Eastern Texas Air Quality Forecasting Systems (ETAQ-F)

Evaluation of Summer 2006 Simulations

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Institute for Multi-dimensional Air Quality Studies (IMAQS)
University of Houston

UH (Univ. of Houston)
AQF (Air Quality Forecasting) Systems

Spatial Resolution

36 km : U.S. Continent

12 km : East Texas (2005) State of TX, LA, OK, AR, and MS (2006)

04 km : Houston and Galveston Area (F1) / HGA & DFW (F2 & F3)

Operation Period and Duration (May 2005 ~ Current)

Spin-up : 6 hrs
(0th day 18 CST – 0th day 23 CST)

Forecasting : 46 hrs
(1st day 00 CST – 2nd day 23 CST)

Two Different Air Quality Forecasting Systems

Forecast 1 (F1) : MM5 modified by UH + TEI imputed for 2000 + CMAQ v4.4

Forecast 2 (F2) : MM5 modified by UH + TEI imputed & projected for 2005 + CMAQ v 4.4

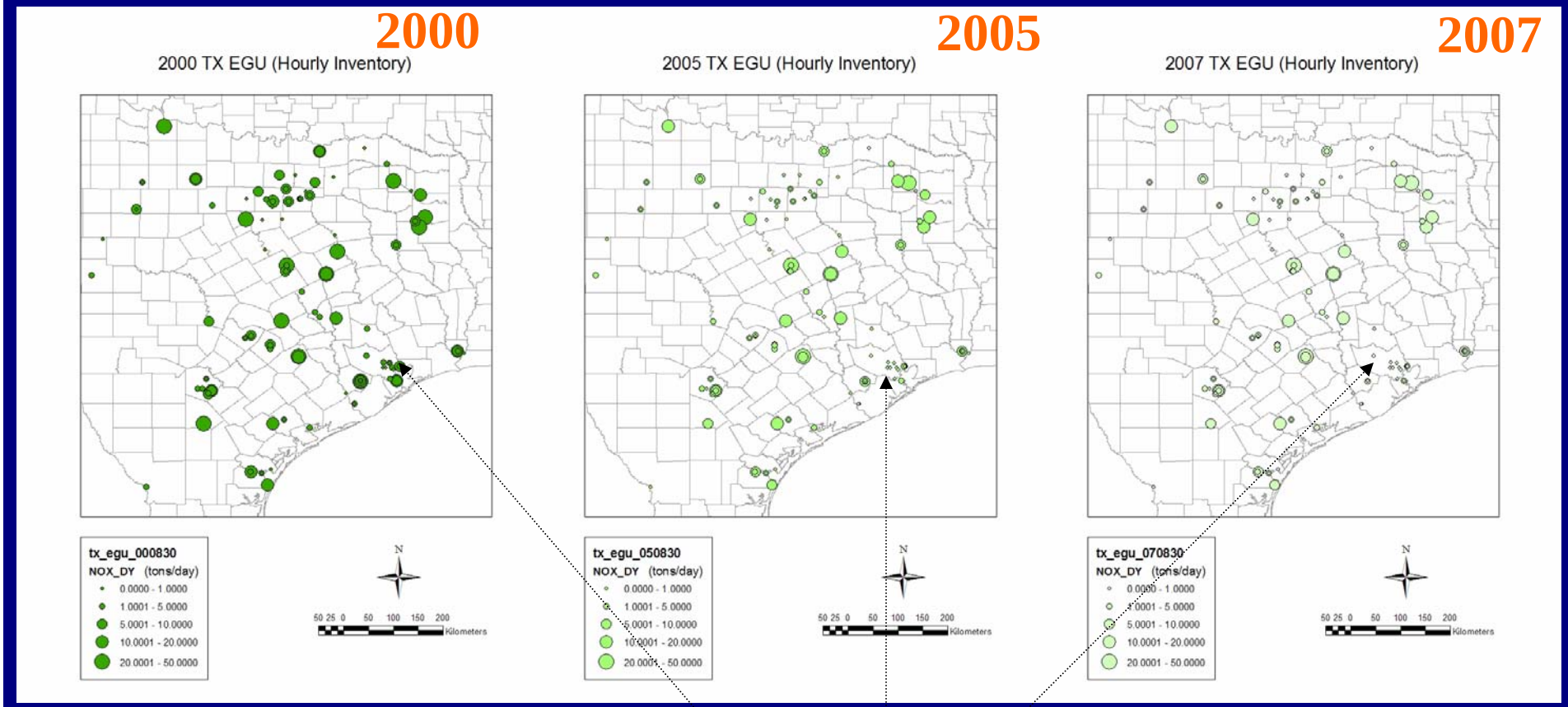
Forecast 3 (F3) : MM5 configured by TAMU + TEI imputed & projected for 2005 + C MAQ v4.4

Anthropogenic Emissions: for F1 (2005/2006)

- TEI 2000 Base5b
  - TexAQS 2000 episode used for State Implementation Plan
  - The day of Week
    - Aug. 25th → Friday, Aug. 26th → Saturday, Aug. 27th → Sunday, Aug. 30th → Monday ~ Thursday
  - CB4, SAPRC99, and RADM2
  - Area & Non-road: 2000 Emissions Inventory
- NEI99 (Final version 3)
  - CONUS 36-km domain
  - Particulate matters and precursors (NH3, SO2)
- Processor: SMOKE version 2.1
  - Internal database: TCEQ's (for spatial and temporal allocation) Default & TCEQ's for chemical speciation

Anthropogenic Emissions for F2/F3 (2006)

Projected Texas EGU NOx emissions after State Implementation Plan (SIP)



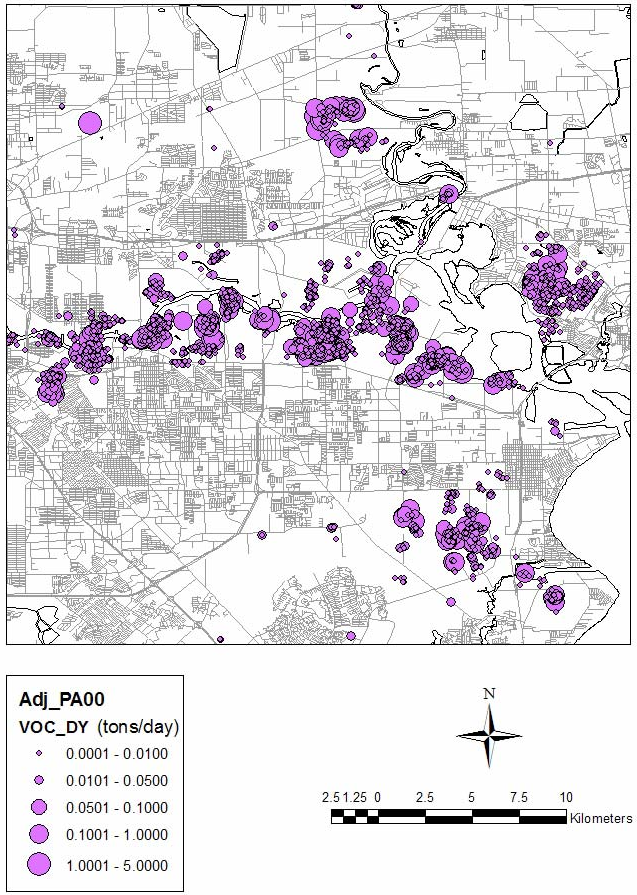
✓ 2007 emissions inventory were projected from 2000 EI with growth and control factors from TCEQ.

✓ For HG NOx emissions for 2005, a factor of 1.747 was applied on 2007 EI based on the 2005/2007 MECT (Mass Emission Cap and Trade) allowances.

Anthropogenic Emissions: for F2/F3 (2006)
VOC emissions for imputation after SIP

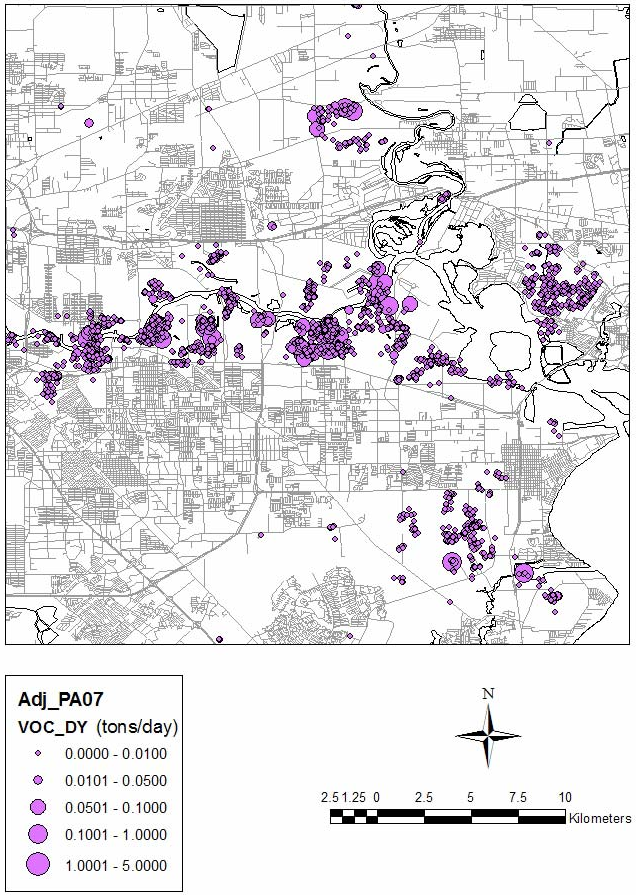
2000

2000 Additonal VOC (Daily Inventory)



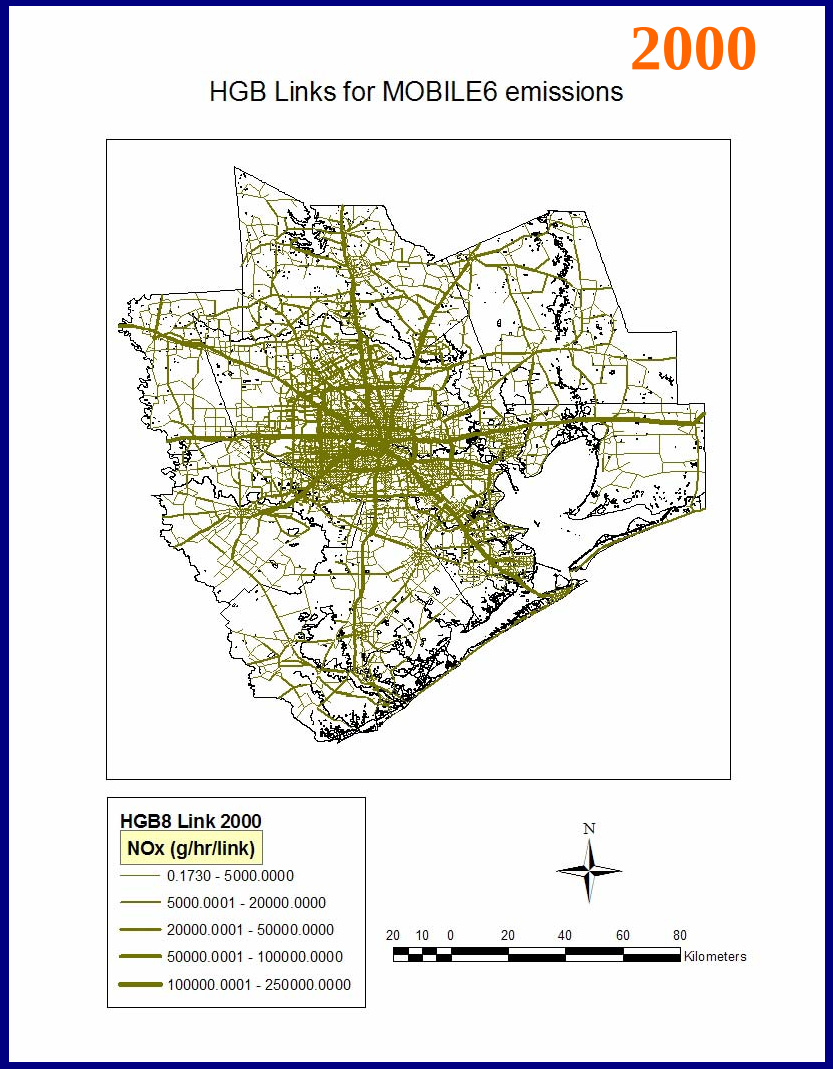
2007

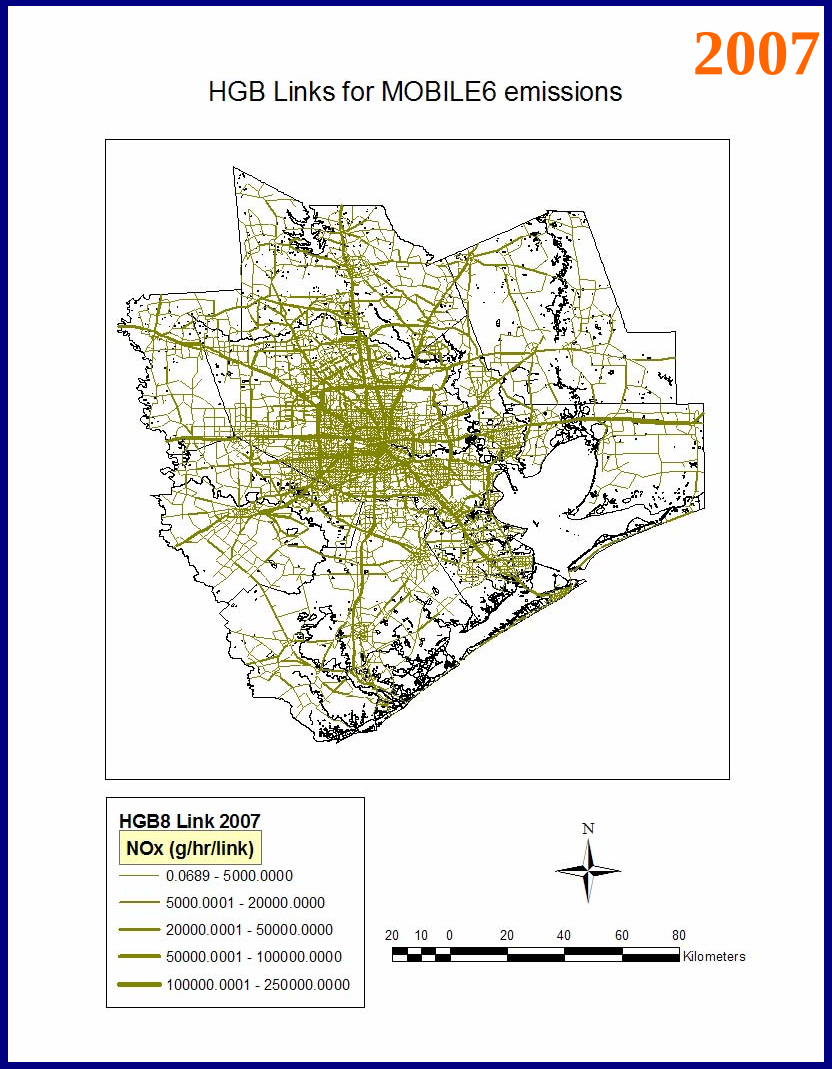
2007 Additonal VOC (Daily Inventory)



✓ UH AQF system uses additional VOC emissions at the 2007 level.

