Model Performance Evaluation Using R. V. Ronald H. Brown Data

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Southeast Texas Photochemical Modeling Technical Committee

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Background

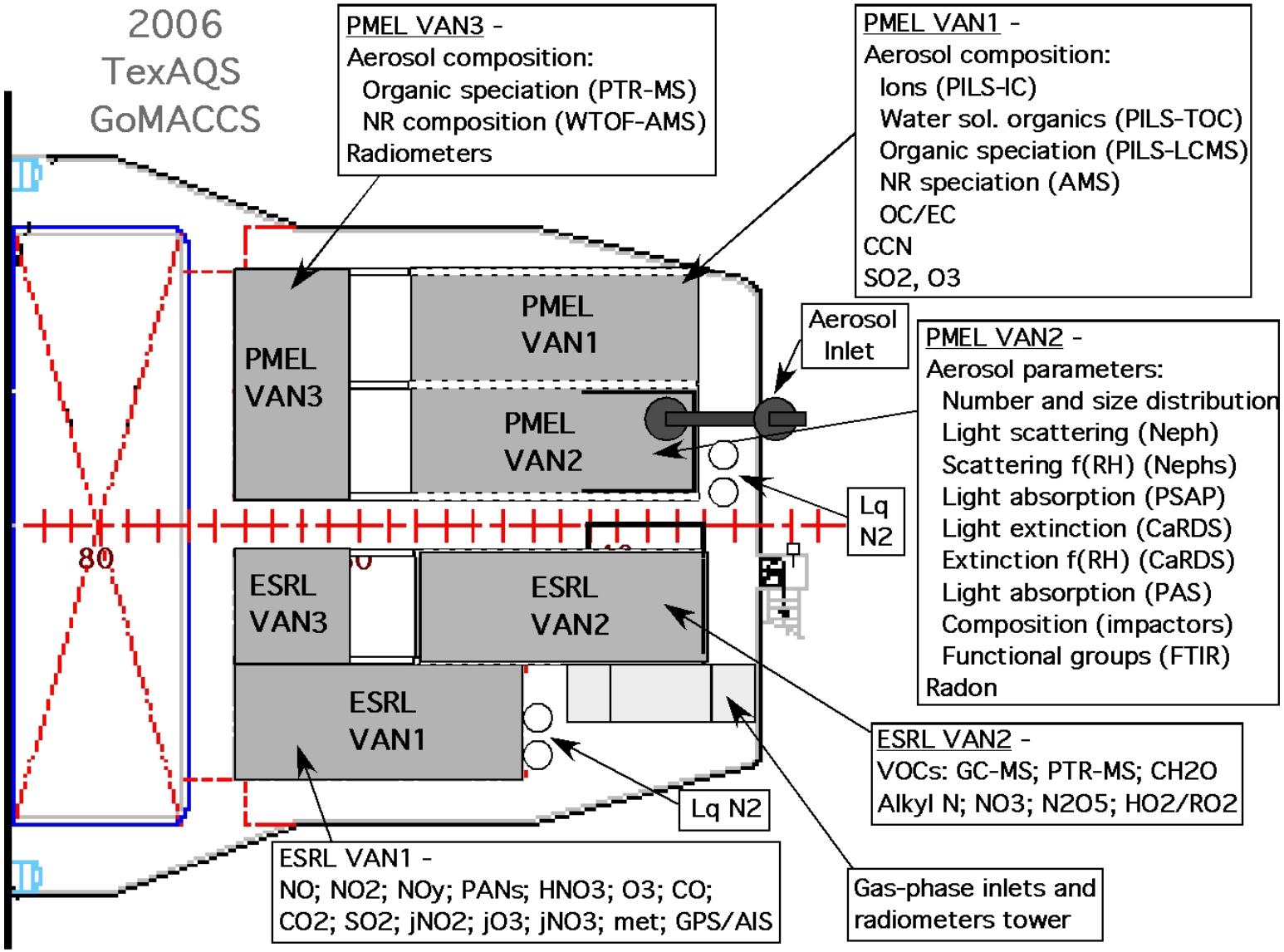
- **The NOAA RV Ron Brown arrived in the HGB area on August 15, 2006, and collected data until its departure on September 13.**

- **The ship carried a wide array of sampling platforms onboard and provided extensive data collected in the Gulf of Mexico, Galveston Bay, and in the Houston Ship Channel.**

- **The Ron Brown data provides a unique opportunity to evaluate CAMx model performance in areas not usually monitored.**

NOAA
R 104

R.V. Ron Brown Instrumentation



R.V. Ron Brown Instrumentation

Parameter	Method
Photolysis rates (j-values)	Spectral radiometer
Ozone (O3)	UV absorbance
Ozone	NO chemiluminescence
Carbon monoxide (CO)	Nondispersive IR
Carbon dioxide (CO2)	Nondispersive IR
Sulfur dioxide (SO2)	Pulsed UV fluorescence
Nitric oxide (NO)	Chemiluminescence
Nitrogen dioxide (NO2)	Photolysis/chemiluminescence
Total reactive nitrogen oxides (NOy)	Au tube/chemiluminescence
Peroxyacyl nitric anhydrides (PANs)	Gas Chromatograph (GC)/ Electron Capture Detector (ECD)
Alkyl nitrates (RONO2)	GC/Mass Spectrometer (GC/MS)
Nitrate radical (NO3); Dinitrogen pentoxide (N2O5)	Cavity ring-down spectrometry
Nitric acid (HNO3)	Mist chamber/Ion Chromatograph
Water vapor (H2O)	Nondispersive IR
Continuous Speciation of VOCs	PTR-MS/Chem Ionization MS

Ron Brown Instrumentation (Cont.)

Parameter	Method
VOC Speciation	GC/MS
Formaldehyde (HCHO)	1,3-cyclohexanedione (CHD) fluorimetry
Radon (Rn)	Radon gas decay
Seawater/atmospheric CO2	Nondispersive IR
Enhanced measurement of radiative fluxes	Spectral radiometers
Aerosol optical depth	Total Ozone Portable Spectrometer (MicroTOPS)
Irradiance	Portable Radiation Package (PRP)
Size-resolved aerosol composition and gravimetric mass	Impactors (Ion Chromatograph (IC), X-Ray Fluoresence (XRF), and thermal-optical OC/EC)
Organic Carbon/Elemental Carbon (OC/EC)	On-line thermal optical
Ionic Aerosol Composition	Particle Into Liquid Sampler (PILS)
Aerosol Size and Composition	Aerosol Mass Spectrometer
Organic function groups	Fourier Transform Infrared spectrometer (FTIR)
Aerosol scattering (400, 550, 700 nm)	TSI Model 3563 Nephelometer

Ron Brown Instrumentation (Cont.)

Parameter	Method
Aerosol absorption (400, 550, 700nm)	Radiance Research Particle Soot Absorption Photometer (PSAP)
Aerosol number	Condensation Nuclei Counter (CNC)
Aerosol size distribution	Twin Differential Mobility Analyzers (DMA) and an Aerodynamic Particle Sizer (APS)
Aerosol light scattering hygroscopic growth f(RH)	Twin TSI 3563 nephelometers
Aerosol size hygroscopic growth g(RH)	Tandem DMAs
Aerosol light extinction hygroscopic growth f(RH)	Cavity ring-down spectrometer
Total and sub-micron aerosol extinction	Cavity ring-down spectrometer
Ozone/aerosol vertical profiles	O3/Aerosol Lidar (OPAL)
Wind/temperature vertical profiles	915 MHz wind Radar
High-resolution Boundary Layer (BL) winds/aerosol	High-Resolution Doppler Lidar (HRDL)
Wind profiles/microscale turbulence	C-band radar
Temperature/relative humidity profiles	Radiosondes
Surface energy balance (fluxes)	Eddy covariance (bow mounted)
High resolution BL turbulence structure	Doppler mini-Sodar

CAMx Ozone Modeling in SIP Development
The Big Picture

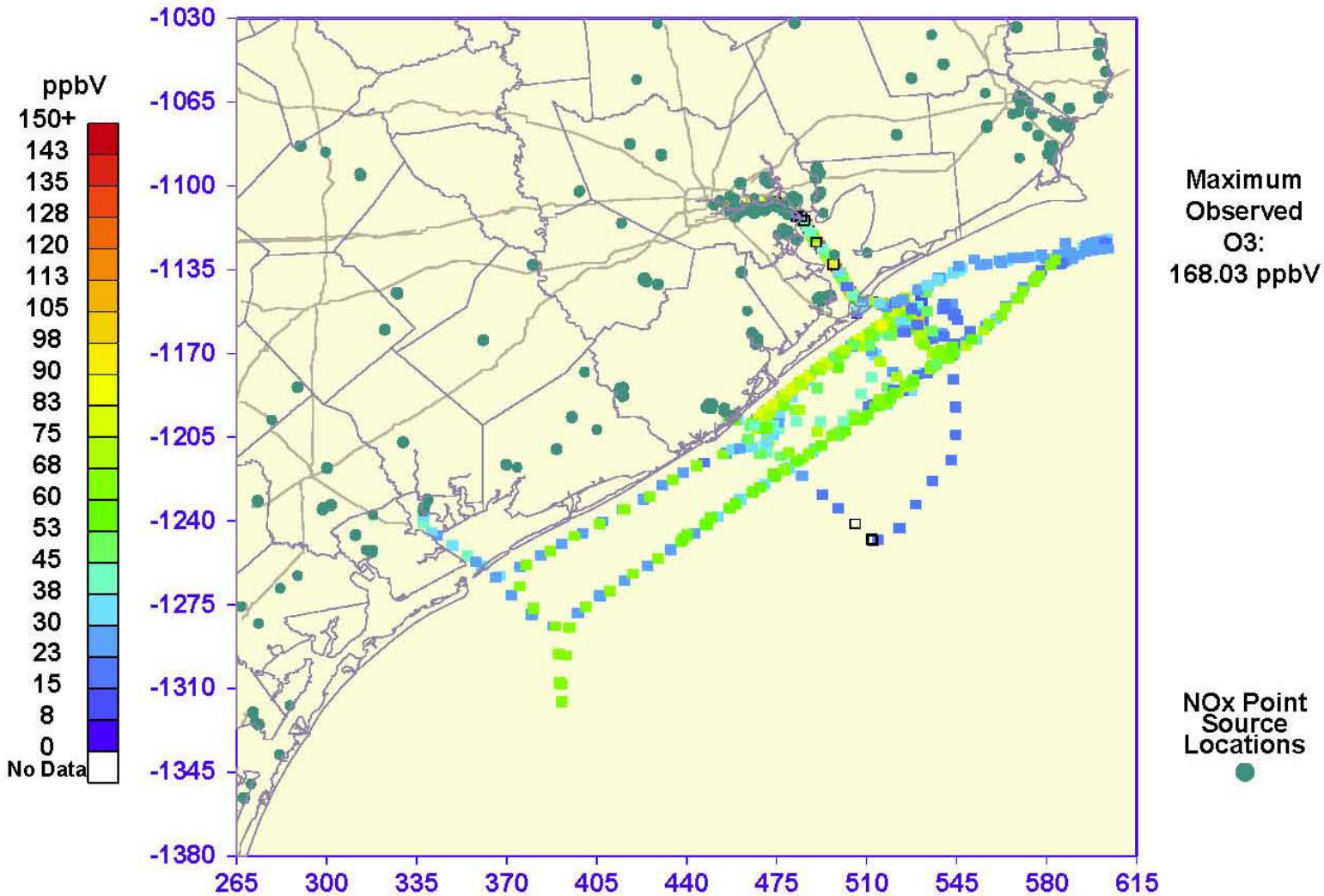
Base Case	**Day-specific emissions; replicate what actually happened**
Baseline Case	**Typical emissions; used in RRF to predict future design values**
Future Base Case	**Apply future growth + on-the-books controls to estimate future ozone**
Control Strategy Testing	**Determine control strategies that will effectively reduce ozone**
SIP	**Document modeling procedures**

The Voyage of the Ron Brown

- Performance analysis using the Ron Brown data was complicated by the course taken by the ship, since it frequently traversed almost identical paths, sometimes several times within a single day.

- Model performance was simplified somewhat by segregating the data into seven distinct analysis zones, allowing model performance to be evaluated in each of seven different environments.

NOAA RV Ron Brown Measured O3 Mixing Ratios
15AUG 00:00 to 11SEP 12:30, 30 Minute Averages



Analysis Zones

- ***Houston Ship Channel***. This zone was defined as consisting of all measurements made to the north and west of Barbour's Cut, and is the portion of the Houston Ship Channel which bisects the main industrial area of eastern Harris County. The Ron Brown made an extended visit to this area on September 6 and 7, including an overnight stay at Jacinto Port.

- ***Barbour's Cut***. The Ron Brown made seven extended visits to Barbour's Cut near the northwestern extremity of Galveston Bay.

- ***Barbour's Cut to Galveston***. The ship made numerous transects of the deepwater channel between Barbour's Cut and the mouth of Galveston Bay located between Galveston Island and Bolivar Peninsula. This channel is actually part of the Houston Ship Channel but is analyzed separately because it is not located directly in the industrial area.

Analysis Zones (cont.)

- ***Galveston Harbor***. The Ron Brown collected data during two overnight stays in Galveston Harbor and also briefly during two other occasions. The ship also remained docked in the Galveston Harbor for three days between August 18 and 21 during which time no data were collected.

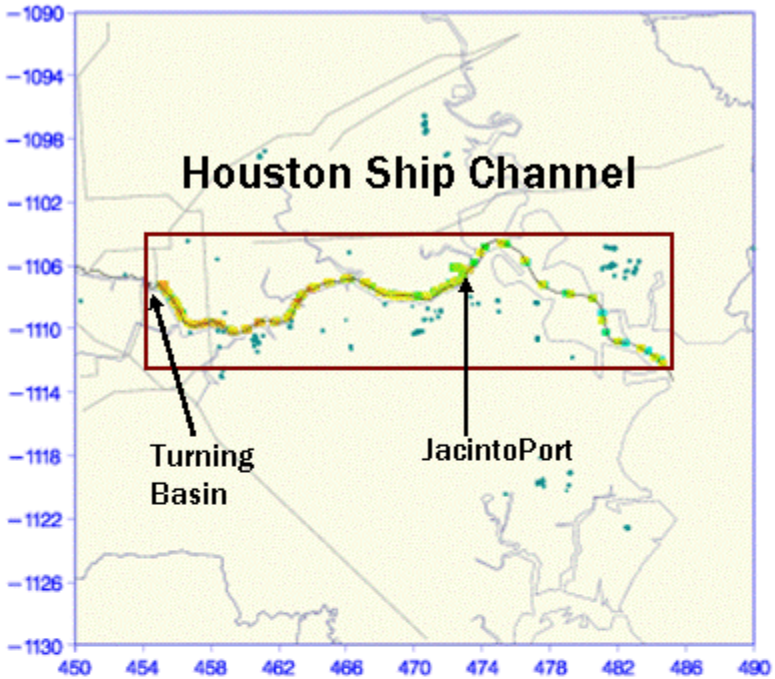
- ***Galveston Entrance/Anchorage***. This zone consists of the main fairway through which ships approach the entrance to Galveston Bay and parts of two anchorage areas lying alongside the fairway. This zone was treated separately from other offshore locations because the Ron Brown conducted extensive sampling of ship emissions in this area.

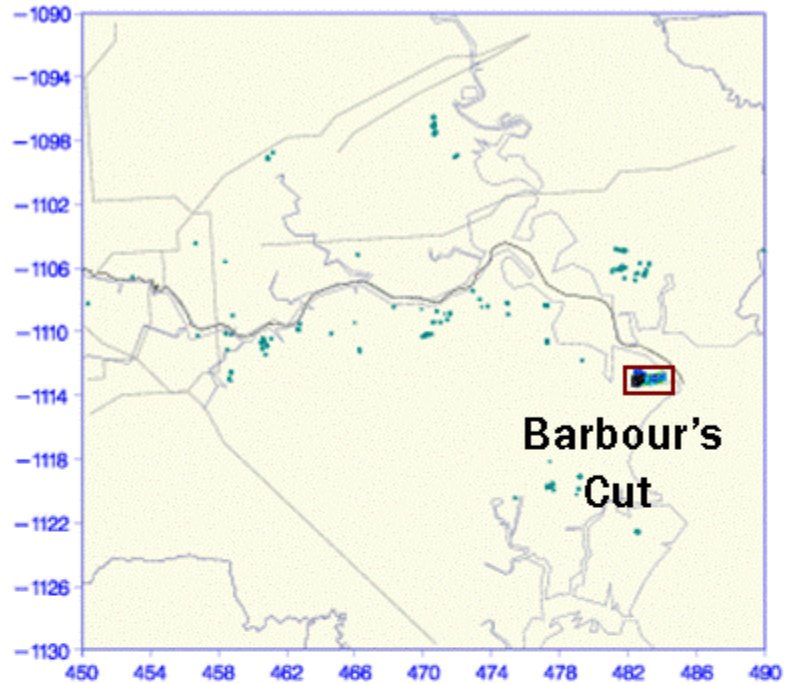
Analysis Zones (cont.)

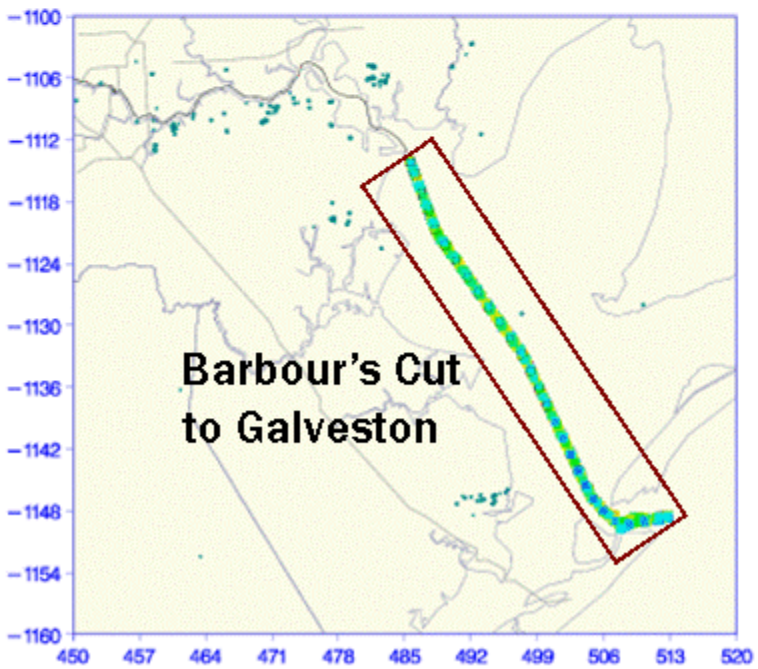
- ***Gulf – Near Shore***. The Near Shore area of the Gulf of Mexico consists of measurements made within approximately 20 kilometers of the Texas Coast (excluding the Galveston Entrance Anchorage area). This zone is intended to represent the offshore areas affected directly by onshore emissions carried out to sea by the land breeze.

