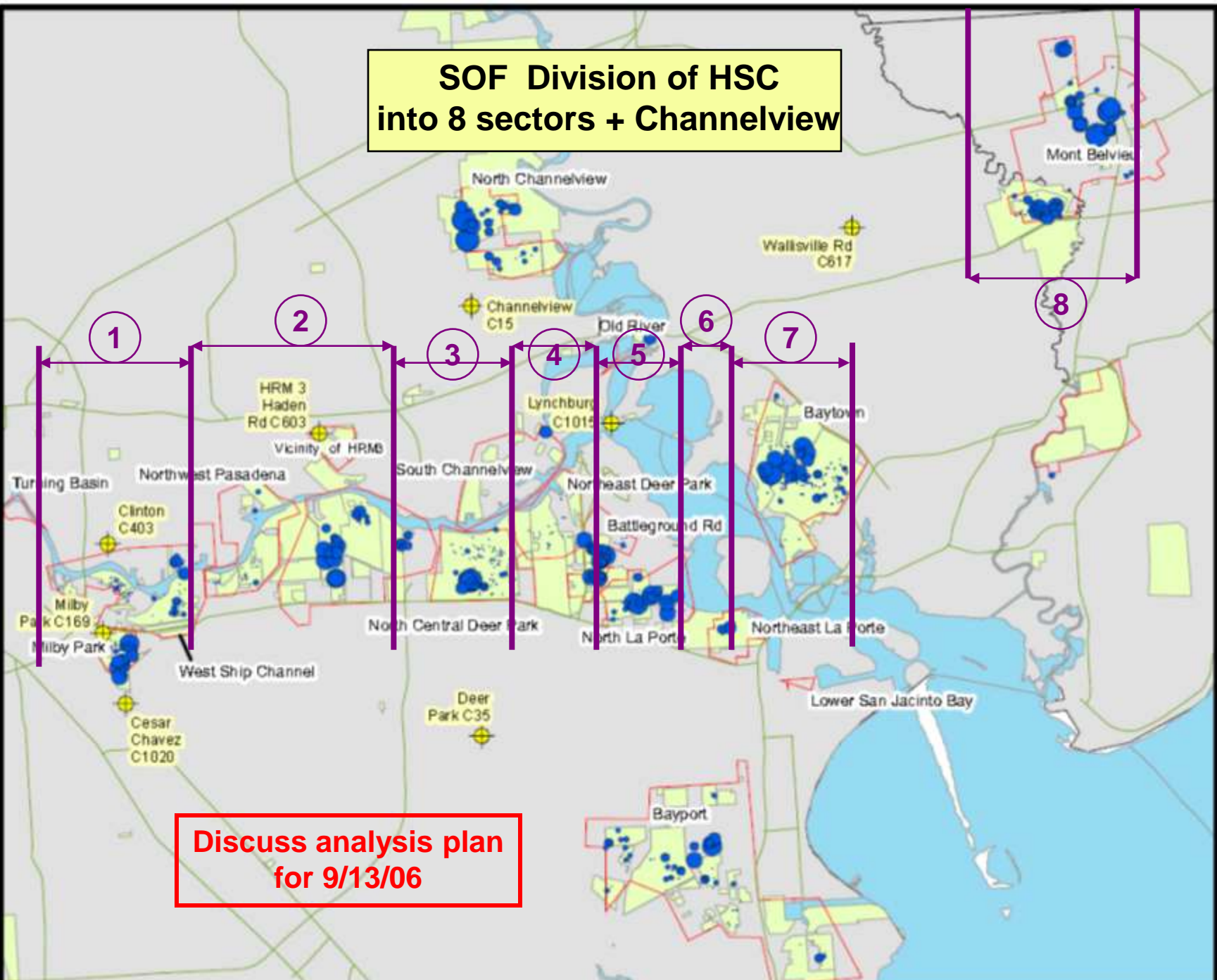
SOF-Box sources

Better SOF data on 8/30/06 than on 9/13/06

Better Aztec data on 9/13/06 than on 8/30/06 (HCHO)

This proposal is for analyses of 8/30, 31 and 9/20,27

**SOF Division of HSC
into 8 sectors + Channelview**



**Discuss analysis plan
for 9/13/06**

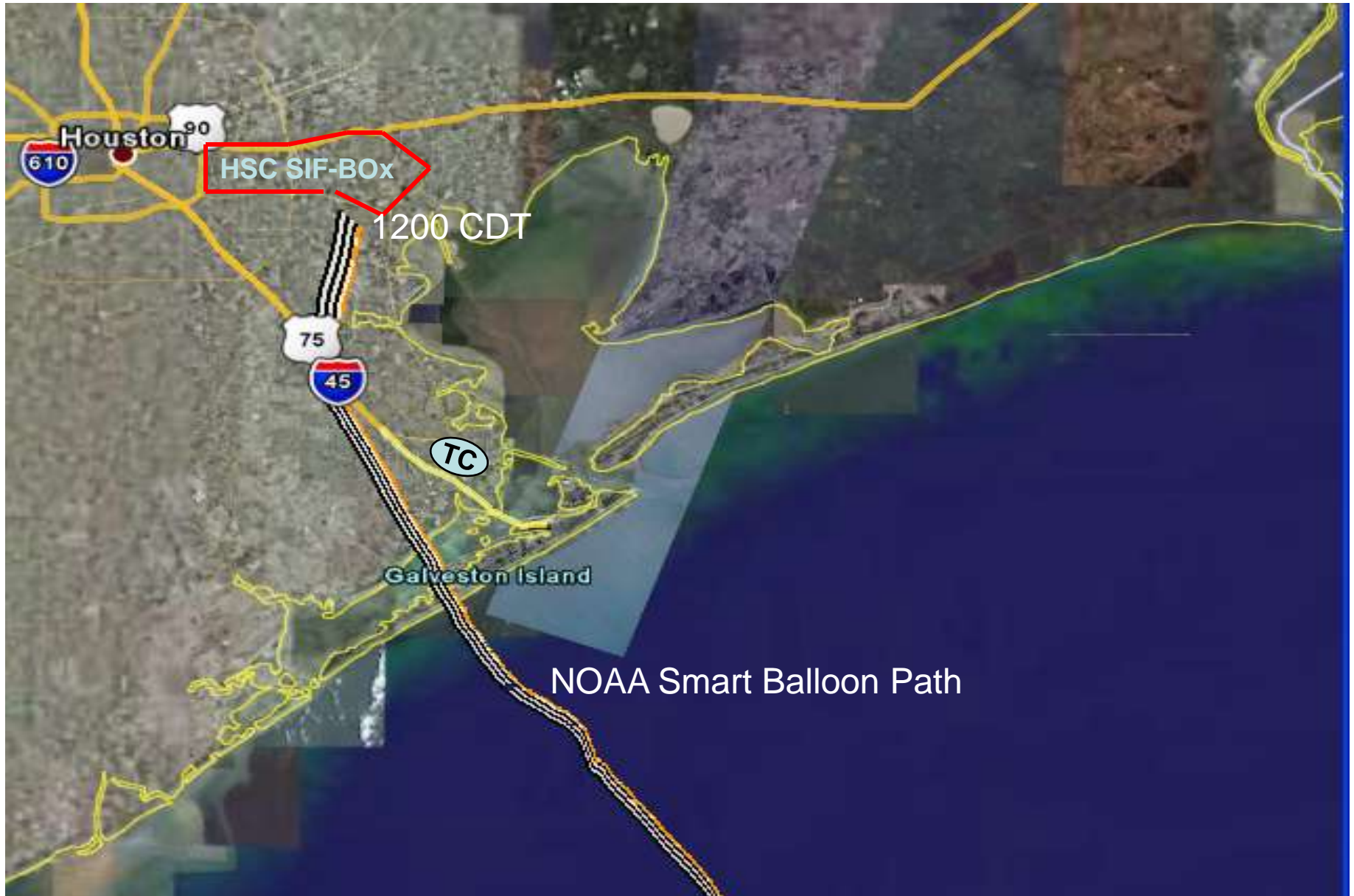
Houston Ship Channel (HSC) TDEV & Plume Transport Mission Plan for Wed 13 Sep 2006

Collaborators

SOF van, Baylor Aztec, NOAA Smart Balloon, UH Met Team

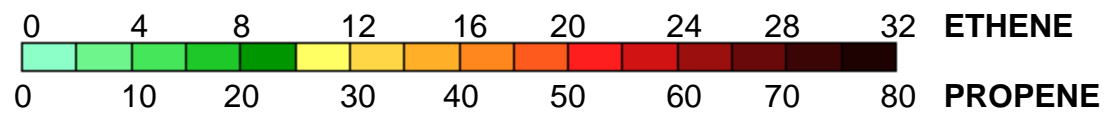
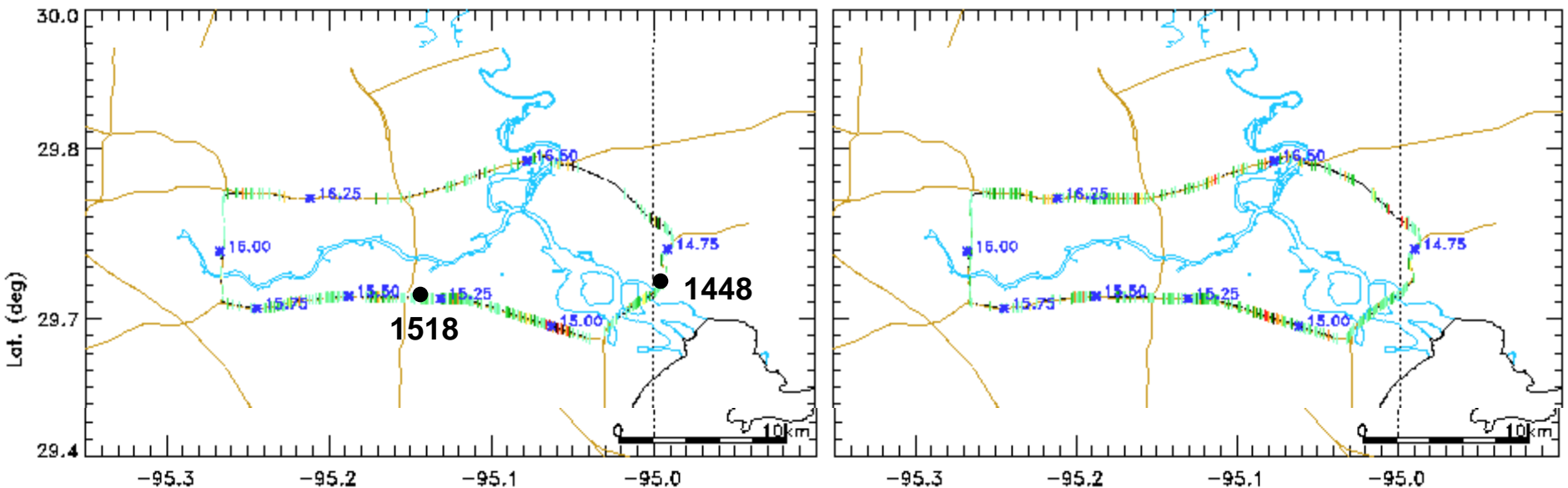
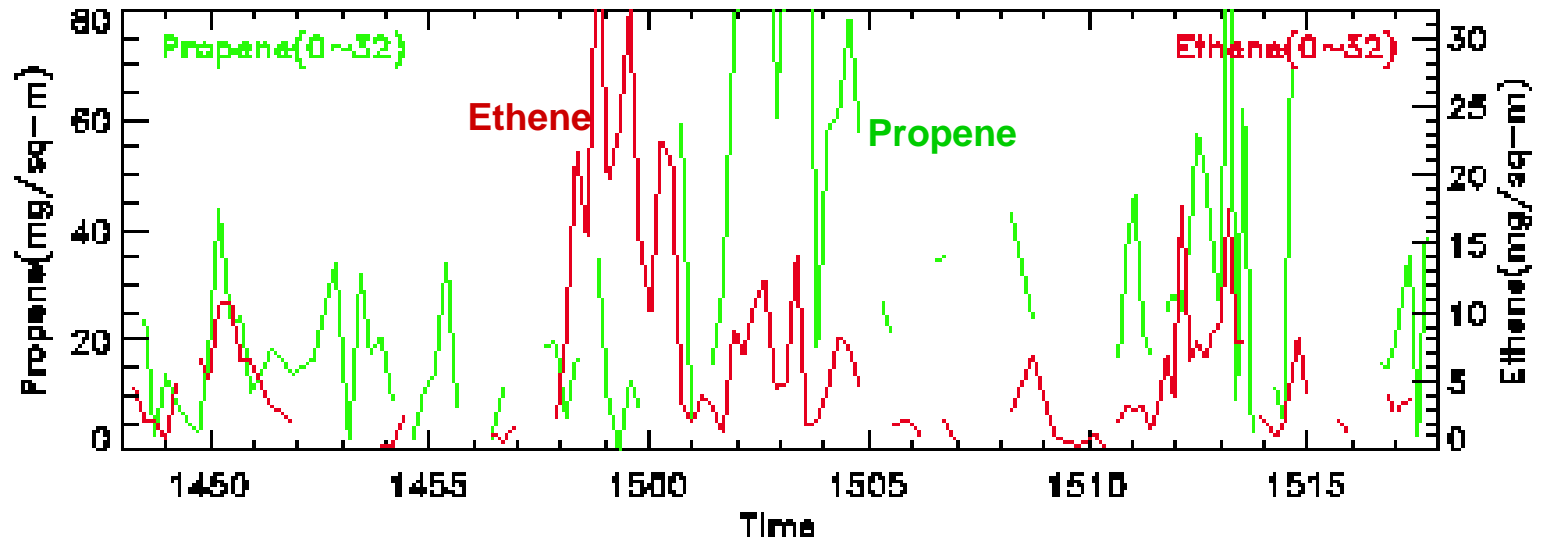


9/13/06 NOAA Smart Balloon Path



SOF Data, 13 Sep 2006

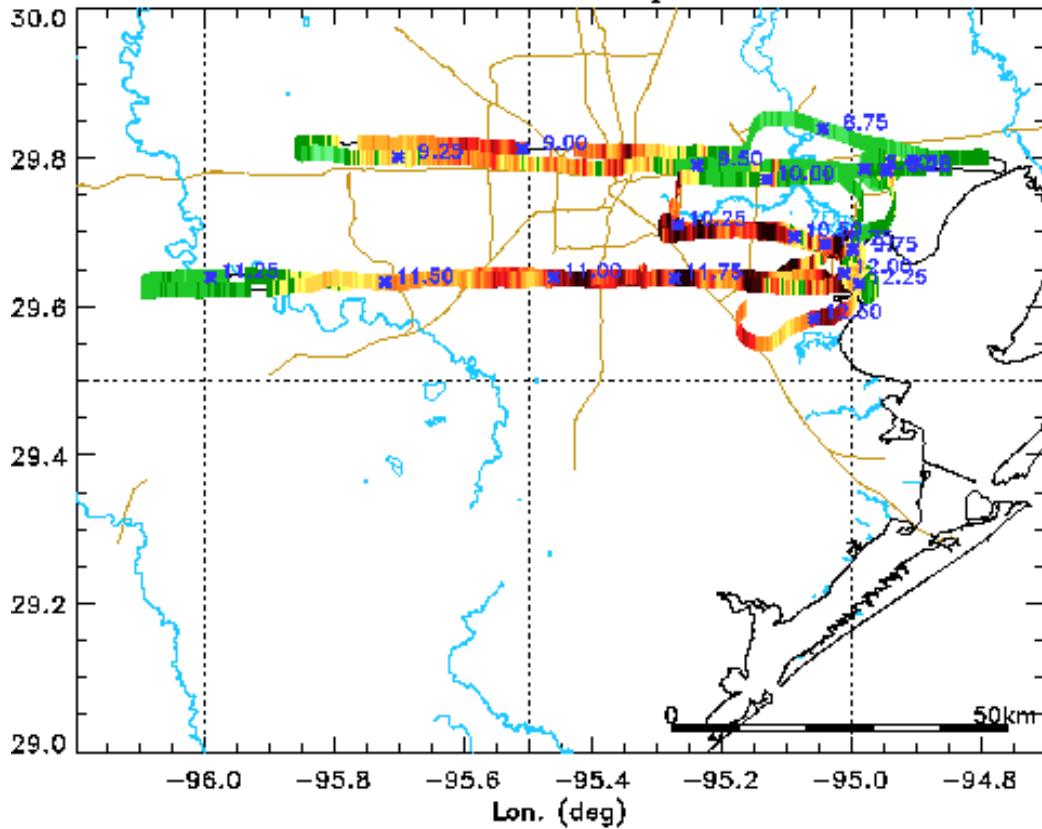
144800-151800



Baylor Aztec Data

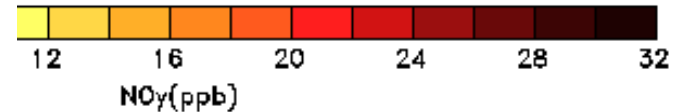
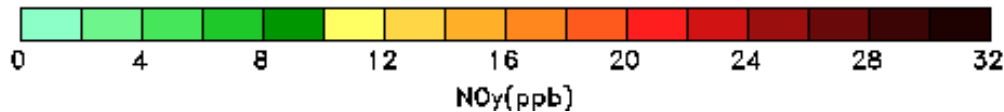
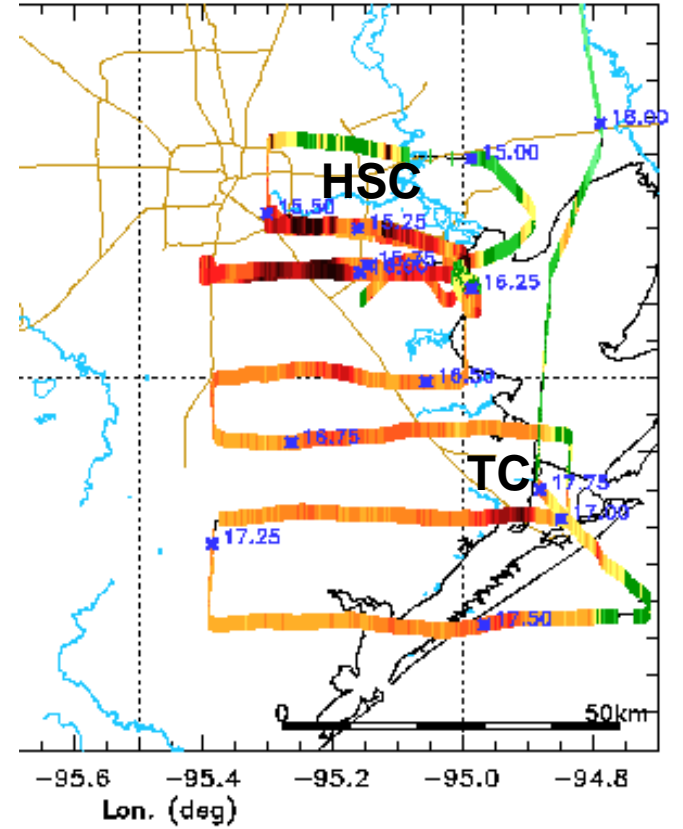
9/13/06, **NO_y**

HARC data: 13 Sep 2006 (0750 – 1236)



SOF: HSC in pm

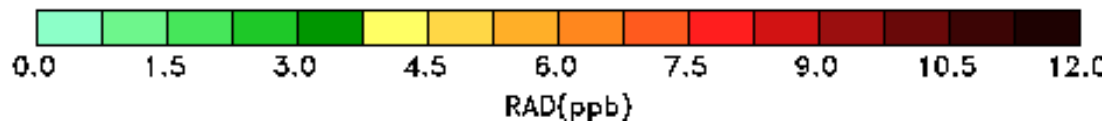
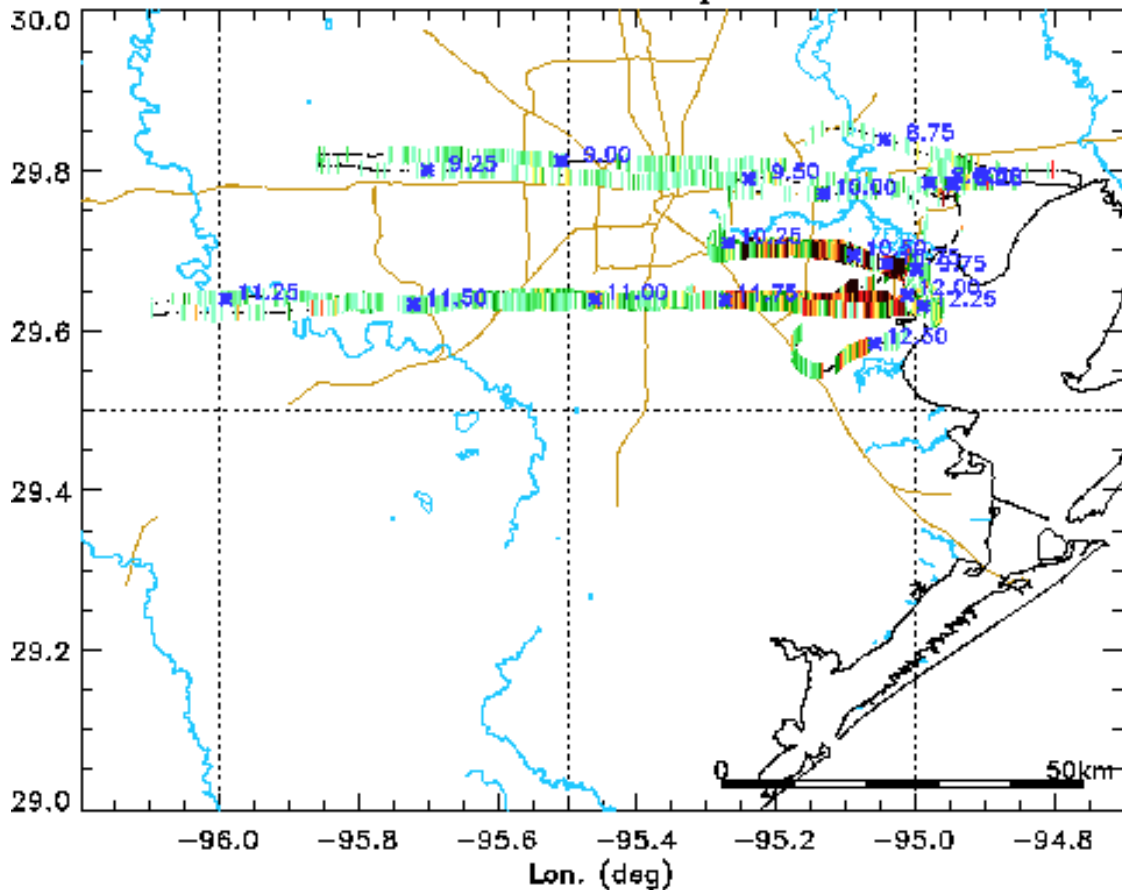
SC data: 13 Sep 2006 (1447 – 1918)