MOBILE6 NOx emissions for 2000 and 2007





✓ The emissions amounts for each county, vehicle type, hour and species were determined for 2005 based on those for 2000 and 2007.

✓ Then, the factor was applied on 2007 MOBILE6 emissions to get 2003 emissions.

What Configurations were used for ETAQ-F 2006?

- For ETAQF 2005, we used TCEQ's 2000 Base5b with imputed HRVOC
  - * Was quite successful
  - * NOx and some VOC emissions might have been too high
- For ETAQF 2006,

Meteorology (F1 = F2=UH MM5 vs. F3 = TAMU config.)

* improved LULC
* improved MRF for stable PBL and transition times (under development)
* cloud; both the subgrid scale explicit scheme at 4-km
* satellite observed sea surface temperature (in preparation for sensitivity testing)

Emissions (F1 = 2000 SIP imputed TEI vs. F2 = F3 = 2005* projected)

* 2005 TEI (projected from 2000 & 2007)
* 2000 HRVOC (instead of 2005 projected)
* Mobile projected for 2003
* satellite-observed fire events (in preparation)

CMAQ (F1 = HGB 4-km vs. F2 = F3 = Extended 4-km (HGB + DFW)

* with and w/o cloud attenuation
* CB4 for forecasting and SAPRC99 for evaluation (on-going)
* Better regional characterization at 12-km resolution

http://www.imaqs.uh.edu/

UNIVERSITY of HOUSTON

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THE INSTITUTE FOR MULTI-DIMENSIONAL AIR QUALITY STUDIES

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- :GIS Analysis
- :Measurement

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  - .CAMX
  - .TFORS
  - .MM5
- :Trajectory
- :Data Analysis
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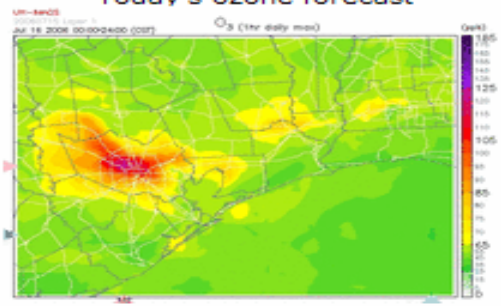
Welcome to the Institute for Multi-dimensional Air Quality Studies. We are a diverse group of researchers from fields of geosciences, math, computer science and chemistry committed to using premier scientific tools to model the complex issues of air quality and climate change. Our modeling efforts address many critical components simultaneously including emissions inventories, meteorology, and atmospheric chemistry. We are currently developing atmospheric boundary layer measurement techniques. We work closely with national, state and local leaders to identify key scenarios to run on our modeling systems so that public policy is guided with the best science.

Today's ozone forecast



RESEARCH PROJECTS

- Tools for creating automated QA in IMAQS
- Development of Joint Multi-Pollutant Air Quality Modeling Facilities
- Development of Texas Emissions Inventory Preparation System for SMOKE
- Photochemical Modeling of Ethylene and Propylene Emissions
- Air Quality Simulation and Forecasting

PRODUCTS

- Trajectory
- Air Quality Forecast
- Emission Processing
- GIS Analysis
- Measurement (Sounding data)

NEWS AND EVENTS

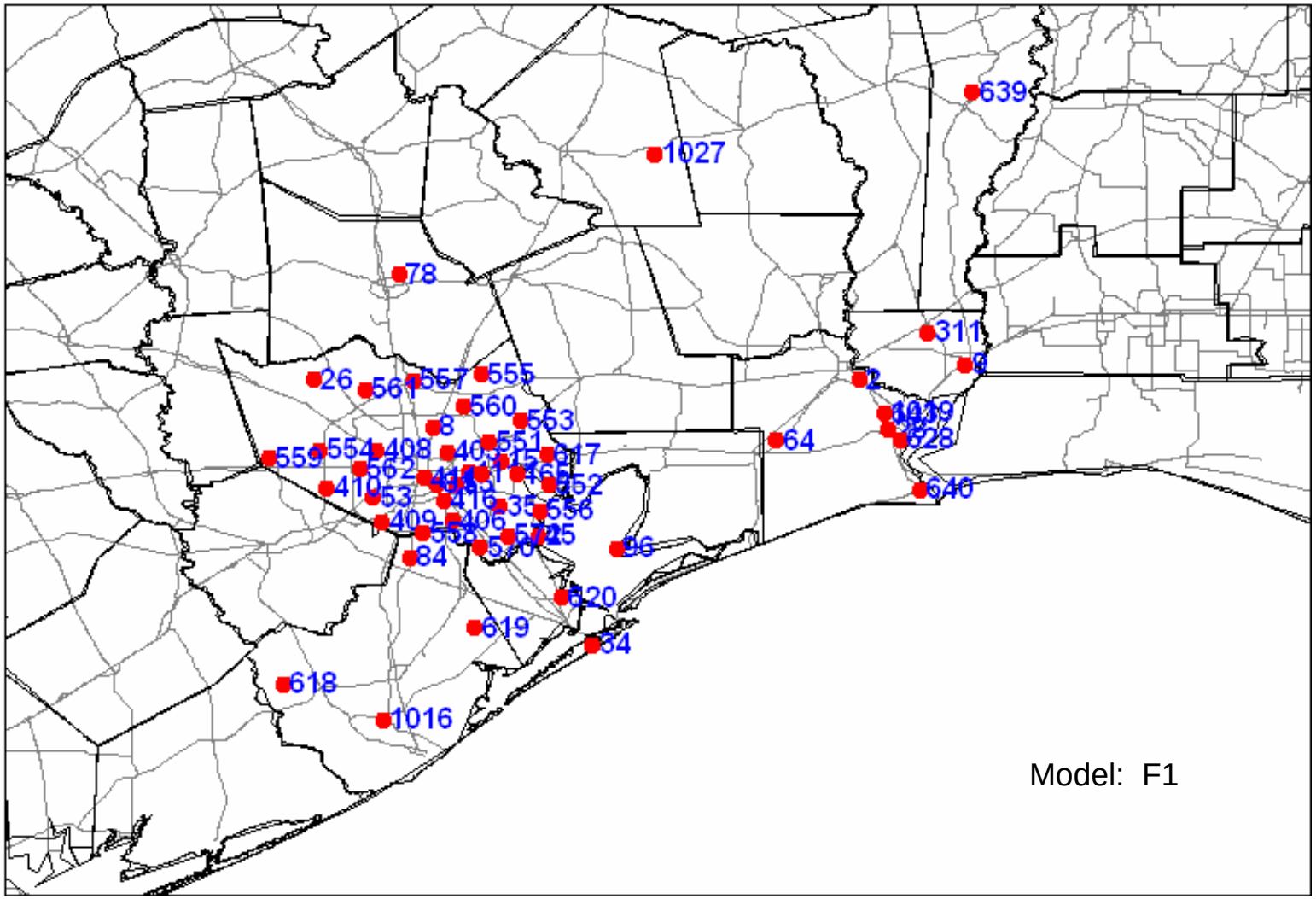
- Meteorological Data During Hurricane Rita
- NSM Momentum: Improving Air Quality in Houston (November 2004) Original Link
- New Real-Time Trajectory Web Interface

Our New Real-Time Trajectory Analysis

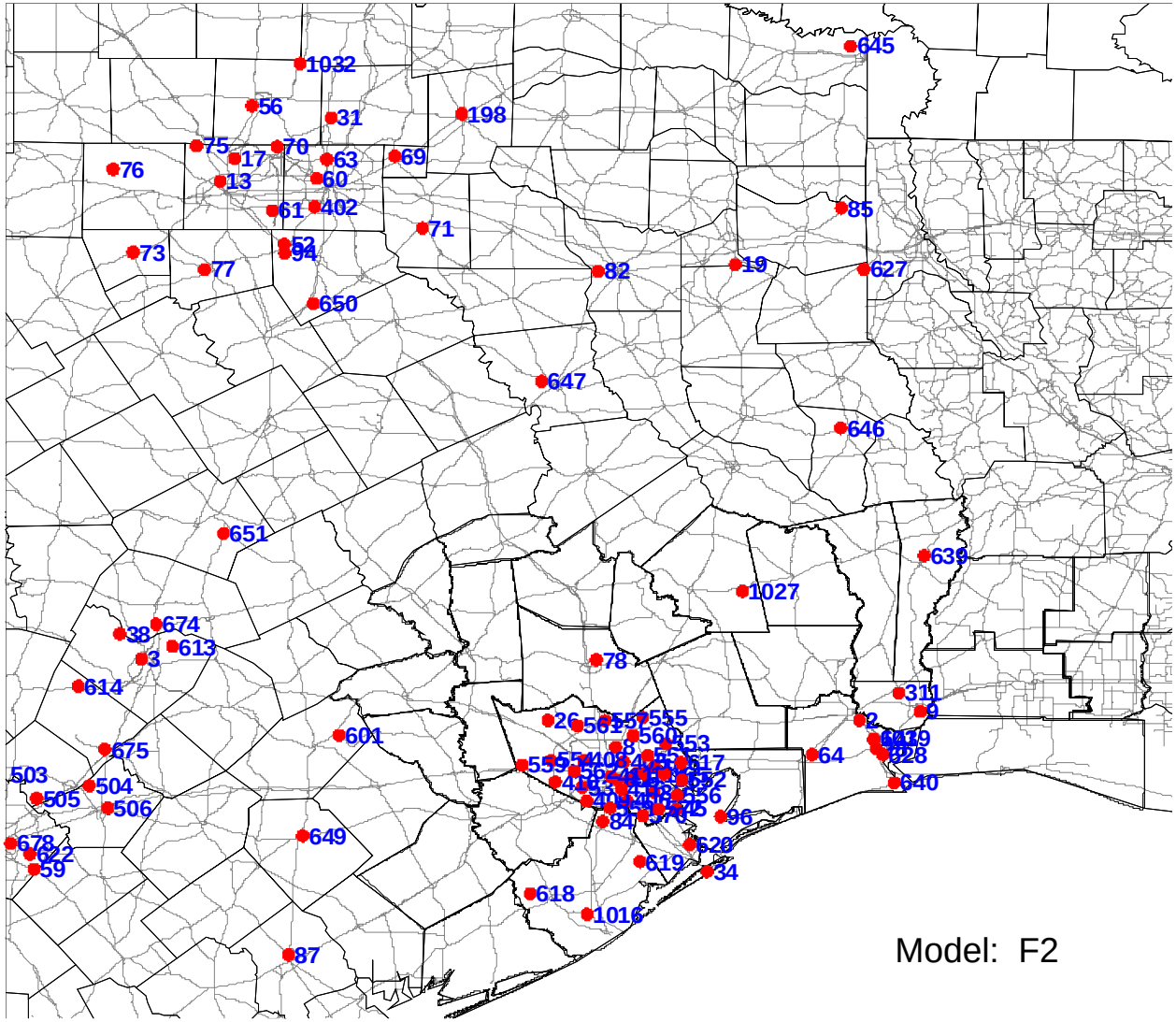
Performance Analysis of 2006 AQF

- Pollutants : O3, NO, NO2, PM2.5
- Period : 2006.06 – 09
- F1 (2000 TEI) & F2 (2005 projected)