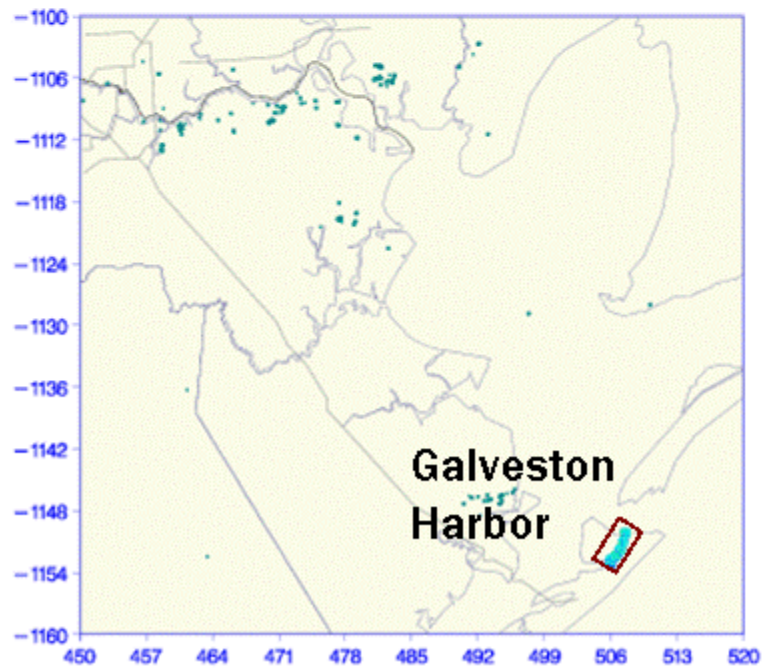
- ***Gulf – Offshore***. This zone is defined by measurements made by the Ron Brown in the Gulf of Mexico farther than approximately 20 kilometers from shore. This area is intended to be representative of marine background.

- The ship made brief visits to ports at Freeport and Palacios, but these small data sets were not included in this analysis.


Houston Ship Channel
Turning Basin
JacintoPort
−1090
−1094
−1098
−1102
−1106
−1110
−1114
−1118
−1122
−1126
−1130
450
454
458
462
466
470
474
478
482
486
490


Barbour's Cut
−1090
−1094
−1098
−1102
−1106
−1110
−1114
−1118
−1122
−1126
−1130
450
454
458
462
466
470
474
478
482
486
490


Barbour's Cut to Galveston
−1100
−1106
−1112
−1118
−1124
−1130
−1136
−1142
−1148
−1154
−1160
450
457
464
471
478
485
492
499
506
513
520


Galveston Harbor
−1100
−1106
−1112
−1118
−1124
−1130
−1136
−1142
−1148
−1154
−1160
450
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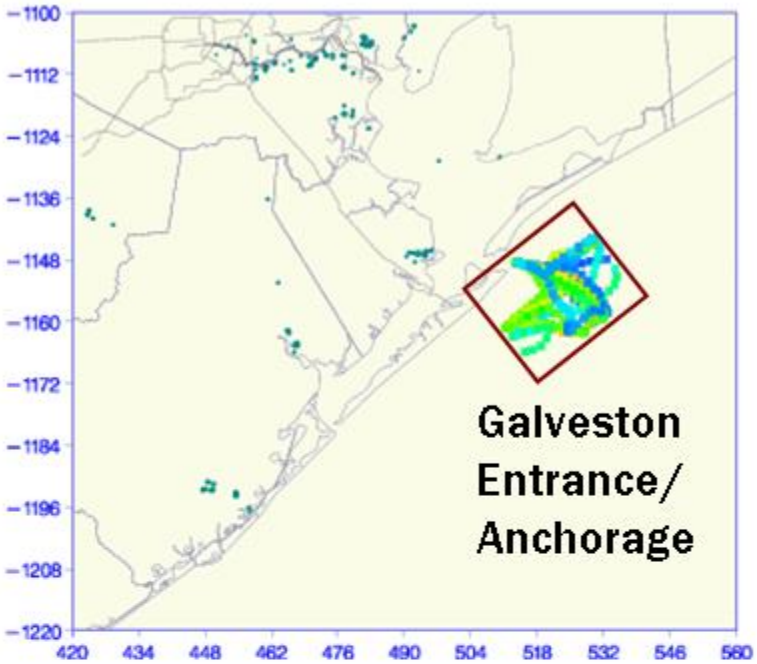
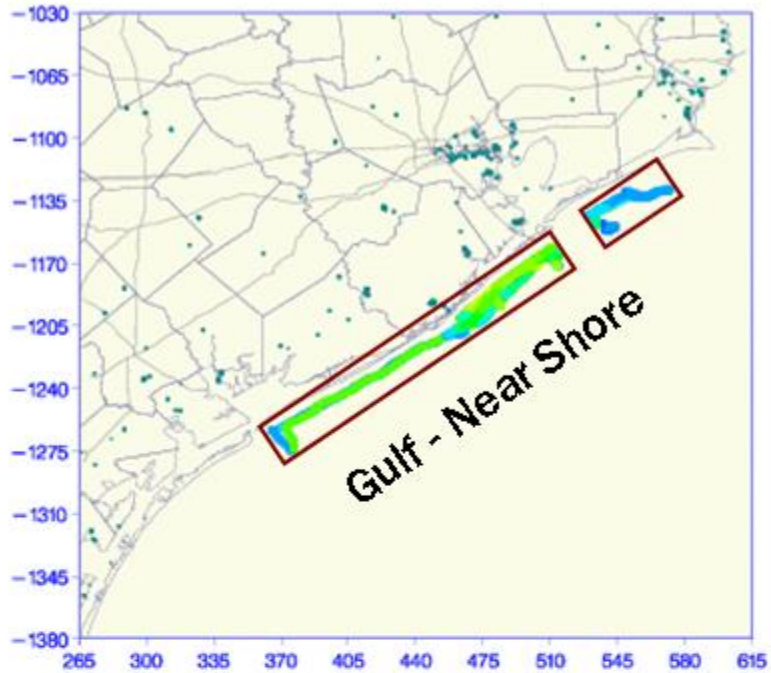
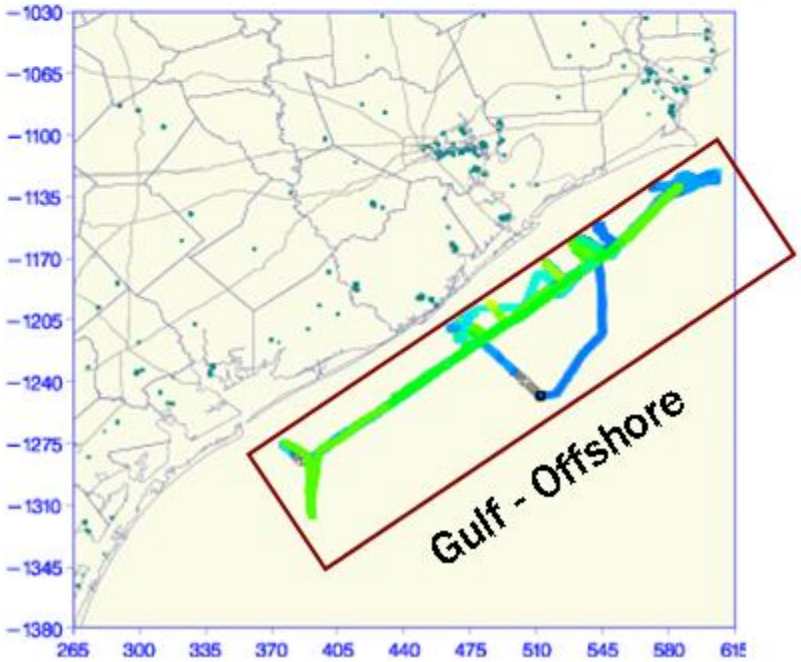
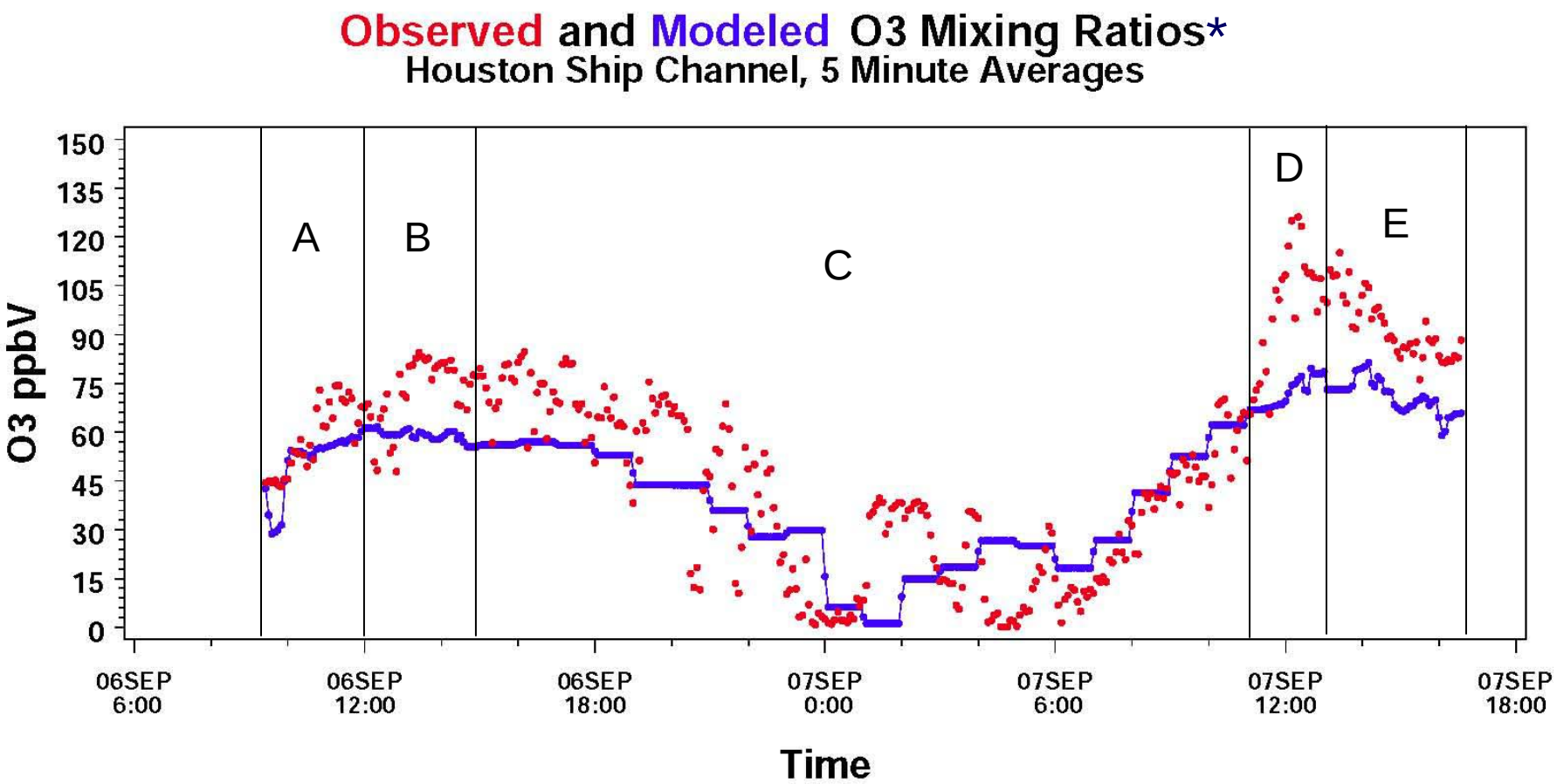
464
471
478
485
492
499
506
513
520


Galveston
Entrance/
Anchorage


Gulf - Near Shore

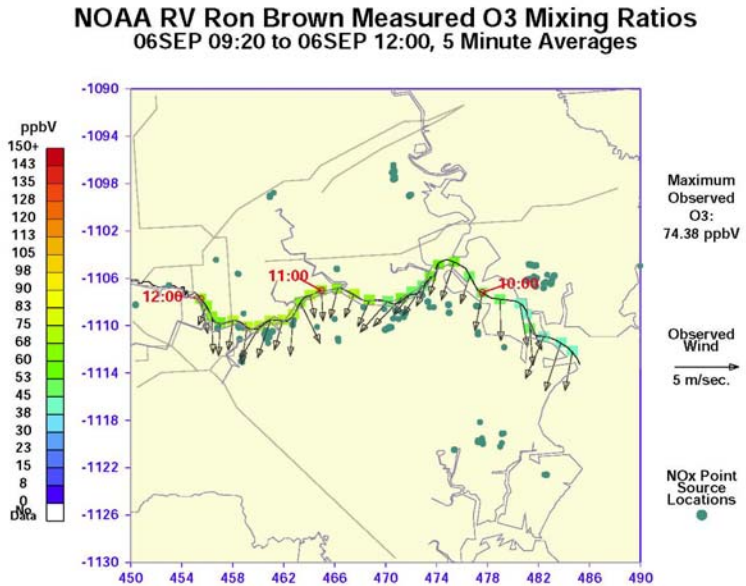

Gulf - Offshore

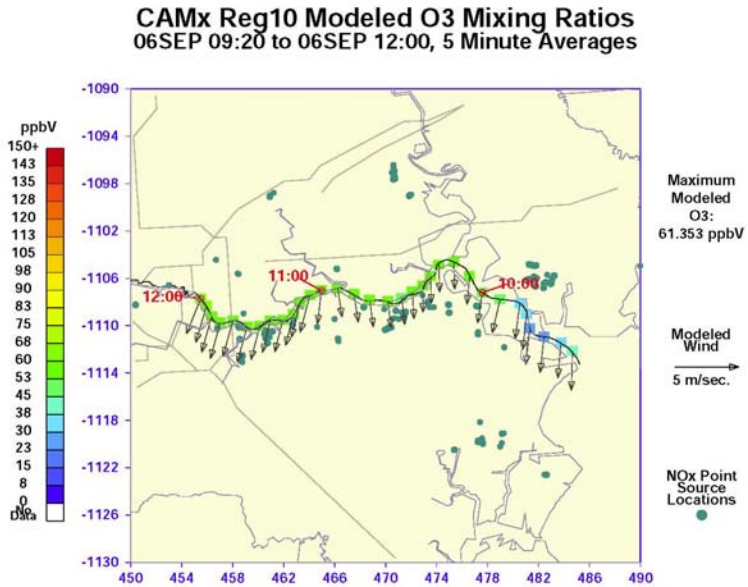
Houston Ship Channel



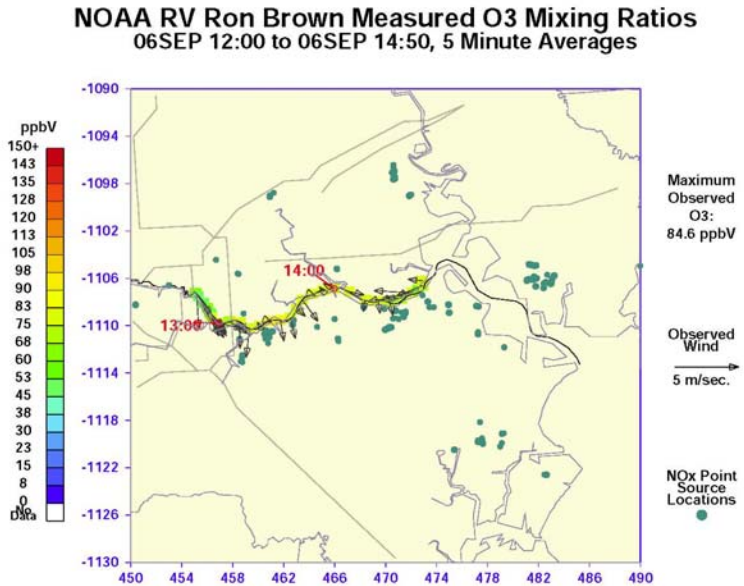
*** Note:** Consistent with NOAA's preferred notation, graphics depicting data from the R.V. Ron Brown use the term "Mixing Ratio" instead of "Concentration". In this context the two terms are interchangeable.