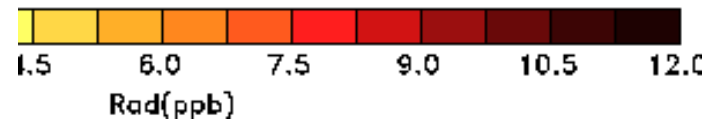
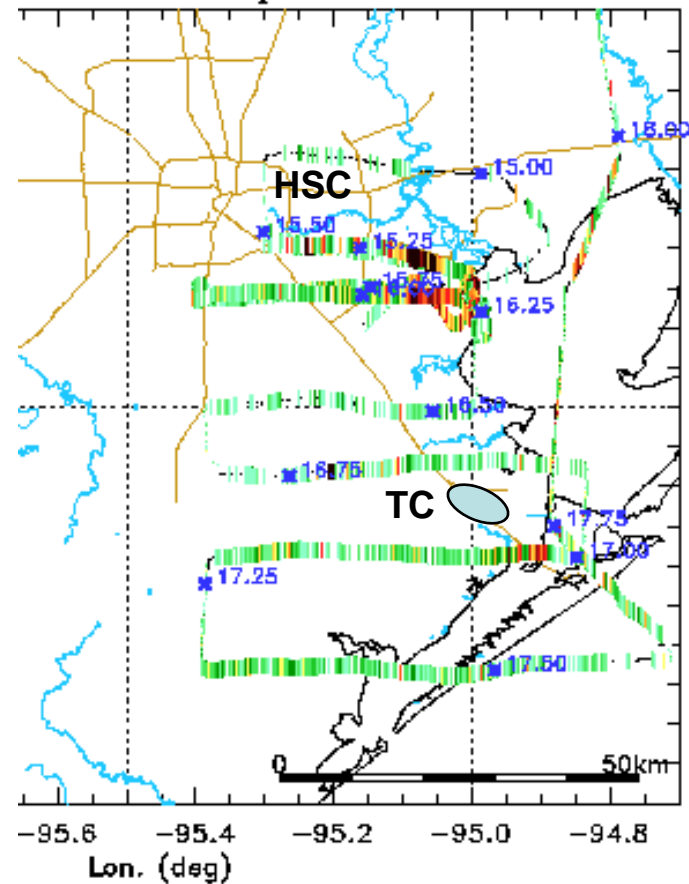
Baylor Aztec Data

9/13/06, **RAD**

HARC data: 13 Sep 2006 (0750 – 1236)



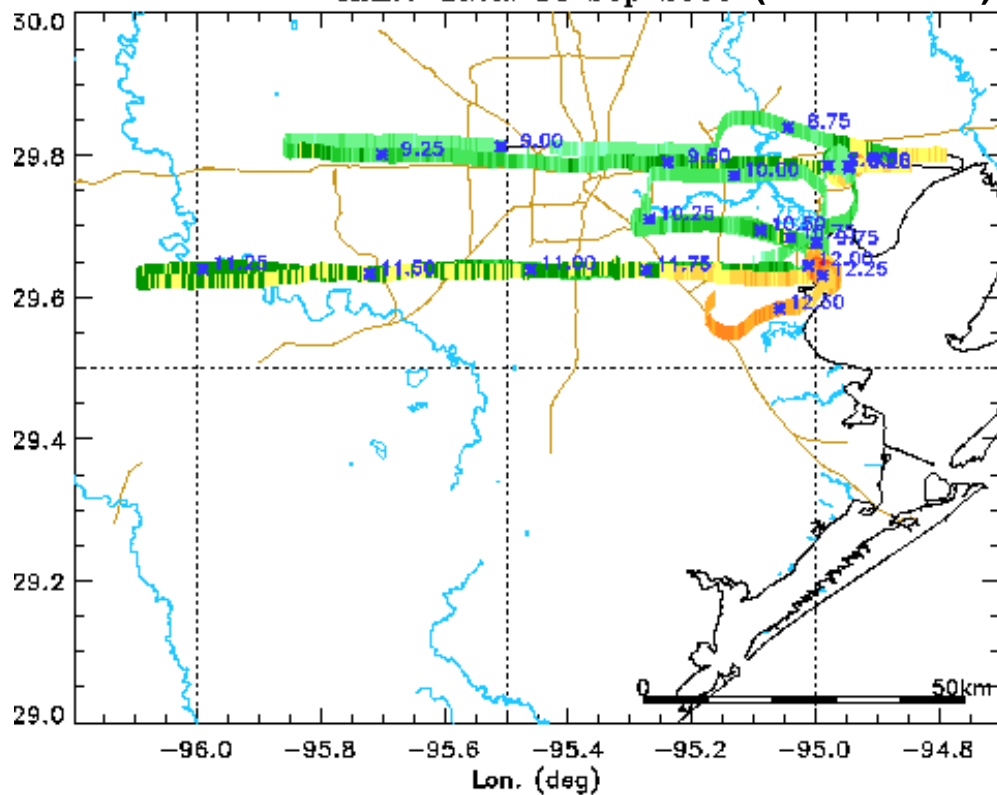
TC data: 13 Sep 2006 (1447 – 1918)



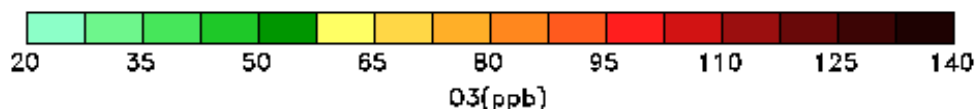
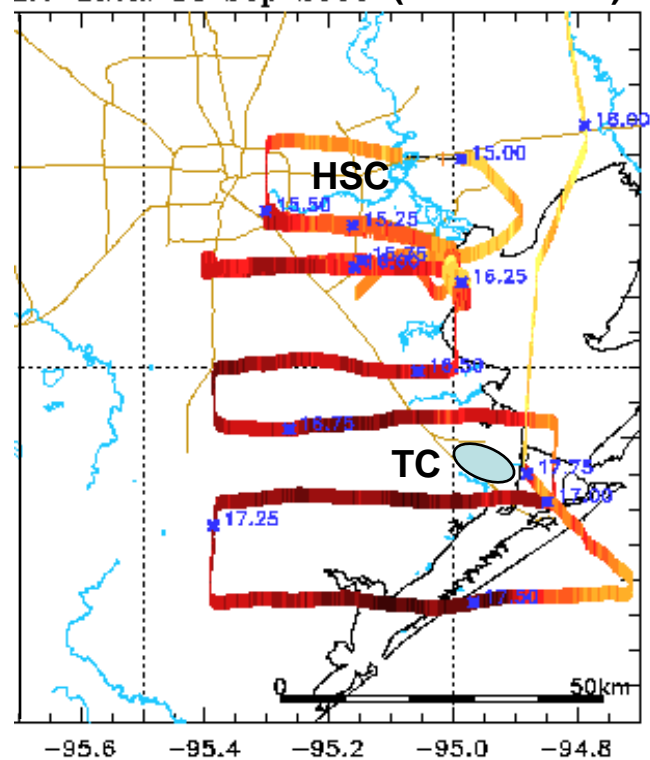
Baylor Aztec Data

9/13/06, **Ozone**

(0750 – 1236)



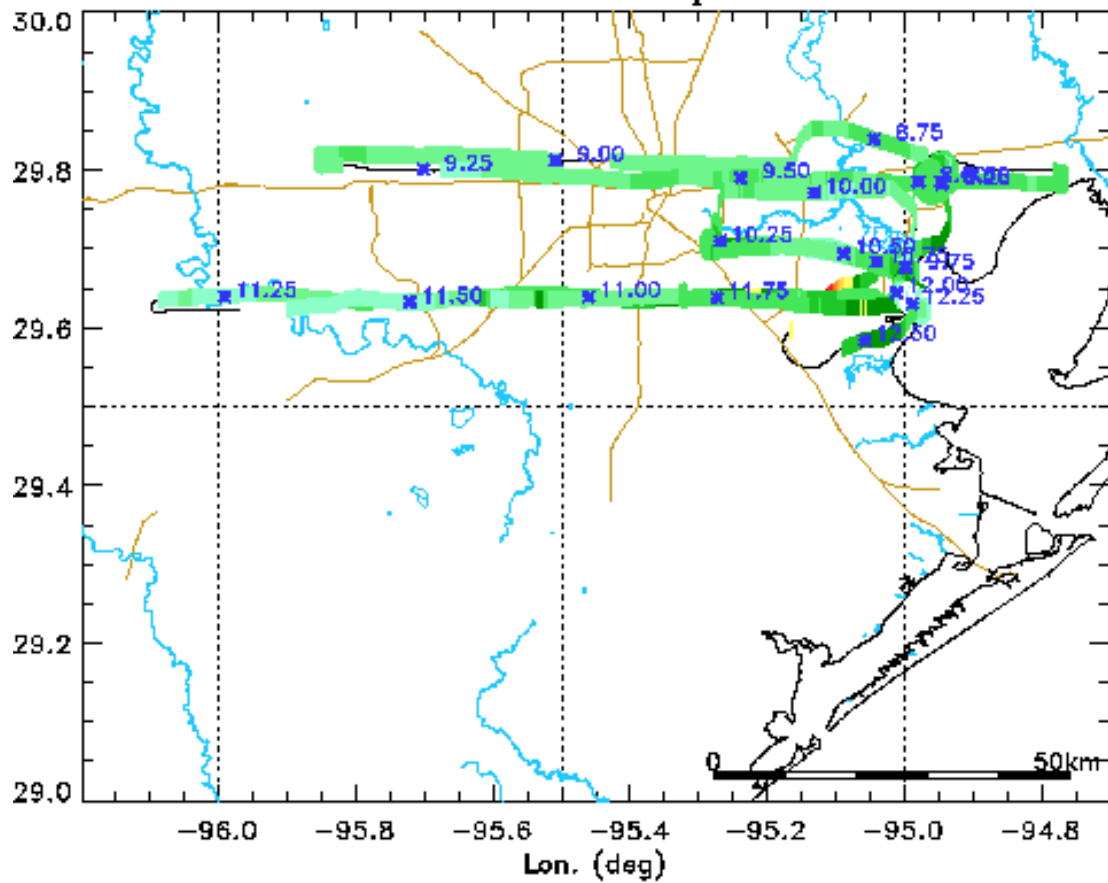
(1447 – 1918)



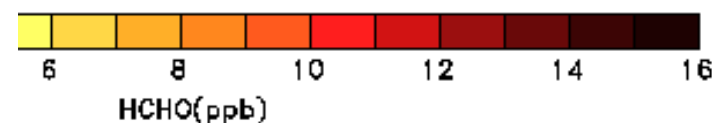
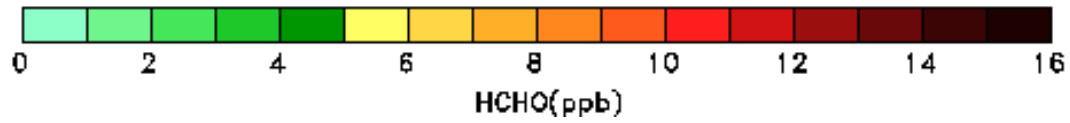
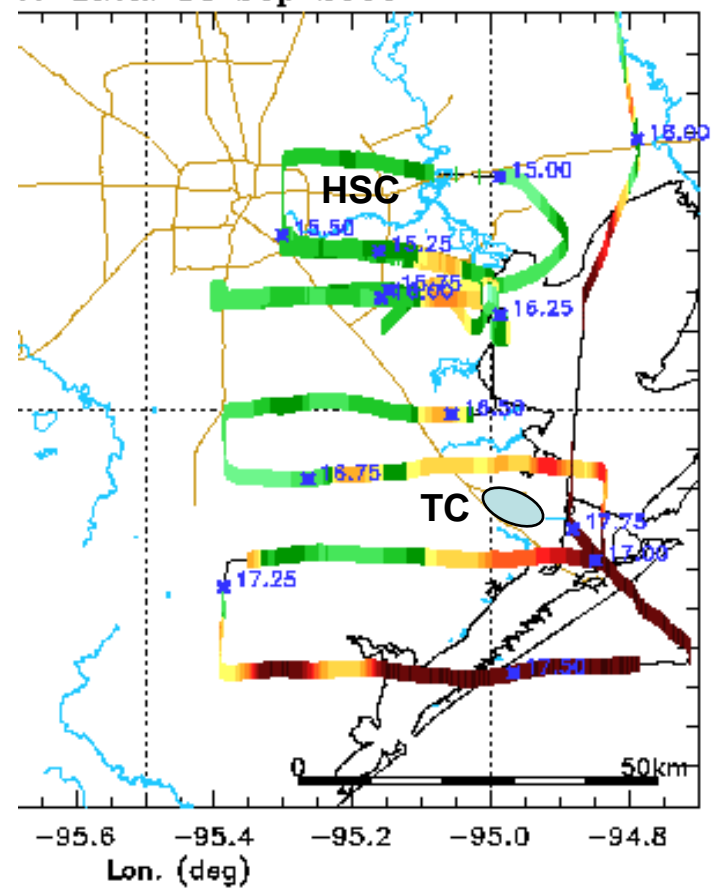
Baylor Aztec Data

9/13/06, **HCHO**

HARC data: 13 Sep 2006 (0750 – 1236)



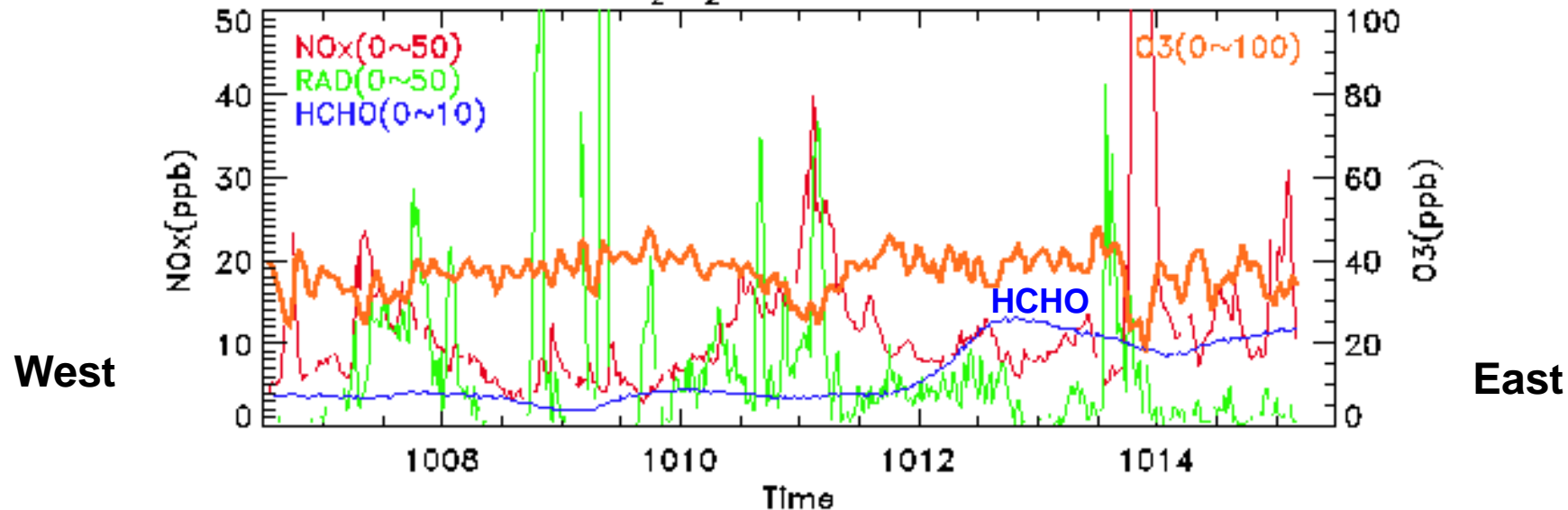
TC data: 13 Sep 2006 (1447 – 1918)