Monitoring site on Houston-Galveston domain F1

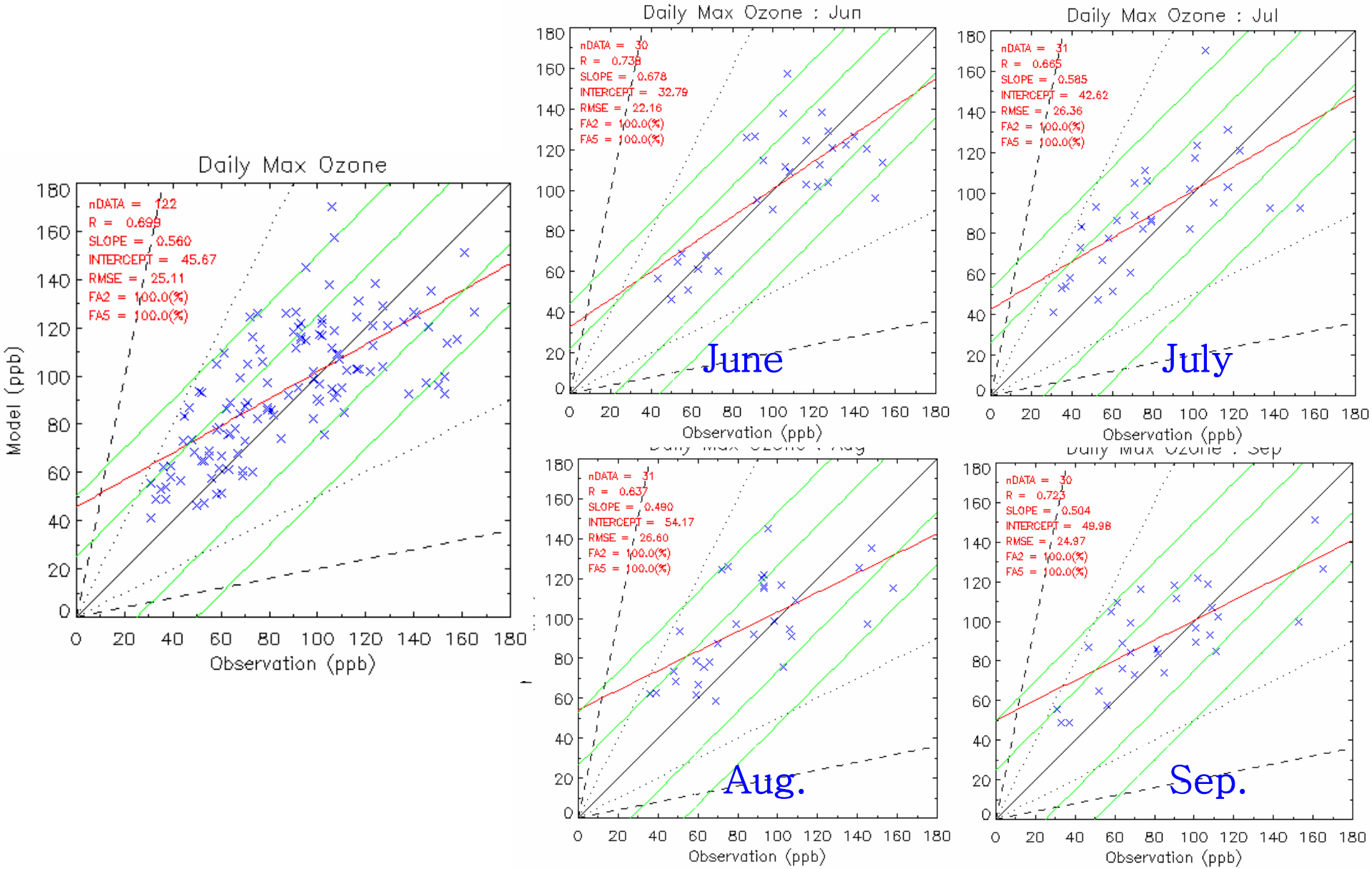


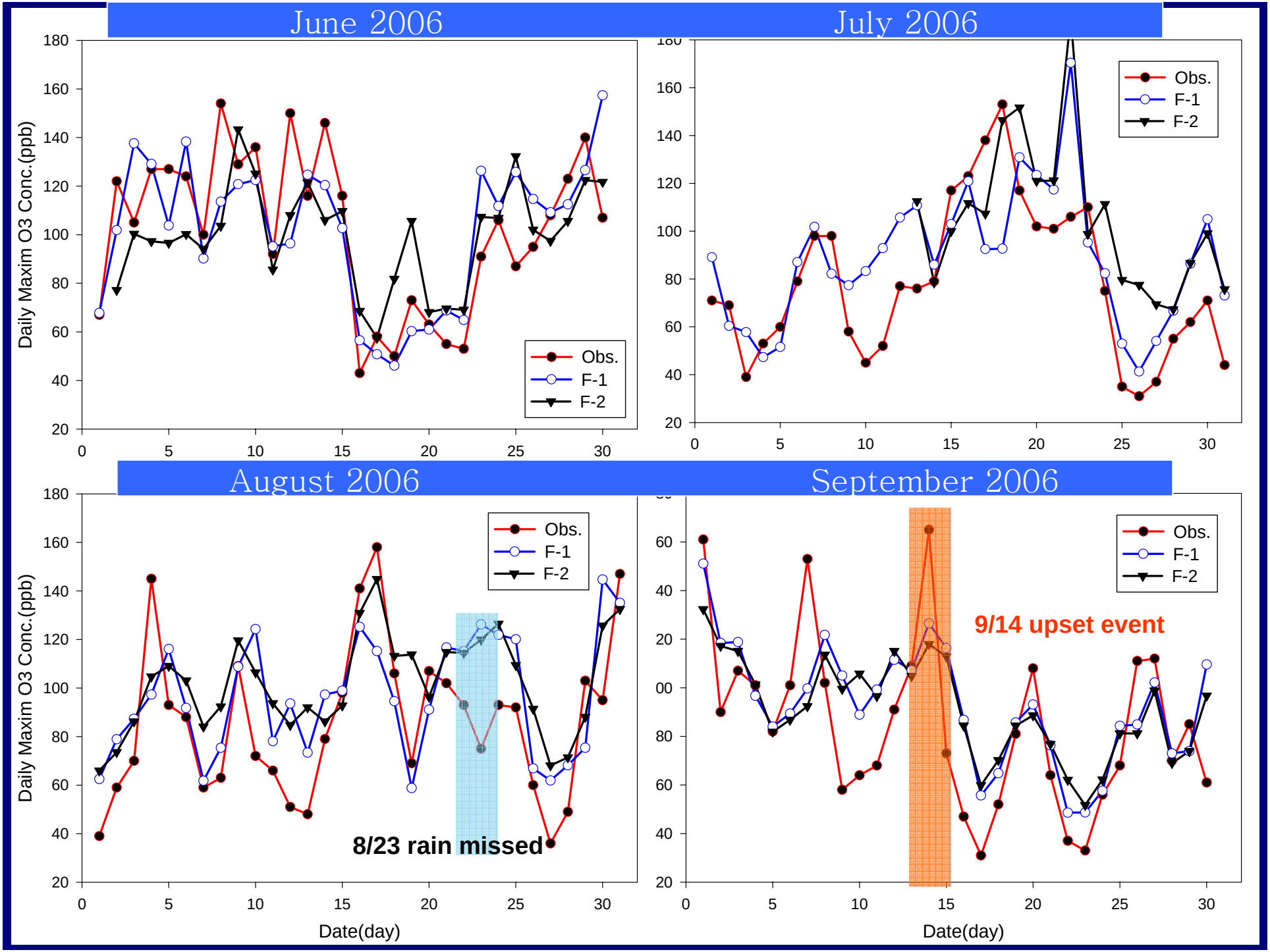
Monitoring sites for Dallas & Houston domain F2



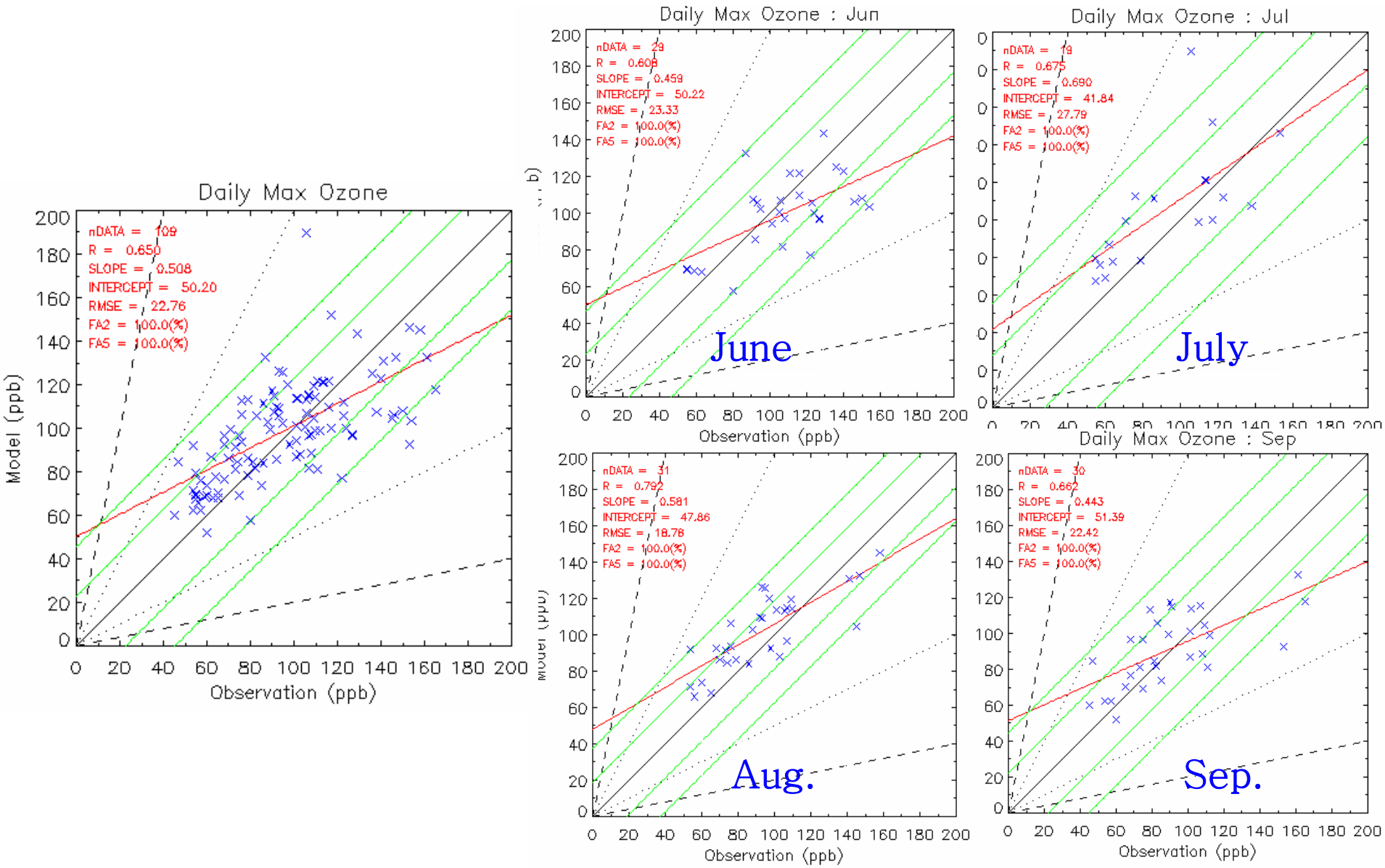
Model: F2

O3 QQ plot for F1 (daily max)

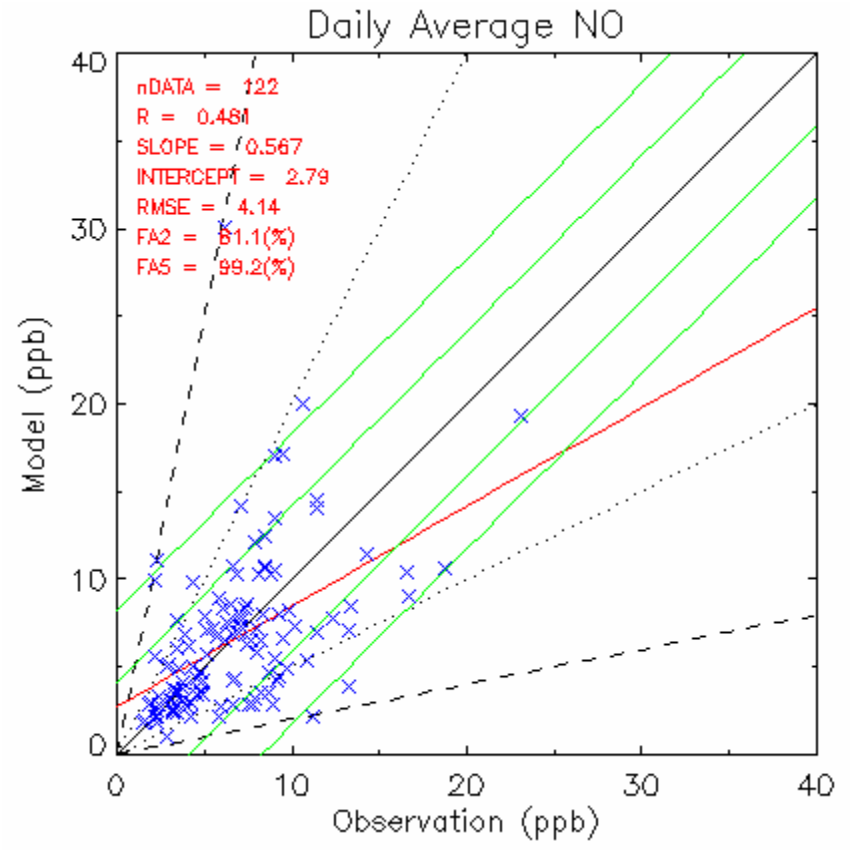



June 2006
July 2006
August 2006
September 2006
Daily Maxim O3 Conc.(ppb)
Date(day)
Obs.
F-1
F-2
8/23 rain missed
9/14 upset event

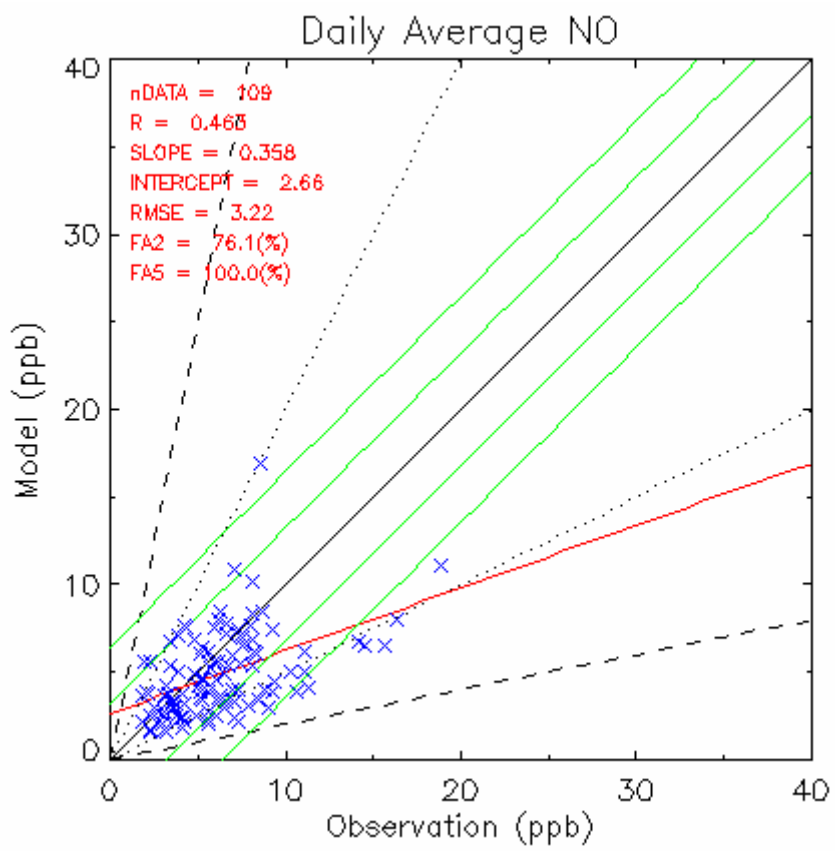
O3 QQ plot for F2 (daily max)