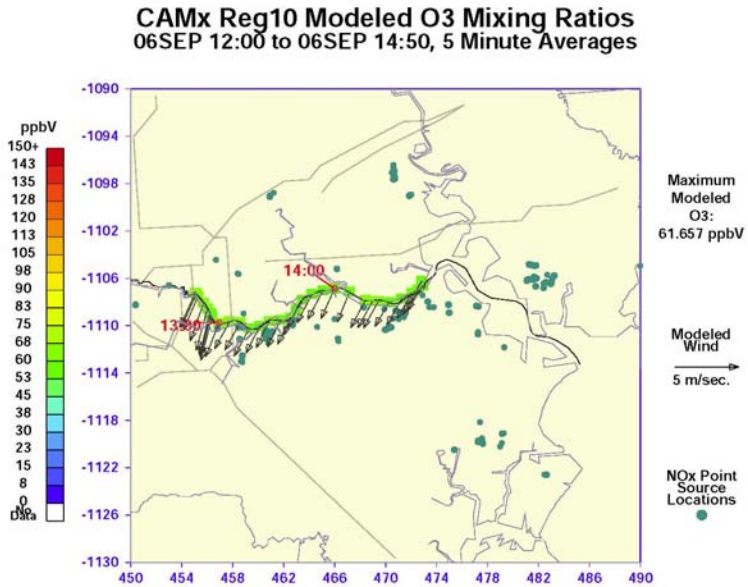
Segment A: Barbour's Cut to Turning Basin



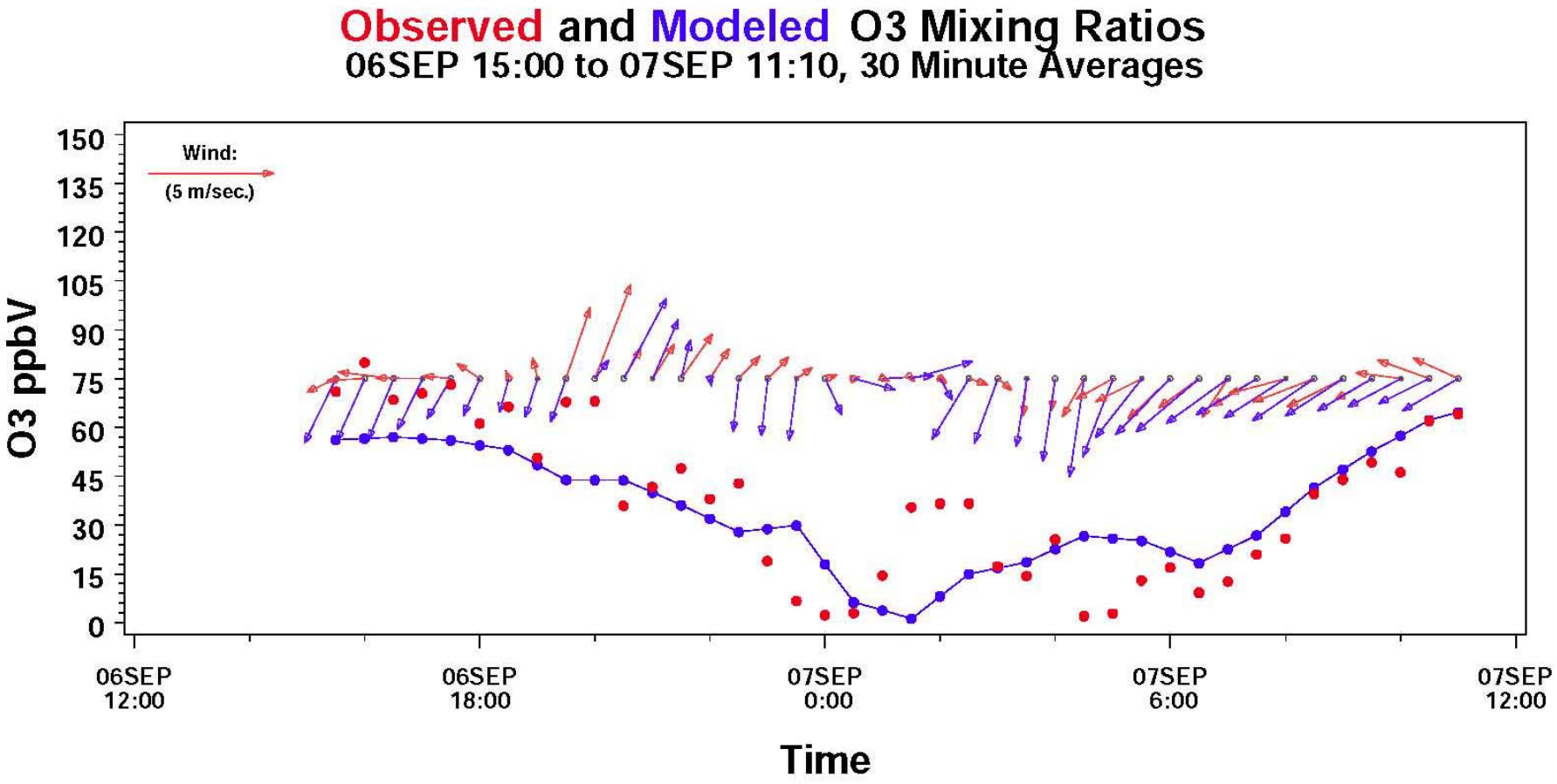


Segment B: Turning Basin to Jacinto Port

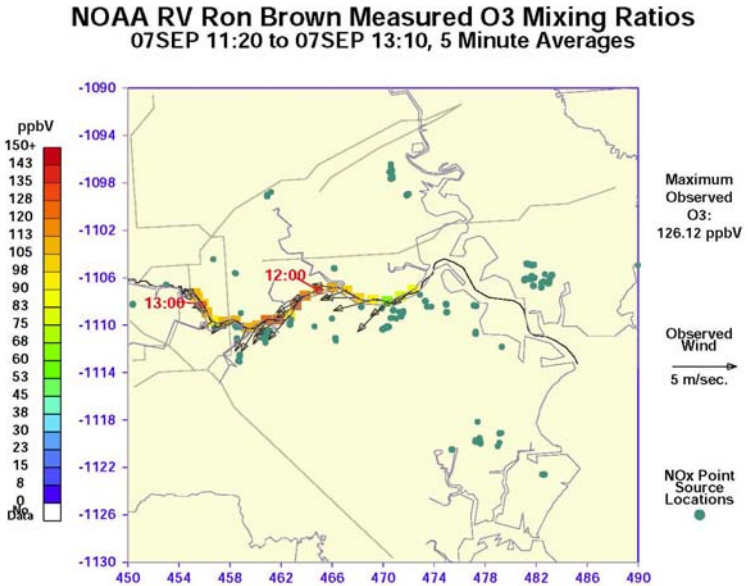


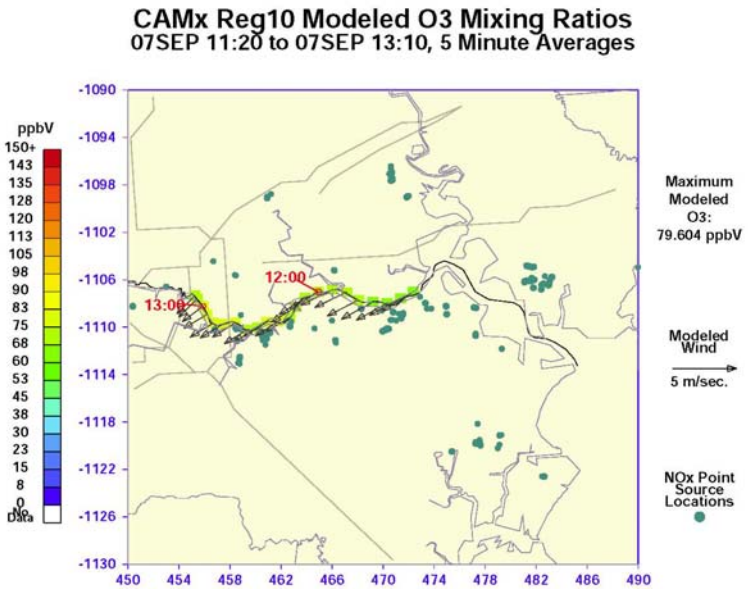


Segment C: Jacinto Port

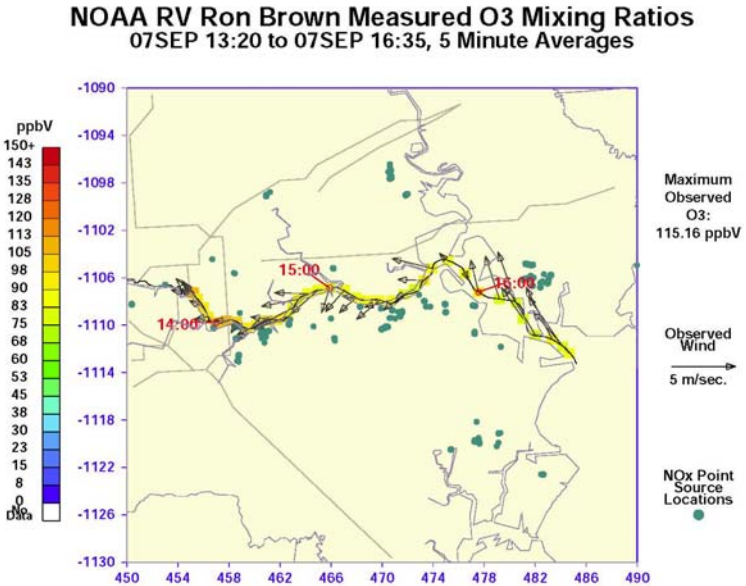


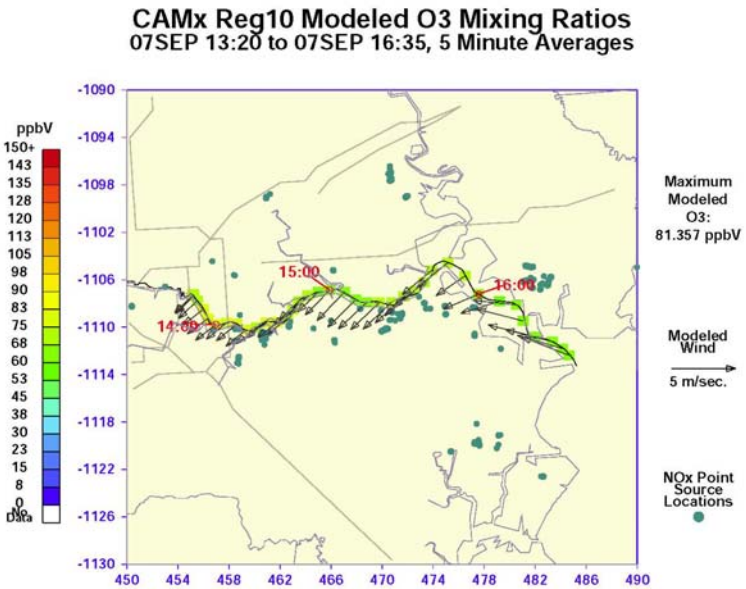
Segment D: Turning Basin to Jacinto Port

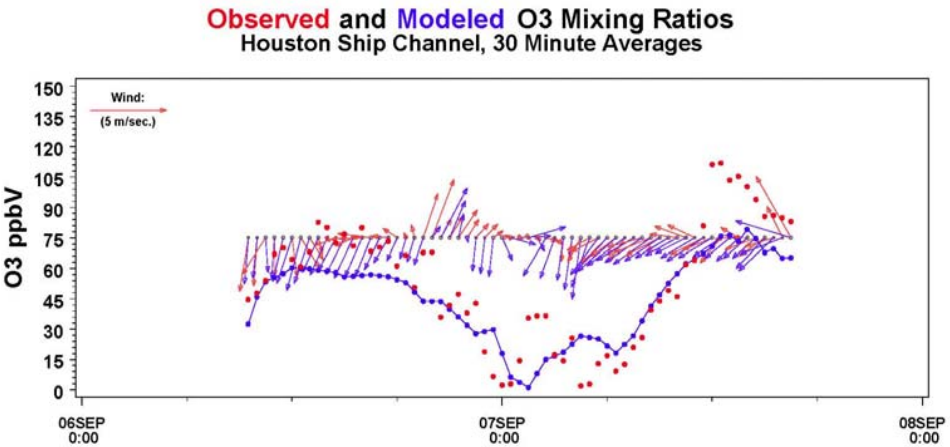


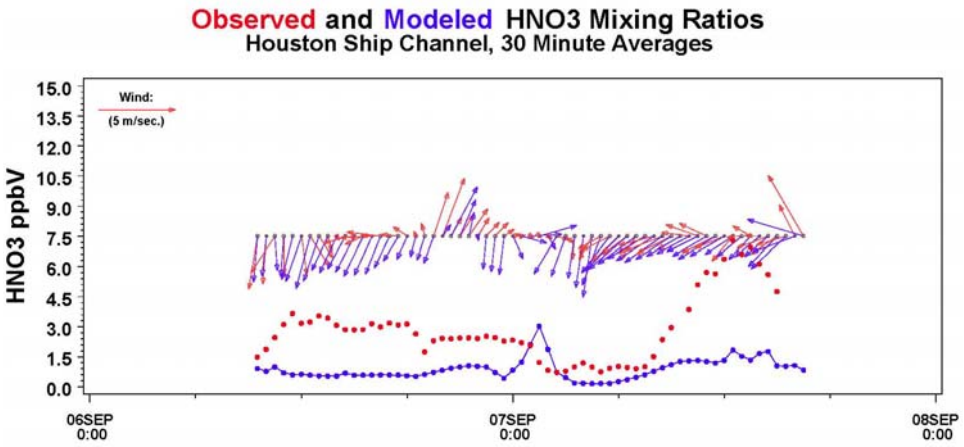


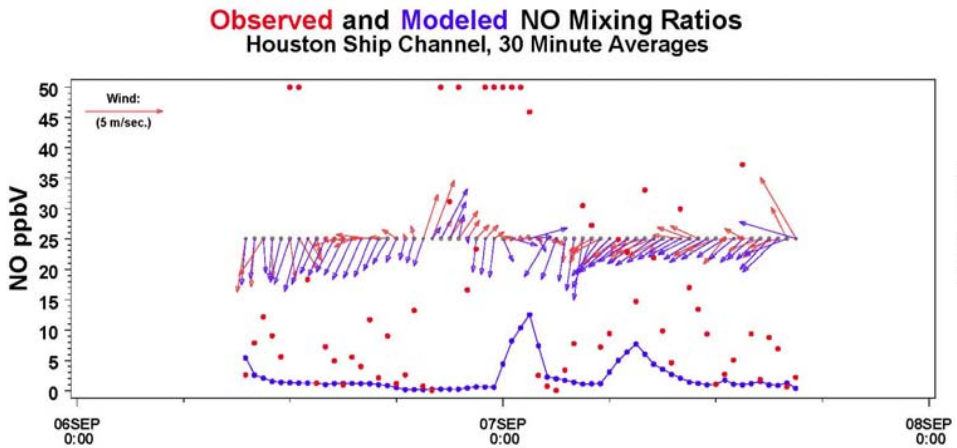
Segment E: Turning Basin to Barbour's Cut

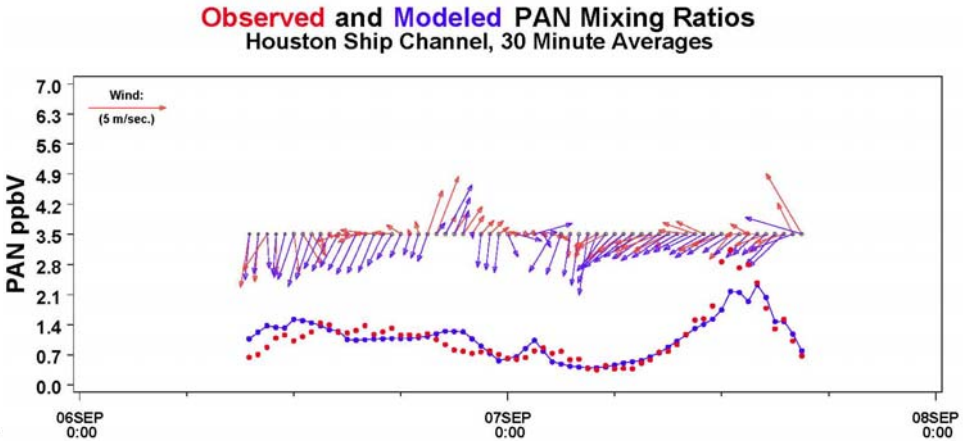


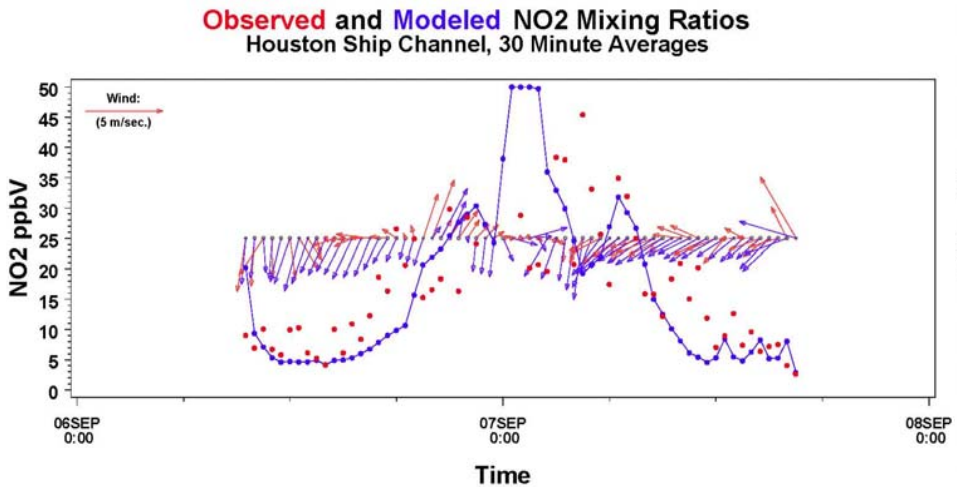


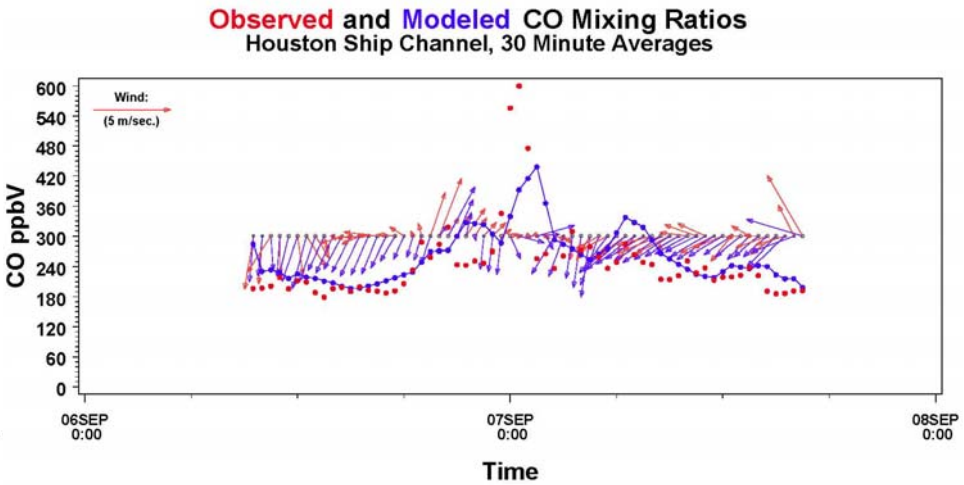

Observed and Modeled O3 Mixing Ratios
Houston Ship Channel, 30 Minute Averages
Wind:
(5 m/sec.)
O3 ppbV
150
135
120
105
90
75
60
45
30
15
0
06SEP 0:00
07SEP 0:00
08SEP 0:00

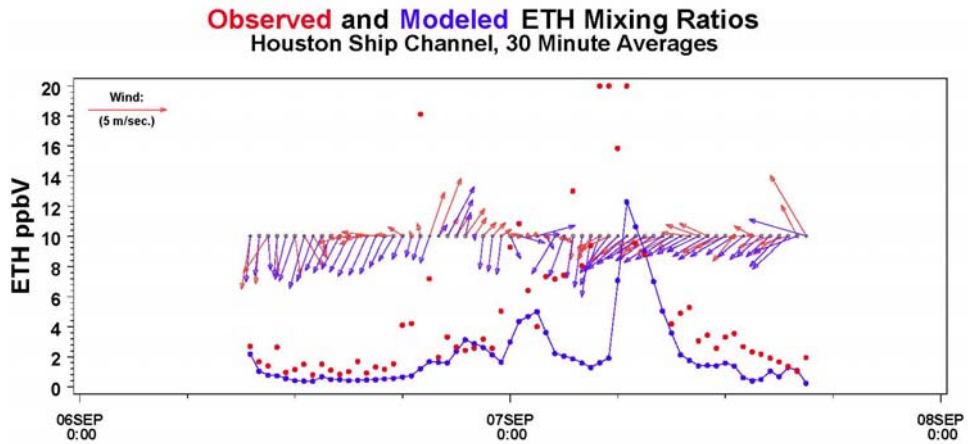

Observed and Modeled HNO3 Mixing Ratios
Houston Ship Channel, 30 Minute Averages
Wind:
(5 m/sec.)
HNO3 ppbV
15.0
13.5
12.0
10.5
9.0
7.5
6.0
4.5
3.0
1.5
0.0
06SEP 0:00
07SEP 0:00
08SEP 0:00