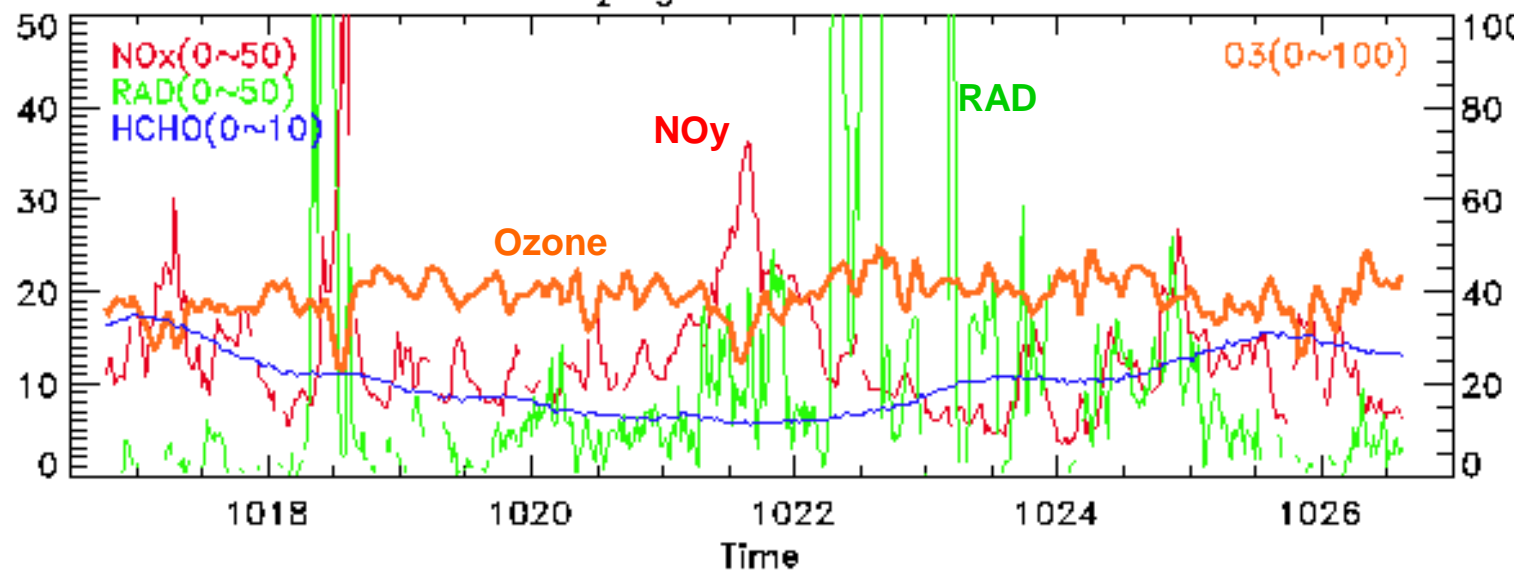
Just downwind
of HSC

HARC data: 13 Sep 2006

X₂ T₂ @ z ~ 162m



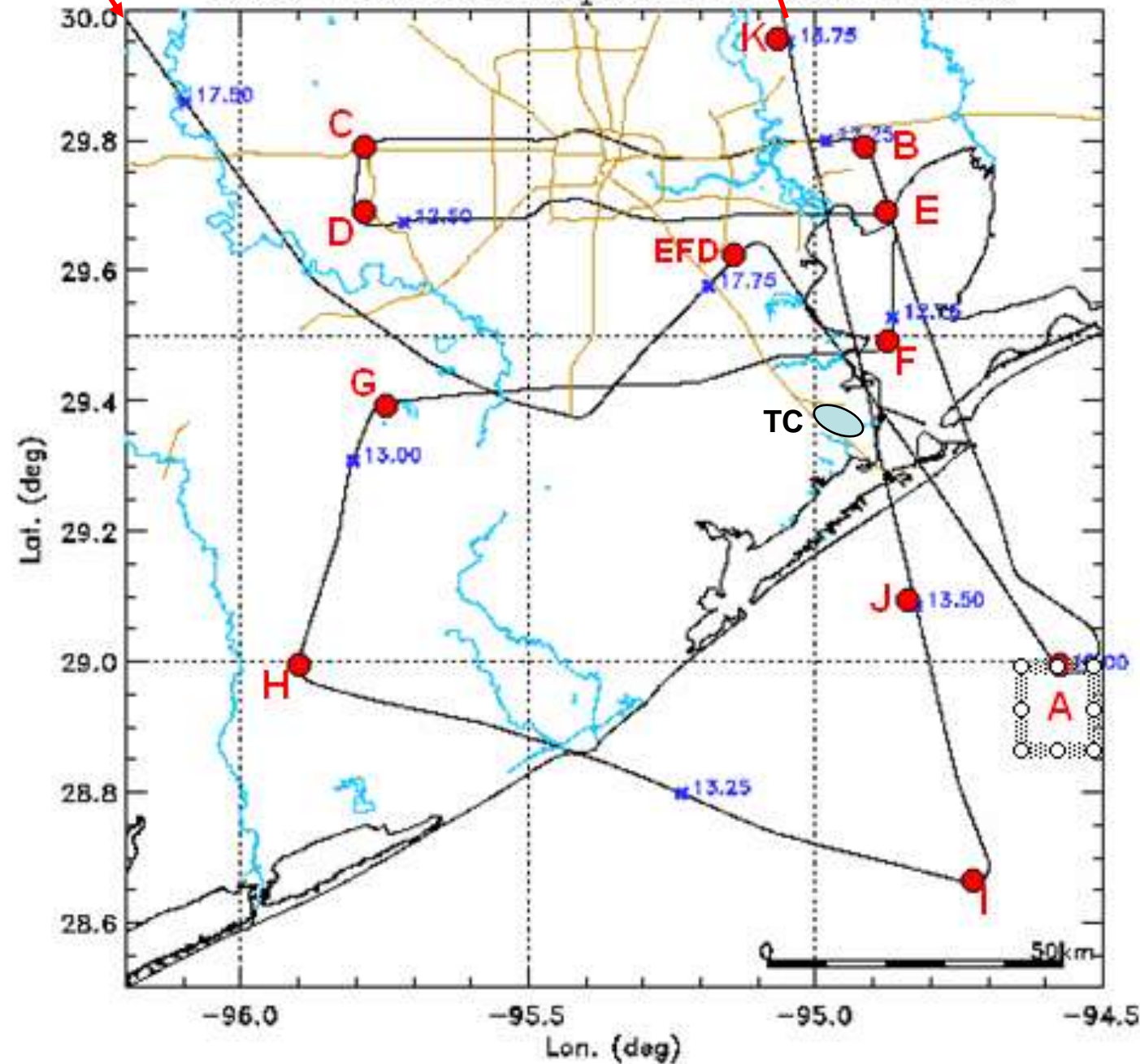
X₂ T₃ @ z ~ 233m



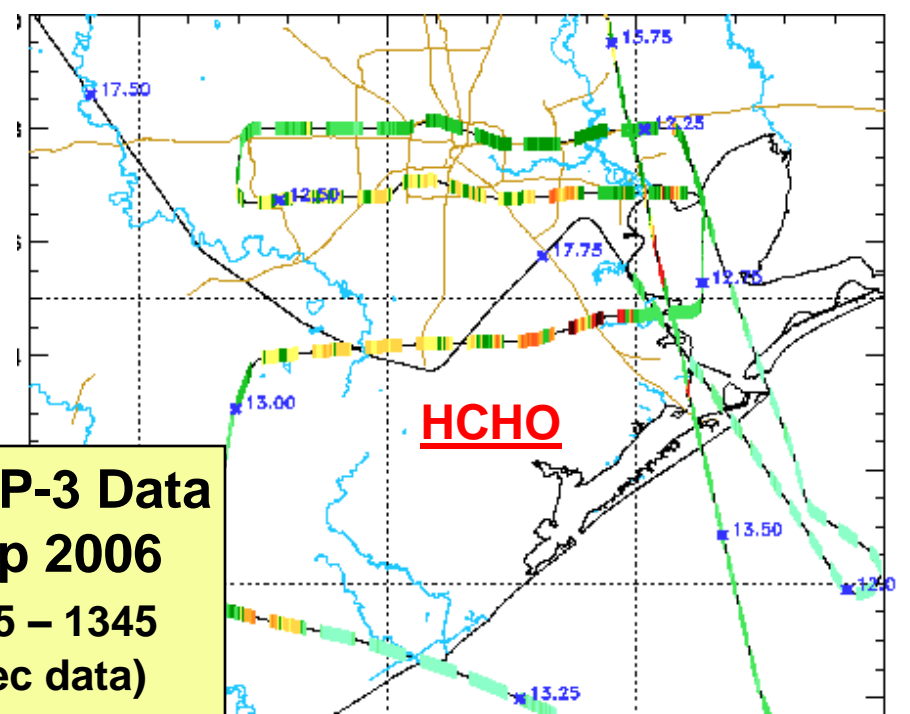
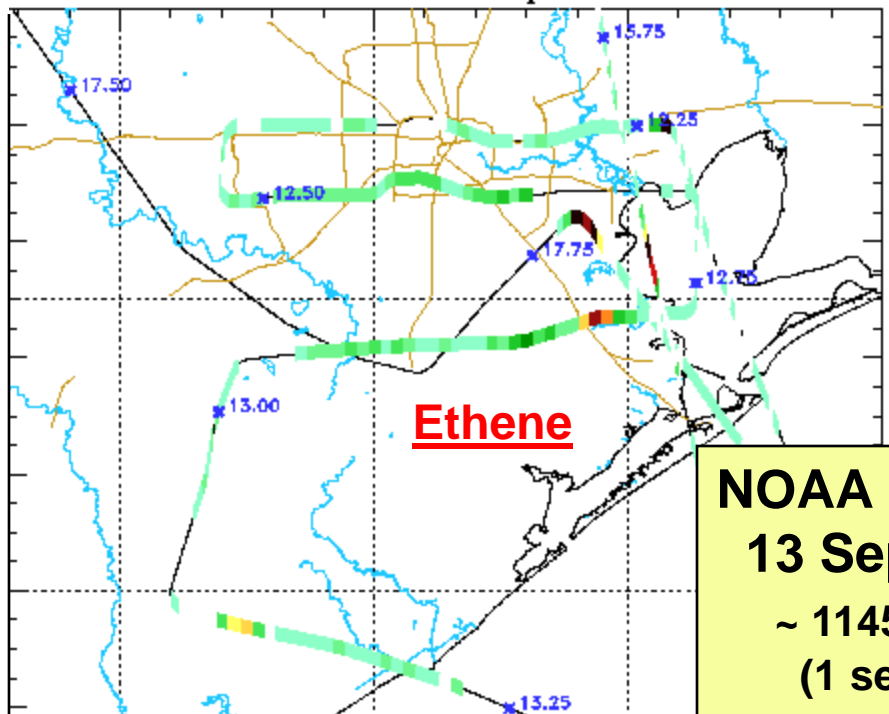
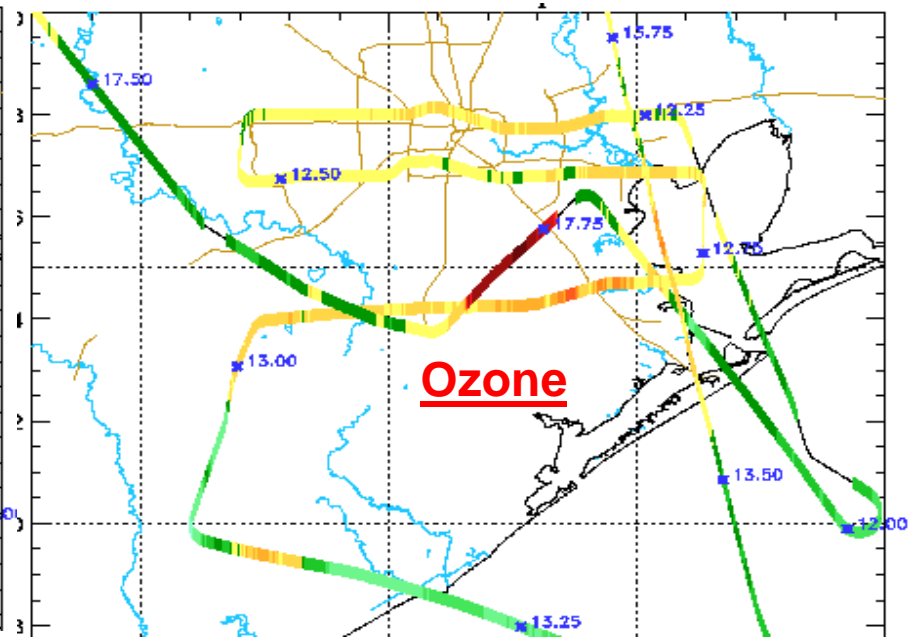
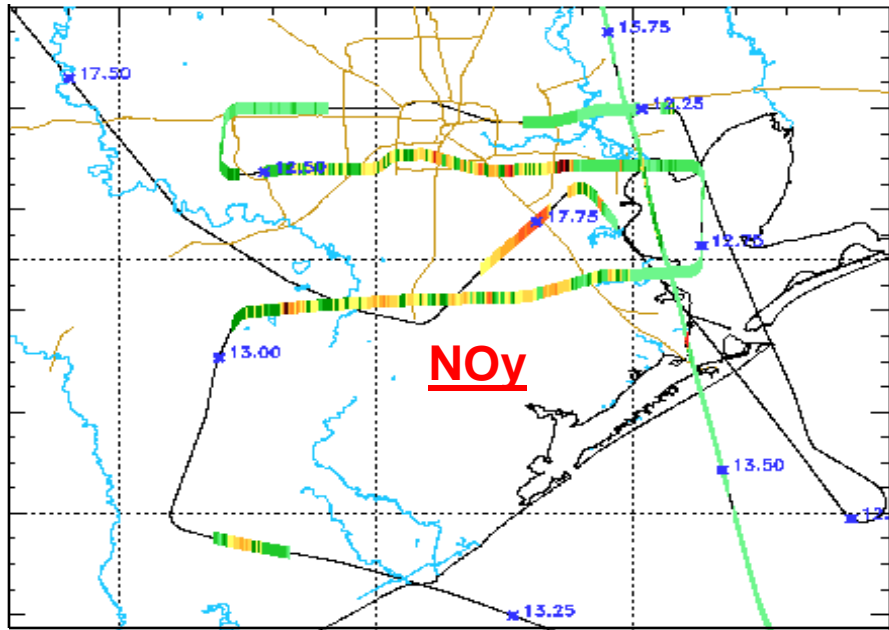
From DFW (~1745)

To DFW (~1345)

NOAA-P3 data: 13 Sep 2006 for Houston Area



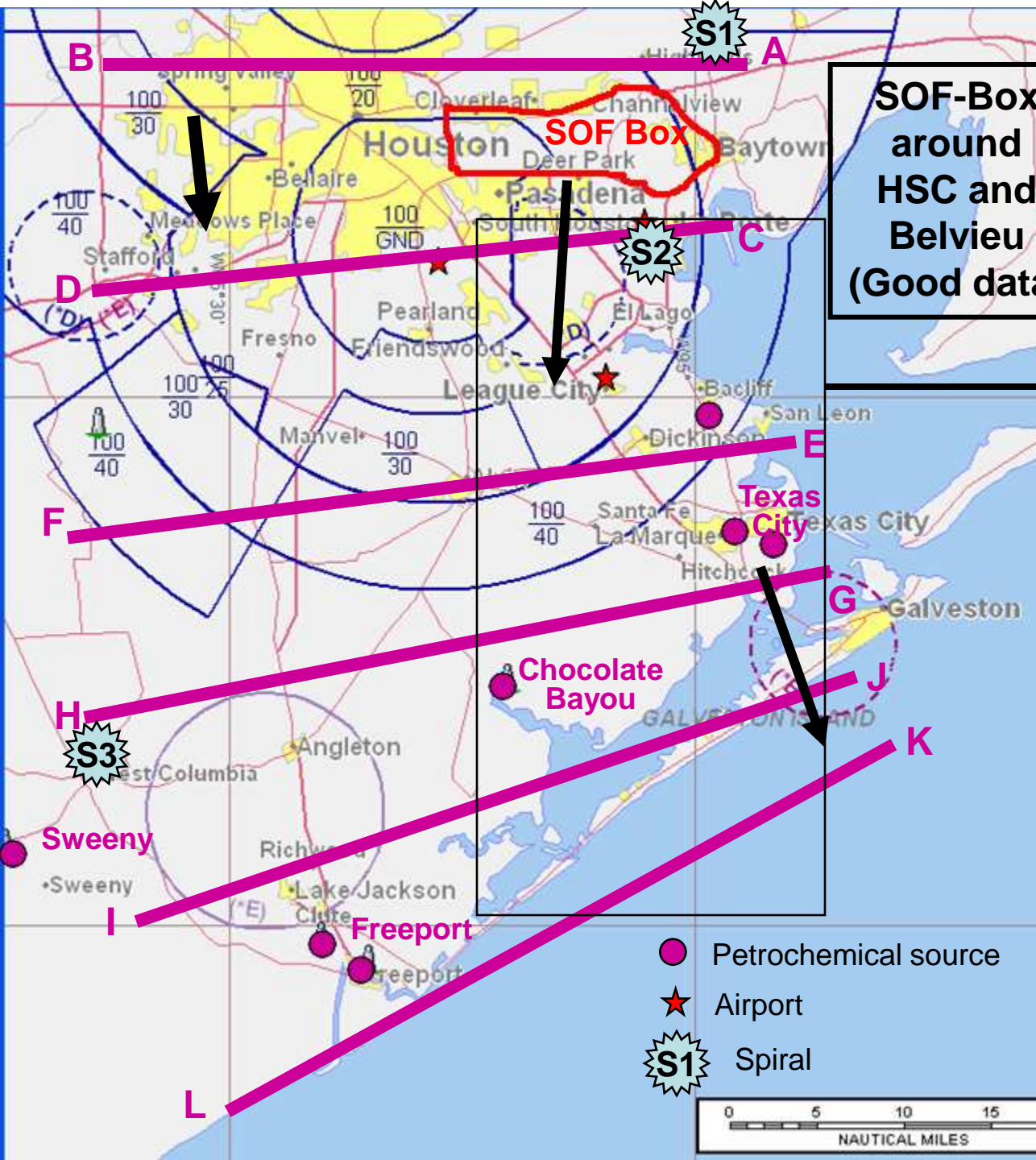
NOAA P-3
flight of
13 sep 06
in the
HOU area



NOAA P-3 Data
13 Sep 2006
~ 1145 – 1345
(1 sec data)

Aztec Flight Plan

30 Aug 2006



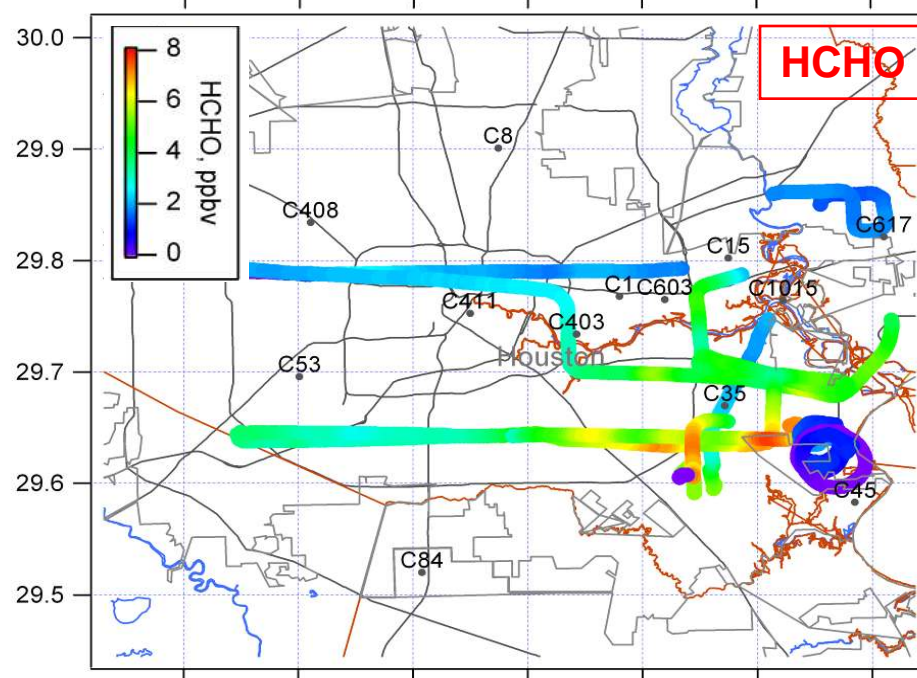
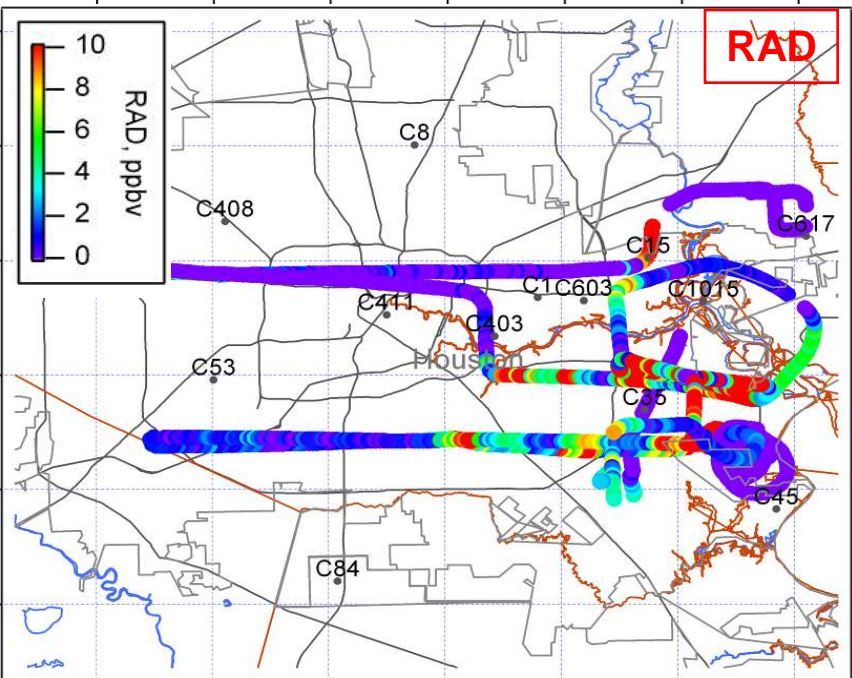
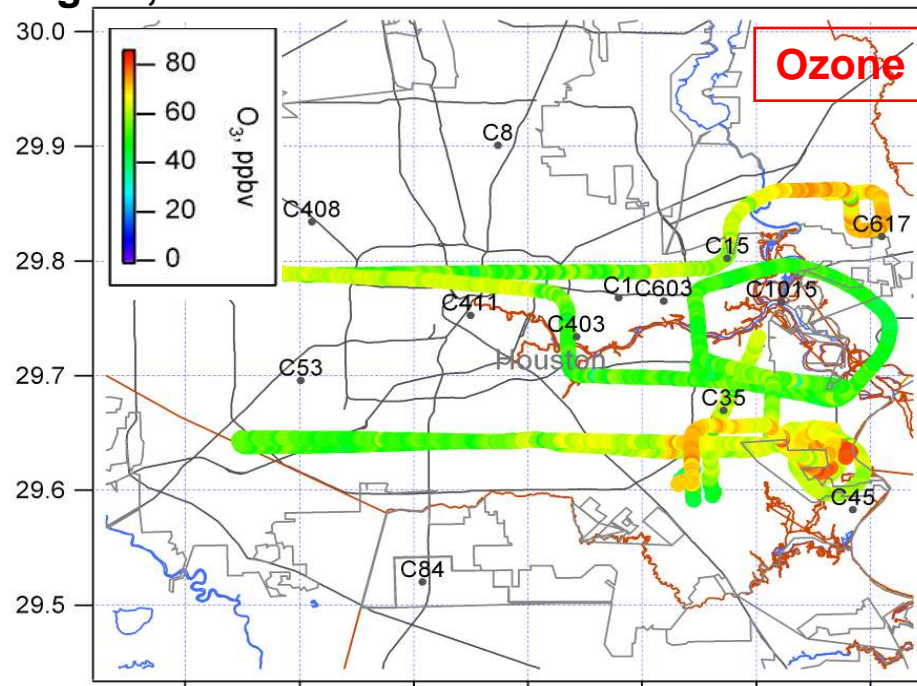
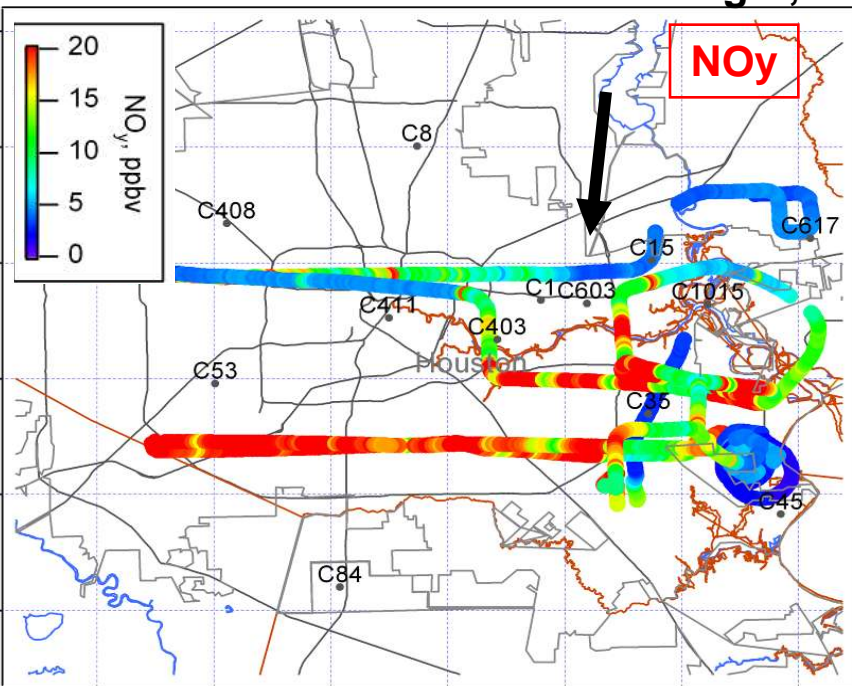
**SOF-Box
around
HSC and
Belvieu
(Good data)**