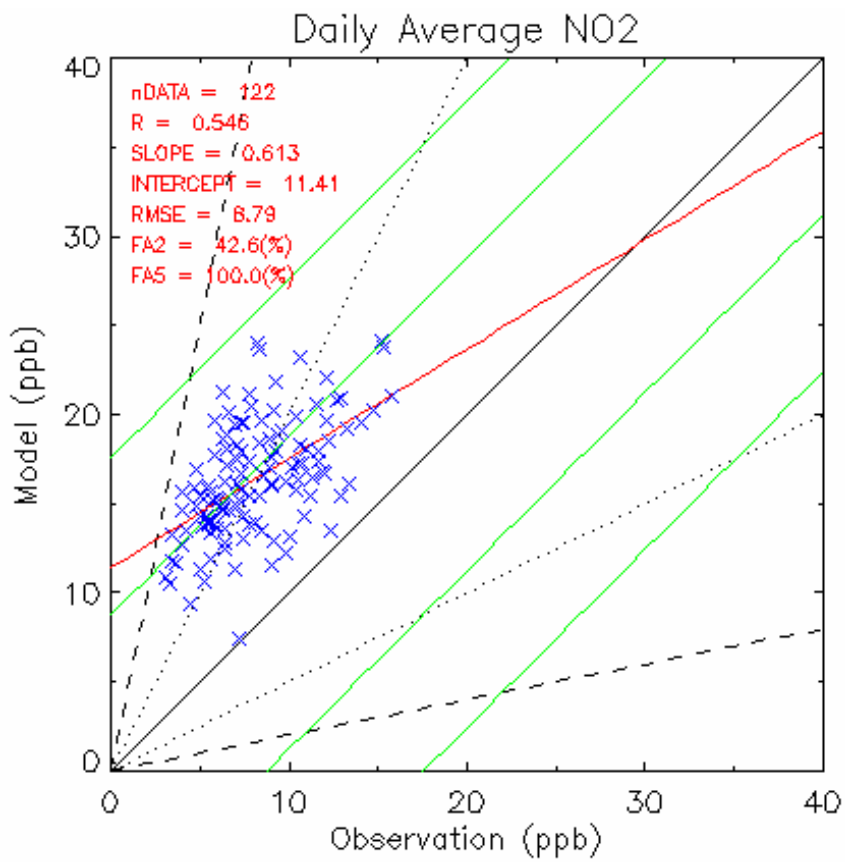
F-1


Daily Average NO
nDATA = 122
R = 0.481
SLOPE = 0.567
INTERCEPT = 2.79
RMSE = 4.14
FA2 = 81.1(%)
FA5 = 99.2(%)
Model (ppb)
Observation (ppb)
0
10
20
30
40

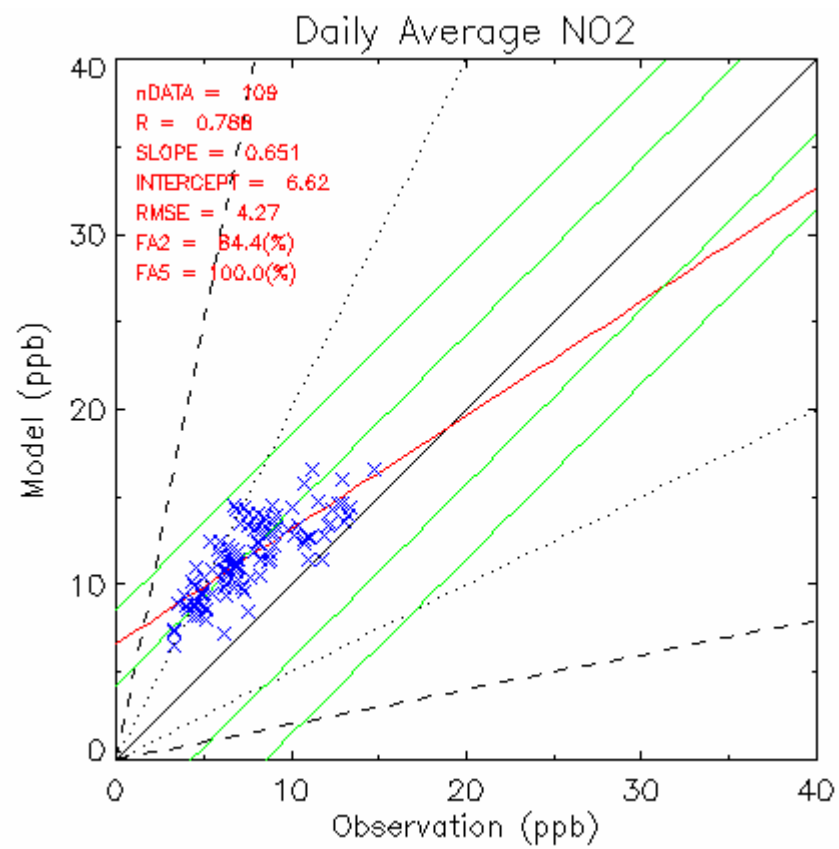
F-2


Daily Average NO
nDATA = 109
R = 0.468
SLOPE = 0.358
INTERCEPT = 2.66
RMSE = 3.22
FA2 = 76.1(%)
FA5 = 100.0(%)
Model (ppb)
Observation (ppb)
0
10
20
30
40

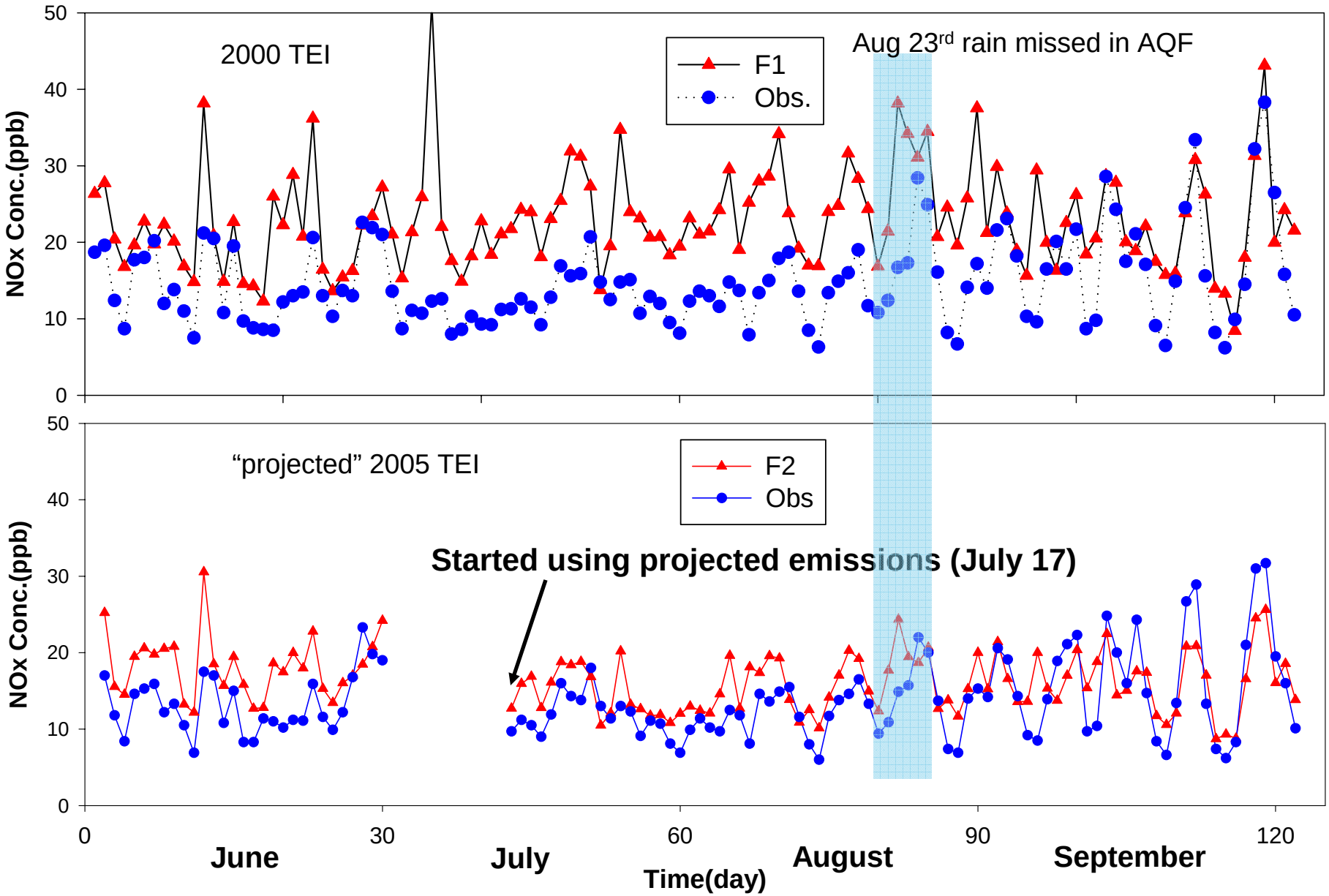
F-1


Daily Average NO2
nDATA = 122
R = 0.546
SLOPE = 0.613
INTERCEPT = 11.41
RMSE = 8.79
FA2 = 42.6(%)
FA5 = 100.0(%)
Model (ppb)
Observation (ppb)
0
10
20
30
40

F-2

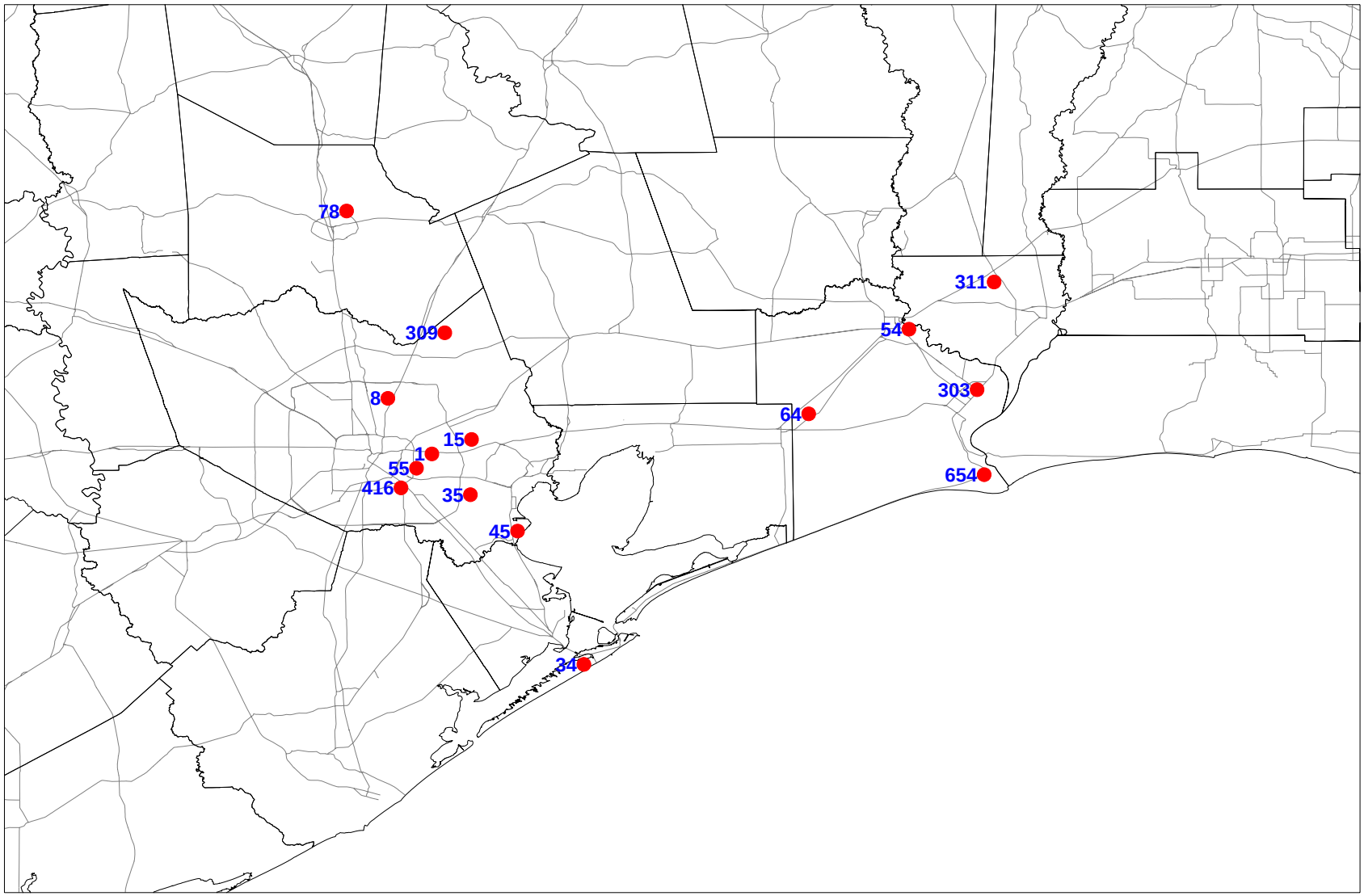

Daily Average NO2
nDATA = 109
R = 0.788
SLOPE = 0.651
INTERCEPT = 6.62
RMSE = 4.27
FA2 = 84.4(%)
FA5 = 100.0(%)
Model (ppb)
Observation (ppb)
0
10
20
30
40