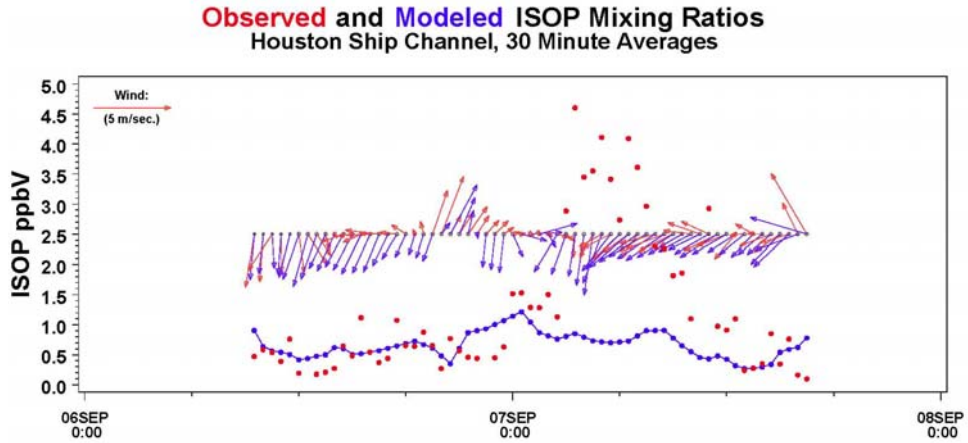

Observed and Modeled NO Mixing Ratios
Houston Ship Channel, 30 Minute Averages
Wind:
(5 m/sec.)
NO ppbV
50
45
40
35
30
25
20
15
10
5
0
06SEP 0:00
07SEP 0:00
08SEP 0:00

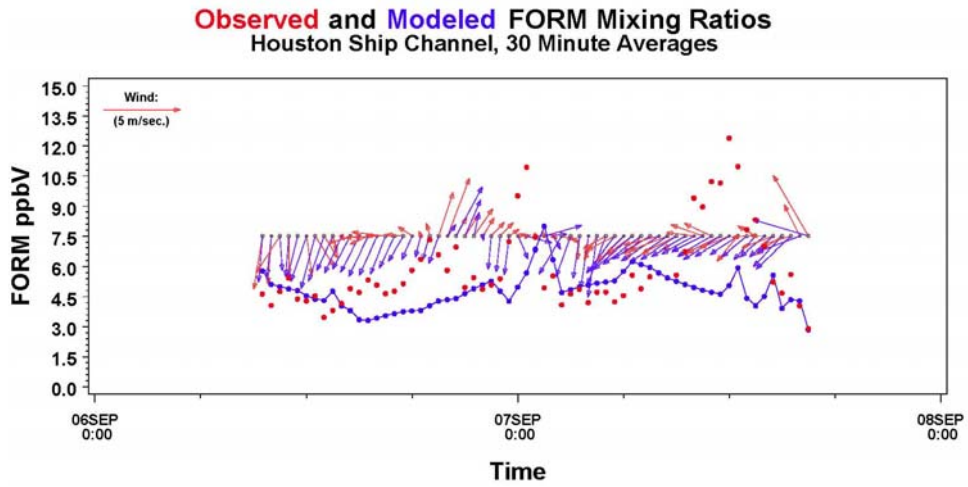

Observed and Modeled PAN Mixing Ratios
Houston Ship Channel, 30 Minute Averages
Wind:
(5 m/sec.)
PAN ppbV
7.0
6.3
5.6
4.9
4.2
3.5
2.8
2.1
1.4
0.7
0.0
06SEP 0:00
07SEP 0:00
08SEP 0:00


Observed and Modeled NO2 Mixing Ratios
Houston Ship Channel, 30 Minute Averages
Wind:
(5 m/sec.)
NO2 ppbV
50
45
40
35
30
25
20
15
10
5
0
06SEP 0:00
07SEP 0:00
08SEP 0:00
Time

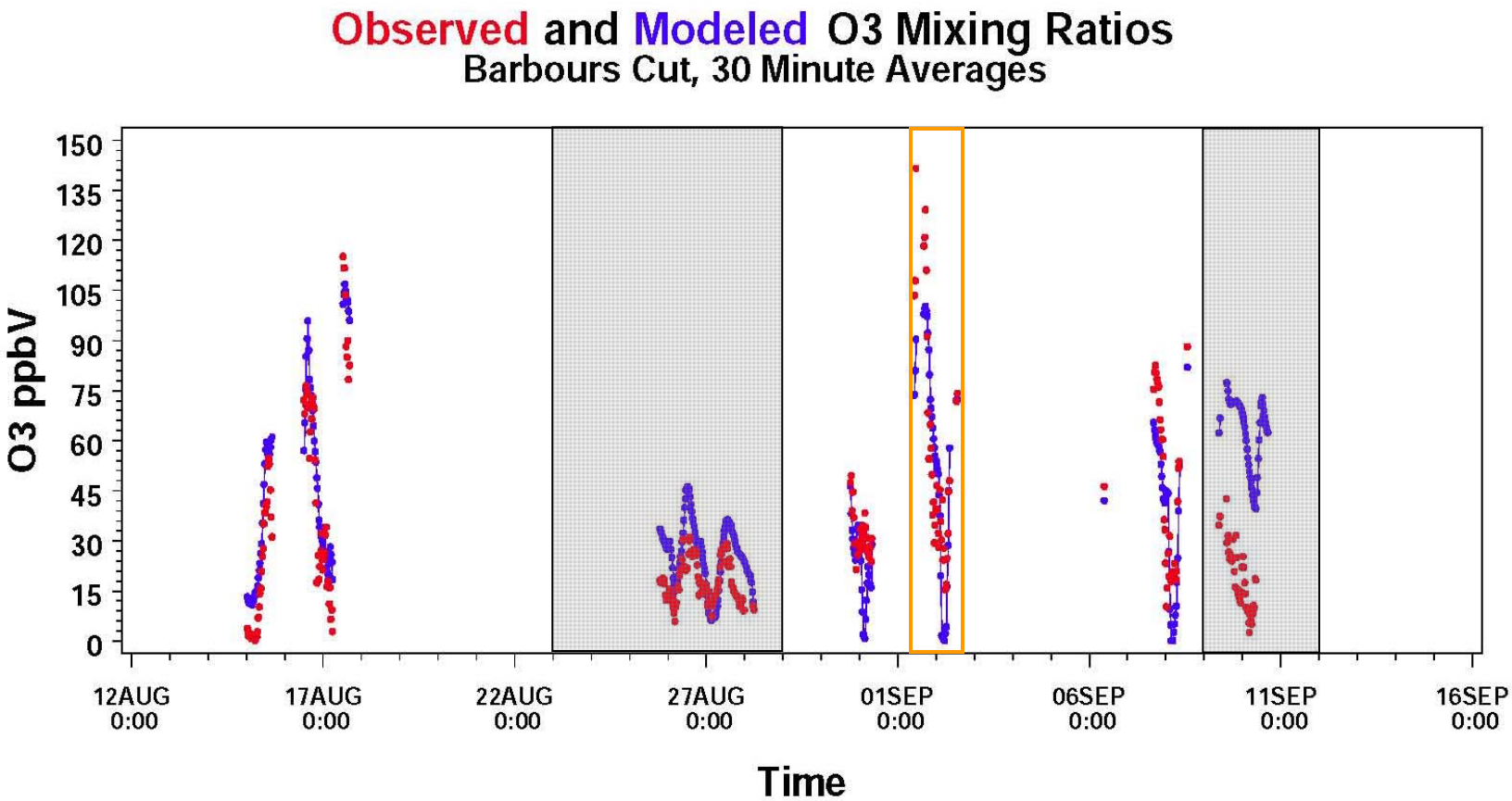

Observed and Modeled CO Mixing Ratios
Houston Ship Channel, 30 Minute Averages
Wind:
(5 m/sec.)
CO ppbV
600
540
480
420
360
300
240
180
120
60
0
06SEP 0:00
07SEP 0:00
08SEP 0:00
Time


Observed and Modeled ETH Mixing Ratios
Houston Ship Channel, 30 Minute Averages
Wind:
(5 m/sec.)
ETH ppbV
20
18
16
14
12
10
8
6
4
2
0
06SEP 0:00
07SEP 0:00
08SEP 0:00

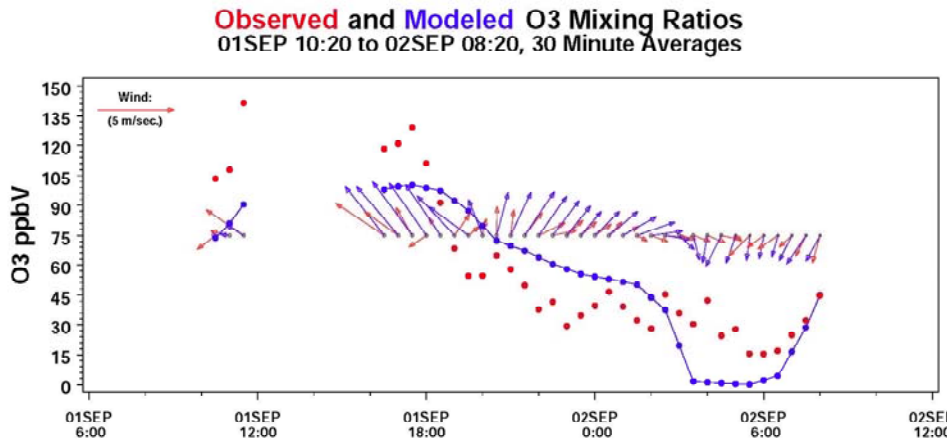

Observed and Modeled ISOP Mixing Ratios
Houston Ship Channel, 30 Minute Averages
Wind:
(5 m/sec.)
ISOP ppbV
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
06SEP 0:00
07SEP 0:00
08SEP 0:00

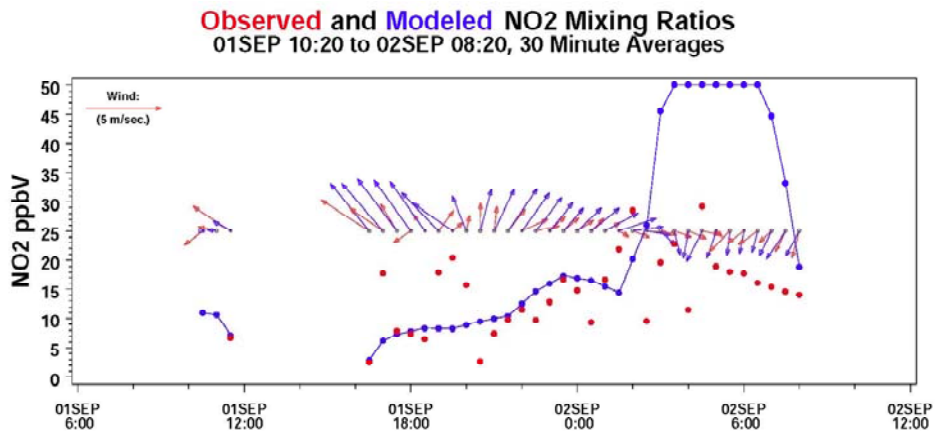

Observed and Modeled FORM Mixing Ratios
Houston Ship Channel, 30 Minute Averages
Wind:
(5 m/sec.)
FORM ppbV
15.0
13.5
12.0
10.5
9.0
7.5
6.0
4.5
3.0
1.5
0.0
06SEP 0:00
07SEP 0:00
08SEP 0:00
Time

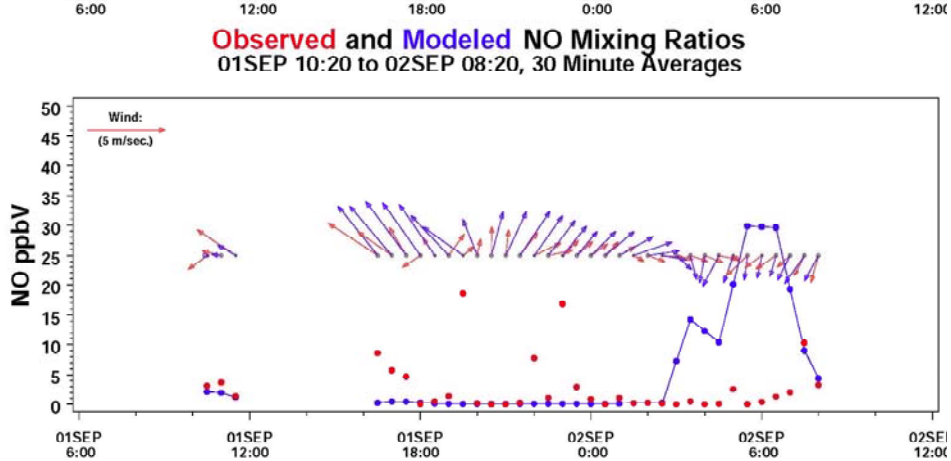
Barbour's Cut

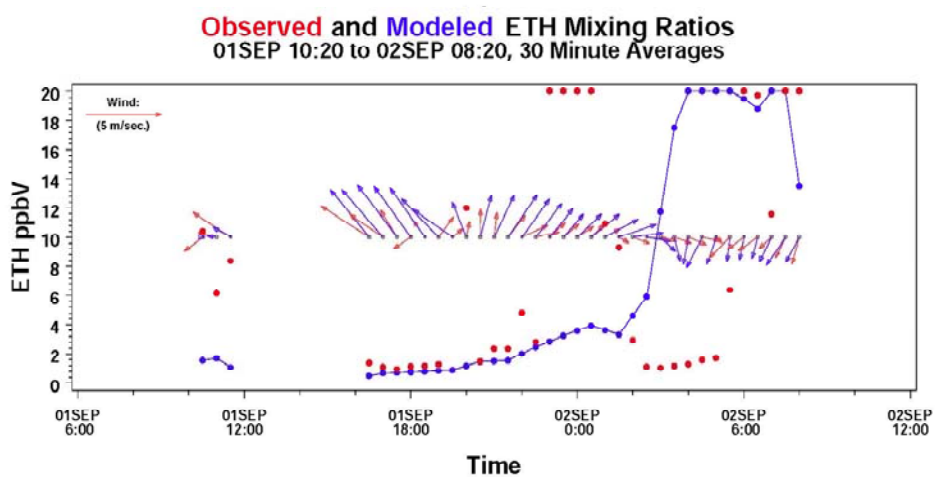


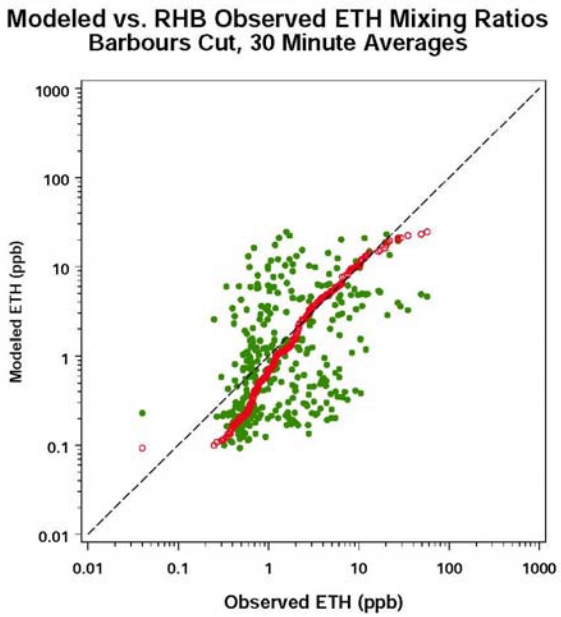
Shaded Areas Represent Periods Modeled Without the 2- and 4-km Fine Grids.

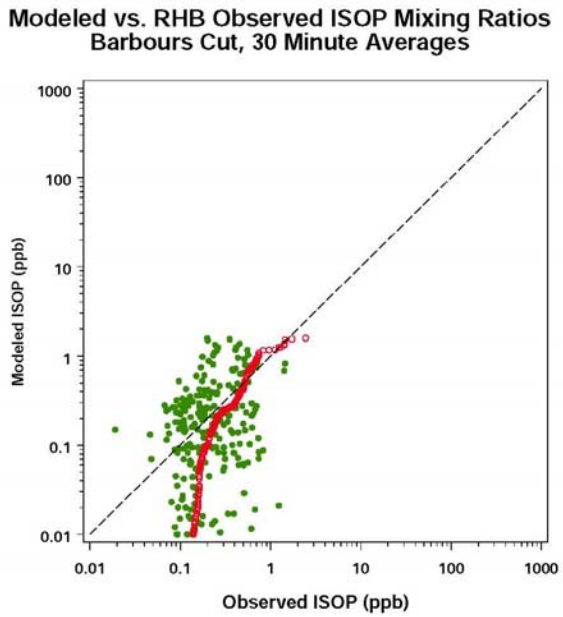

Observed and Modeled O3 Mixing Ratios
01SEP 10:20 to 02SEP 08:20, 30 Minute Averages
Wind:
(5 m/sec.)
O3 ppbV
150
135
120
105
90
75
60
45
30
15
0
01SEP 6:00
01SEP 12:00
01SEP 18:00
02SEP 0:00
02SEP 6:00

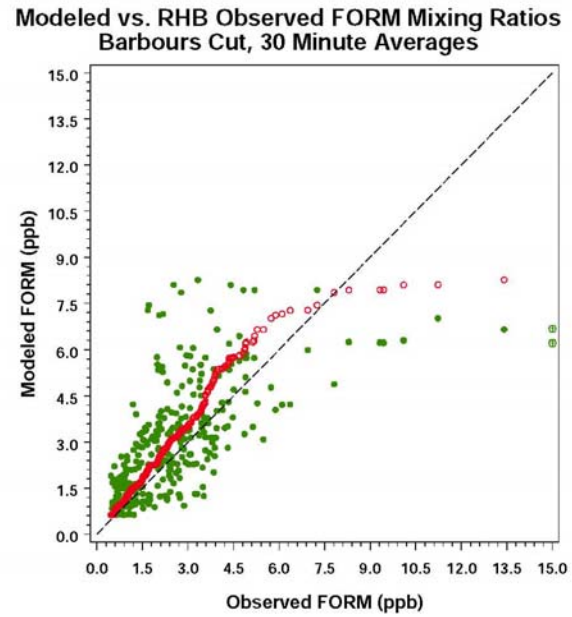

Observed and Modeled NO2 Mixing Ratios
01SEP 10:20 to 02SEP 08:20, 30 Minute Averages
Wind:
(5 m/sec.)
NO2 ppbV
50
45
40
35
30
25
20
15
10
5
0
01SEP 6:00
01SEP 12:00
01SEP 18:00
02SEP 0:00
02SEP 6:00
02SEP 12:00