TexAQS II Smart Balloon Flight ID 2



- Petrochemical source
- ★ Airport
- S1** Spiral

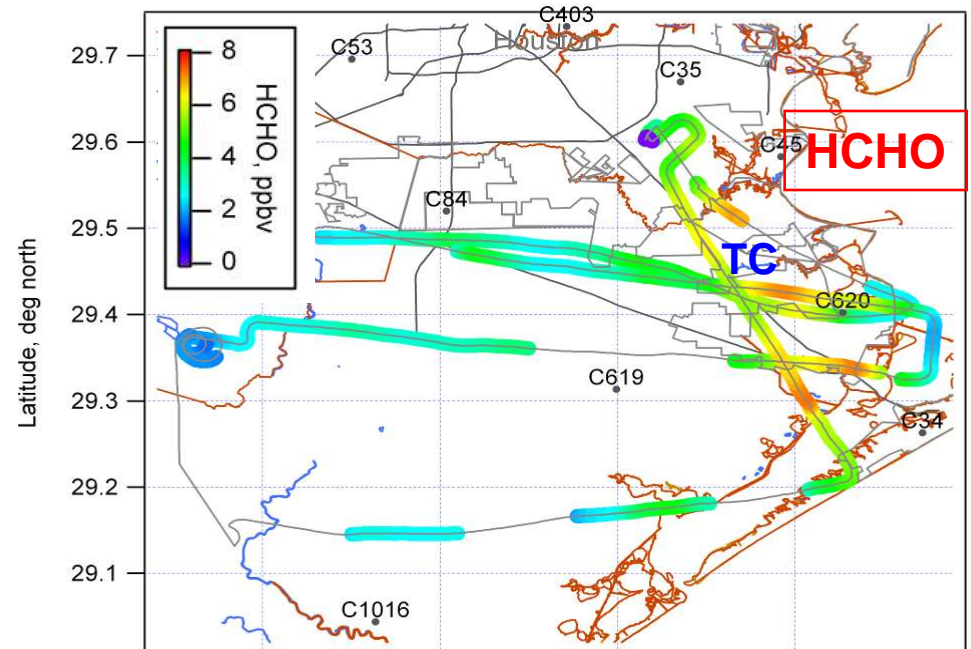
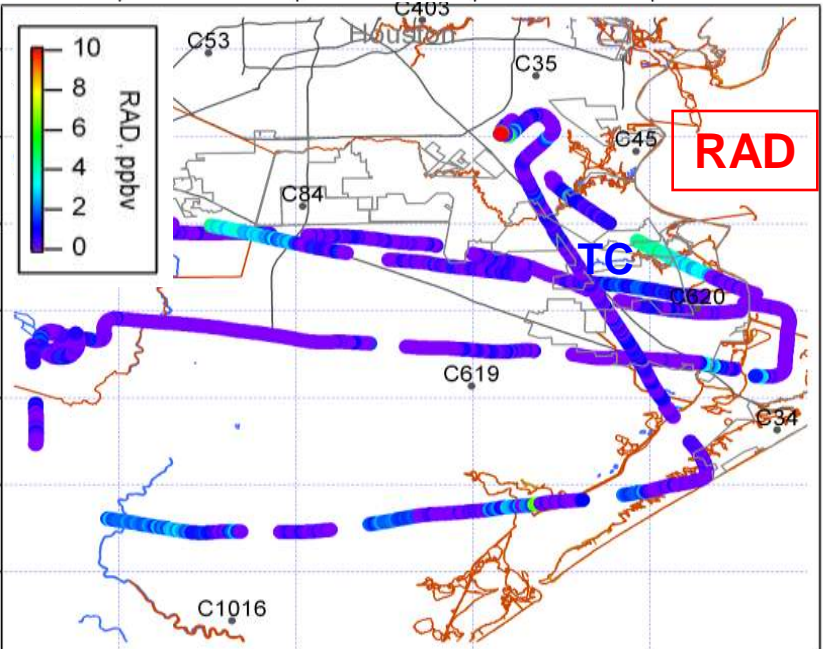
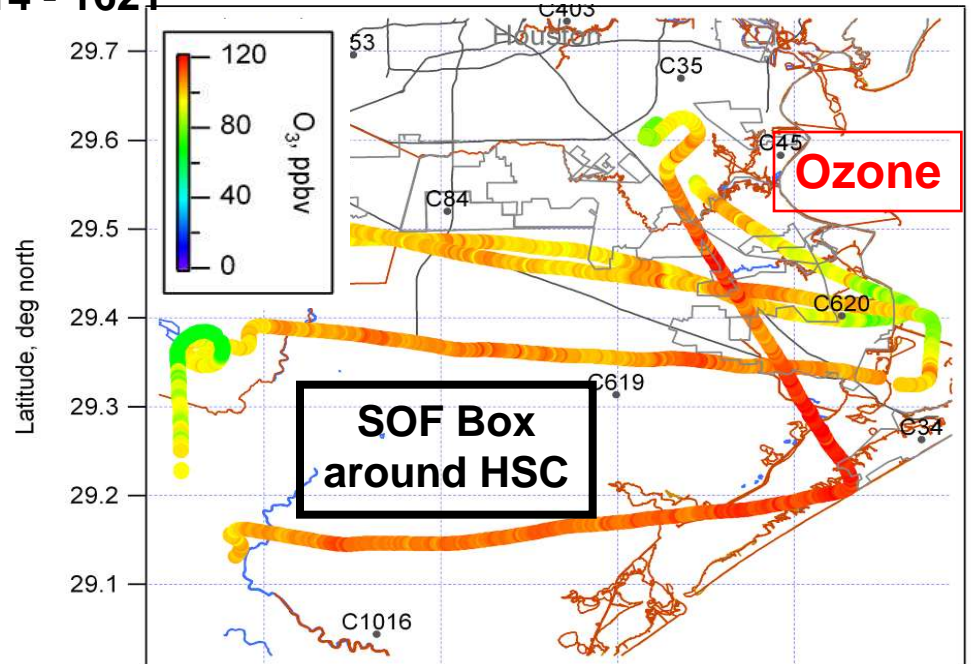
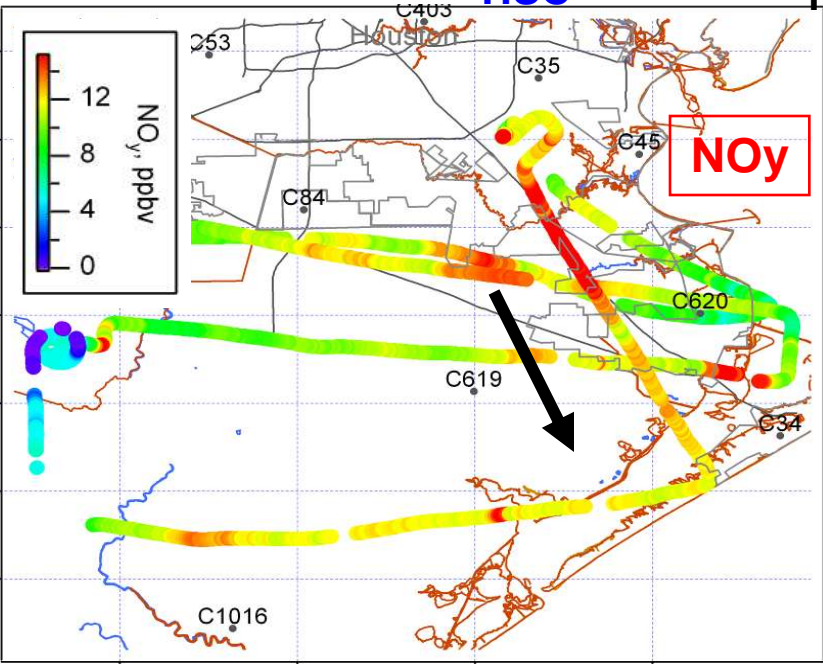
Aztec Flight, 30 August, 0858 - 1105



Aztec Flight, 30 August 1414 - 1621

HSC

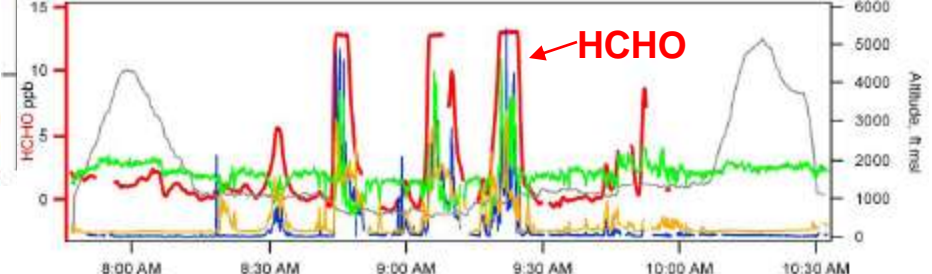
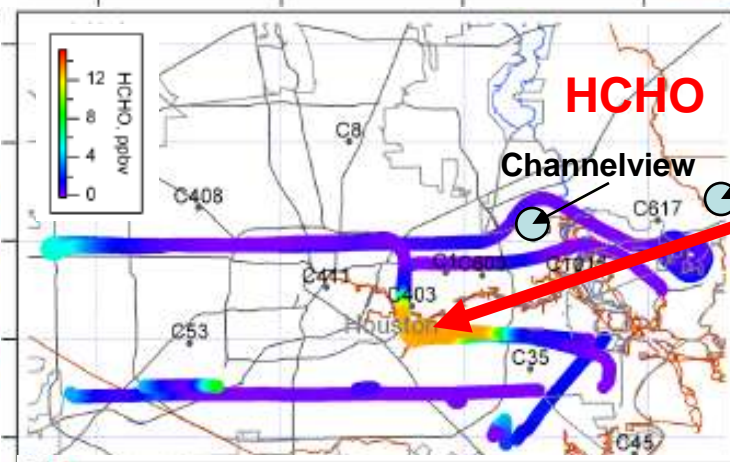
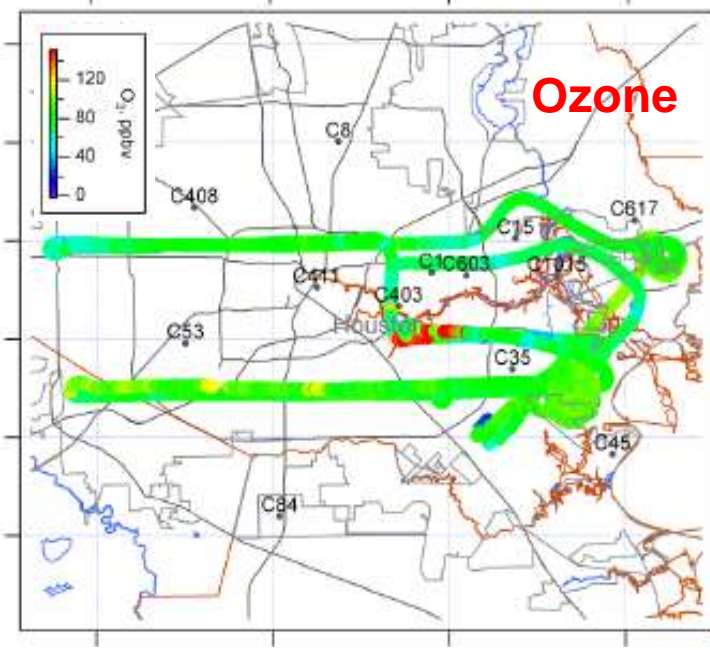
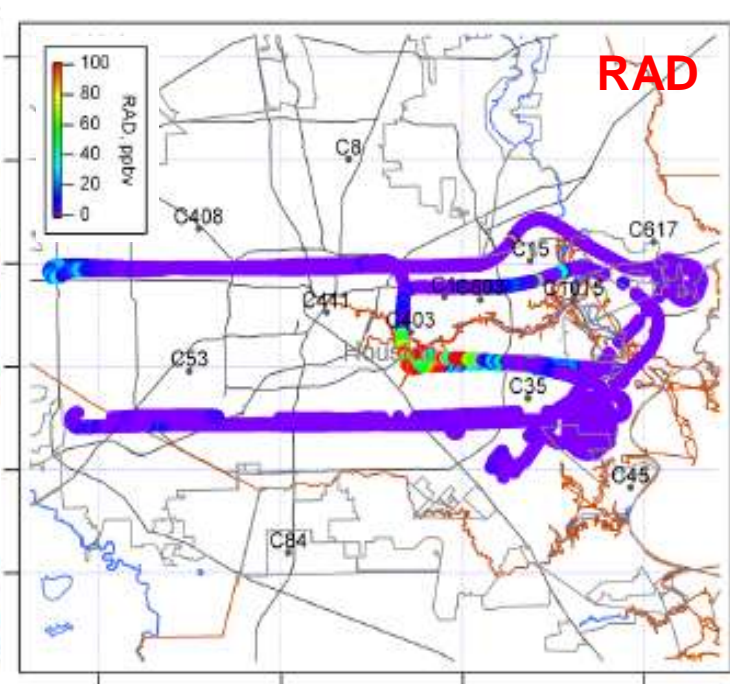
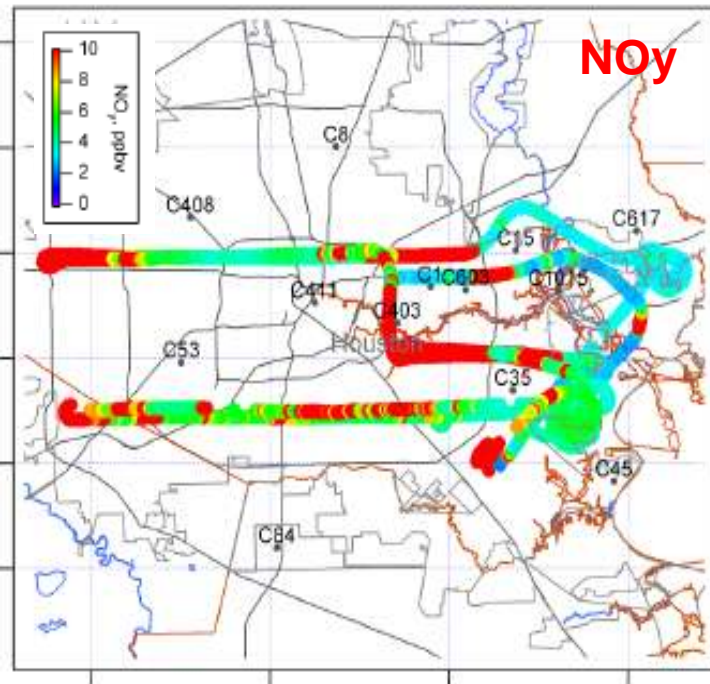
HSC



Aztec Flight 31 Aug 2006

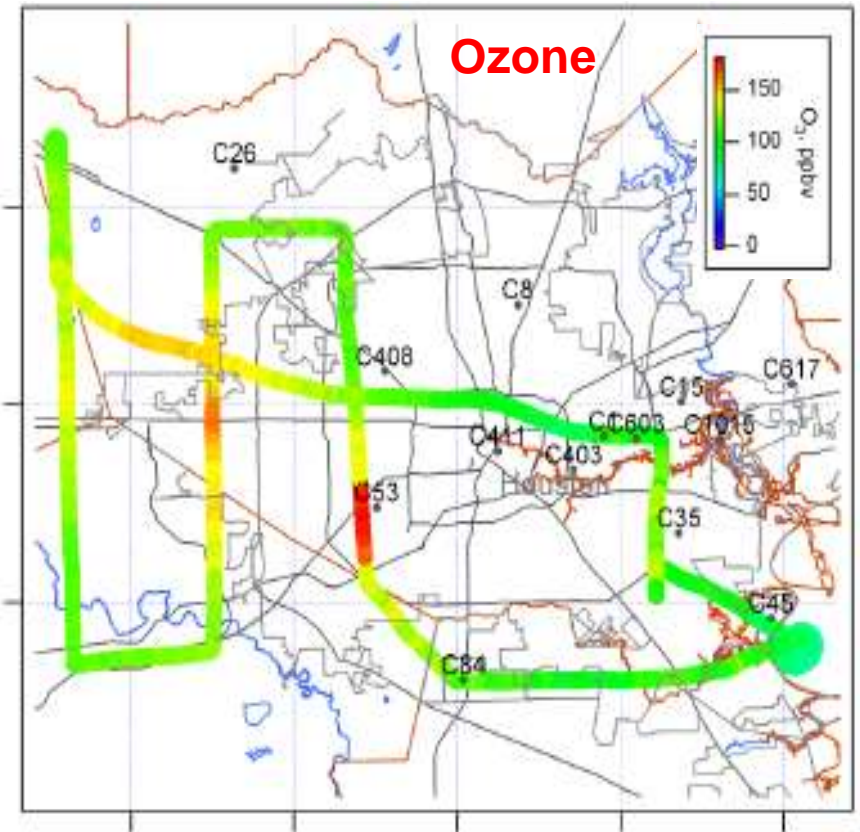
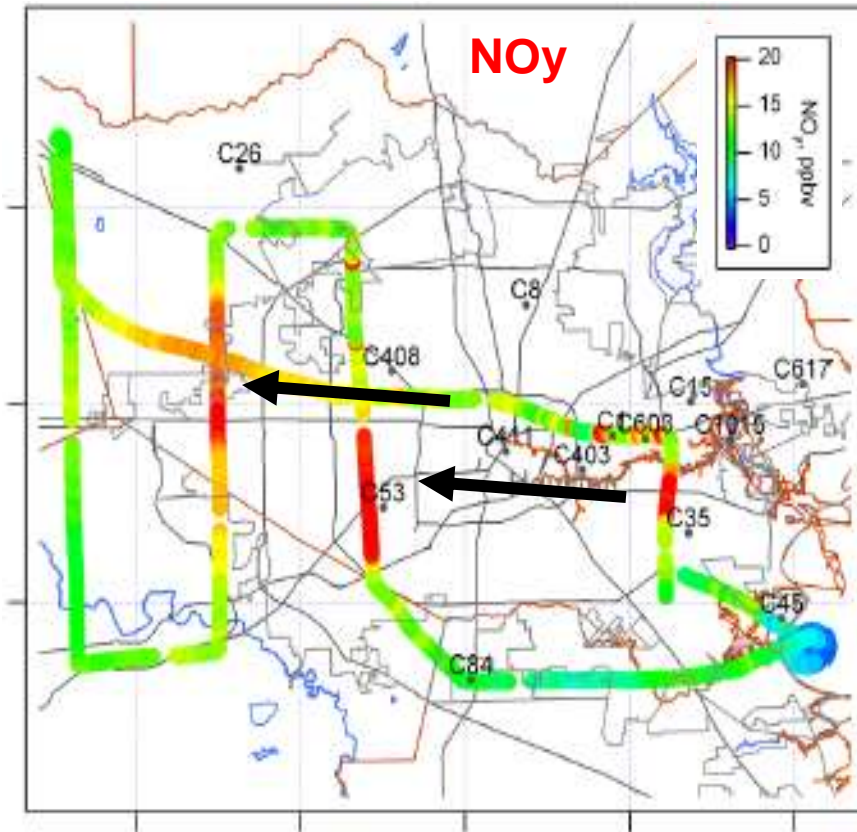
Morning
(0745 – 1032)

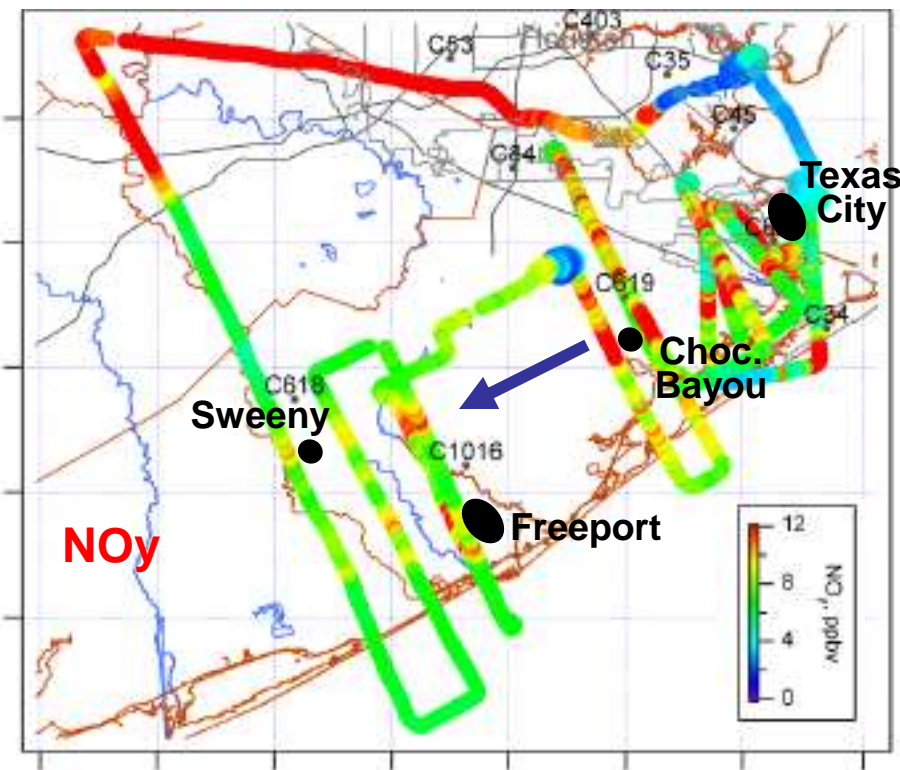
SOF-Box
around
Channelview



Aztec Flight 31 Aug 2006

Afternoon
(1418 – 1618)

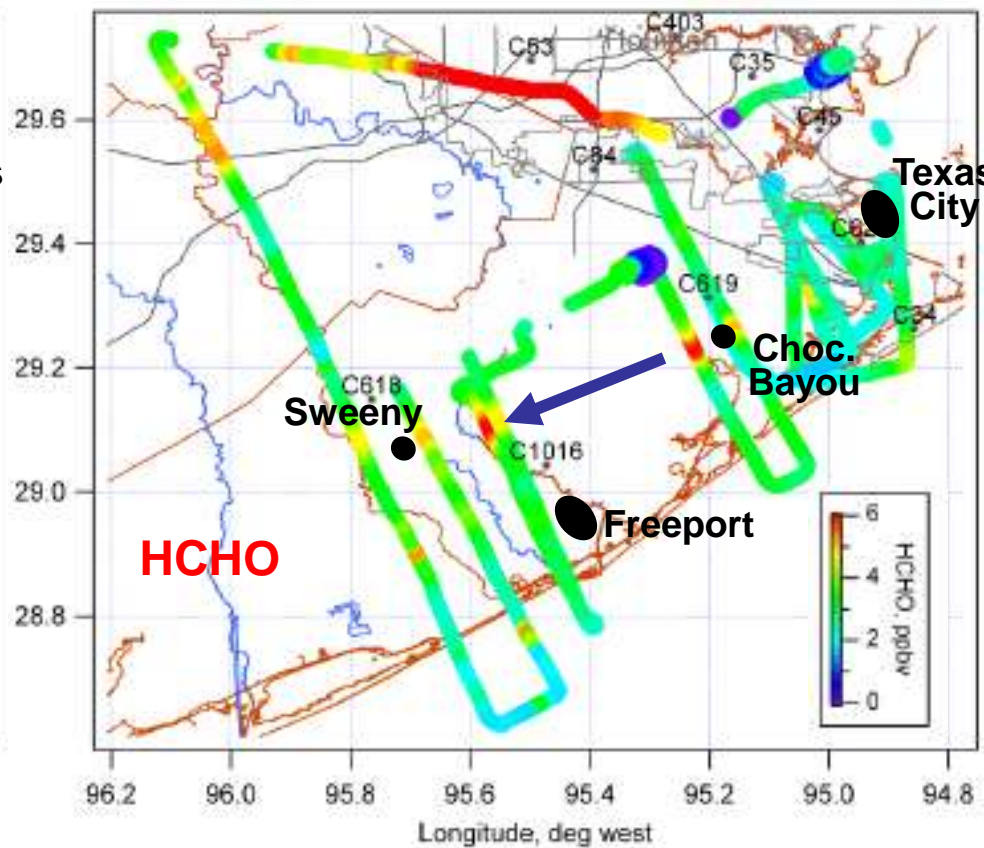




NO_y

**Aztec Flight
20 Sep 2006**

0814 - 1344

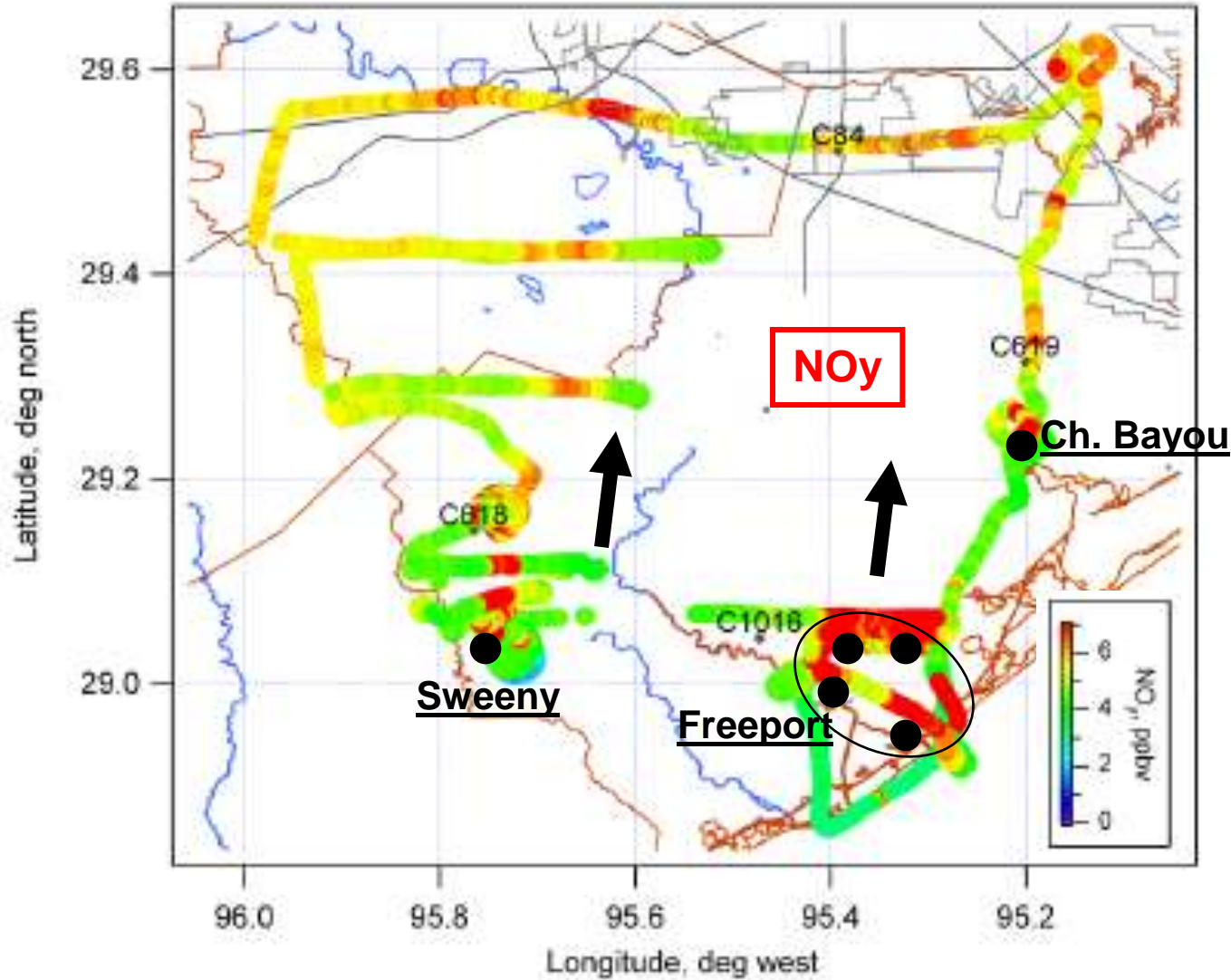


HCHO

**SOF-Box
around
Texas City**

Aztec Flight, 27 Sep 2006

1213 - 1739



**SOF-Boxes
around
Ch. Bayou,
Freeport,
and
Sweeny**

Analysis can include:

1. **LES-chem or LRPM in the near field to characterize actual emissions based on SOF data and aircraft data**

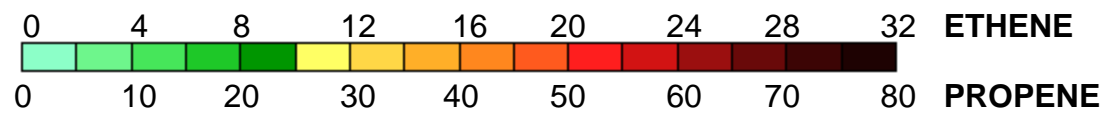
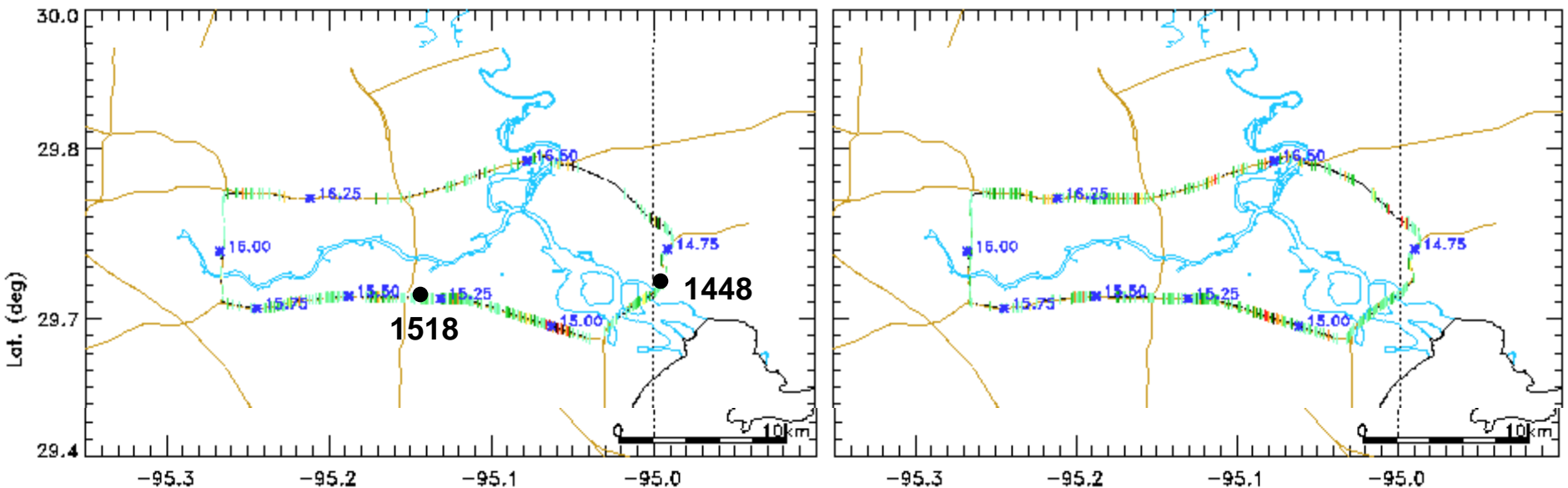
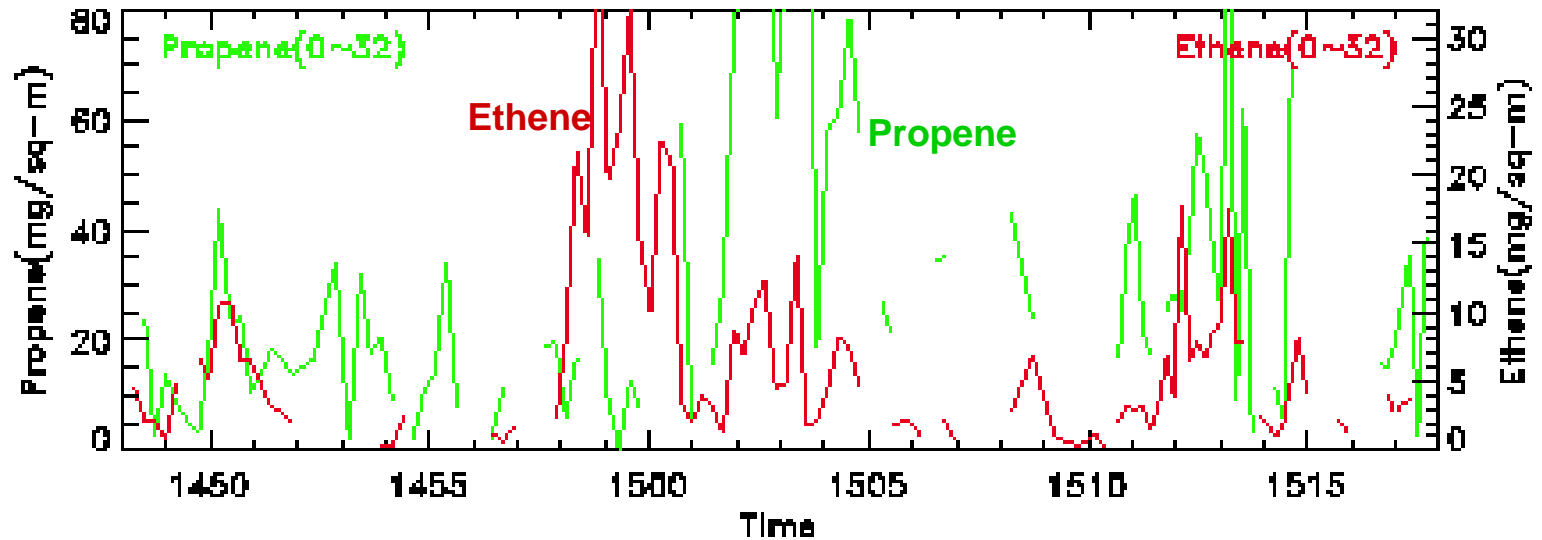
(LESchem fine-resolves dynamics and chemistry vertically and horizontally in the near-field; LRPM fine-resolves, but with parameterized mixing (Ky, Kz))

Main goals of LRPM diagnostic study for TERC

2. **LRPM in the near-field to estimate primary emissions of NO_x and HRVOC, with guidance also from the LES study of 9/13/06, and farther downwind for second TDEV based on secondary formations, and to quantitatively study the impact of secondary products formation, including O₃, NO_z, and HCHO (and H₂O₂/HNO₃ for ozone sensitivity analysis)**
3. **LRPM analysis can also explore primary/secondary HCHO, and HONO production, and their relevance to radical chemistry.**

SOF Data, 13 Sep 2006

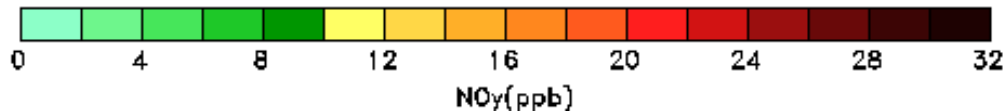
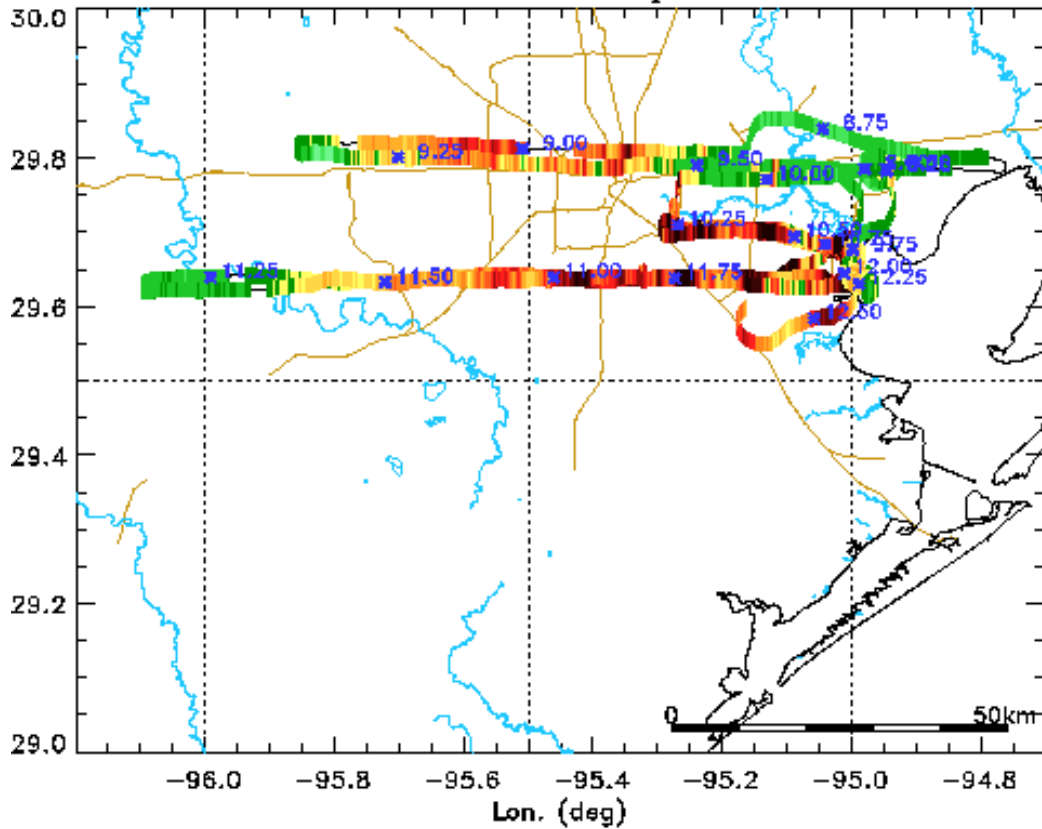
144800-151800



Baylor Aztec Data

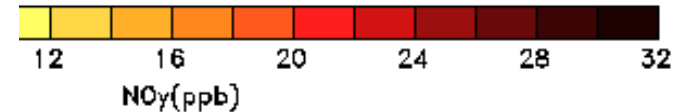
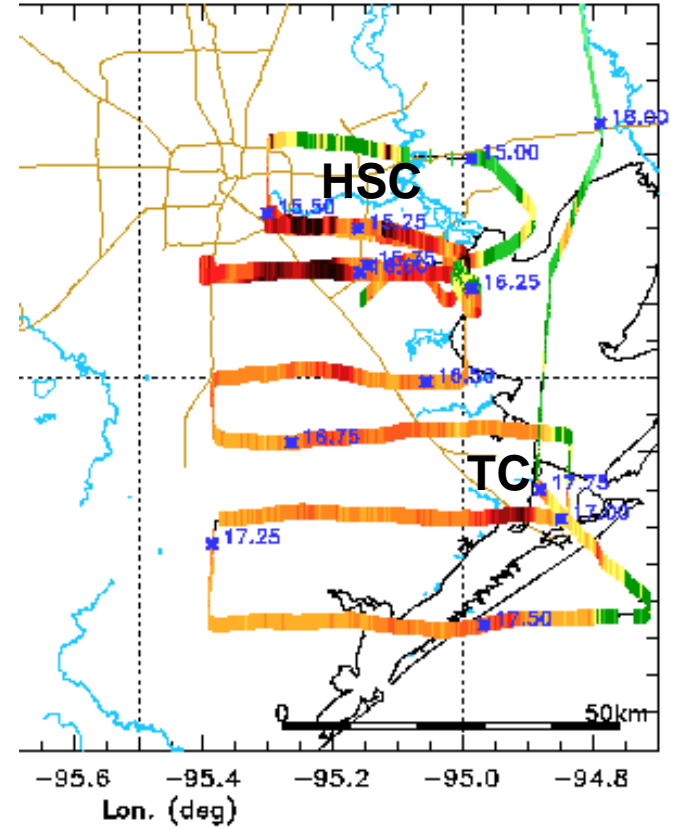
9/13/06, **NO_y**

HARC data: 13 Sep 2006 (0750 – 1236)



SOF: HSC in pm

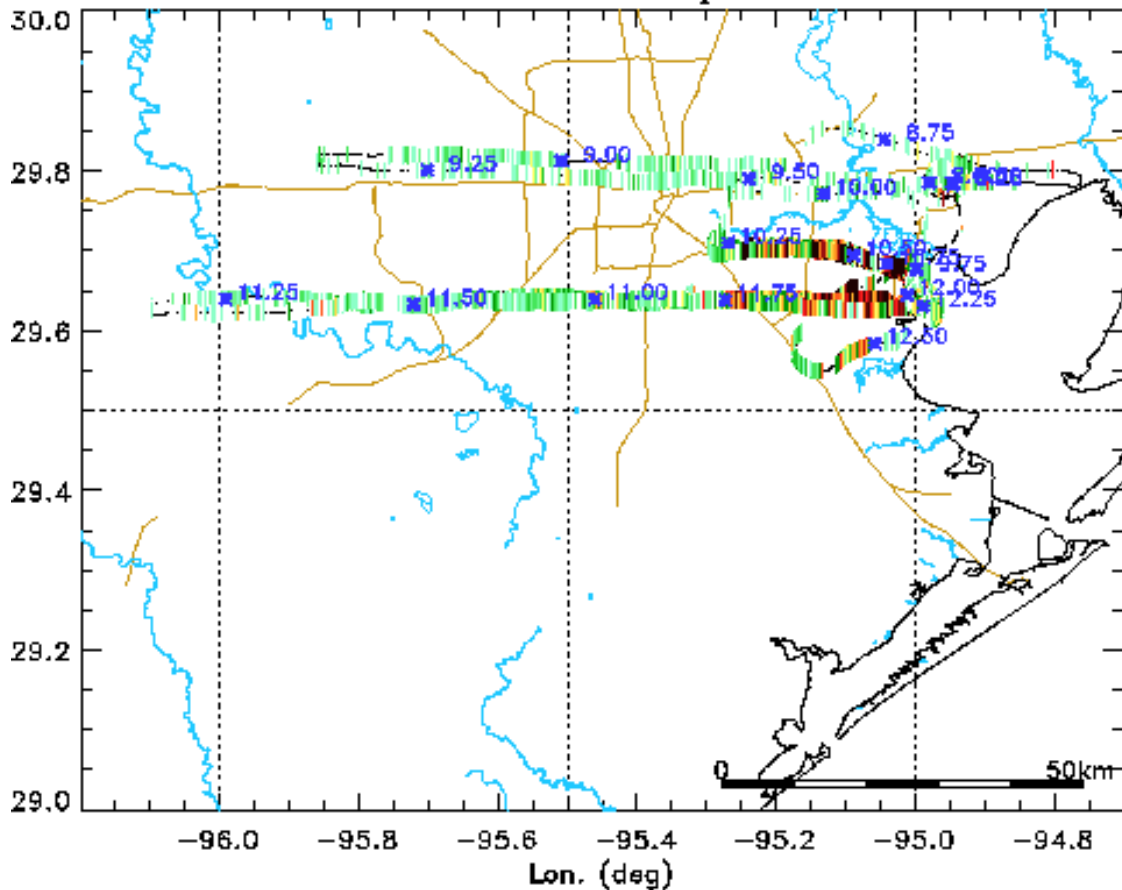
SC data: 13 Sep 2006 (1447 – 1918)



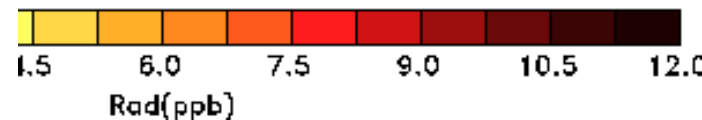
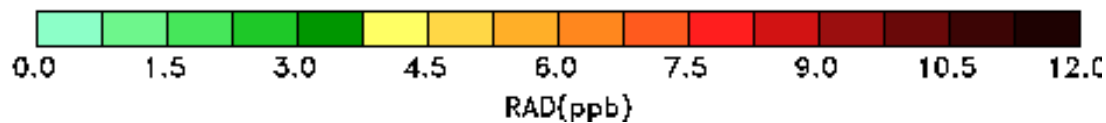
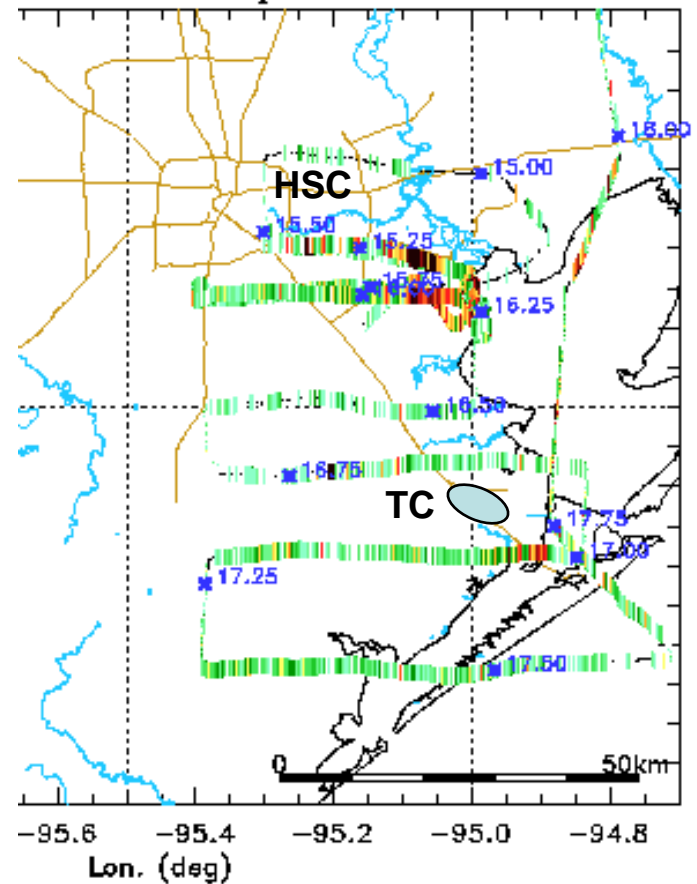
Baylor Aztec Data

9/13/06, **RAD**

HARC data: 13 Sep 2006 (0750 – 1236)



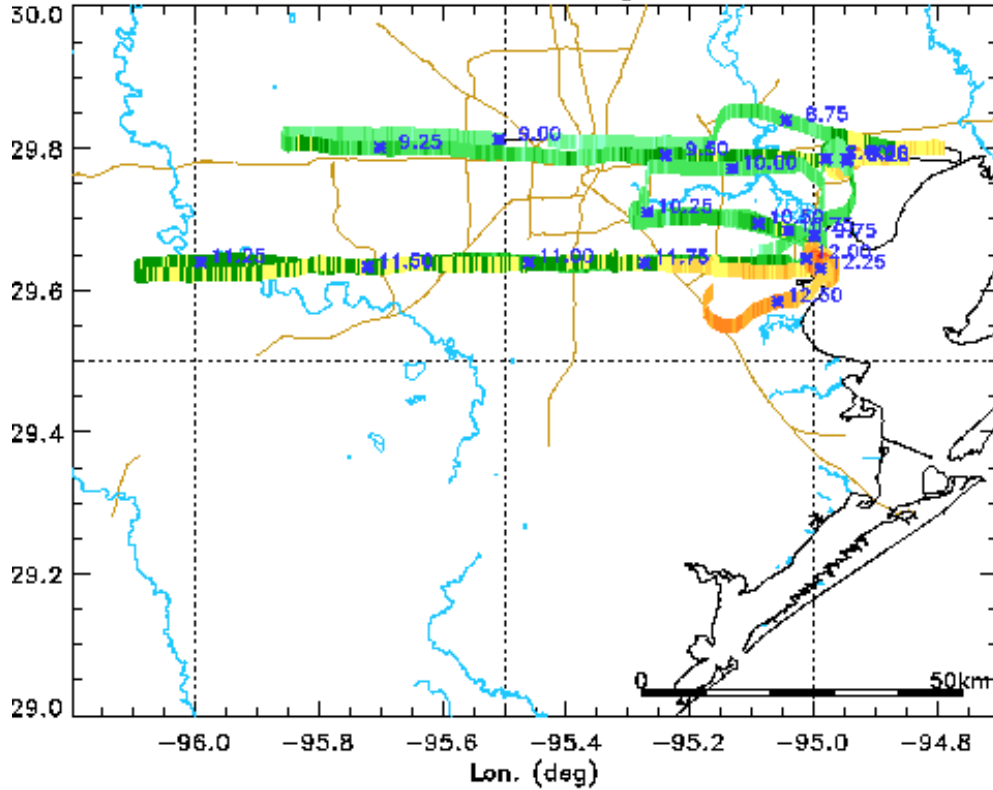
TC data: 13 Sep 2006 (1447 – 1918)