NOx daily mean time series for F1 & F2



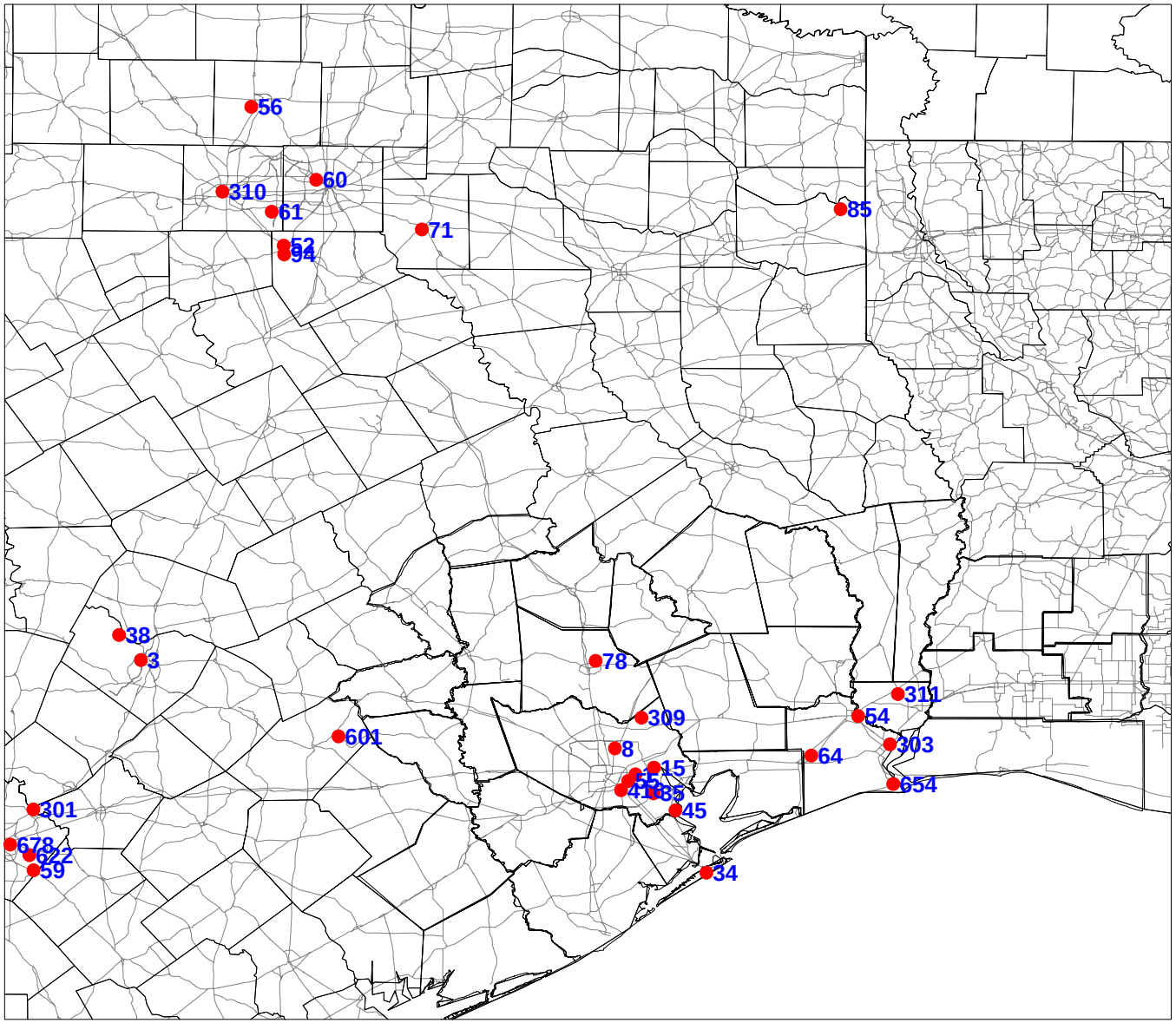
PM2.5 CAMS site location

F-1 : 15 sites

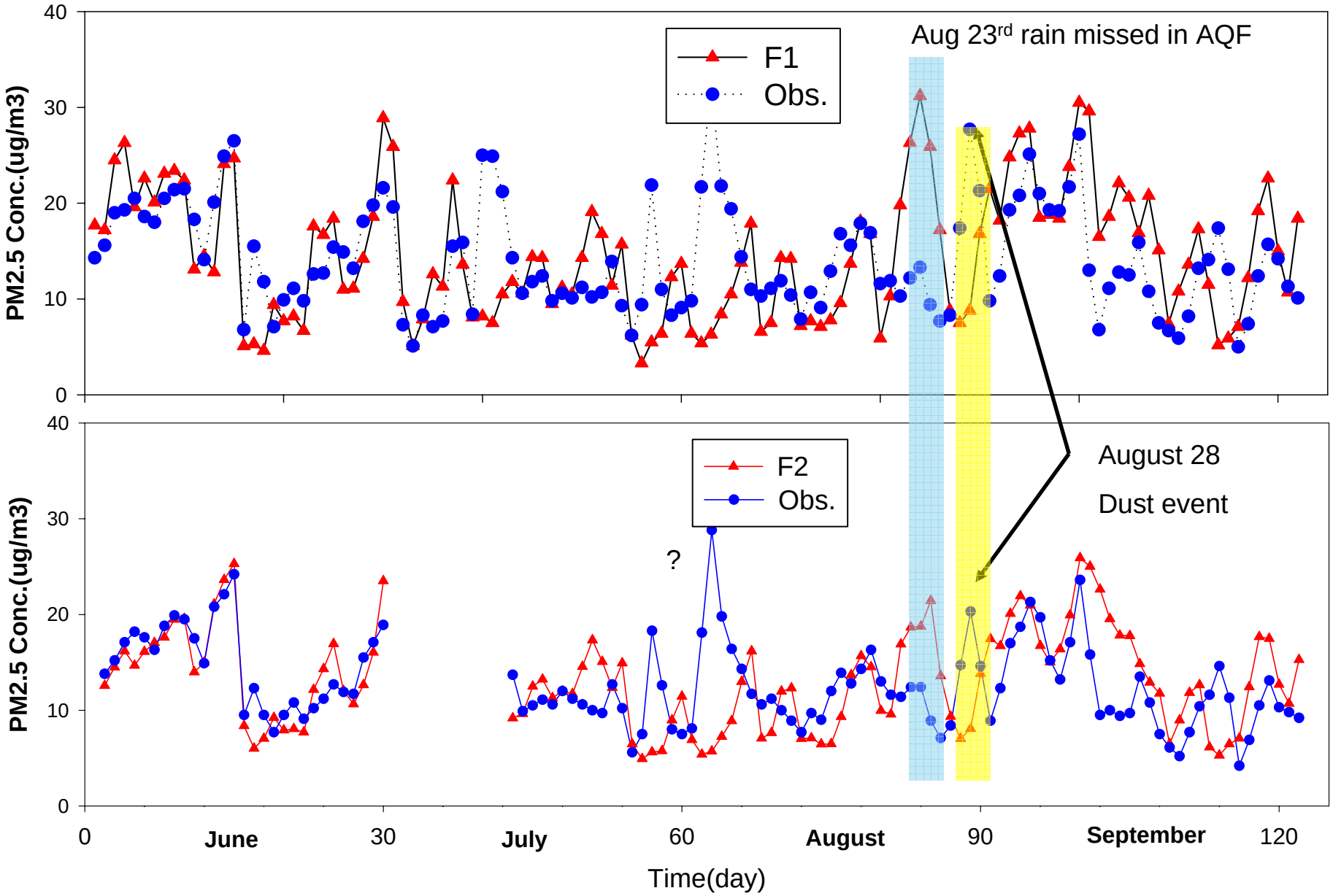


PM2.5 CAMS site location

F-2 : 30 sites

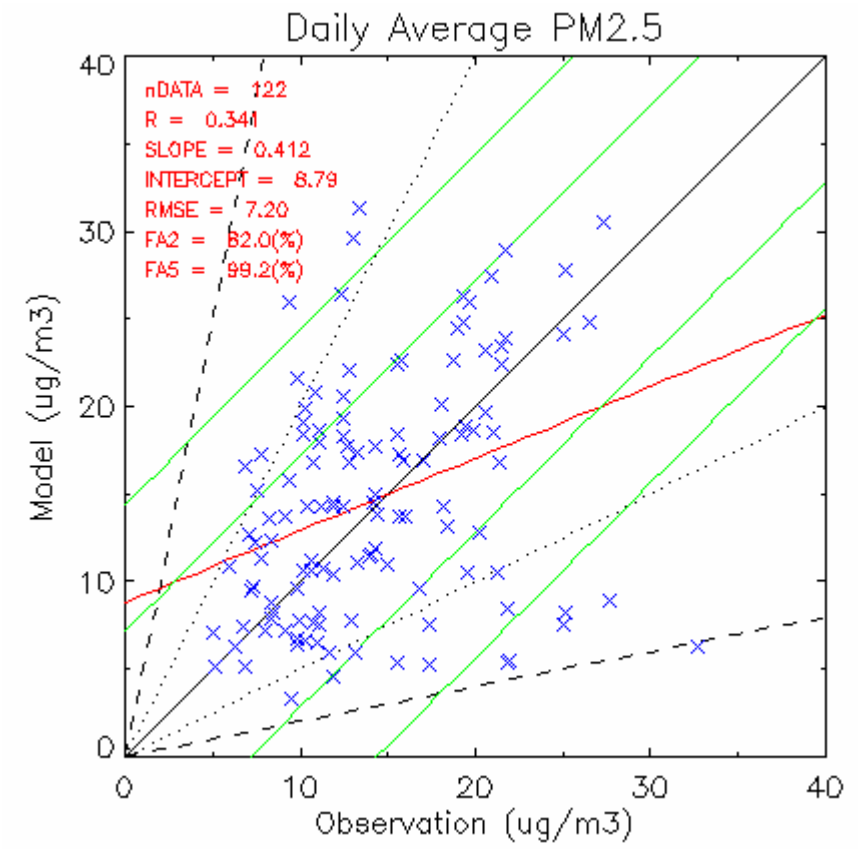


Time series for PM2.5
(Daily average)

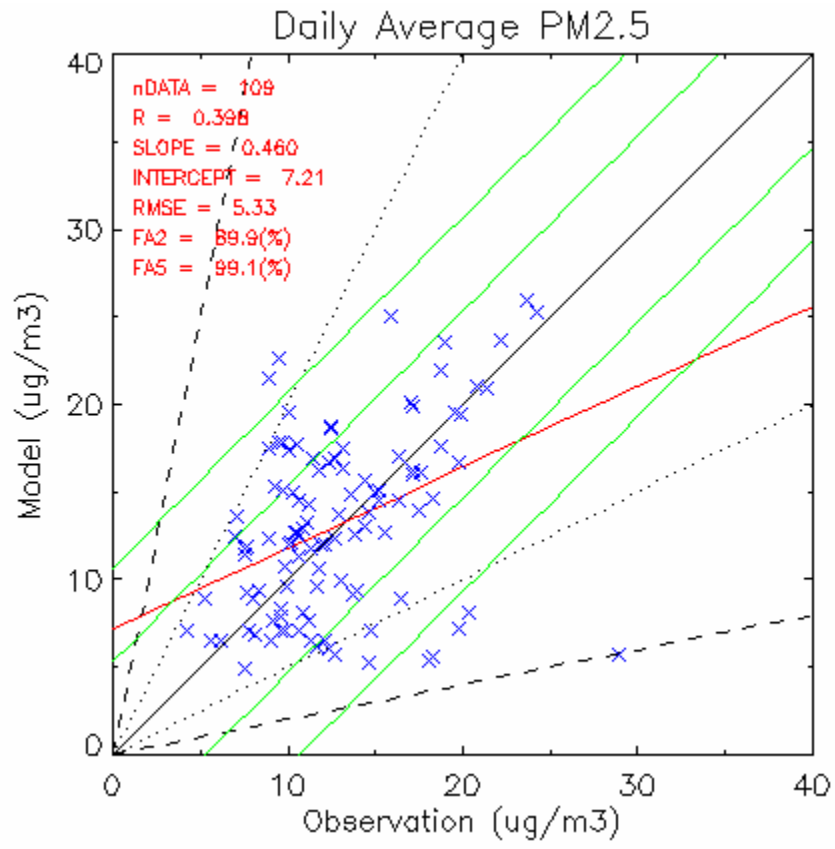


Scatter diagram for PM2.5
(Daily average)

F−1



F−2



Preliminary Sensitivity Study

- 2006 forecasting seems more difficult than 2005

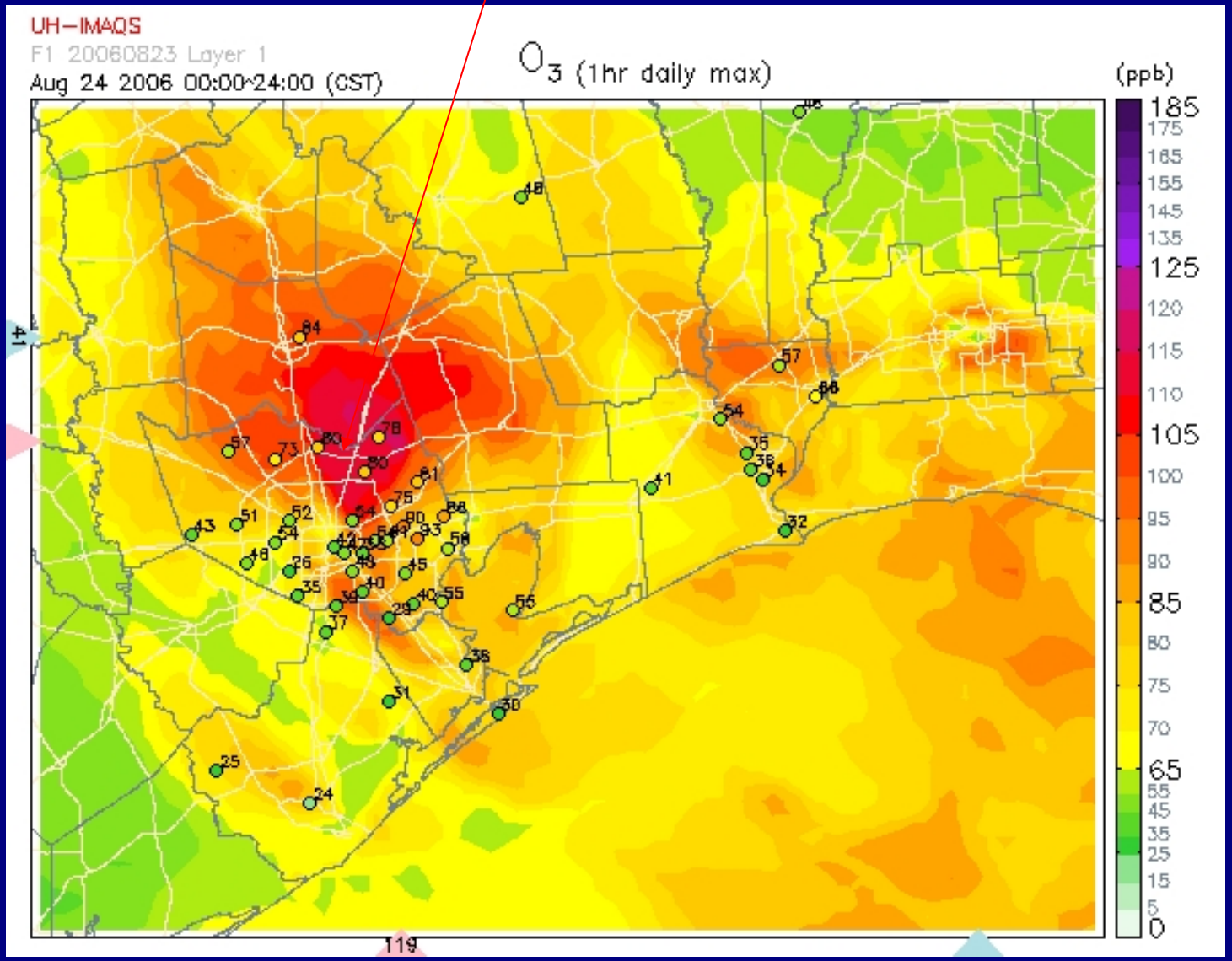
(is it real or perception?)