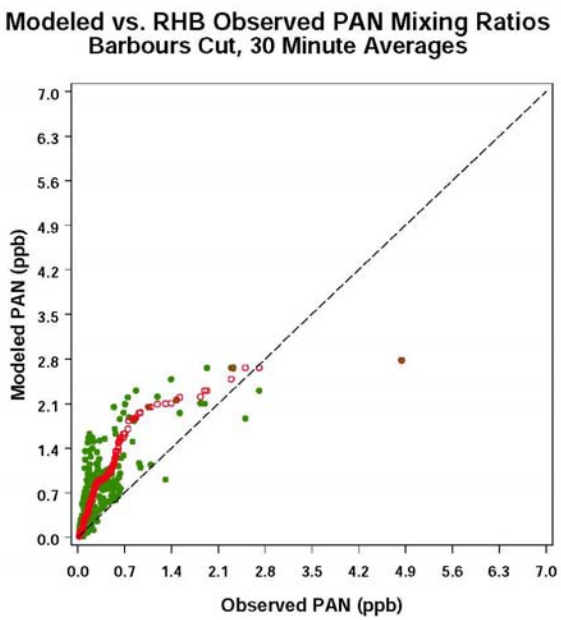

Observed and Modeled NO Mixing Ratios
01SEP 10:20 to 02SEP 08:20, 30 Minute Averages
Wind:
(5 m/sec.)
NO ppbV
50
45
40
35
30
25
20
15
10
5
0
01SEP 6:00
01SEP 12:00
01SEP 18:00
02SEP 0:00
02SEP 6:00

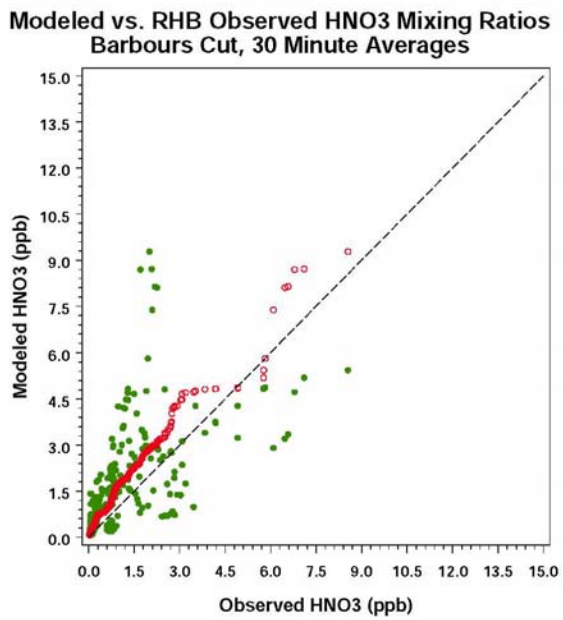

Observed and Modeled ETH Mixing Ratios
01SEP 10:20 to 02SEP 08:20, 30 Minute Averages
Wind:
(5 m/sec.)
ETH ppbV
20
18
16
14
12
10
8
6
4
2
0
01SEP 6:00
01SEP 12:00
01SEP 18:00
02SEP 0:00
02SEP 6:00
02SEP 12:00
Time

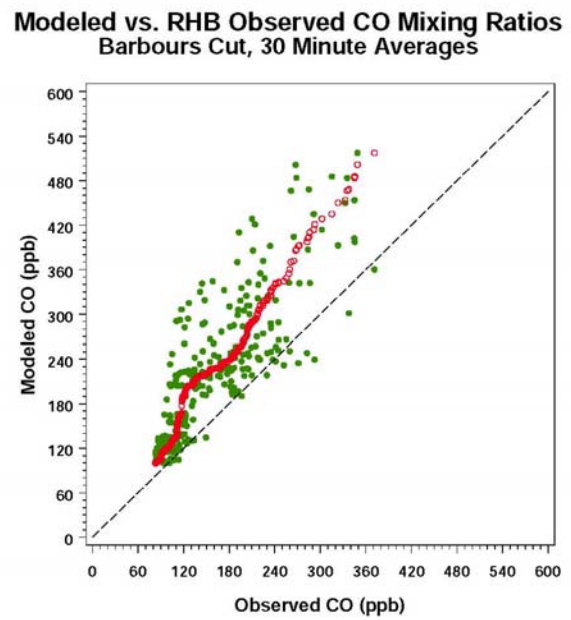

Modeled vs. RHB Observed ETH Mixing Ratios
Barbours Cut, 30 Minute Averages
Modeled ETH (ppb)
Observed ETH (ppb)
1000
100
10
1
0.1
0.01


Modeled vs. RHB Observed ISOP Mixing Ratios
Barbours Cut, 30 Minute Averages
Modeled ISOP (ppb)
Observed ISOP (ppb)
1000
100
10
1
0.1
0.01

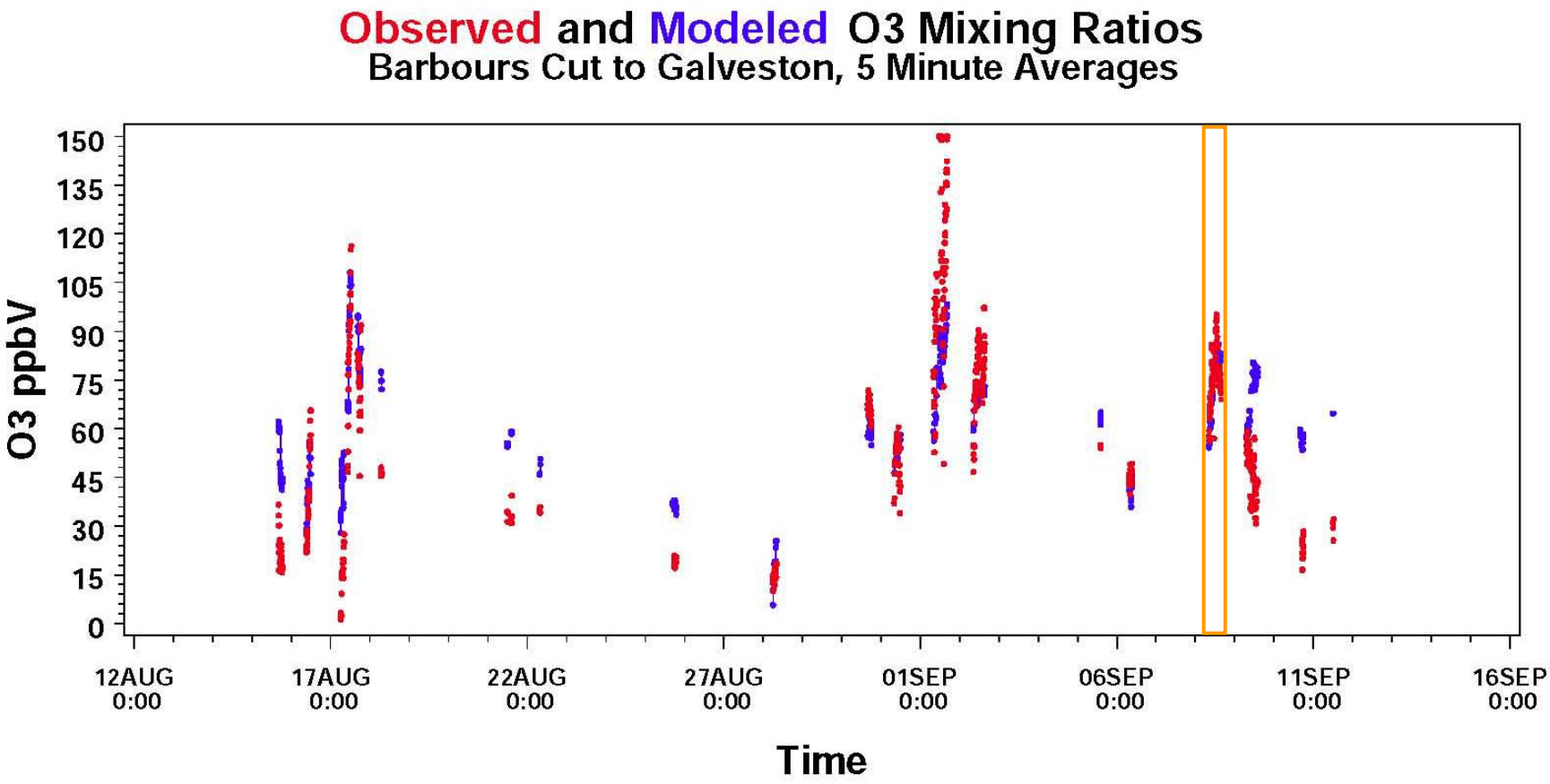

Modeled vs. RHB Observed FORM Mixing Ratios
Barbours Cut, 30 Minute Averages
Modeled FORM (ppb)
Observed FORM (ppb)
15.0
13.5
12.0
10.5
9.0
7.5
6.0
4.5
3.0
1.5
0.0


Modeled vs. RHB Observed PAN Mixing Ratios
Barbours Cut, 30 Minute Averages
Modeled PAN (ppb)
Observed PAN (ppb)
7.0
6.3
5.6
4.9
4.2
3.5
2.8
2.1
1.4
0.7
0.0

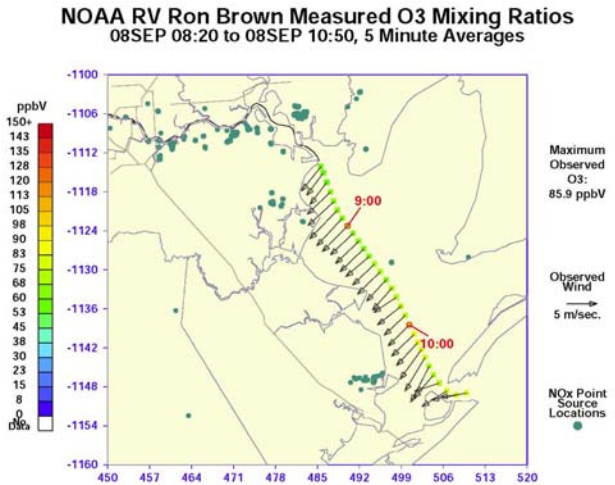

Modeled vs. RHB Observed HNO3 Mixing Ratios
Barbours Cut, 30 Minute Averages
Modeled HNO3 (ppb)
Observed HNO3 (ppb)
15.0
13.5
12.0
10.5
9.0
7.5
6.0
4.5
3.0
1.5
0.0

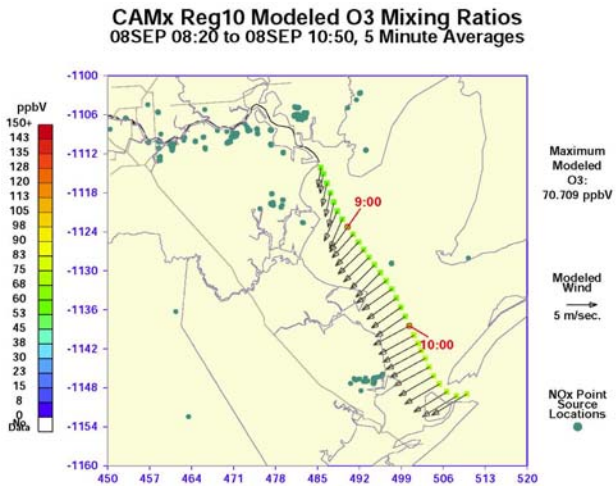

Modeled vs. RHB Observed CO Mixing Ratios
Barbours Cut, 30 Minute Averages
Modeled CO (ppb)
Observed CO (ppb)
600
540
480
420
360
300
240
180
120
60
0