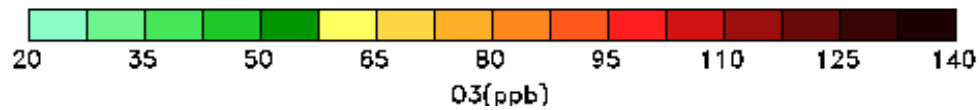
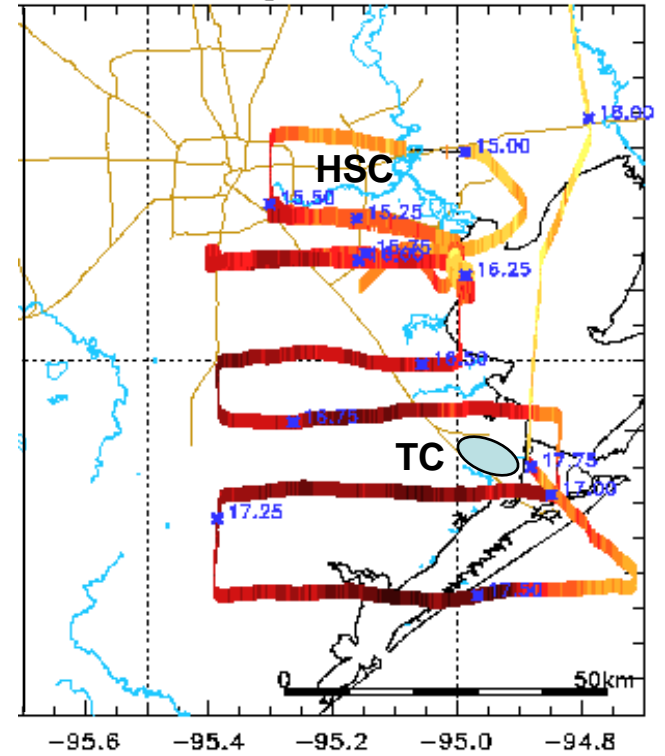
Baylor Aztec Data

9/13/06, **Ozone**

(0750 – 1236)



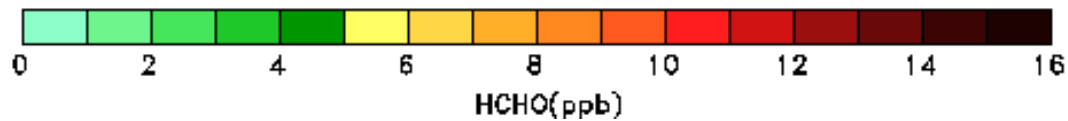
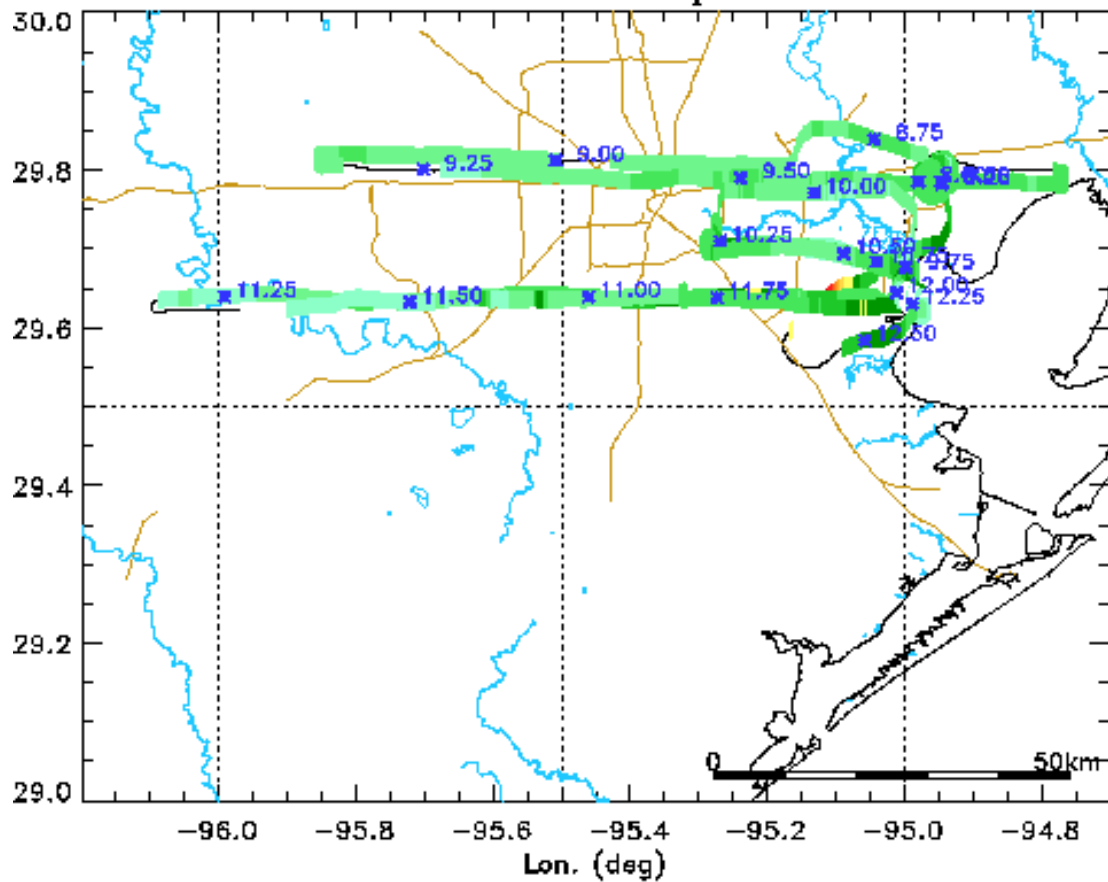
(1447 – 1918)



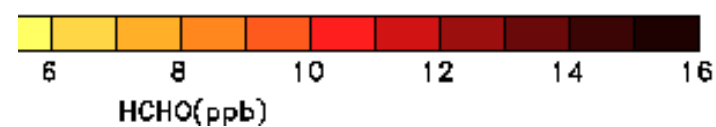
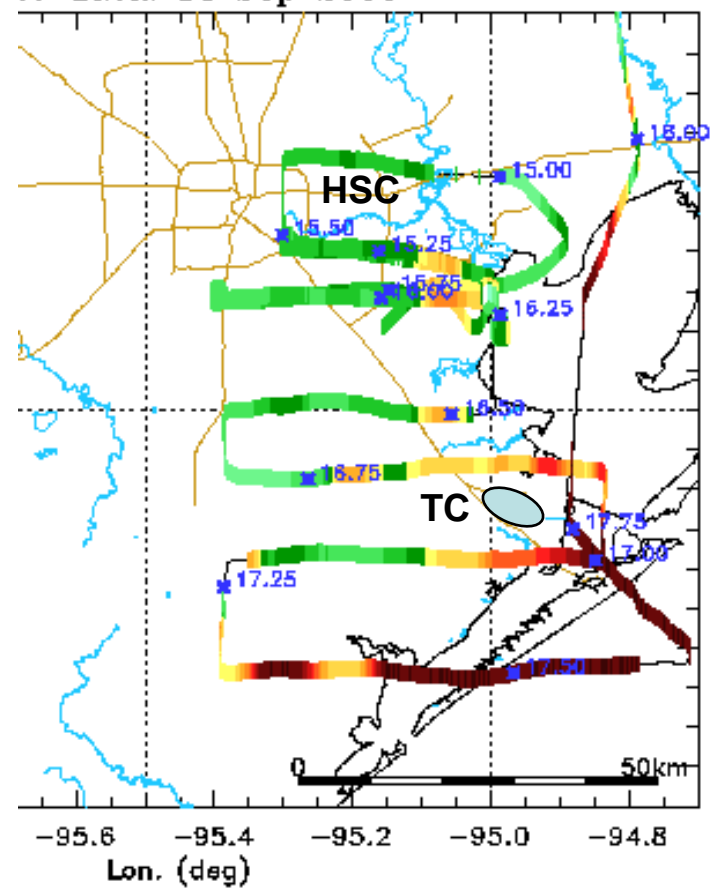
Baylor Aztec Data

9/13/06, **HCHO**

HARC data: 13 Sep 2006 (0750 – 1236)



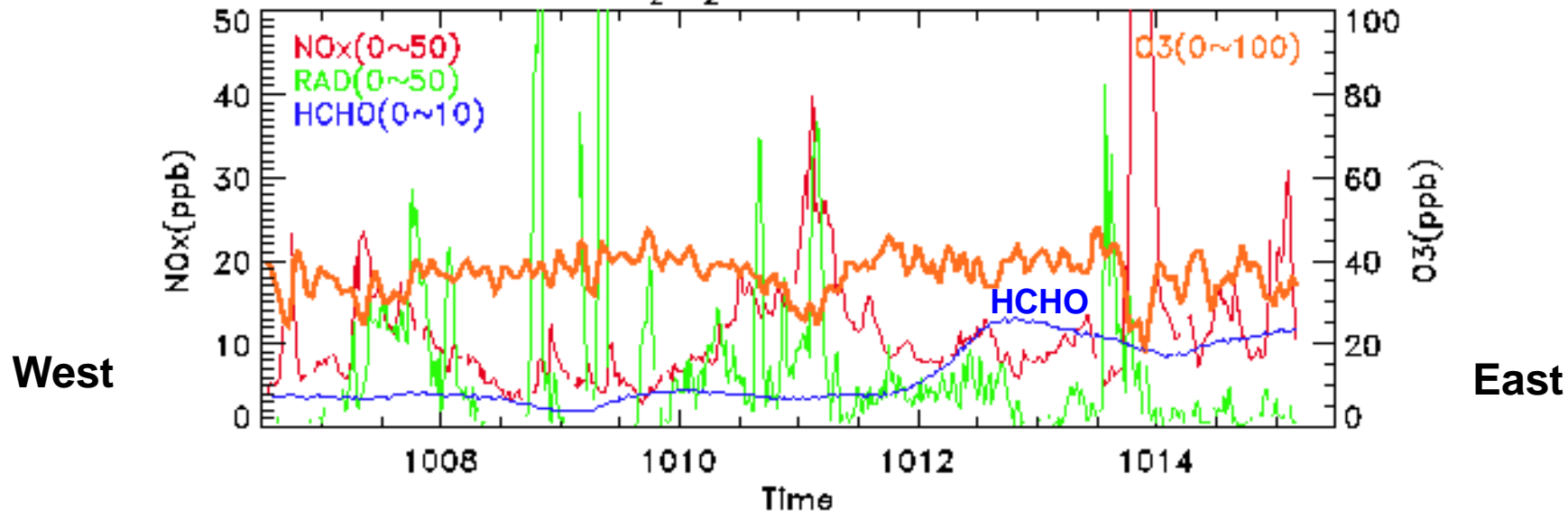
TC data: 13 Sep 2006 (1447 – 1918)