  - Using new NCEP WRF/NMM output for MM5
  - Stable PBL heights
  - Wind speed and direction
  - Projected emissions

- Two bad forecasting events tested
  - After rain, bad IC conditions (Aug 24 & 25)
  - Upset emissions case (Sept 14)

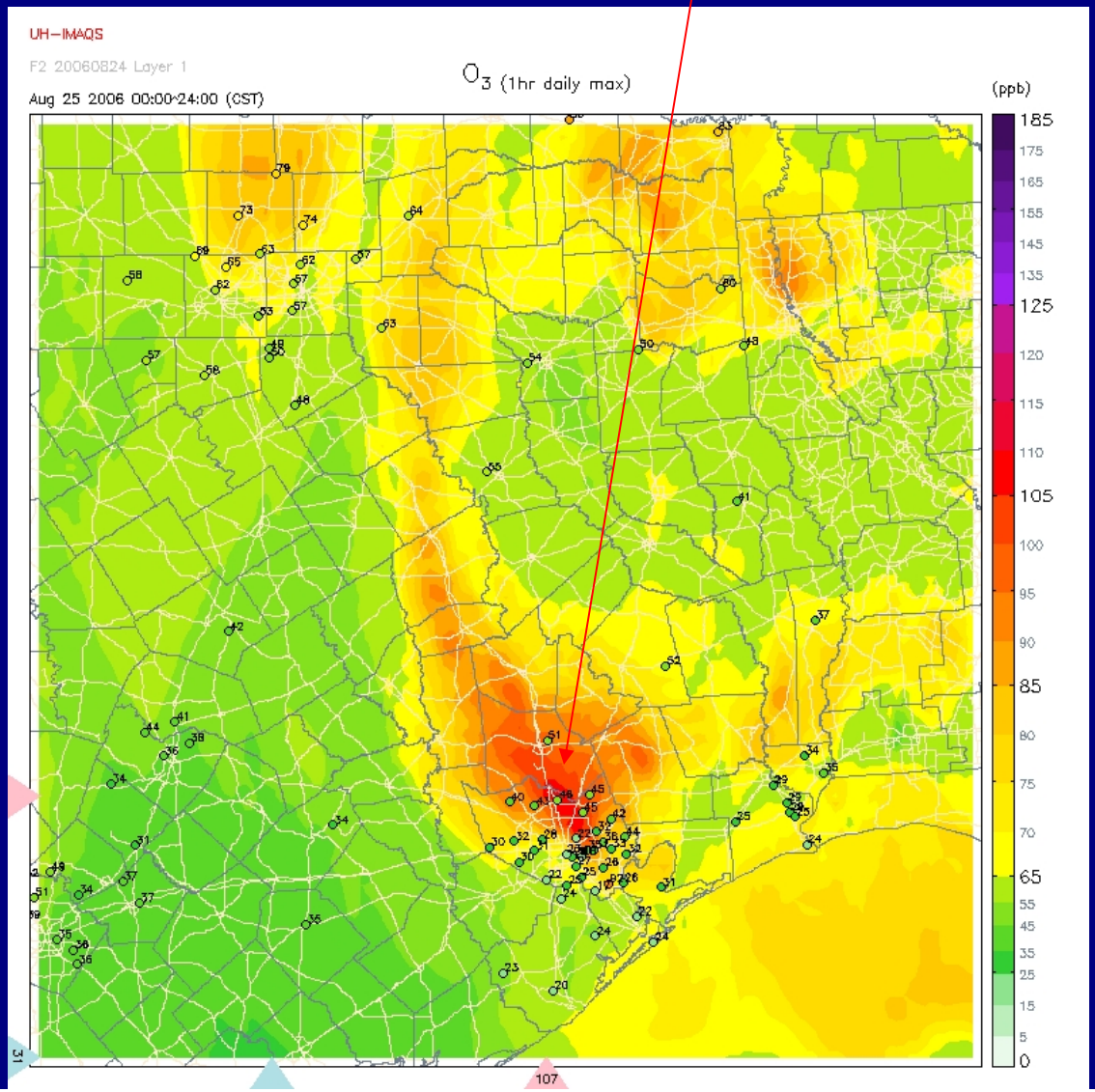
Daily maximum 1-hr O3 for August 24th, 2006: F1

AQF missed rain event during the previous day afternoon (Aug. 23rd), forcing ozone over-prediction on the next day (Aug. 24th).



Daily maximum 1-hr O3 for August 25th, 2006: F2

Ozone over-prediction on August 23rd had an influence on August 25th over the Houston area.



Test Setup

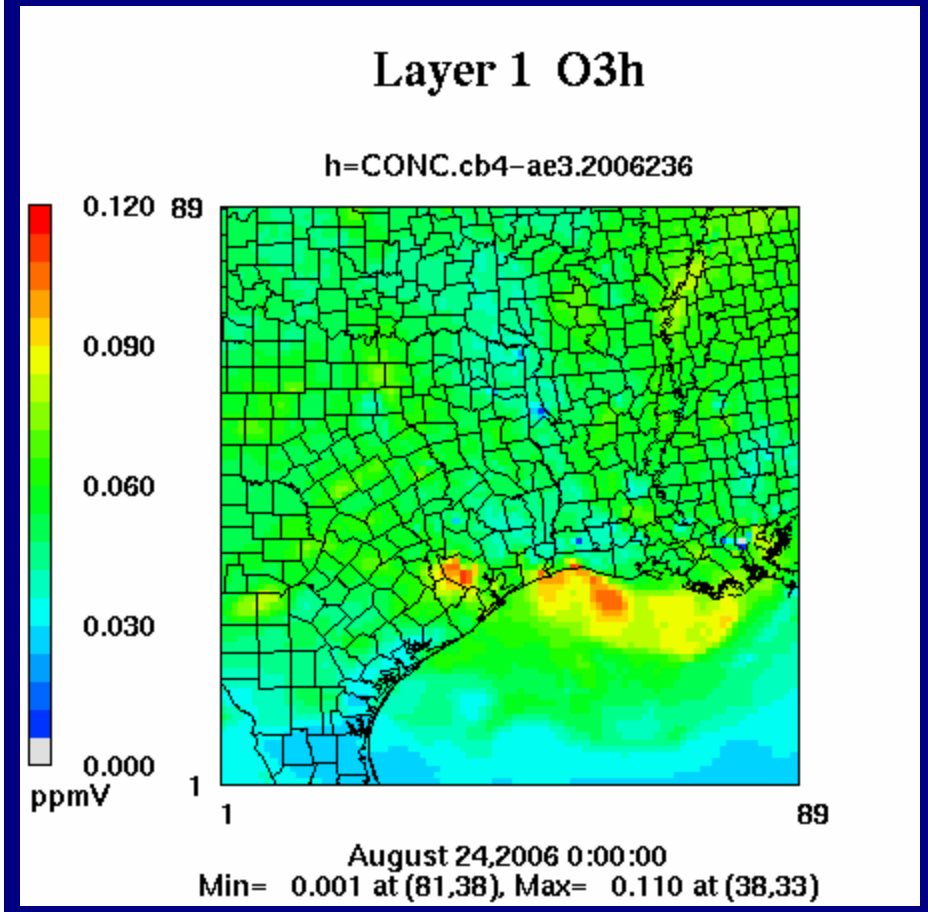
- Goal: To see how a “Clean” IC can help AQF on a day when AQF highly over-predicted ozone concentrations for its previous day, possibly due to rain event.
- AQF: F1
- Test dates: August 24th & 25th, 2006 (Rain on August 23rd)
- Domains: 12k and 4k

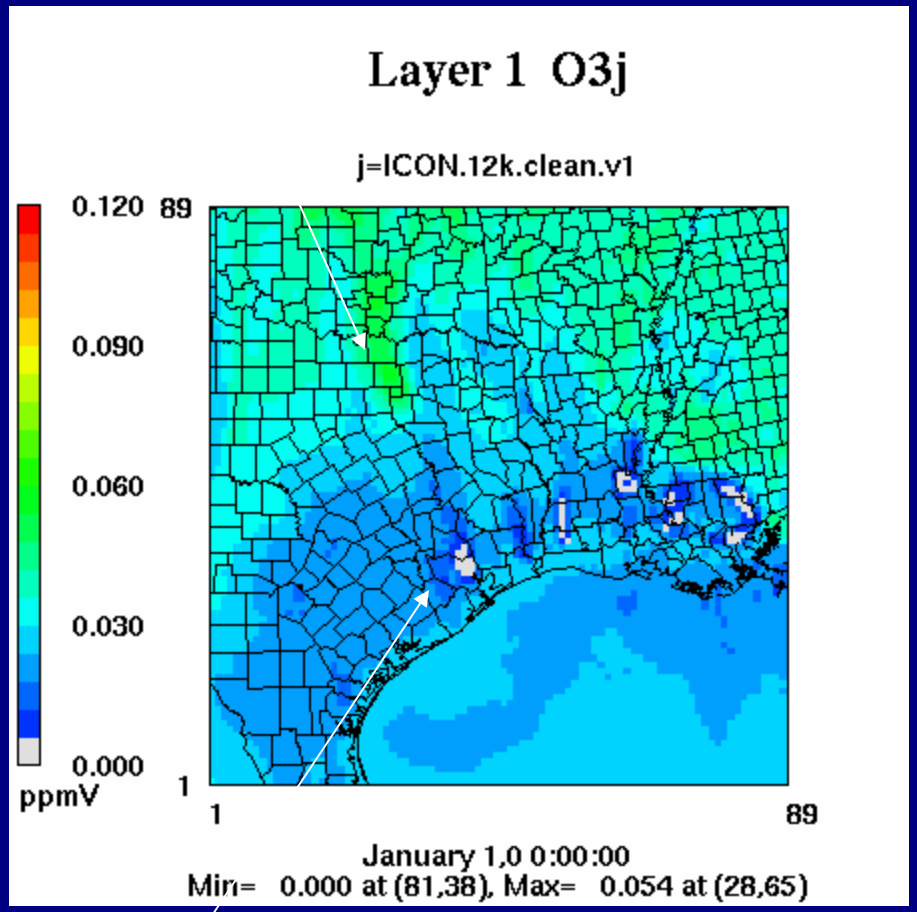
- First day (Aug. 24th)
  IC: a “Clean” IC for both 12k and 4k.
  12k - ICON.12k.clean.v1
  04k - ICON.12k.clean.v1
  BC: For 12k, use profile (The profile would provide the “clean” conditions).
  For 4k, BC w/ CONC for 12k after new simulation for this case.

- Second day (Aug. 25th)
  IC: CONC files for the previous day in this new simulation
  BC: 12k – nested BC from original F1 36k,
  4k- nested BC from new simulation for 12k

Initial Condition (12km)

Somewhat higher O3 over DFW



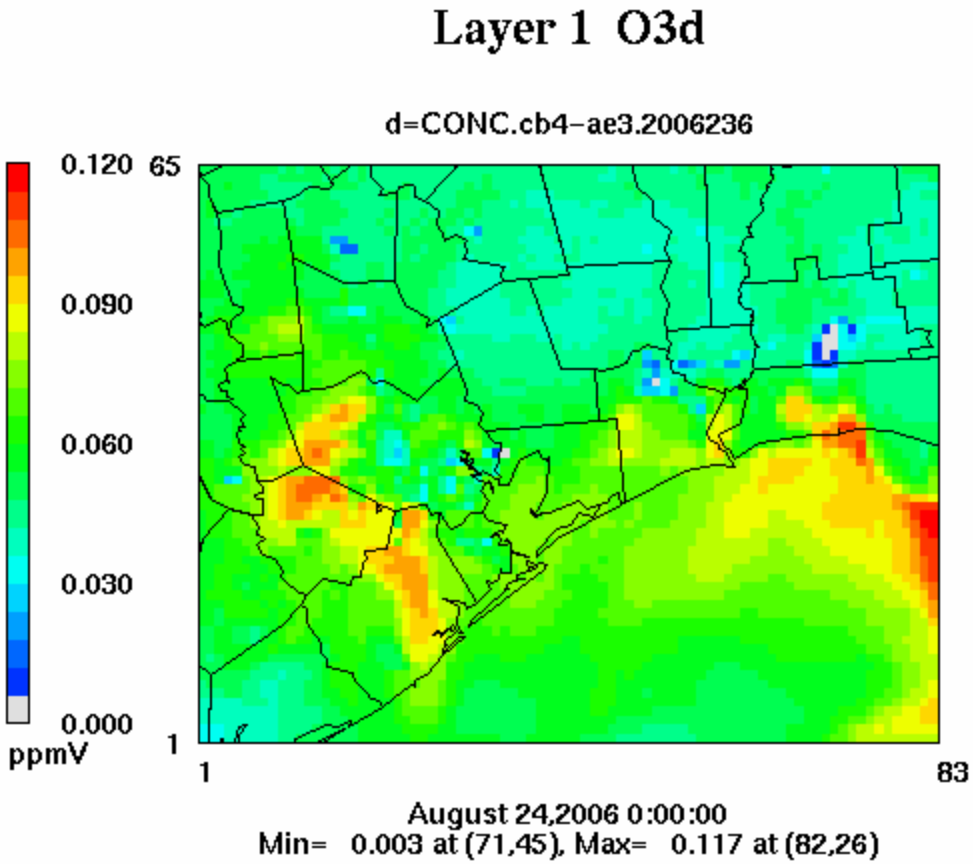


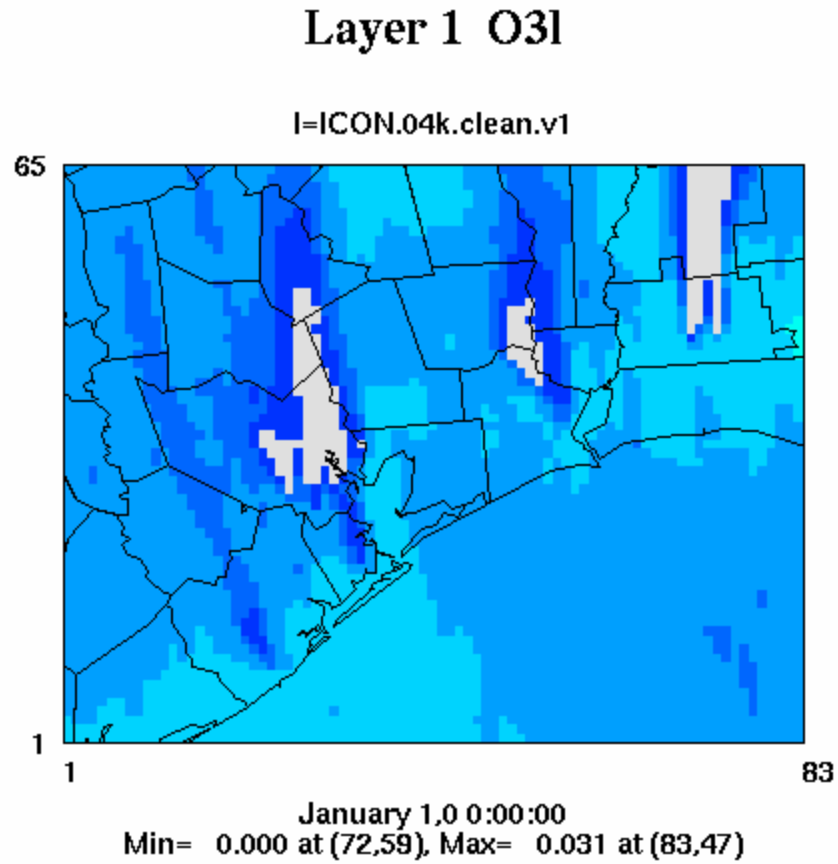
F1 12k IC for Aug. 24th

12k IC for a clean day

Low O3 over Houston

Initial Condition (04km)