Barbour's Cut to Galveston

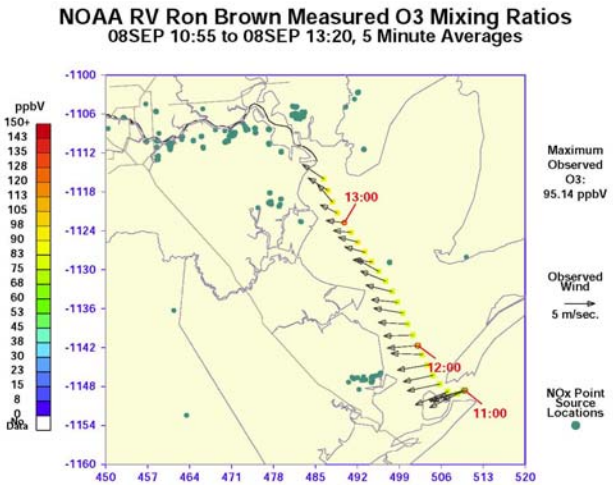


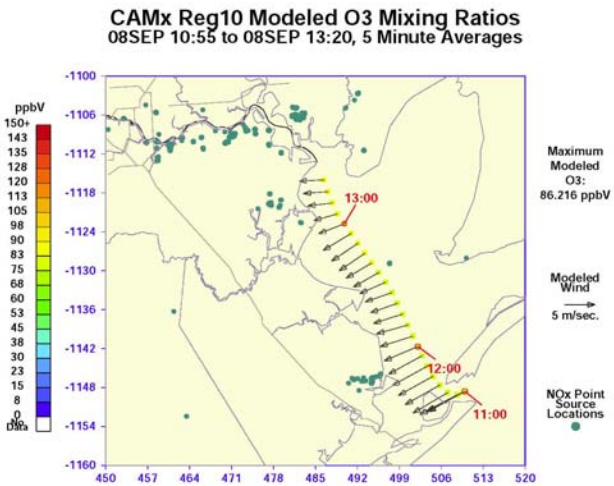
Sept. 8, 08:20 to 10:50 Outbound



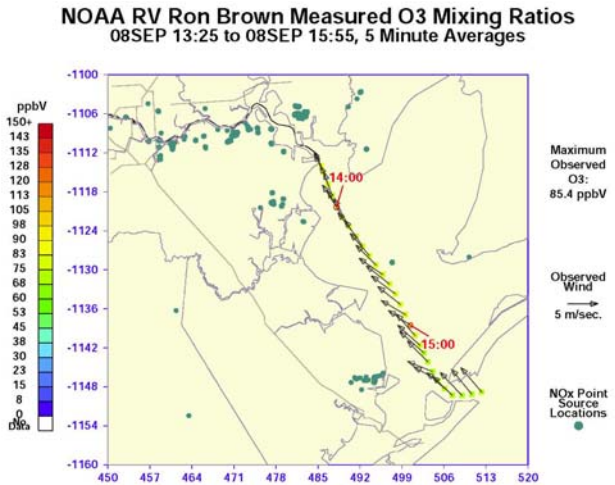


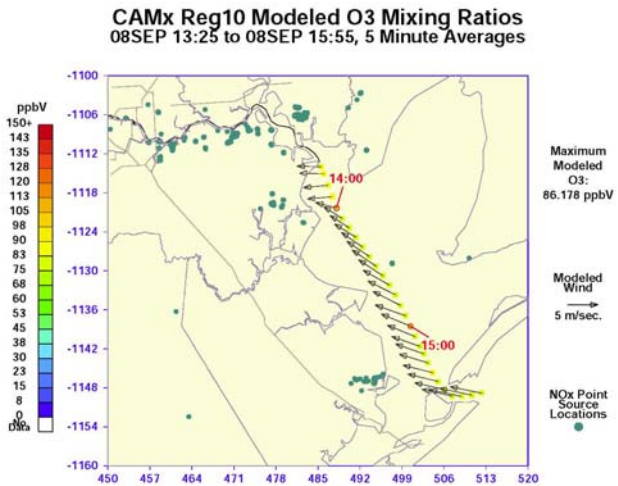
Sept. 8, 10:55 to 13:20 Inbound



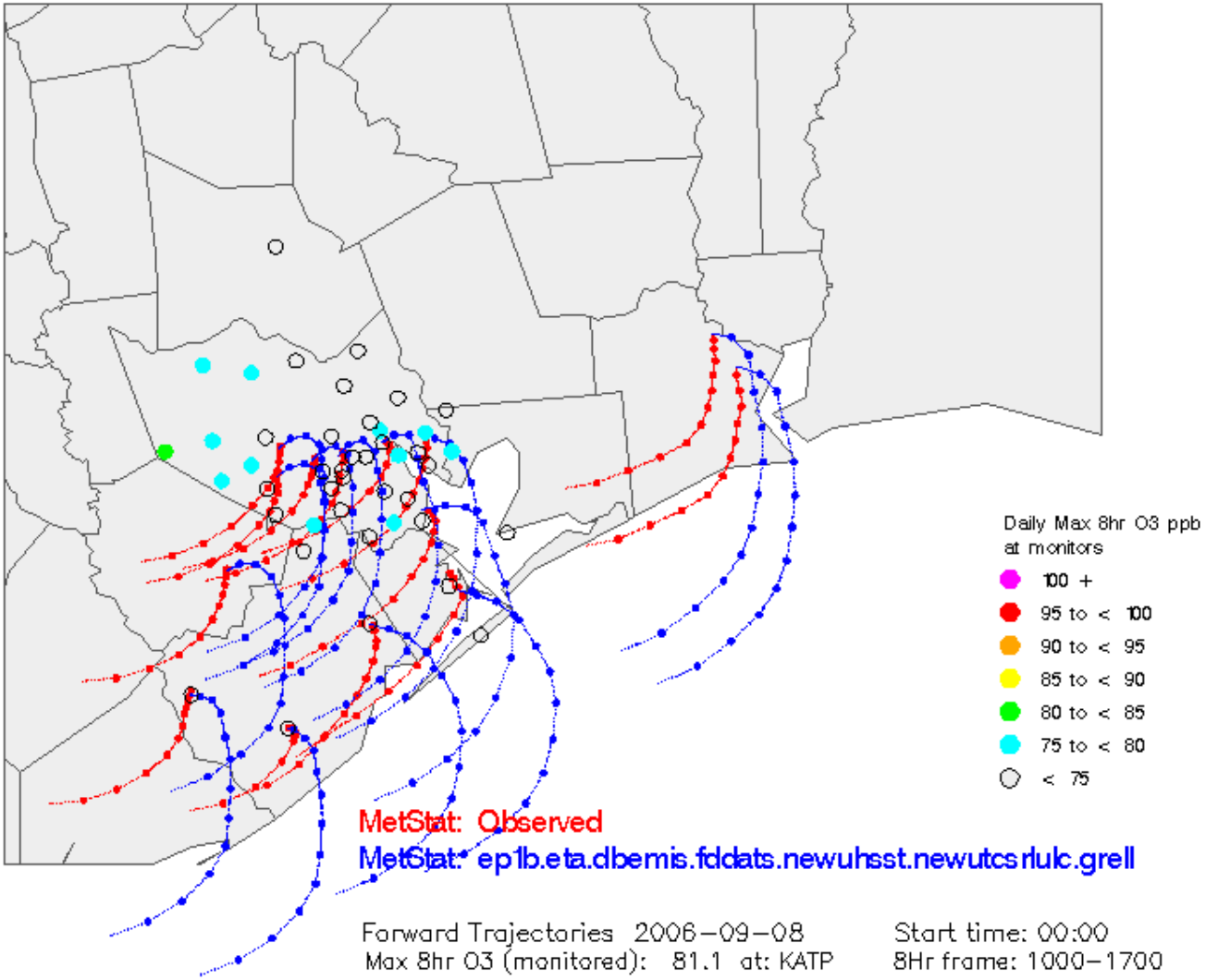


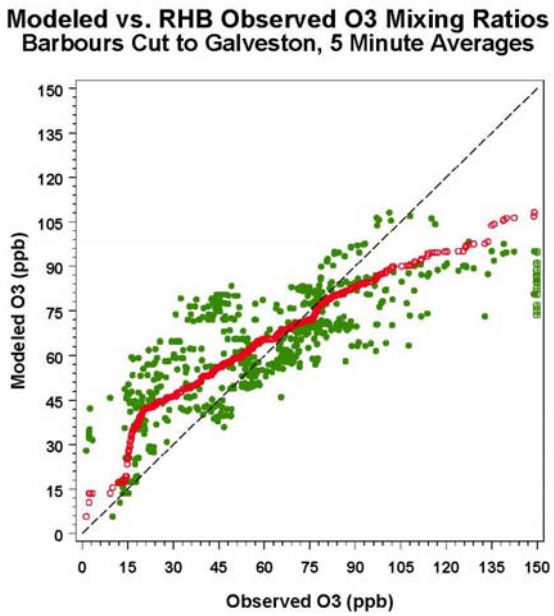
Sept. 8, 13:25 to 15:55 Outbound

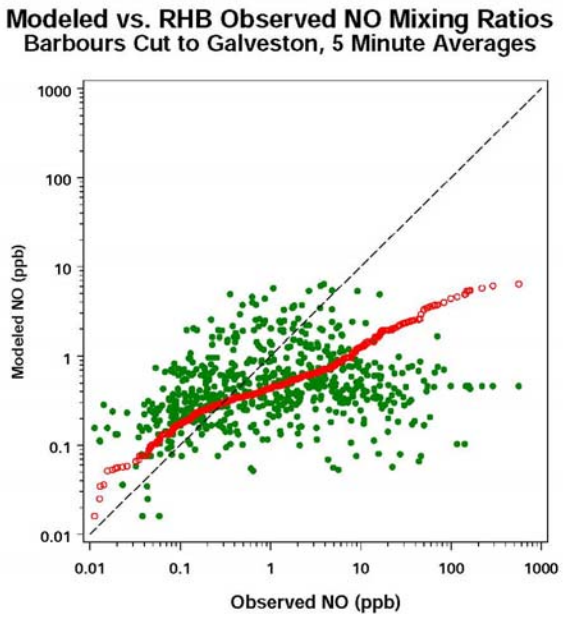


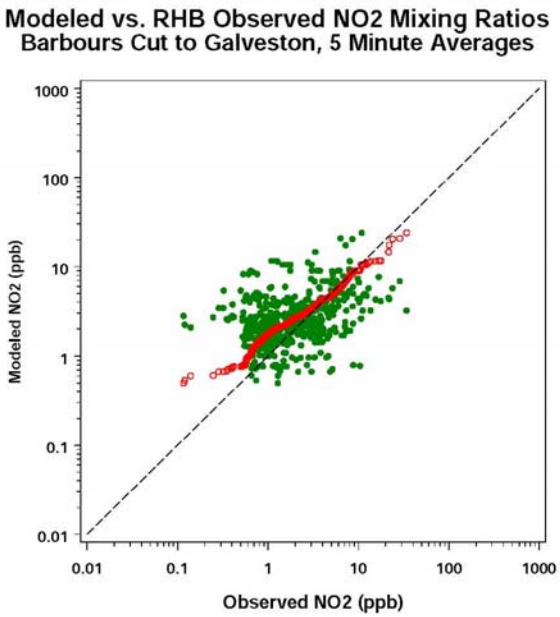


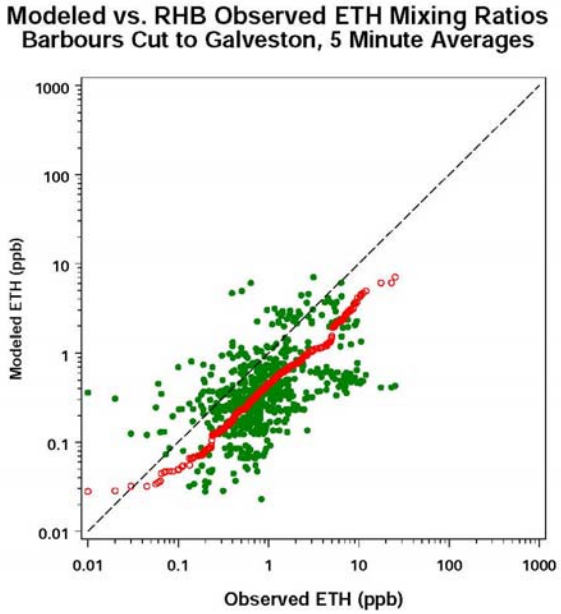
12-Hour Forward Trajectories
Beginning 00:00, August 8, 2006

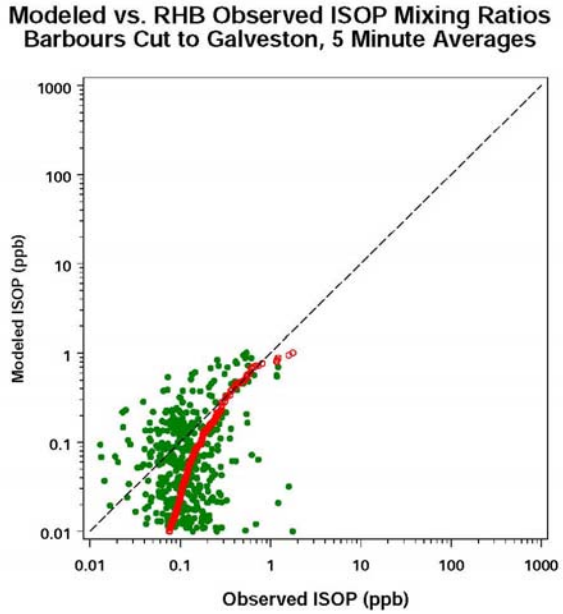


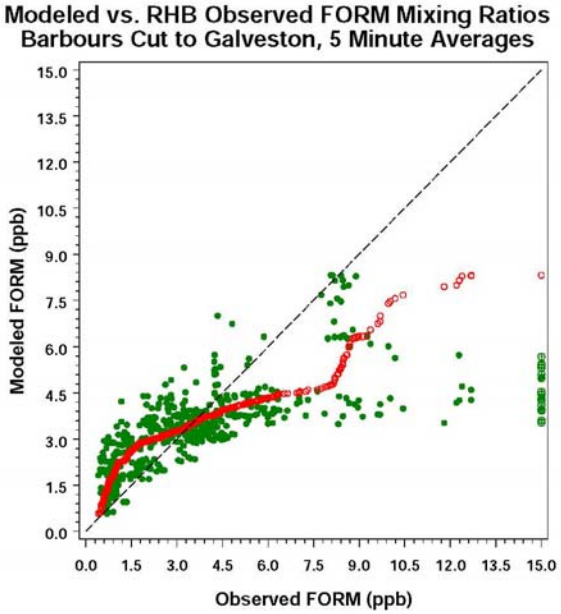

Modeled vs. RHB Observed O3 Mixing Ratios
Barbours Cut to Galveston, 5 Minute Averages
Modeled O3 (ppb)
Observed O3 (ppb)


Modeled vs. RHB Observed NO Mixing Ratios
Barbours Cut to Galveston, 5 Minute Averages
Modeled NO (ppb)
Observed NO (ppb)

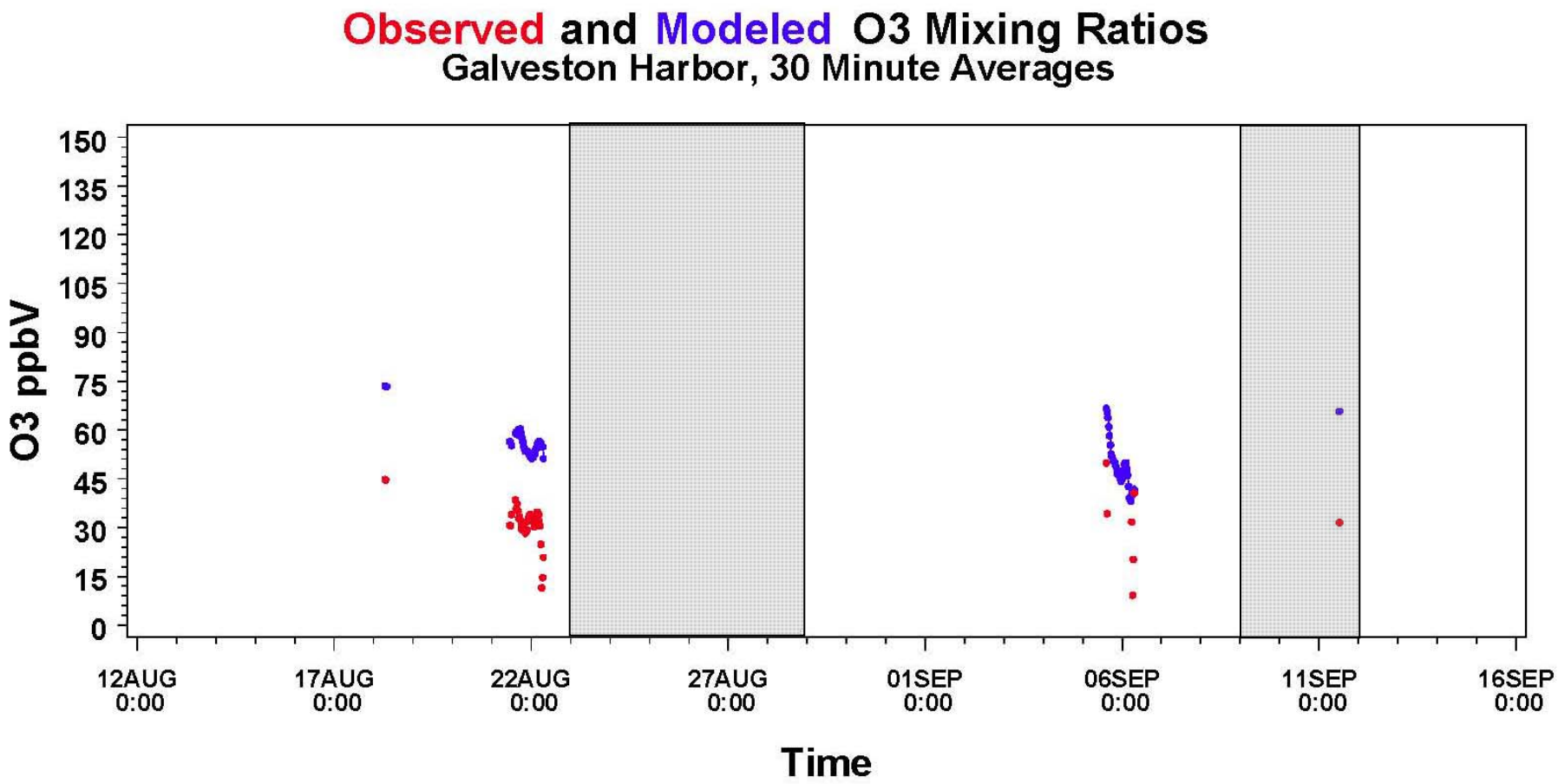

Modeled vs. RHB Observed NO2 Mixing Ratios
Barbours Cut to Galveston, 5 Minute Averages
Modeled NO2 (ppb)
Observed NO2 (ppb)


Modeled vs. RHB Observed ETH Mixing Ratios
Barbours Cut to Galveston, 5 Minute Averages
Modeled ETH (ppb)
Observed ETH (ppb)

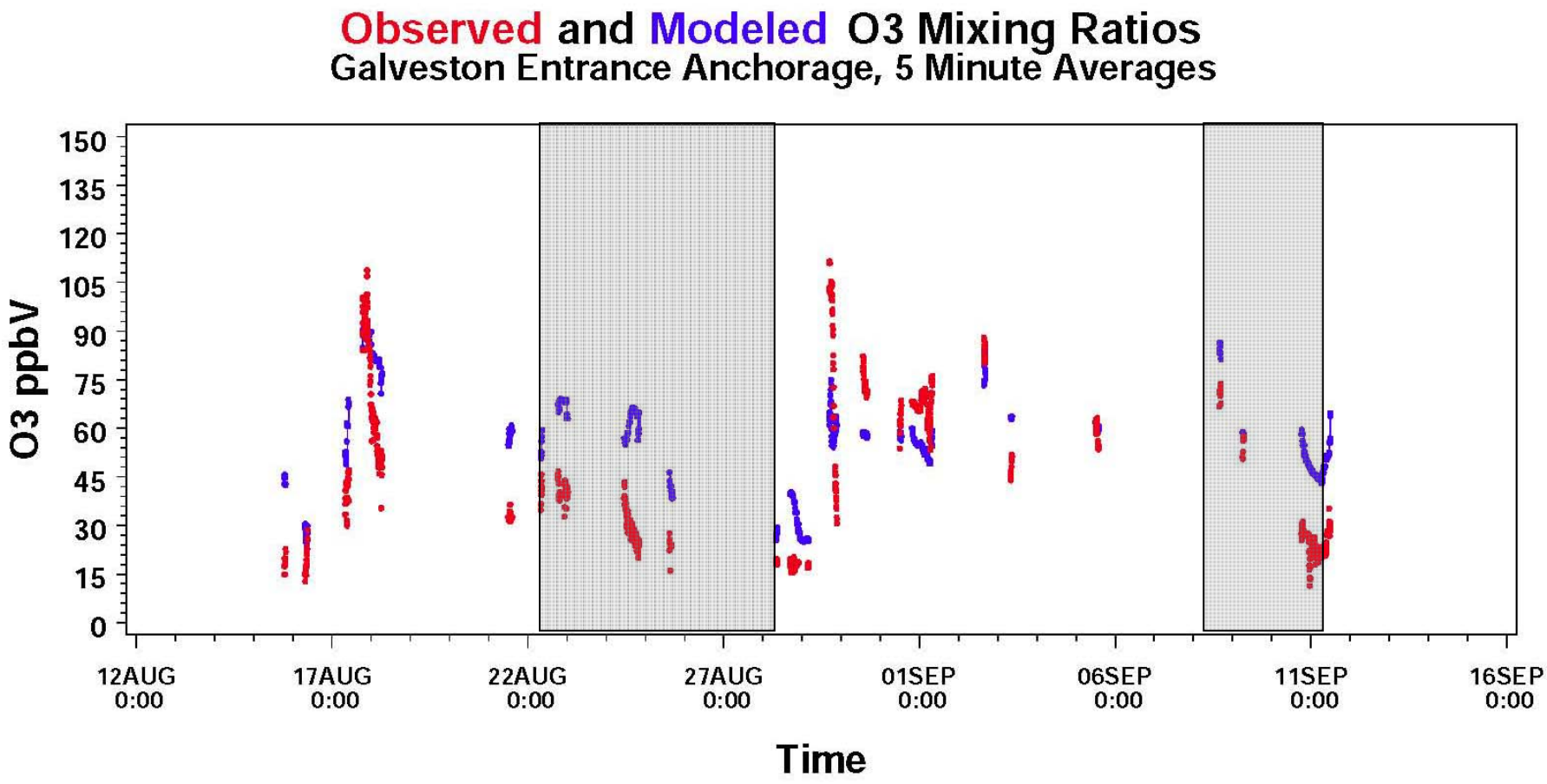

Modeled vs. RHB Observed ISOP Mixing Ratios
Barbours Cut to Galveston, 5 Minute Averages
Modeled ISOP (ppb)
Observed ISOP (ppb)

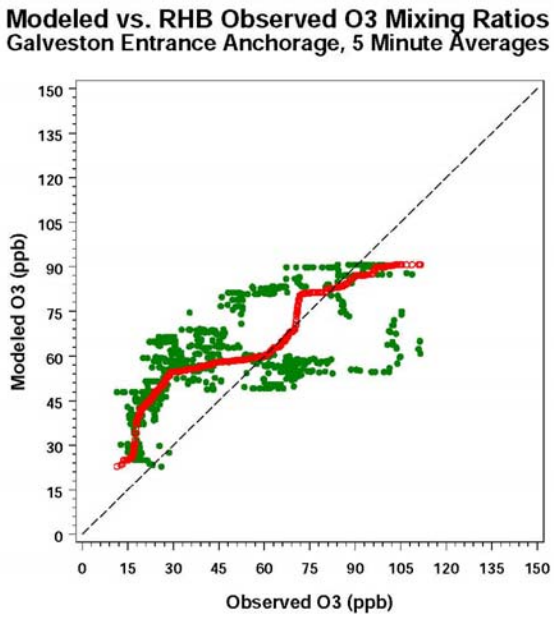

Modeled vs. RHB Observed FORM Mixing Ratios
Barbours Cut to Galveston, 5 Minute Averages
Modeled FORM (ppb)
Observed FORM (ppb)