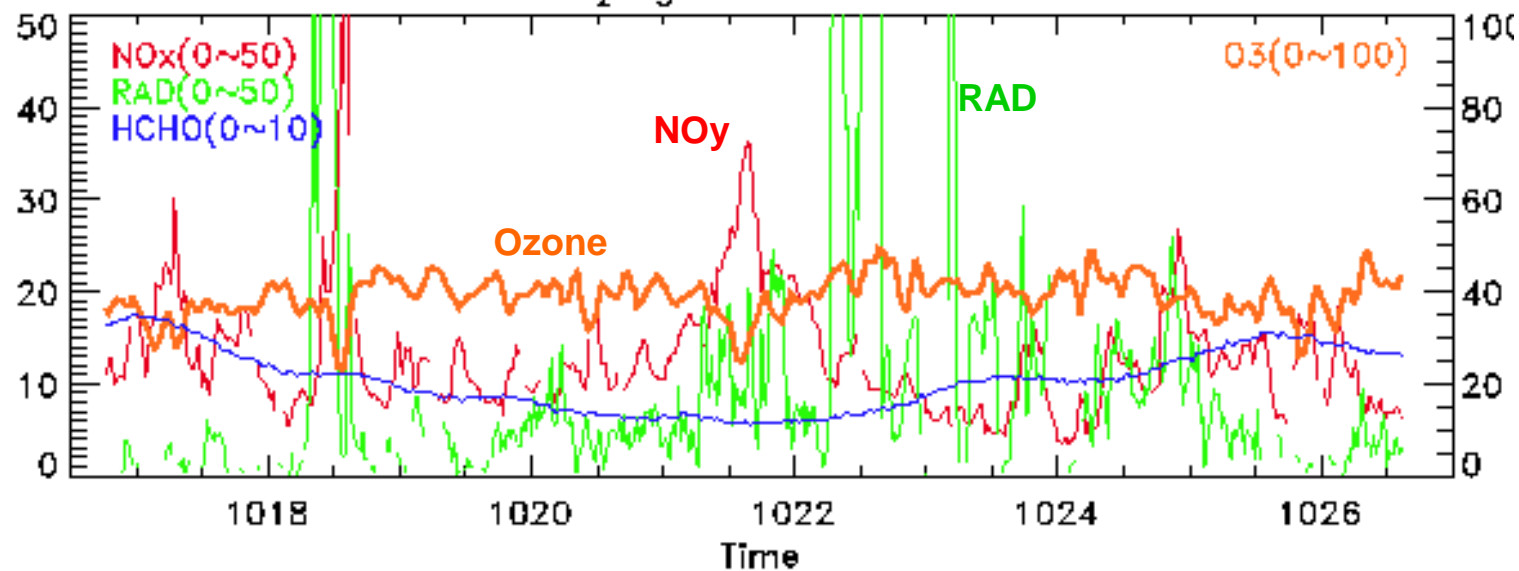
Just downwind
of HSC

HARC data: 13 Sep 2006

X₂ T₂ @ z ~ 162m



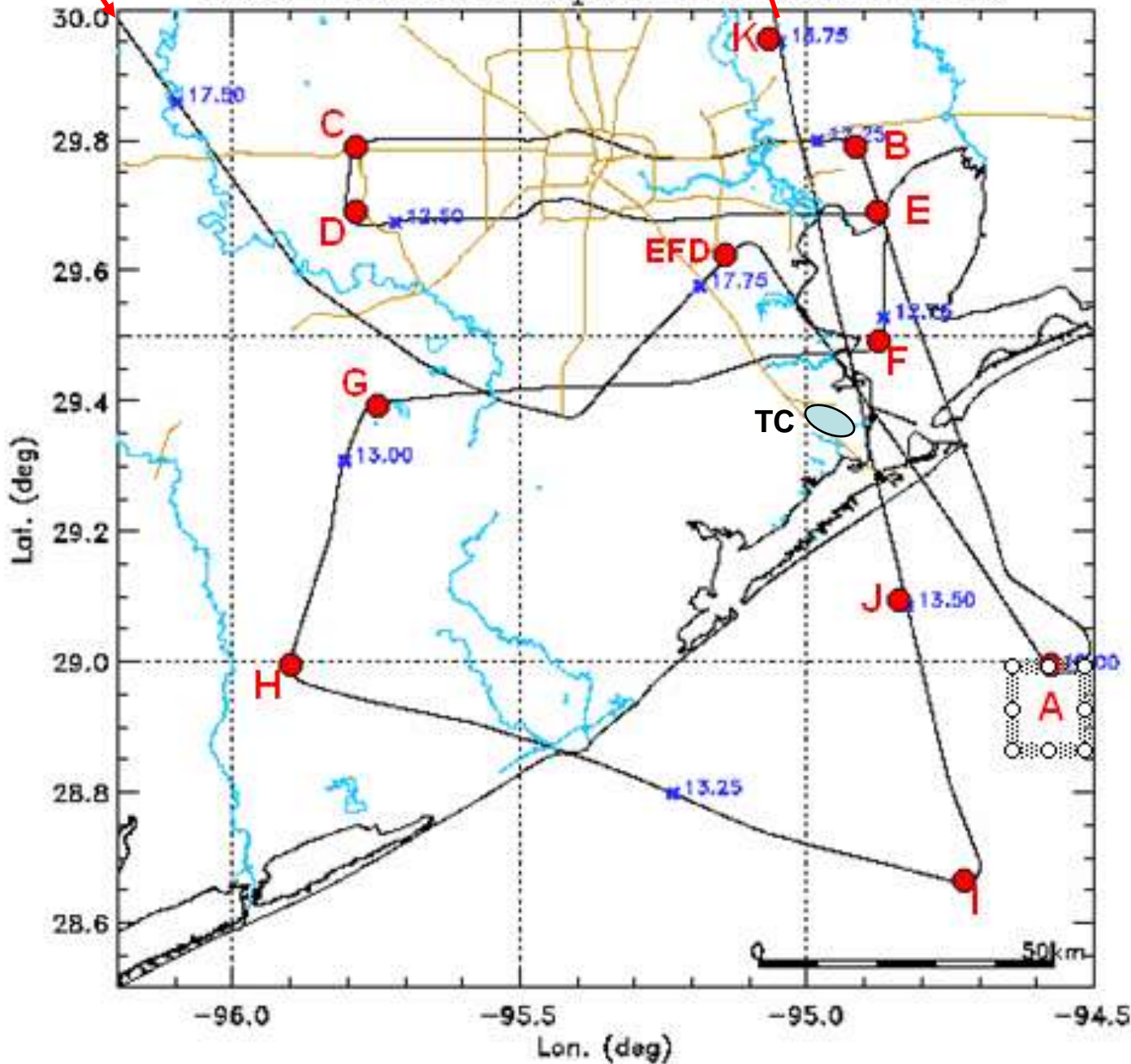
X₂ T₃ @ z ~ 233m



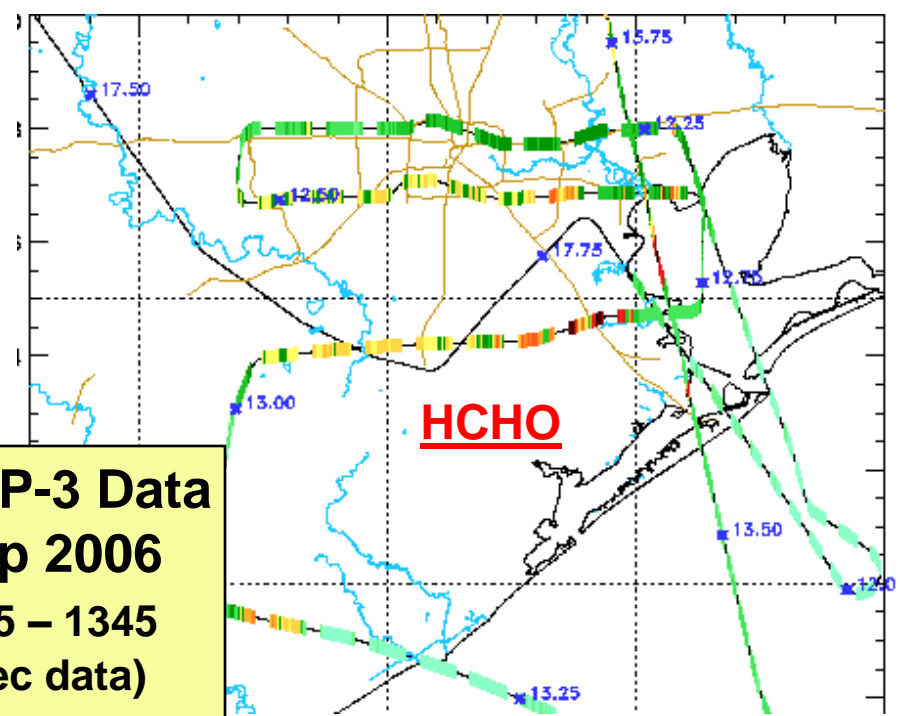
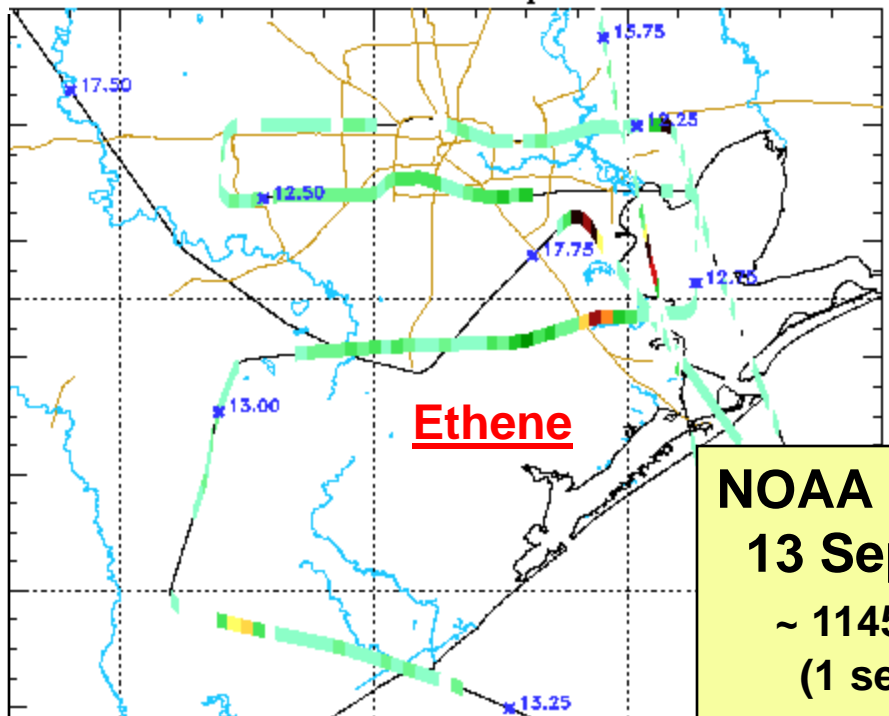
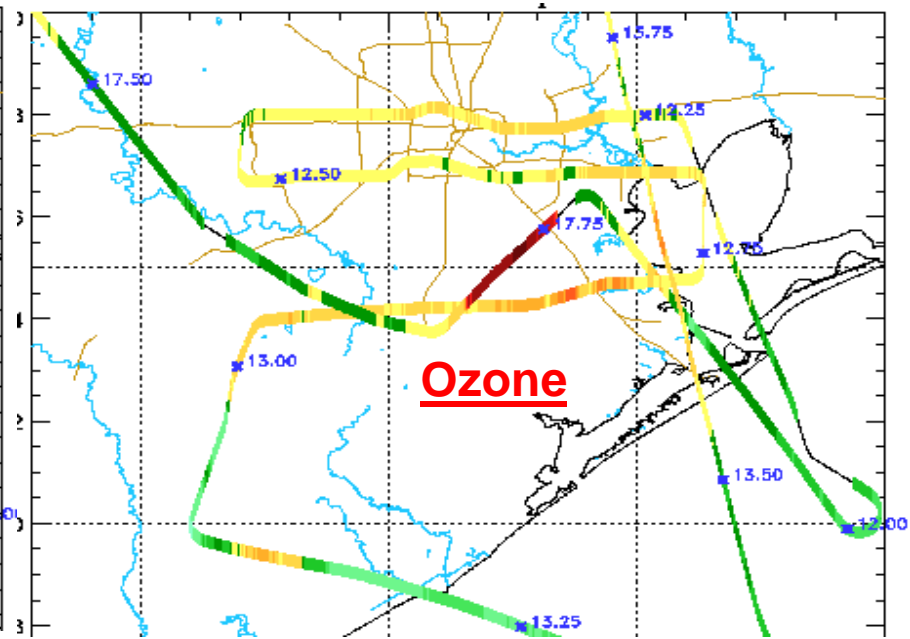
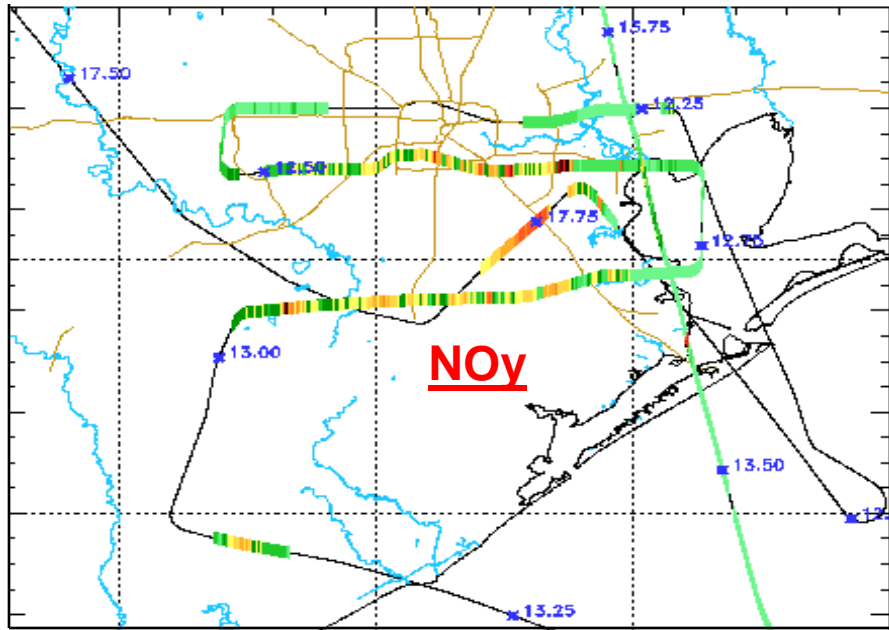
From DFW (~1745)

To DFW (~1345)

NOAA-P3 data: 13 Sep 2006 for Houston Area



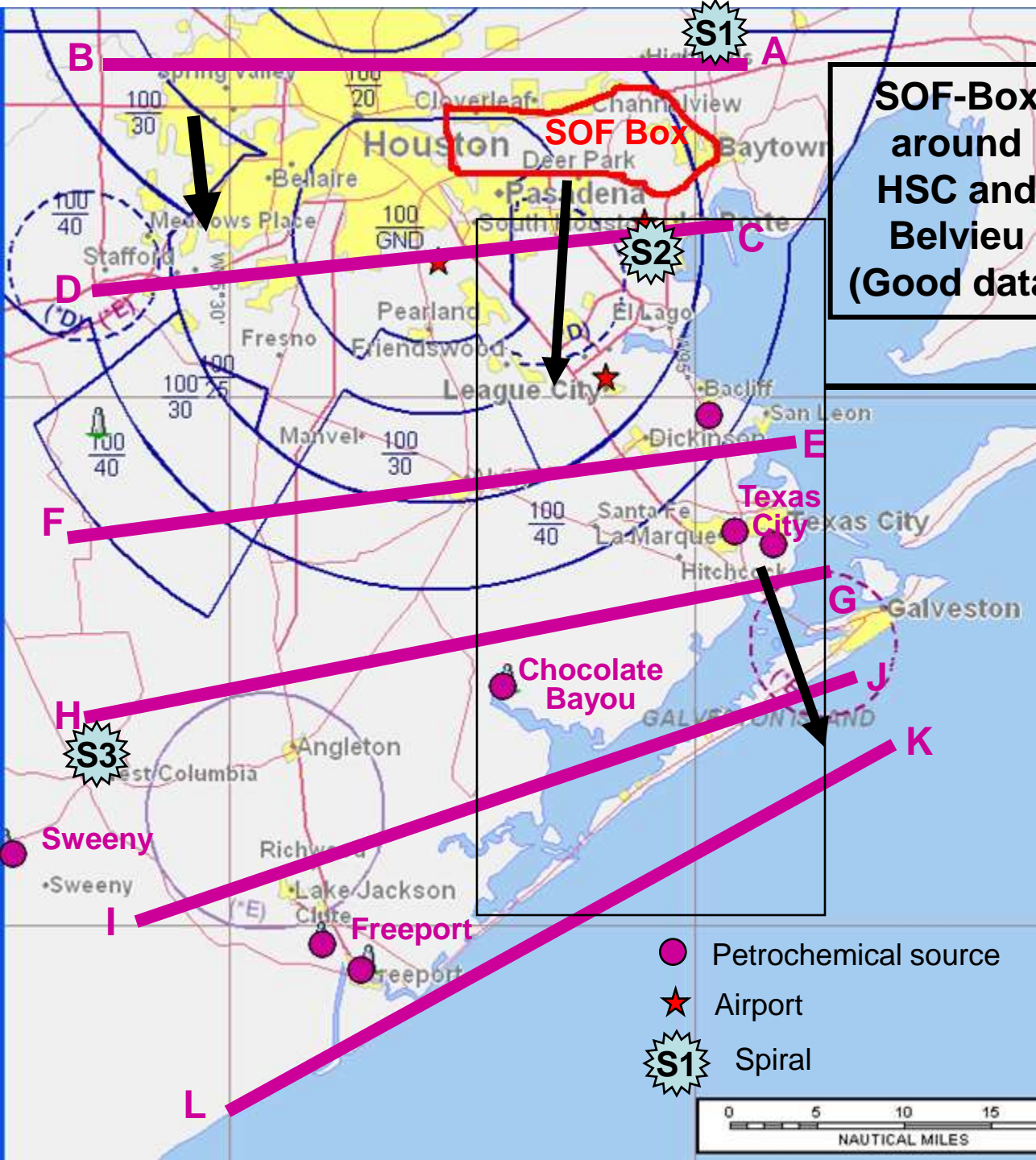
NOAA P-3
flight of
13 sep 06
in the
HOU area



**NOAA P-3 Data
13 Sep 2006
~ 1145 – 1345
(1 sec data)**

Aztec Flight Plan

30 Aug 2006

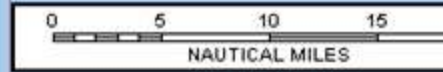


**SOF-Box
around
HSC and
Belvieu
(Good data)**

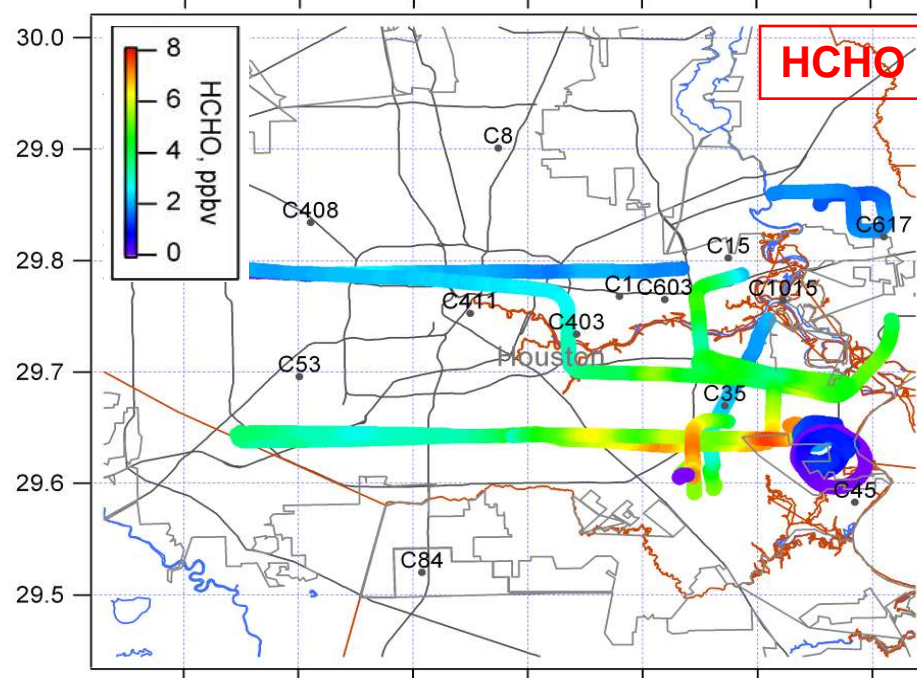
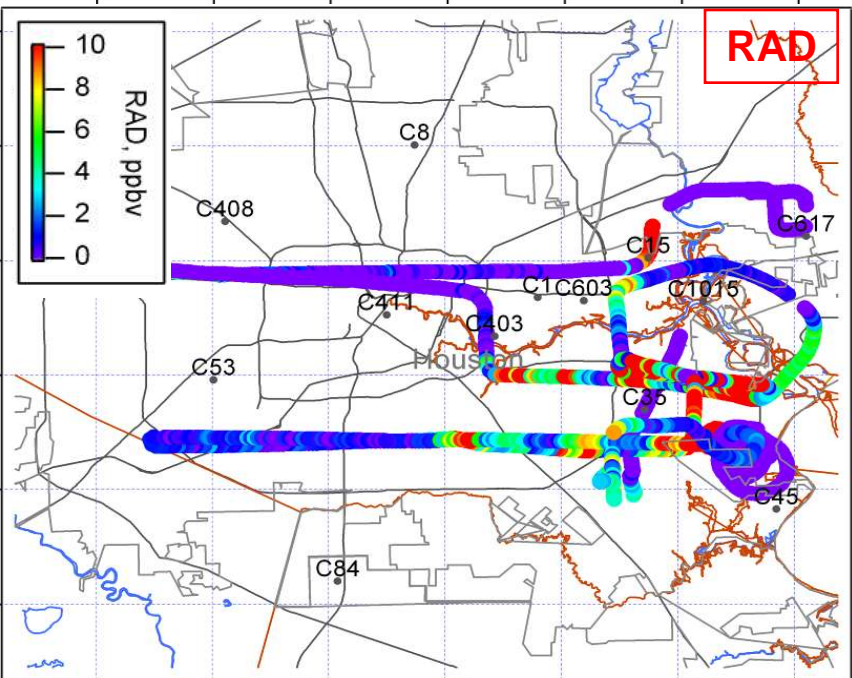
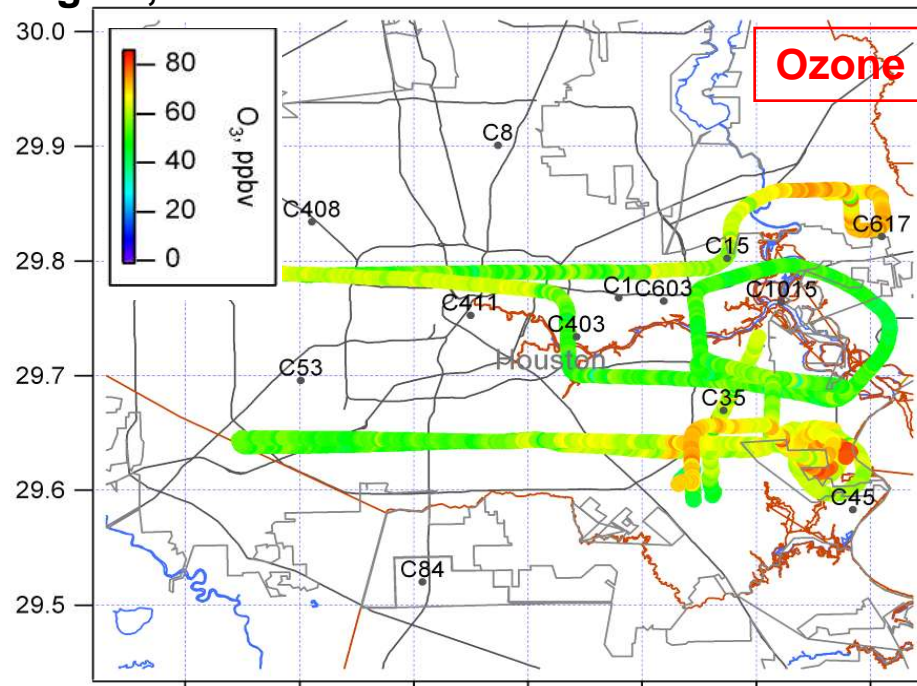
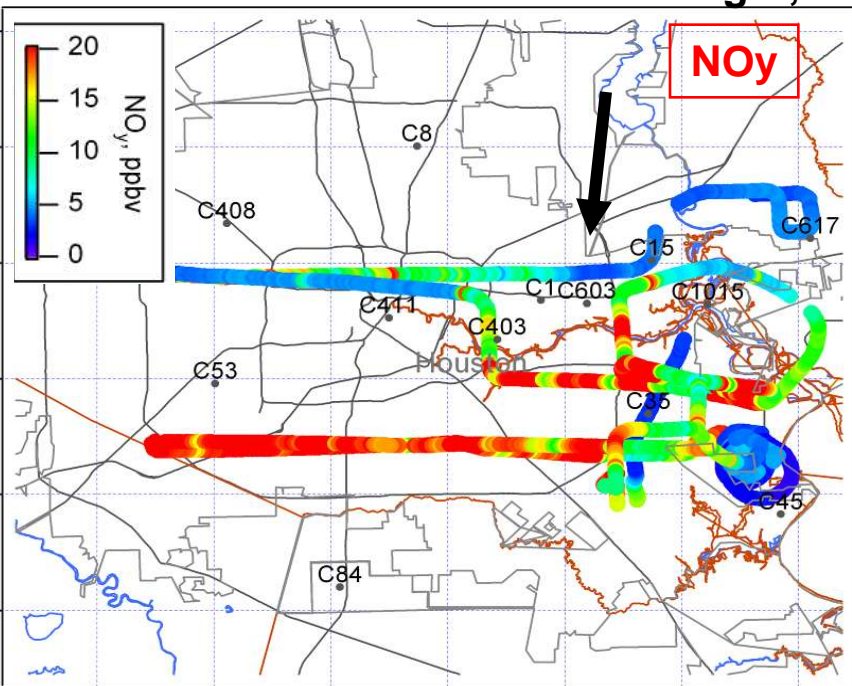
TexAQS II Smart Balloon Flight ID 2



- Petrochemical source
- ★ Airport
- S1 Spiral



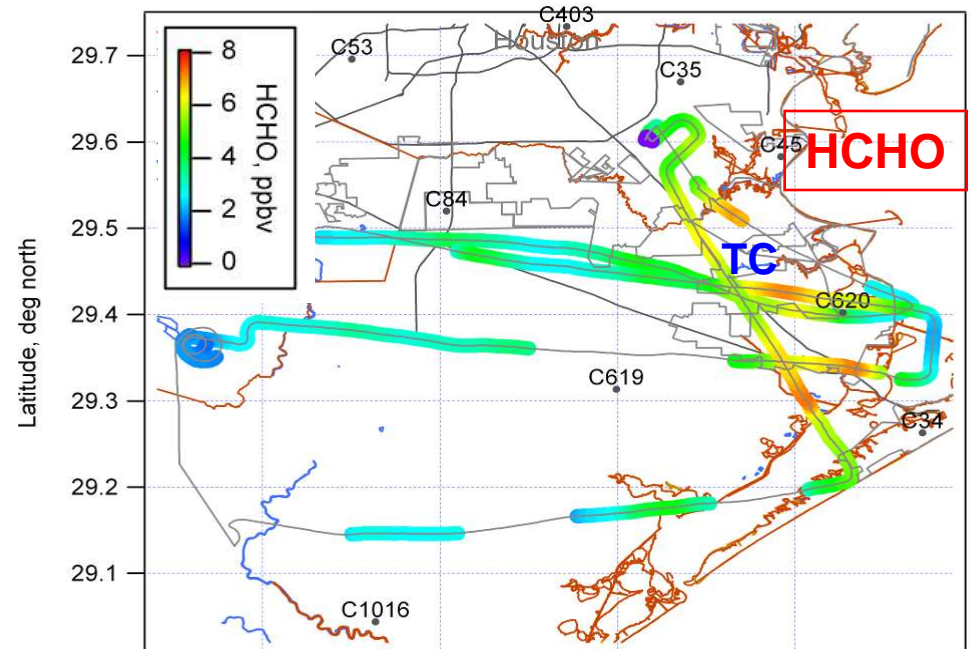
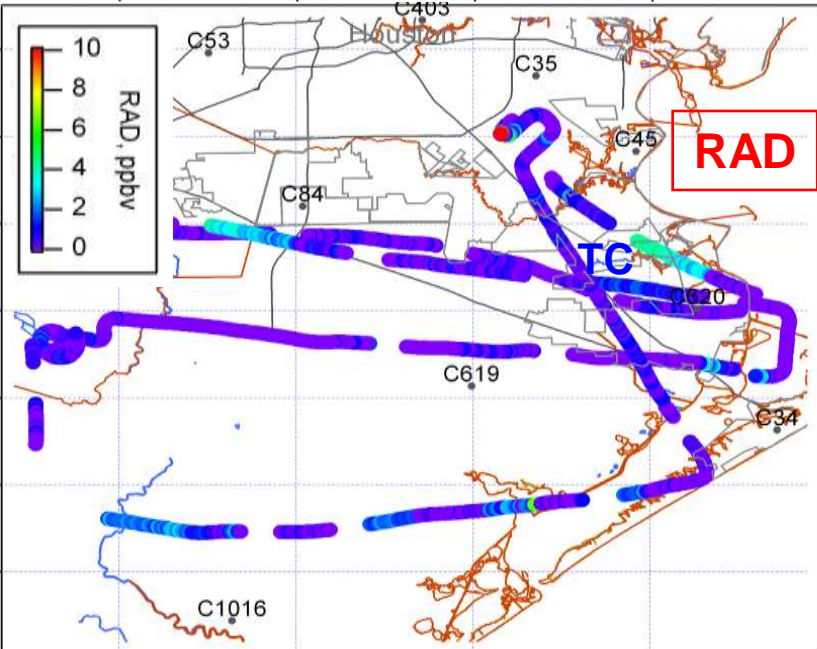
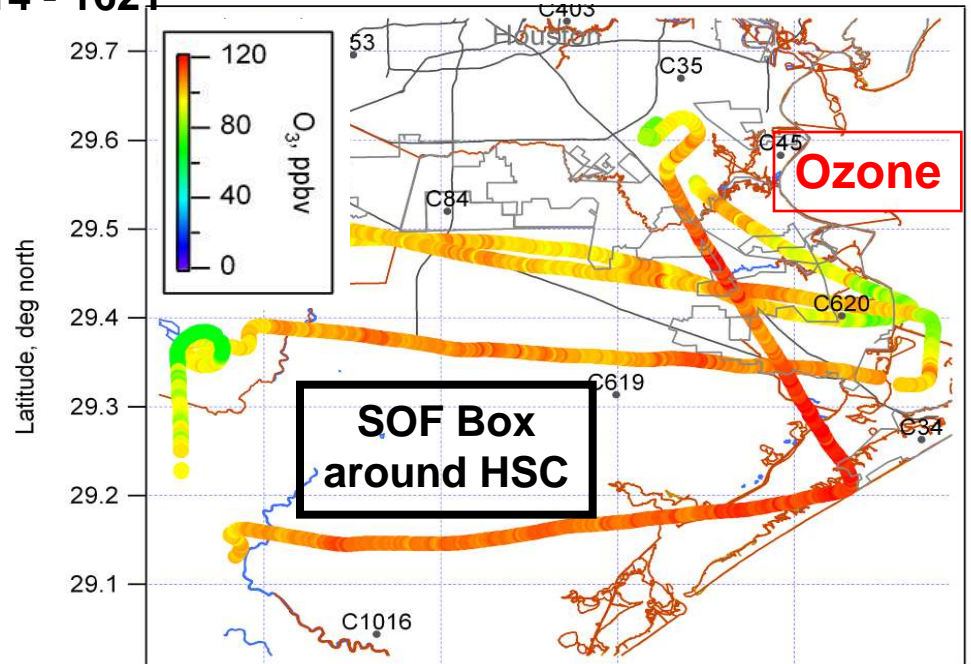
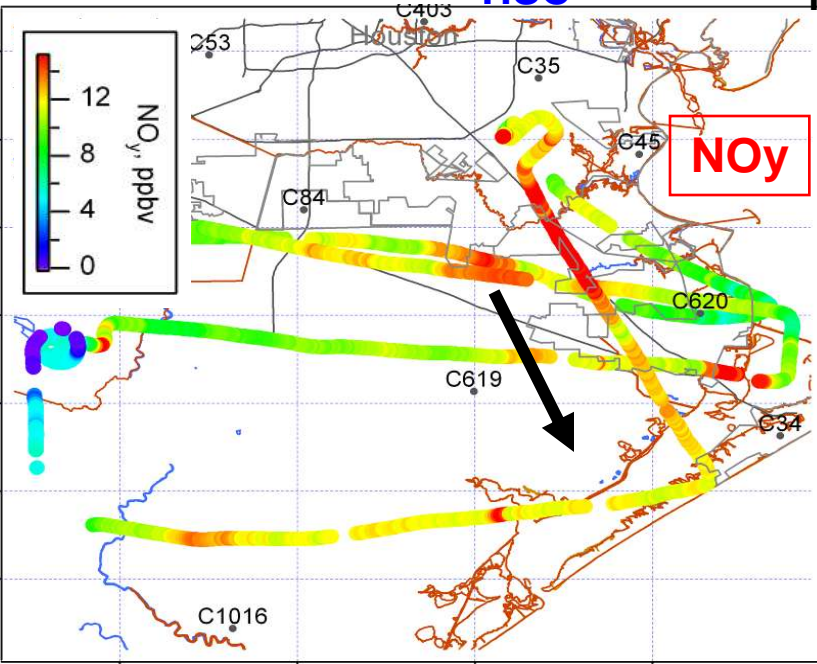
Aztec Flight, 30 August, 0858 - 1105