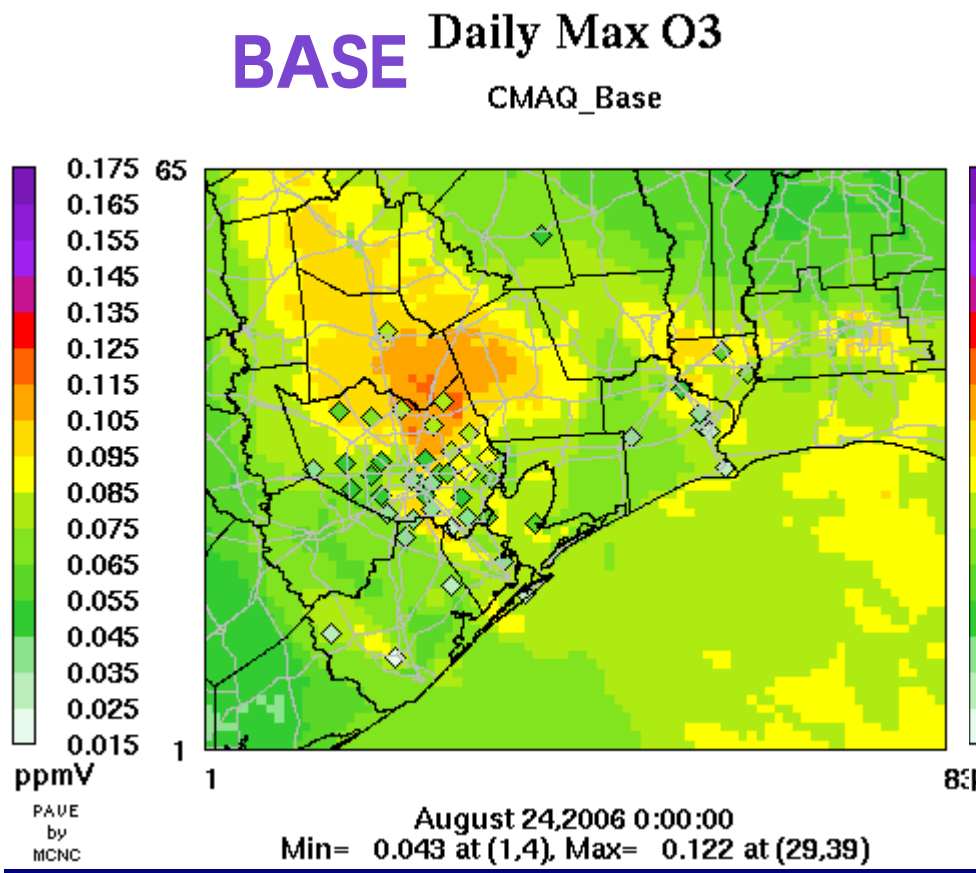


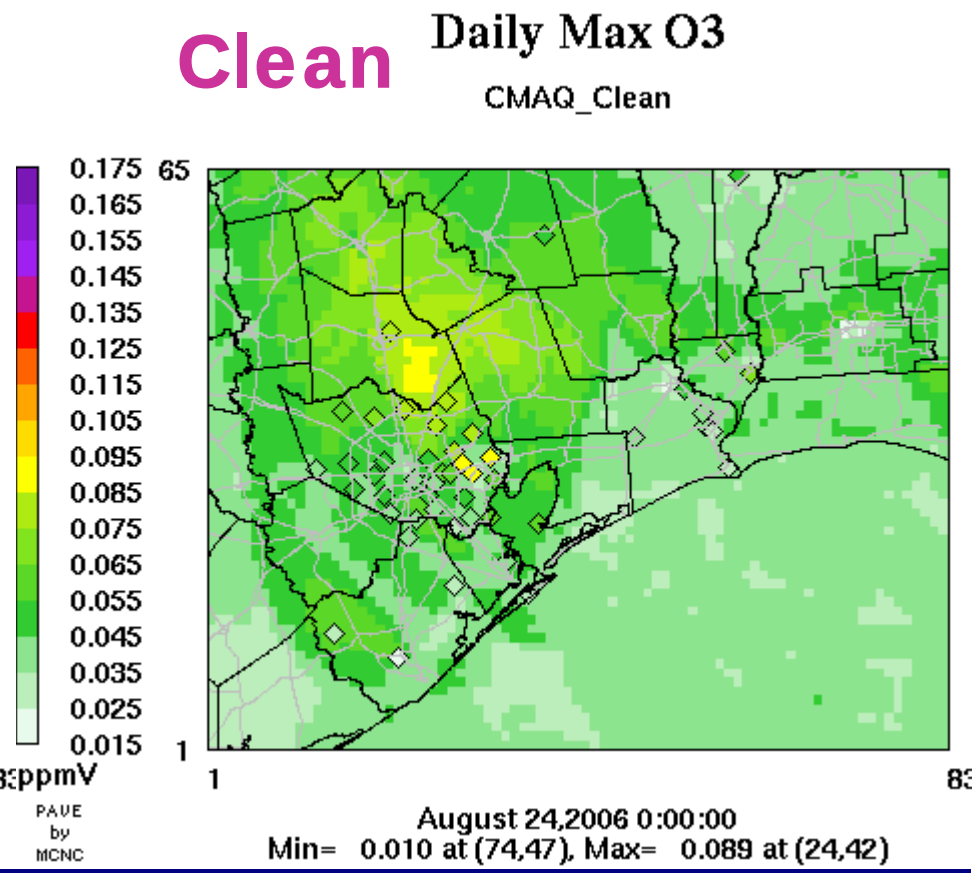
F1 04k IC for Aug. 24th

04k IC for a clean day

Daily maximum 1-hr O3 for August 24th, 2006

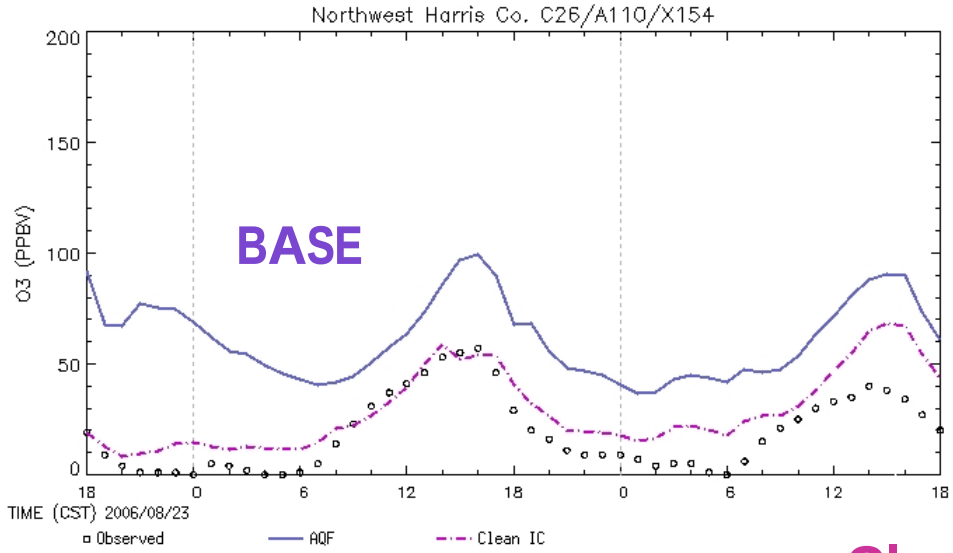
BASE: AQF F1
Clean: Rerun with a clean IC

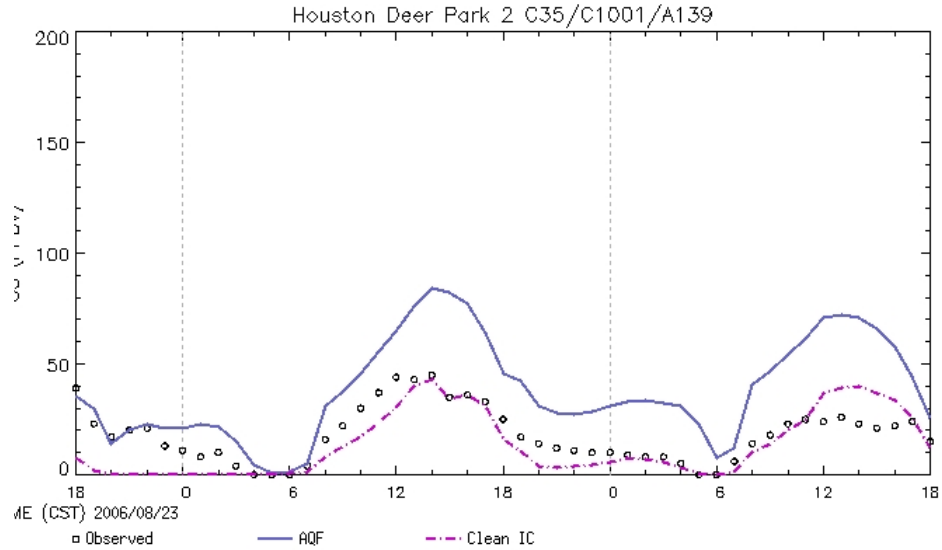




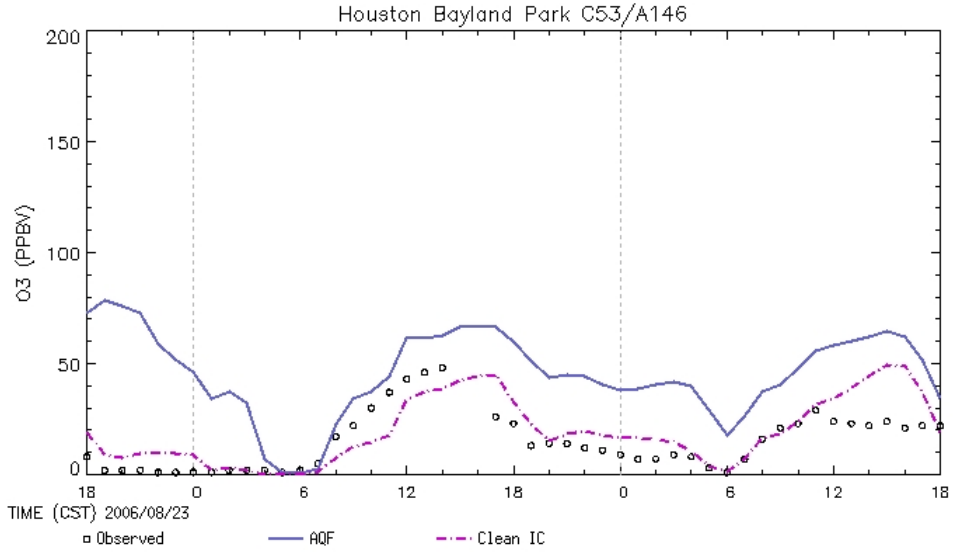
CAMS: 1-hr O3 for August 24th ~ 25th, 2006

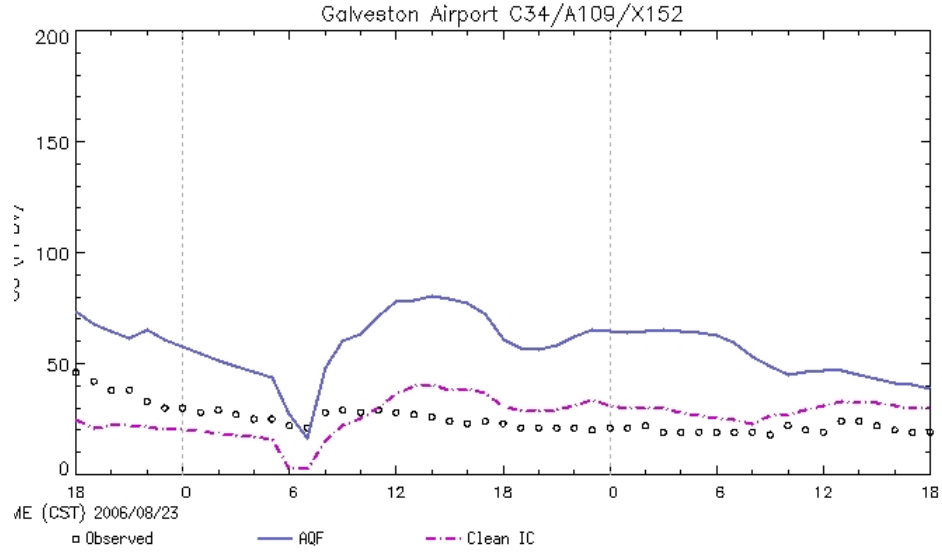
http://geossun2.geosc.uh.edu/web/skim/graph/ambi/cams/F1/20060824_1/0CMAQ.CAMS.Base.2.O3.htm