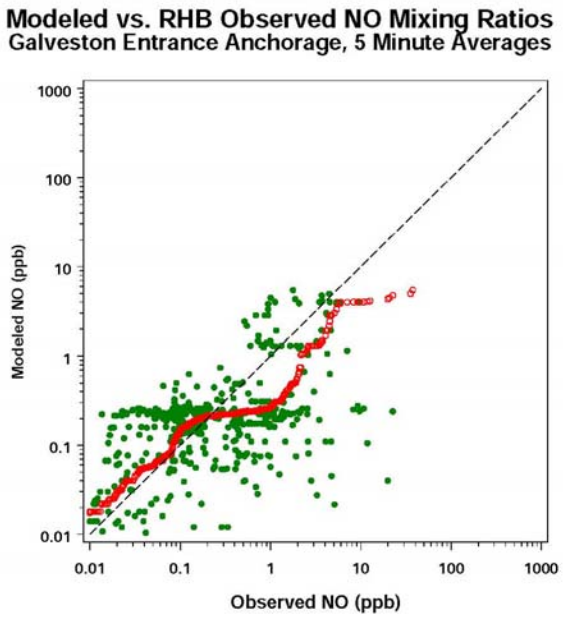
Galveston Harbor

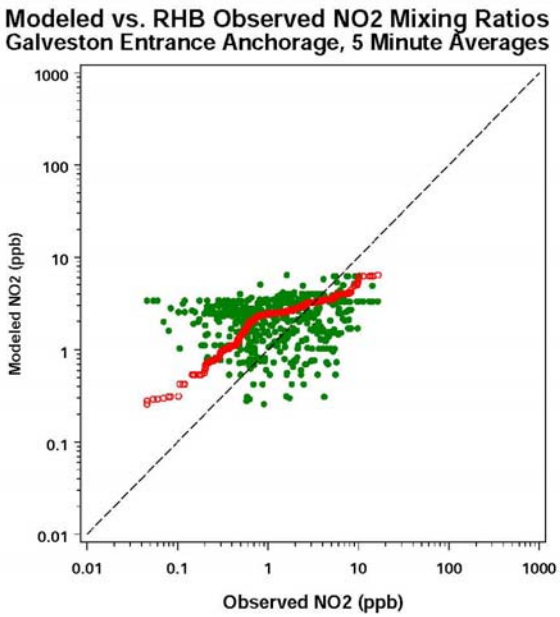


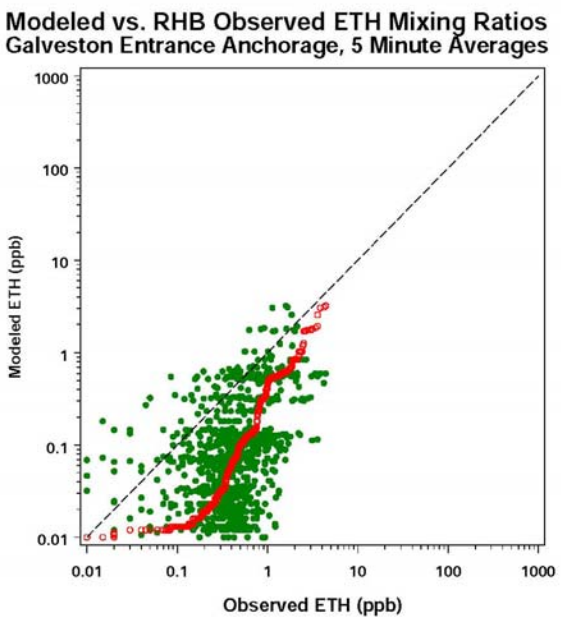
Galveston Entrance/Anchorage

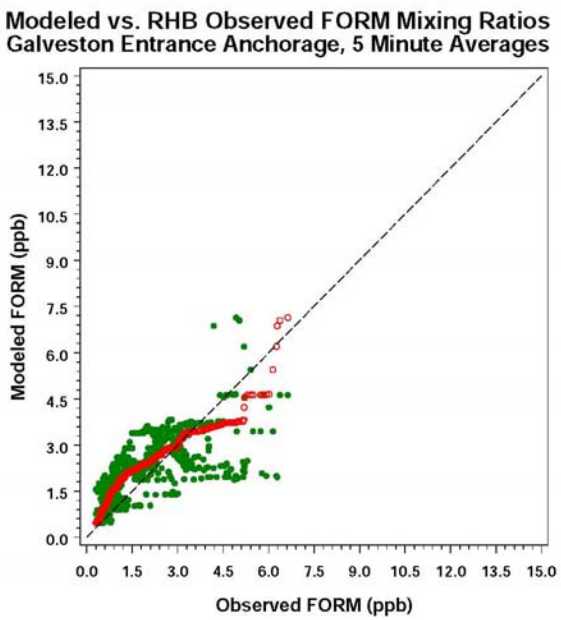



Modeled vs. RHB Observed O3 Mixing Ratios
Galveston Entrance Anchorage, 5 Minute Averages
Modeled O3 (ppb)
Observed O3 (ppb)

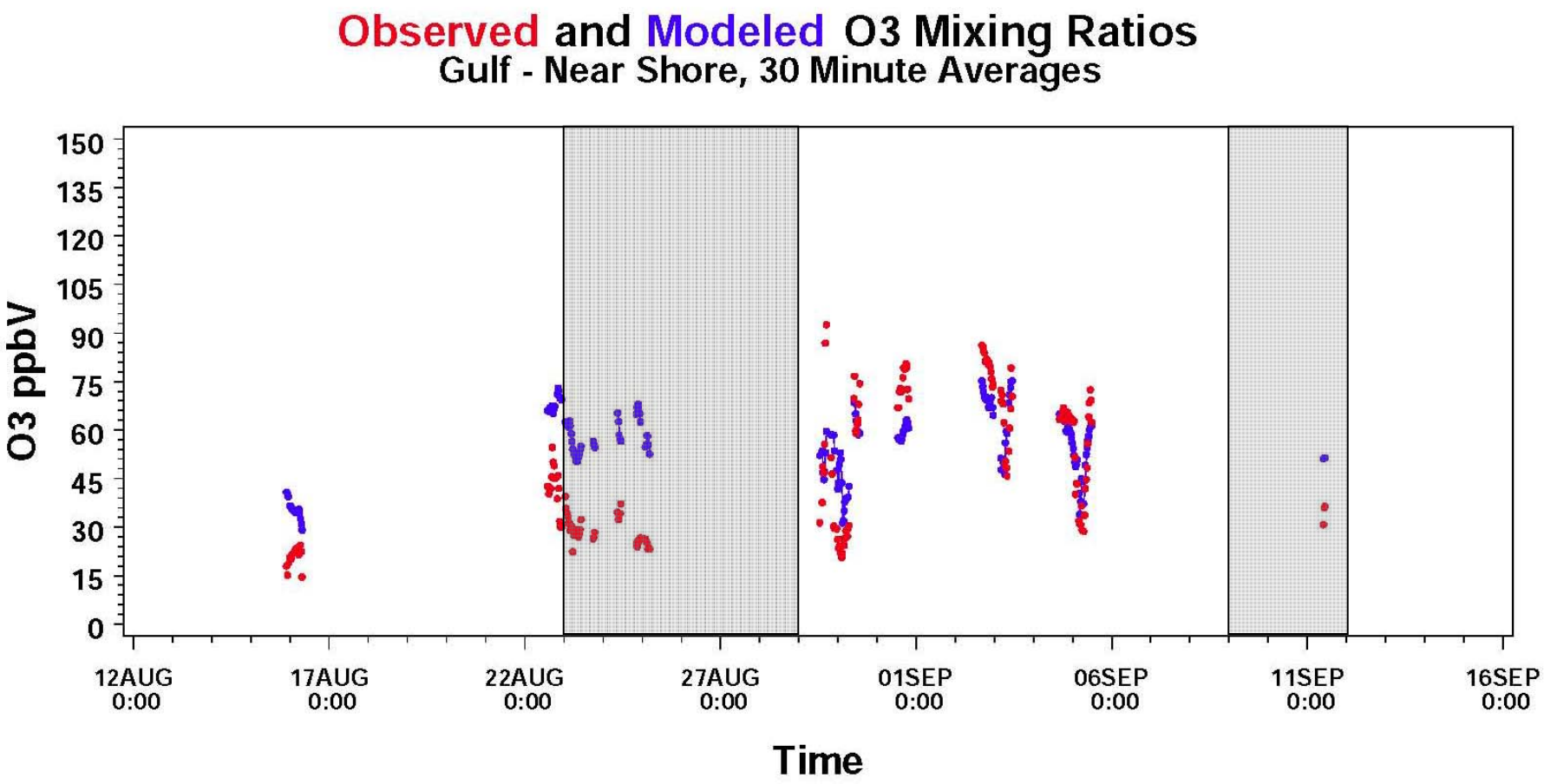

Modeled vs. RHB Observed NO Mixing Ratios
Galveston Entrance Anchorage, 5 Minute Averages
Modeled NO (ppb)
Observed NO (ppb)

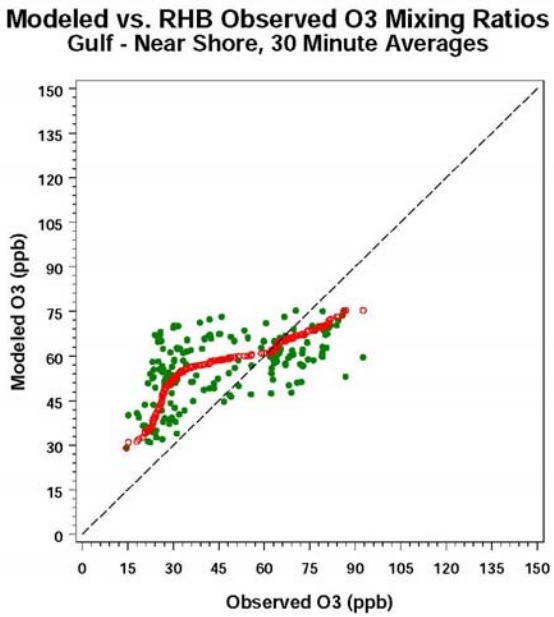

Modeled vs. RHB Observed NO2 Mixing Ratios
Galveston Entrance Anchorage, 5 Minute Averages
Modeled NO2 (ppb)
Observed NO2 (ppb)

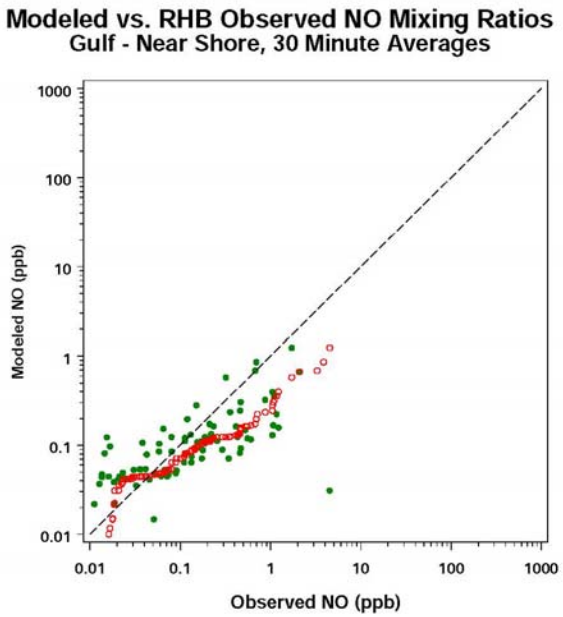

Modeled vs. RHB Observed ETH Mixing Ratios
Galveston Entrance Anchorage, 5 Minute Averages
Modeled ETH (ppb)
Observed ETH (ppb)

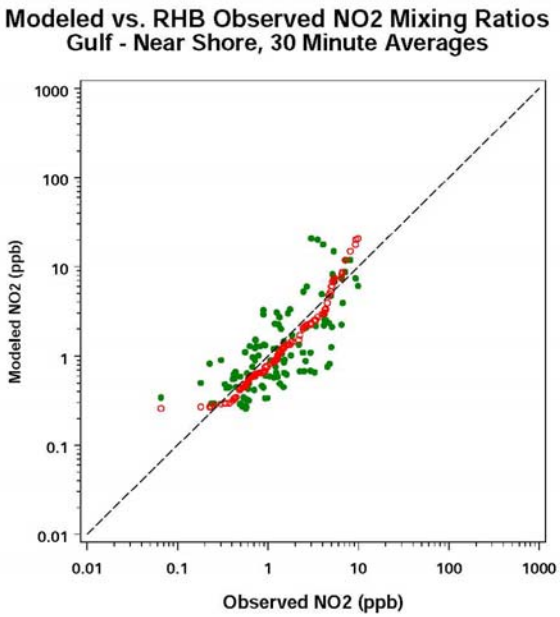

Modeled vs. RHB Observed FORM Mixing Ratios
Galveston Entrance Anchorage, 5 Minute Averages
Modeled FORM (ppb)
Observed FORM (ppb)

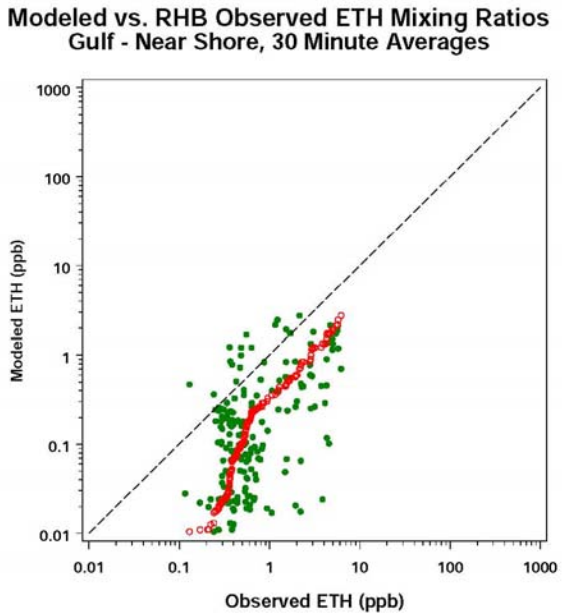
Gulf-Near Shore

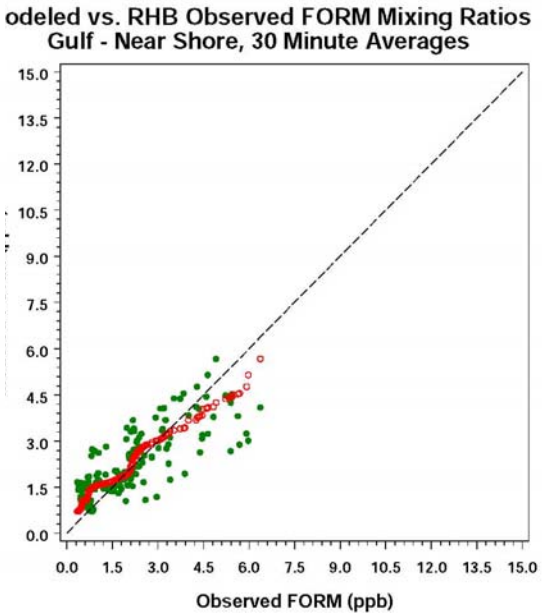



Modeled vs. RHB Observed O3 Mixing Ratios
Gulf - Near Shore, 30 Minute Averages
Modeled O3 (ppb)
Observed O3 (ppb)

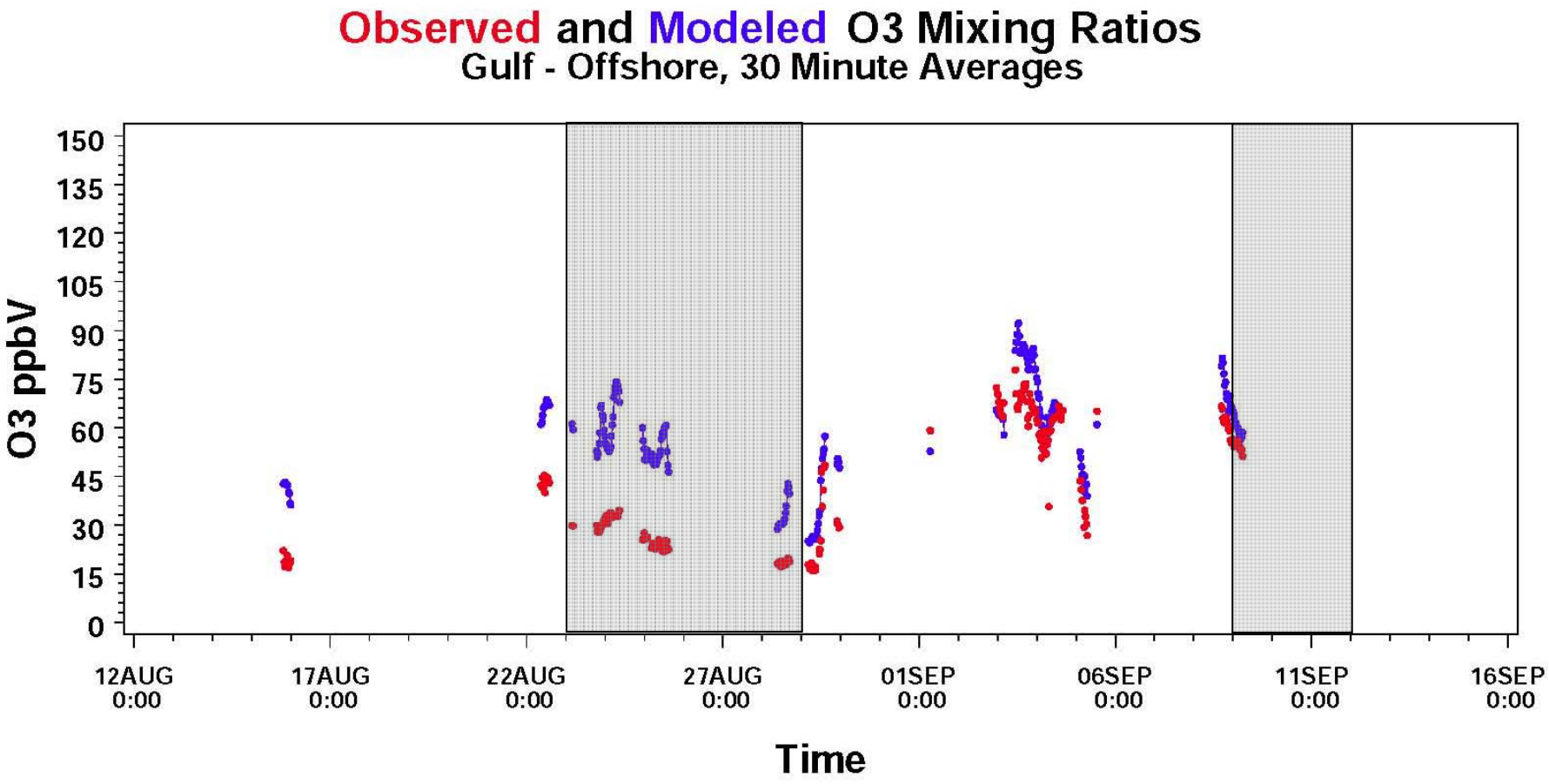

Modeled vs. RHB Observed NO Mixing Ratios
Gulf - Near Shore, 30 Minute Averages
Modeled NO (ppb)
Observed NO (ppb)

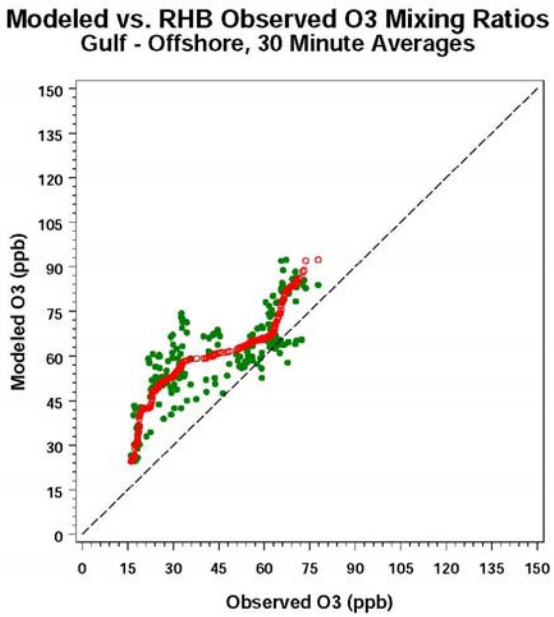

Modeled vs. RHB Observed NO2 Mixing Ratios
Gulf - Near Shore, 30 Minute Averages
Modeled NO2 (ppb)
Observed NO2 (ppb)