Aztec Flight, 30 August 1414 - 1621

HSC

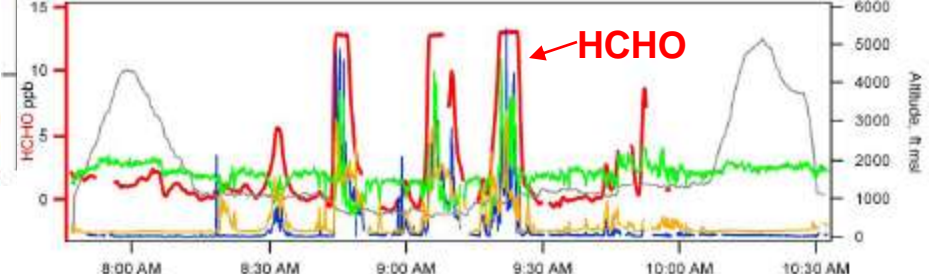
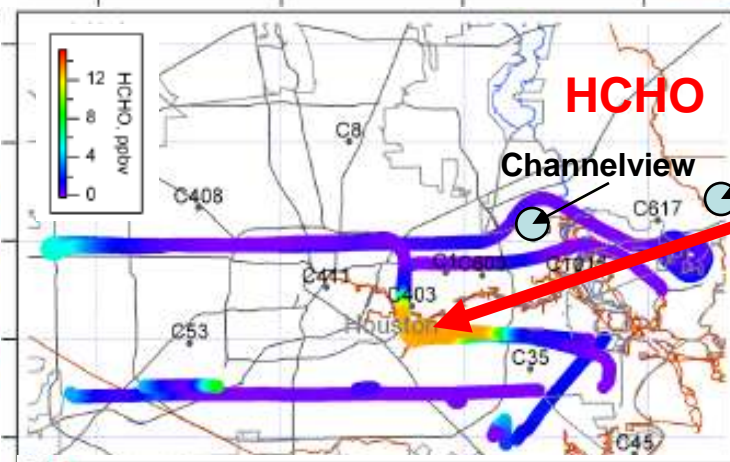
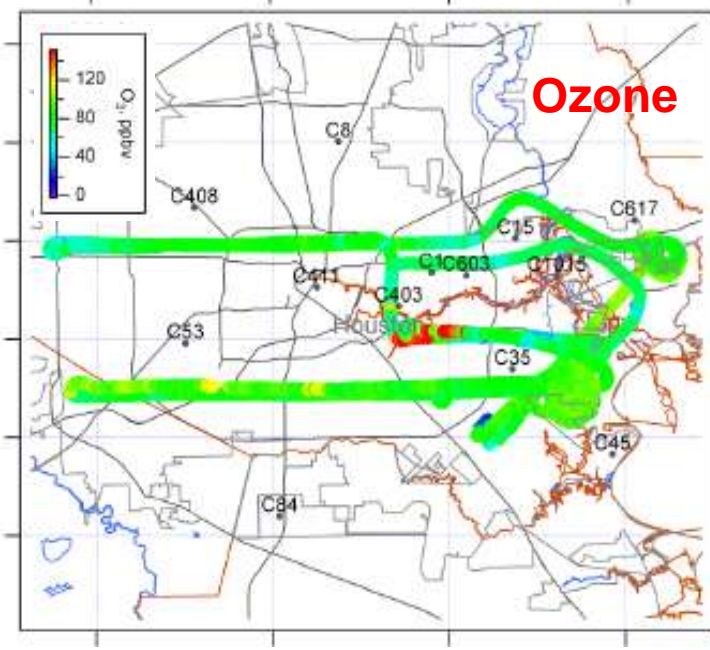
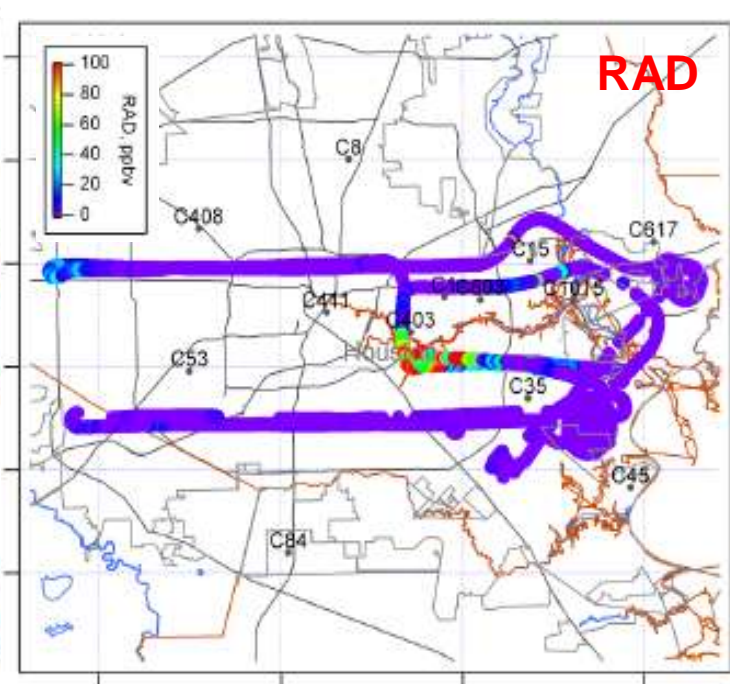
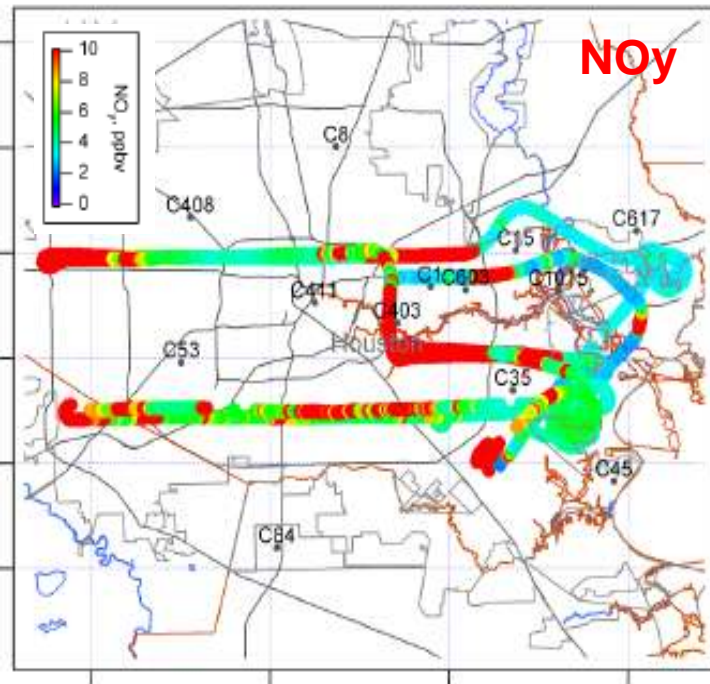
HSC



Aztec Flight 31 Aug 2006

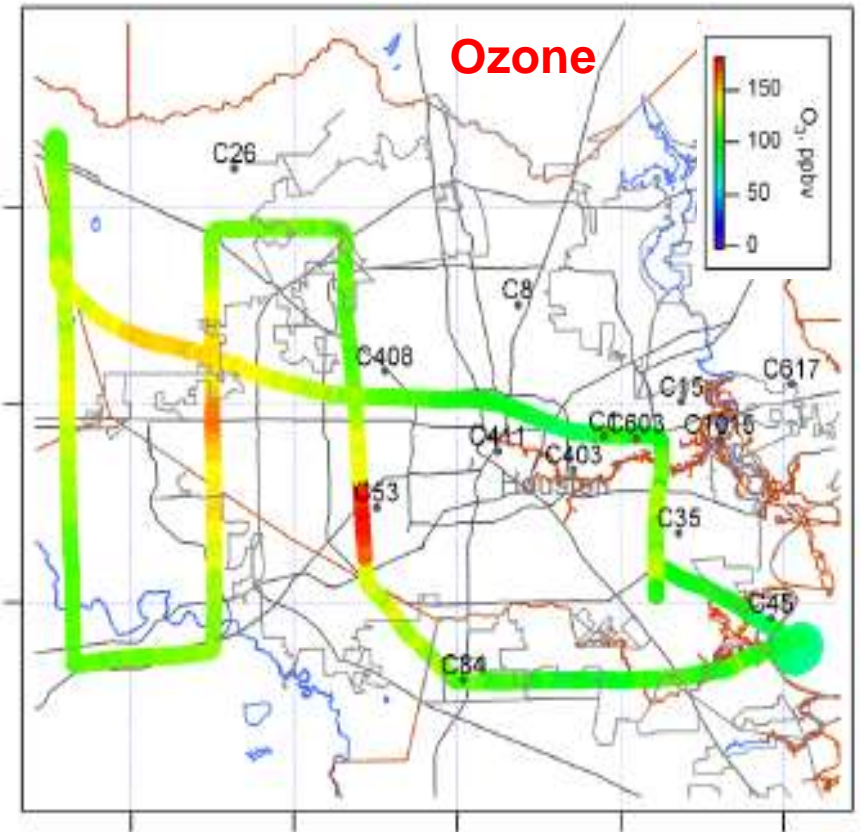
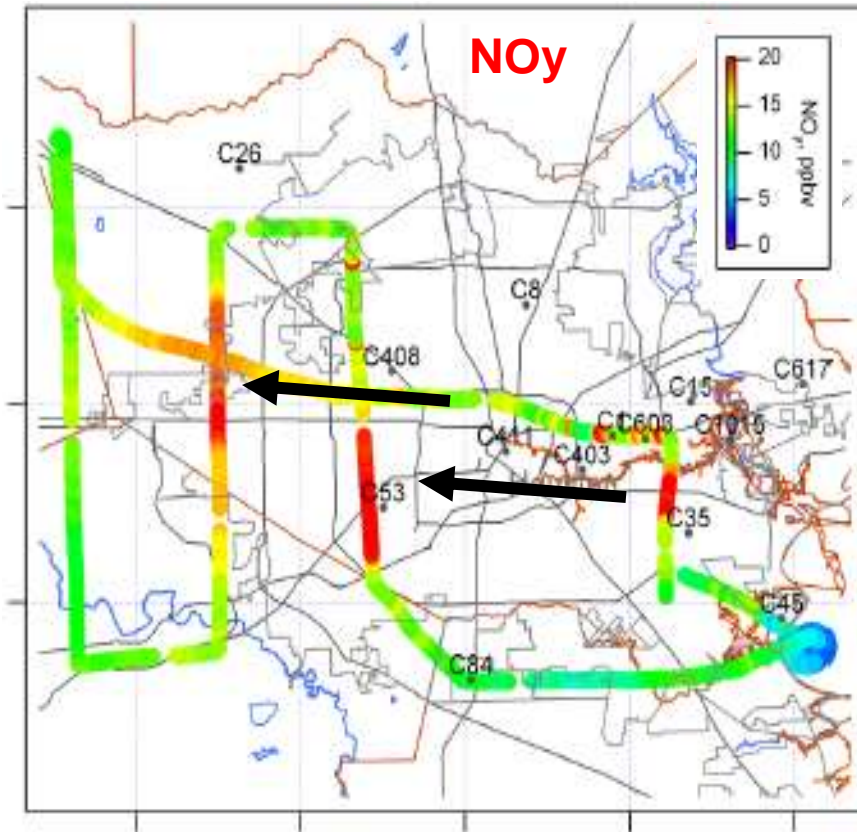
Morning
(0745 – 1032)

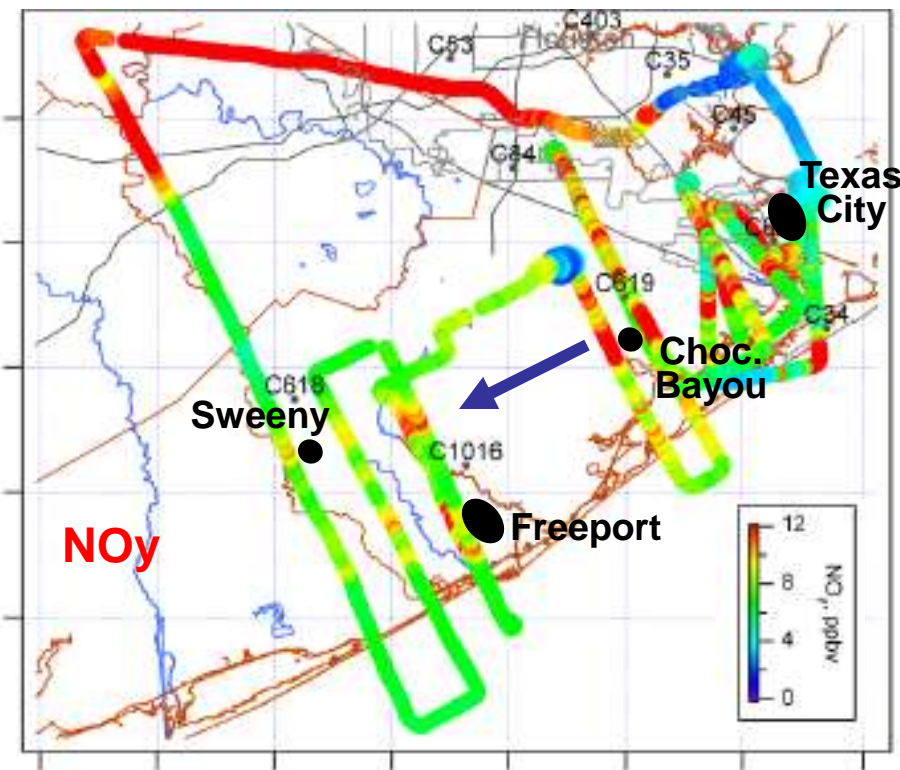
SOF-Box
around
Channelview



Aztec Flight 31 Aug 2006

Afternoon
(1418 – 1618)

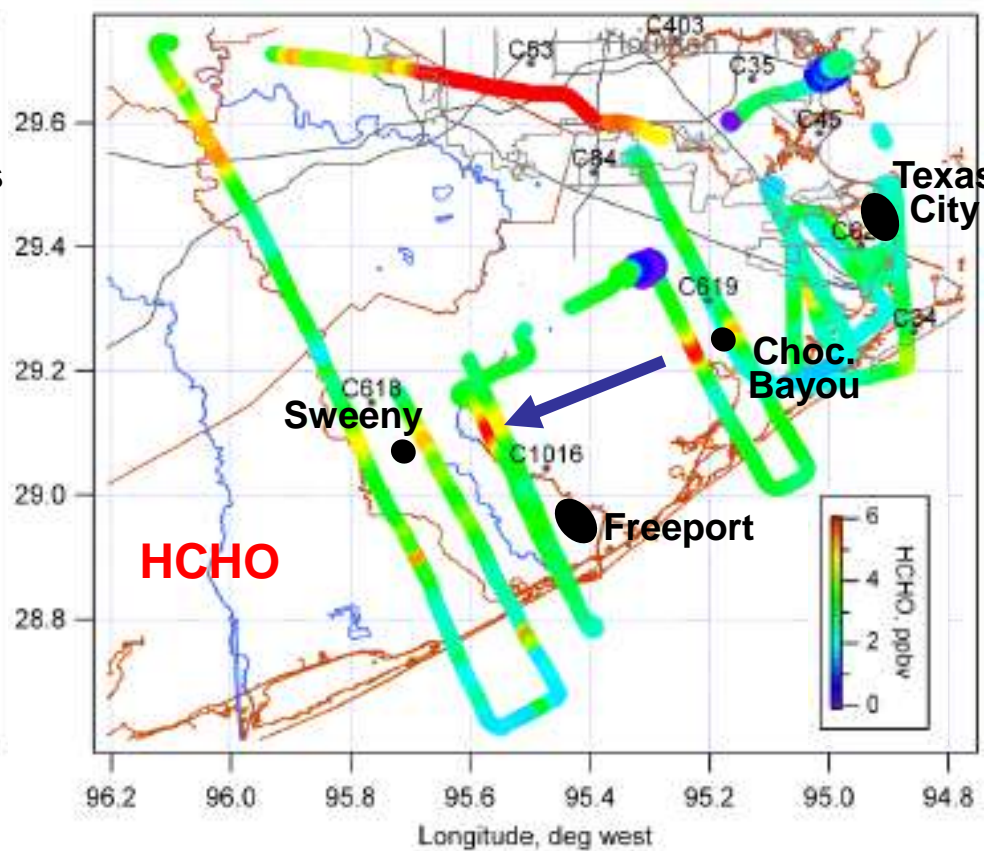




NO_y

**Aztec Flight
20 Sep 2006**

0814 - 1344

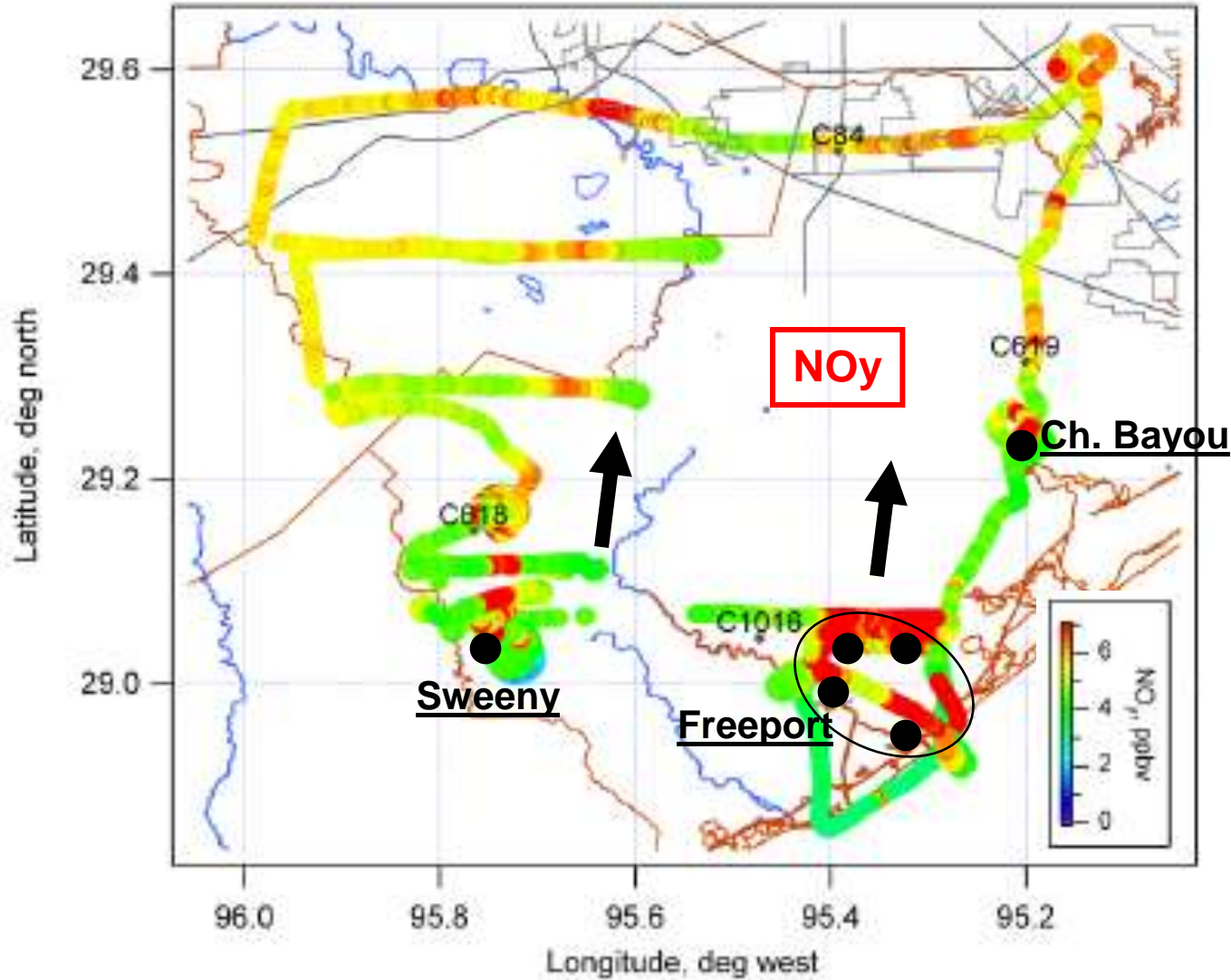


HCHO

**SOF-Box
around
Texas City**

Aztec Flight, 27 Sep 2006

1213 - 1739



**SOF-Boxes
around
Ch. Bayou,
Freeport,
and
Sweeny**

Analysis can include:

1. **LES-chem or LRPM in the near field to characterize actual emissions based on SOF data and aircraft data**

(LESchem fine-resolves dynamics and chemistry vertically and horizontally in the near-field; LRPM fine-resolves, but with parameterized mixing (Ky, Kz))

Main goals of LRPM diagnostic study for TERC

2. **LRPM in the near-field to estimate primary emissions of NO_x and HRVOC, with guidance also from the LES study of 9/13/06, and farther downwind for second TDEV based on secondary formations, and to quantitatively study the impact of secondary products formation, including O₃, NO_z, and HCHO (and H₂O₂/HNO₃ for ozone sensitivity analysis)**
3. **LRPM analysis can also explore primary/secondary HCHO, and HONO production, and their relevance to radical chemistry.**