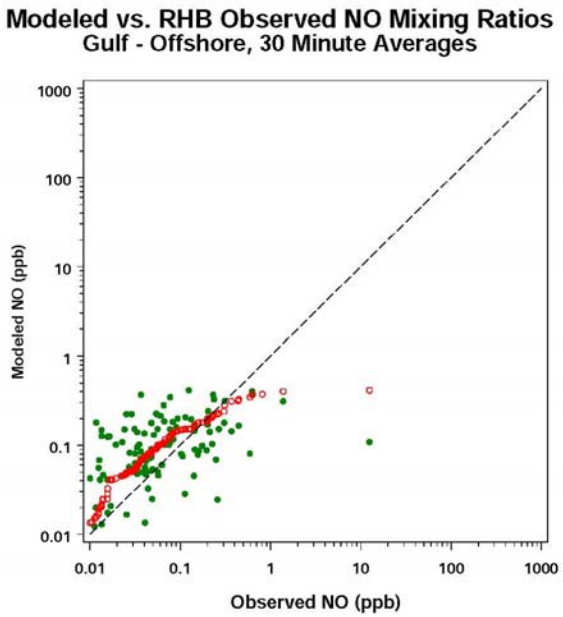

Modeled vs. RHB Observed ETH Mixing Ratios
Gulf - Near Shore, 30 Minute Averages
Modeled ETH (ppb)
Observed ETH (ppb)

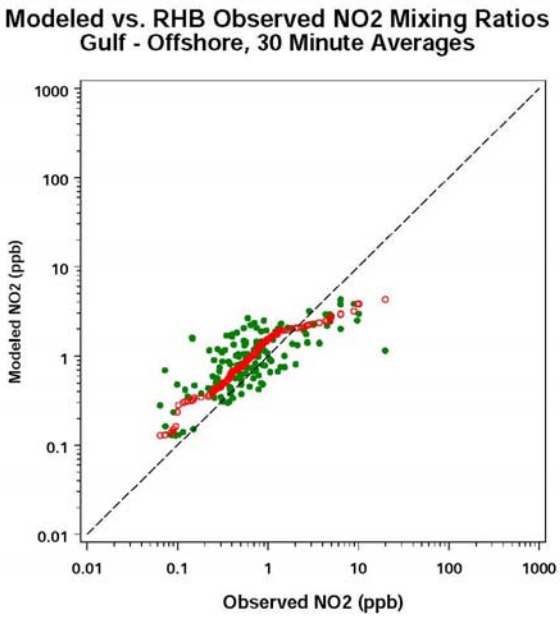

odeled vs. RHB Observed FORM Mixing Ratios
Gulf - Near Shore, 30 Minute Averages
Observed FORM (ppb)

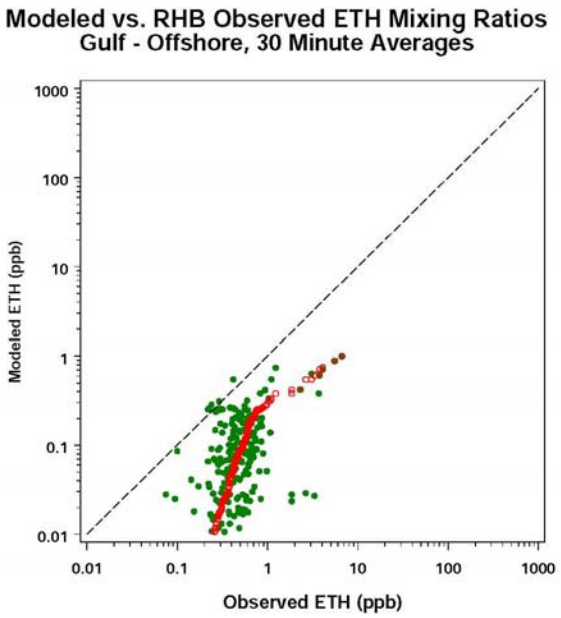
Gulf-Offshore

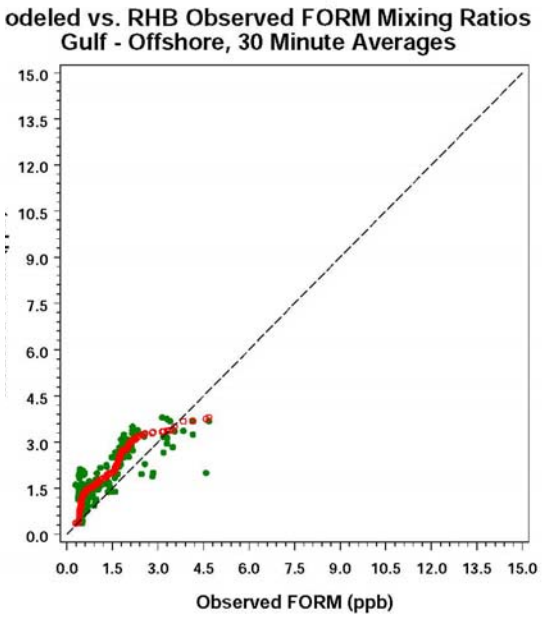



Modeled vs. RHB Observed O3 Mixing Ratios
Gulf - Offshore, 30 Minute Averages
Modeled O3 (ppb)
Observed O3 (ppb)


Modeled vs. RHB Observed NO Mixing Ratios
Gulf - Offshore, 30 Minute Averages
Modeled NO (ppb)
Observed NO (ppb)


Modeled vs. RHB Observed NO2 Mixing Ratios
Gulf - Offshore, 30 Minute Averages
Modeled NO2 (ppb)
Observed NO2 (ppb)


Modeled vs. RHB Observed ETH Mixing Ratios
Gulf - Offshore, 30 Minute Averages
Modeled ETH (ppb)
Observed ETH (ppb)

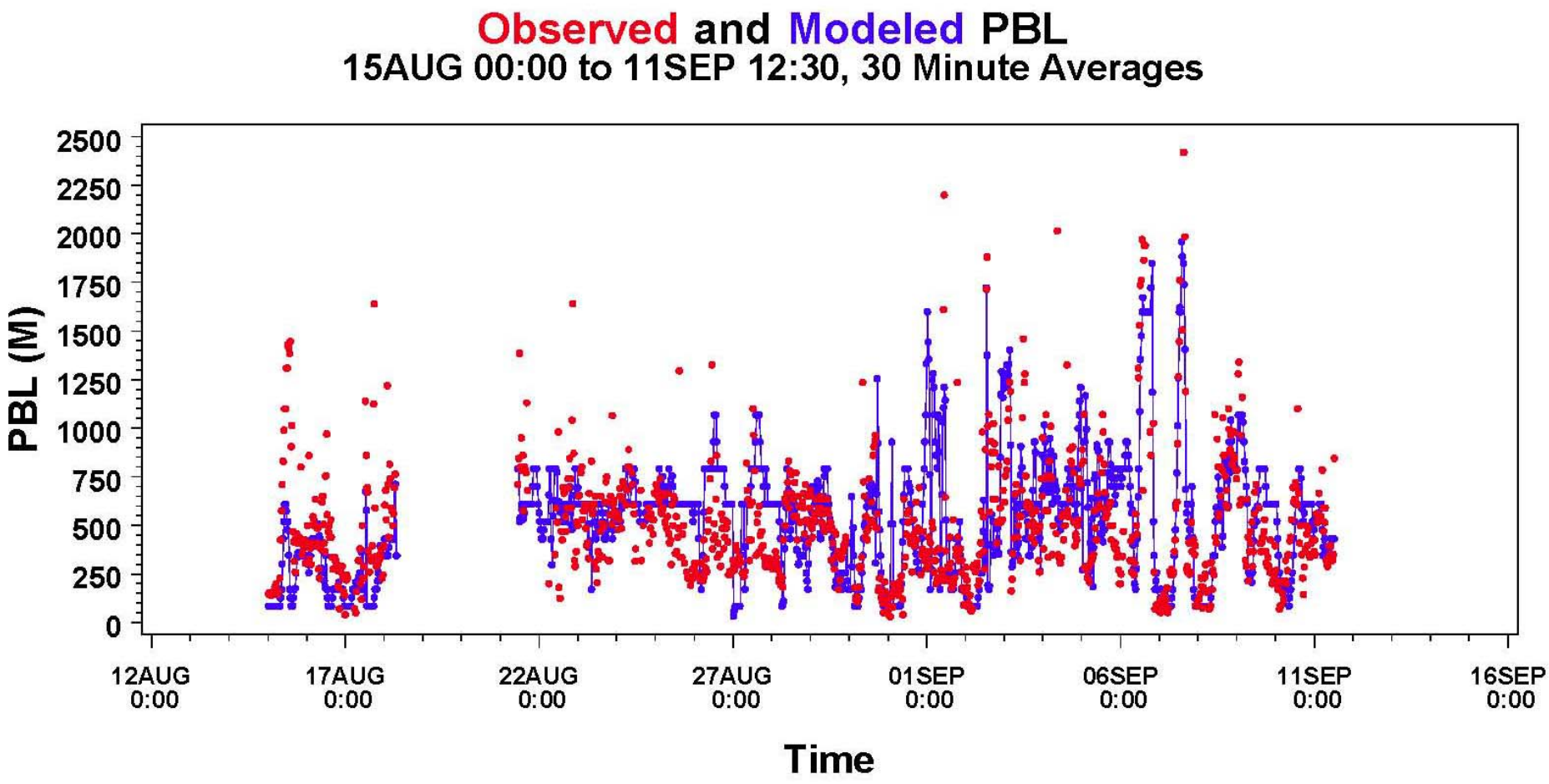

odeled vs. RHB Observed FORM Mixing Ratios
Gulf - Offshore, 30 Minute Averages
Observed FORM (ppb)

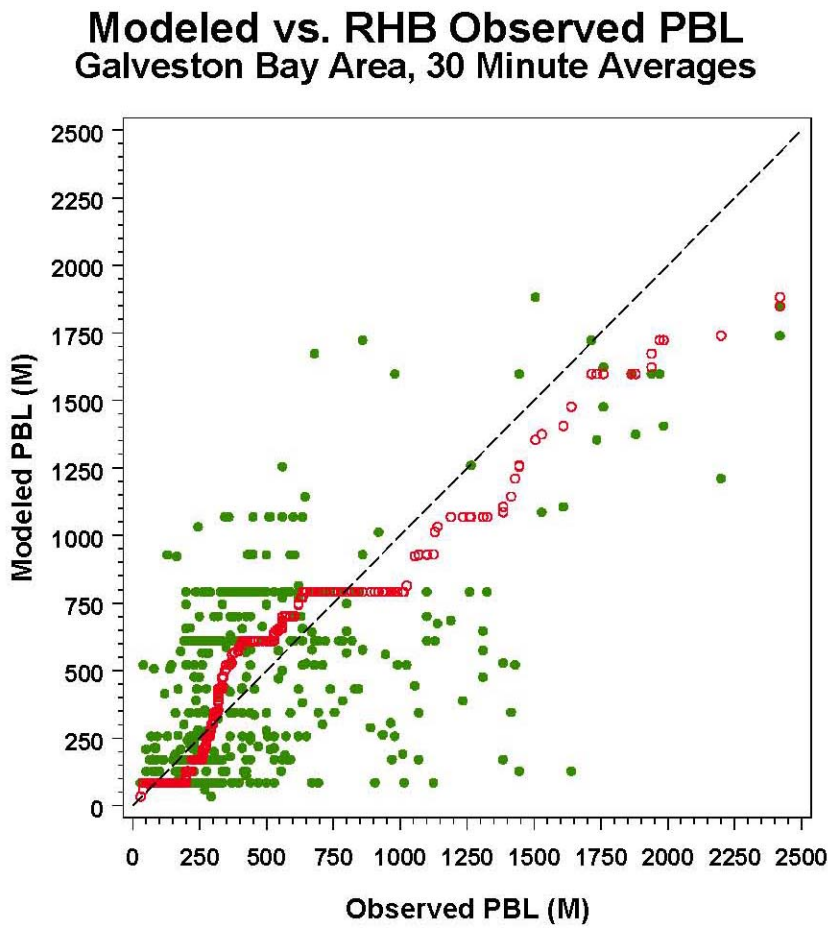
PBL Analysis

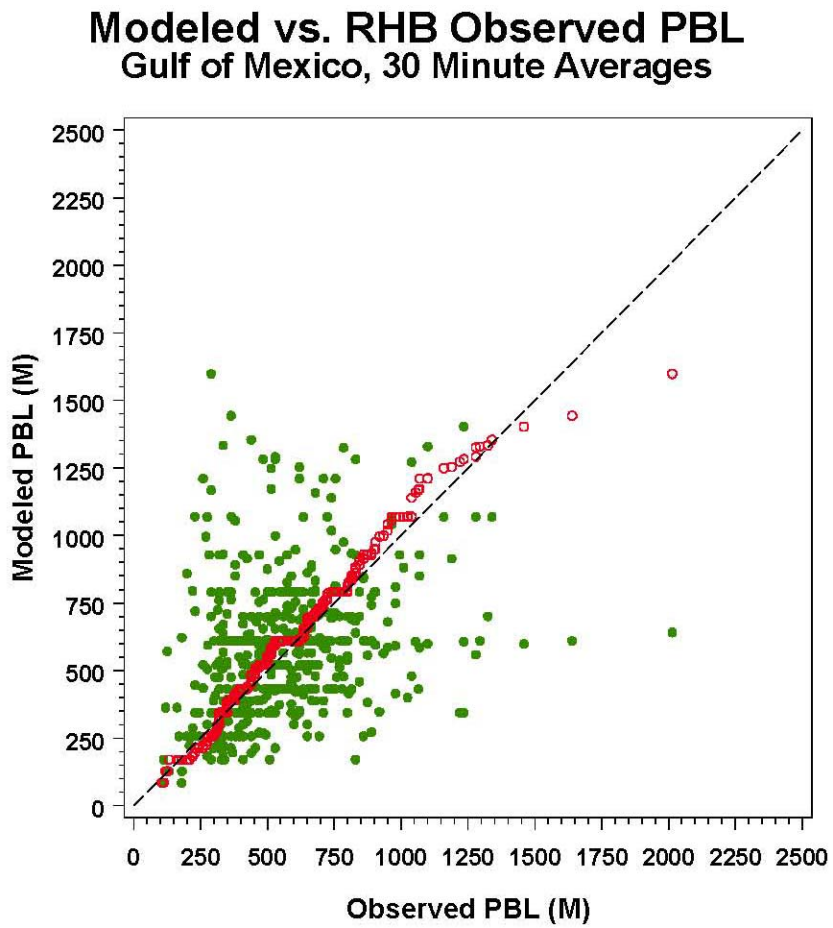
- TCEQ recently received planetary boundary layer (PBL) depth estimates from Dr. Sara Tucker at NOAA, derived using the High-Resolution Doppler LiDAR (HRDL) instrument located on the stern of the Brown.

- These data were compared with modeled PBL depths to see how well the model captures this important meteorological parameter.

- Two analysis zones were used:
  - **Gulf** = Galveston Entrance/Anchorage ∪ Near Shore ∪ Offshore
  - **Galveston Bay** = Houston Ship Channel ∪ Barbour's Cut ∪ Barbour's Cut to Galveston ∪ Galveston Harbor


Observed and Modeled PBL
15AUG 00:00 to 11SEP 12:30, 30 Minute Averages
PBL (M)
2500
2250
2000
1750
1500
1250
1000
750
500
250
0
12AUG 0:00
17AUG 0:00
22AUG 0:00
27AUG 0:00
01SEP 0:00
06SEP 0:00
11SEP 0:00
16SEP 0:00
Time


Modeled vs. RHB Observed PBL
Galveston Bay Area, 30 Minute Averages
Modeled PBL (M)
Observed PBL (M)
0
250
500
750
1000
1250
1500
1750
2000
2250
2500


Modeled vs. RHB Observed PBL
Gulf of Mexico, 30 Minute Averages
Modeled PBL (M)
Observed PBL (M)
0
250
500
750
1000
1250
1500
1750
2000
2250
2500

Summary

- **Ozone**
  - The model tended to over-predict observed ozone concentrations below 50 to 60 ppb in all areas.
  - In the Galveston Bay area, the model under-predicted higher ozone concentrations, including some very high observed concentrations ranging up to 180 ppb+.
  - Outside Galveston Bay, the model was relatively unbiased for higher observed concentrations, and slightly over-predicted ozone concentrations in the Offshore zone.
- **NO**
  - The model under-predicted observed NO concentrations within the Galveston Bay area, especially large NO “spikes” apparently associated with local sources.
  - Outside the Bay, NO predictions were relatively unbiased.

Summary (cont.)

- **NO_2**
  - The model overall performed quite well for NO_2 in all areas.
- **HNO_3**
  - A large amount of scatter in the data pairs means that the model did not predict individual points very well, but the model showed little evidence of overall bias in its nitric acid predictions.
- **PAN**
  - In the Houston Ship Channel, measured PAN concentrations were close to the modeled values.
  - In most other situations, modeled PAN values showed a small positive bias, excepting a couple of dozen very high measured values in the Barbour's Cut to Galveston zone.
  - In the Offshore region, modeled PAN concentrations were on the order of 2-3 times the observations.

Summary (cont.)

- **CO**
  - The model showed a positive bias of ~ 40% in most areas.
  - Model bias was ~10% during a brief visit to the Ship Channel.

- **ETH**
  - The model under-predicted ethylene concentrations by around a factor of two in the Ship Channel and in the Barbour's Cut to Galveston zones.
  - The model was unbiased in Barbour's cut except for concentrations < 1 ppb.
  - Modeled and observed concentrations of ethylene outside Galveston Bay were fairly low, with only a few observations > 2 ppb.

Summary (cont.)

- **ISOP**
  - Unusually high isoprene concentrations measured in the Ship Channel were not replicated by the model.
  - Otherwise, the model showed little bias in the Ship Channel and in Barbour's Cut.
  - Elsewhere, both observed and modeled concentrations were generally very low (< 1 ppb).

- **FORM**
  - Overall model performance was good, except for some very high observations in the Galveston Bay area which were not captured by the model.

Summary (cont.)

- **PBL**
  - Modeled PBL shows little evidence of bias.
  - In Galveston Bay area, both modeled and observed PBLs have a wider dynamic range than in the Gulf.
  - Large (> 800 m) values of modeled and observed PBL in the Gulf are often associated with land breeze advection.