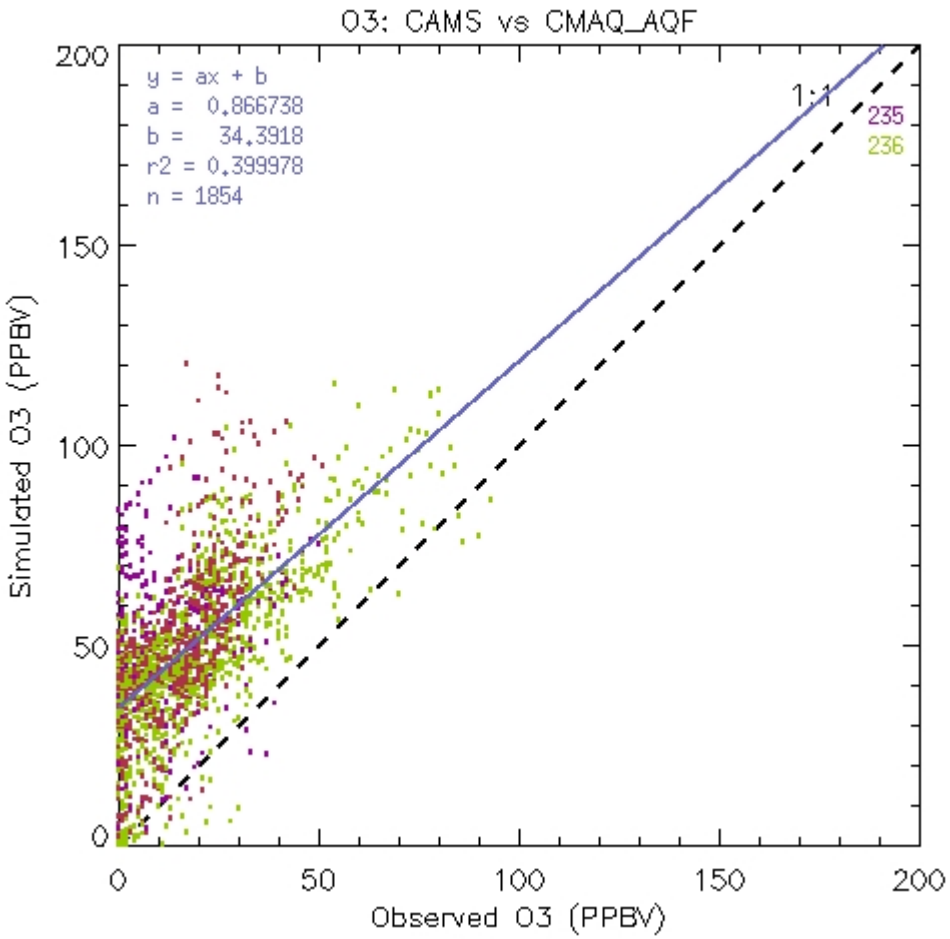
Clean

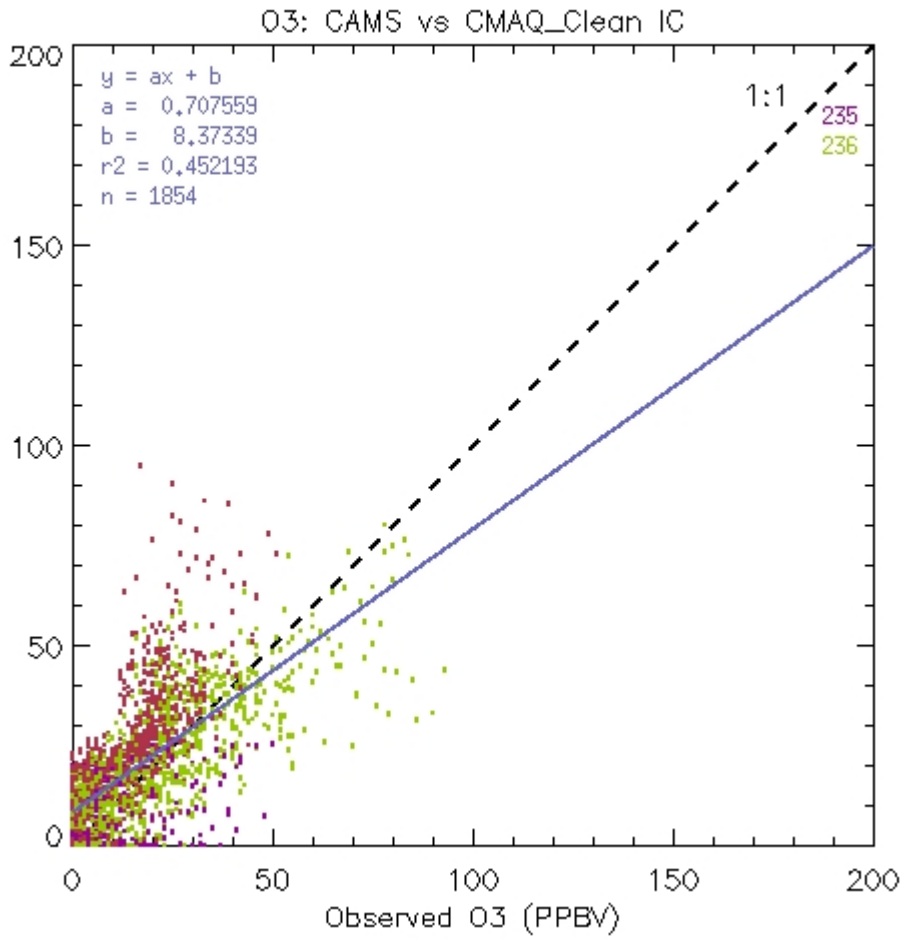




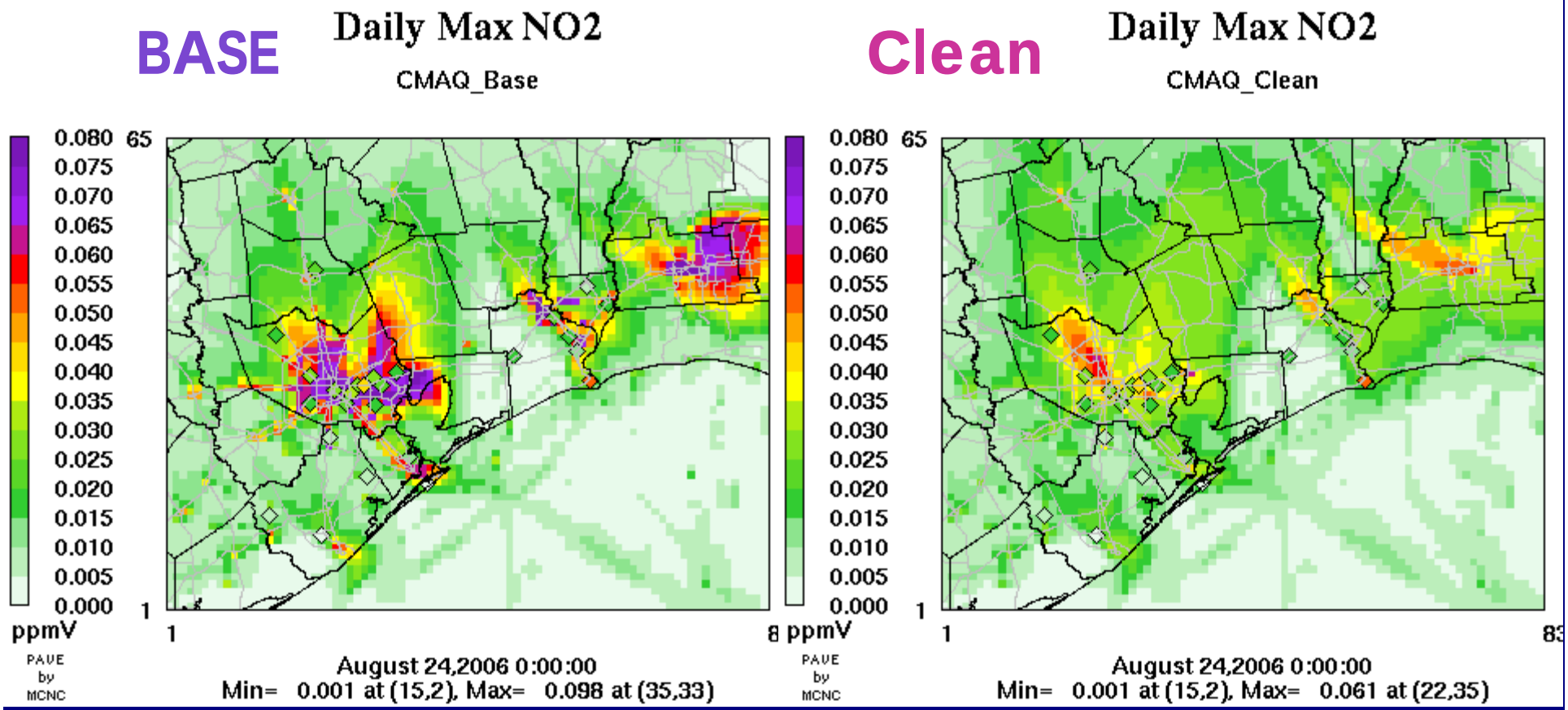
CAMS: 1-hr O3 for August 24th ~ 25th, 2006

BASE **Clean**



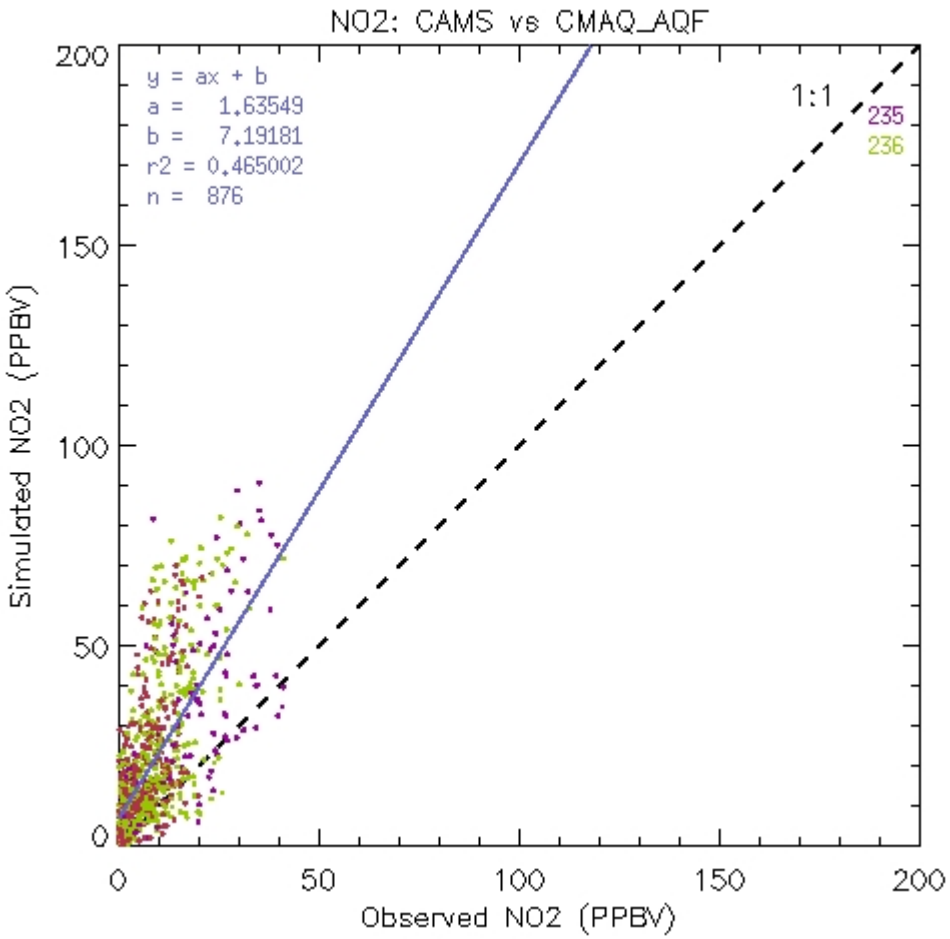


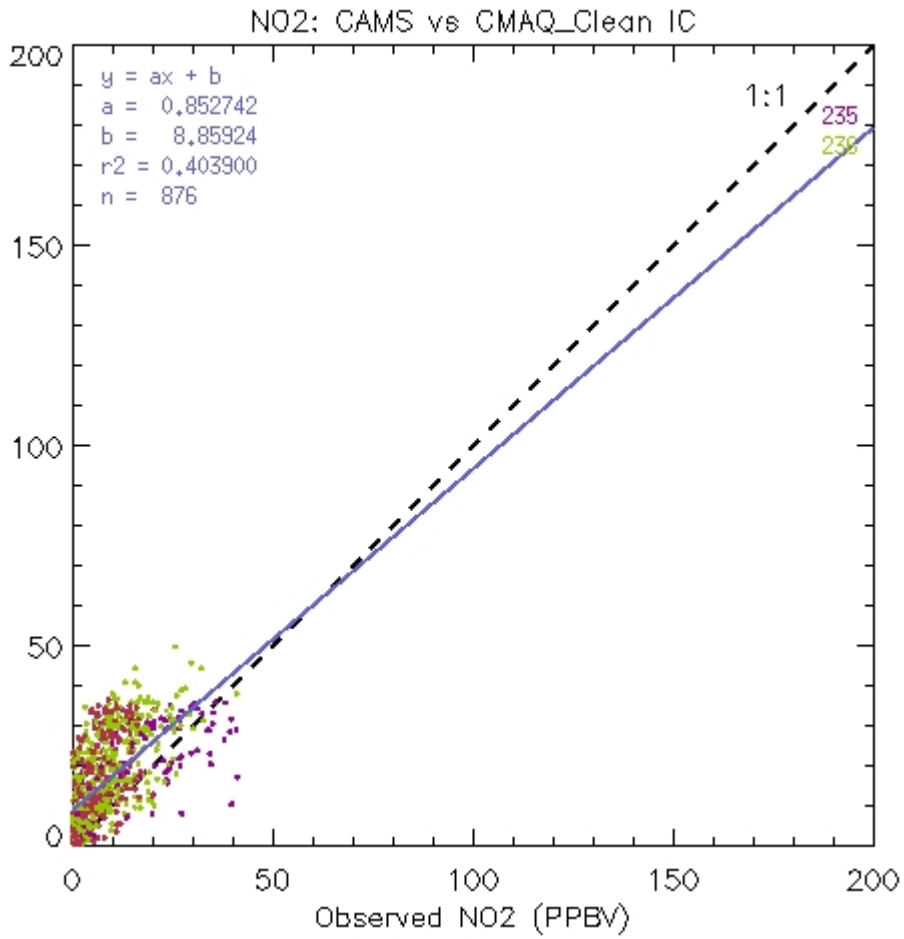
Daily maximum 1-hr NO2 for August 24th, 2006



CAMS: 1-hr NO2 for August 24th ~ 25th, 2006

BASE **Clean**





Summary of clean IC runs

1. Clean IC is able to help get better overall AQF performance for the next day when AQF unreasonably over-predicted ozone concentrations for a day.

2. Not only ozone but also other precursor concentrations such as NO2 can be improved.

3. The IC correction can affect more than one day under a given condition.

4. However, some sites may show poor performance when new IC is applied as shown in the next slide. Supposedly, it depends on where and how much we need to rely on new IC.

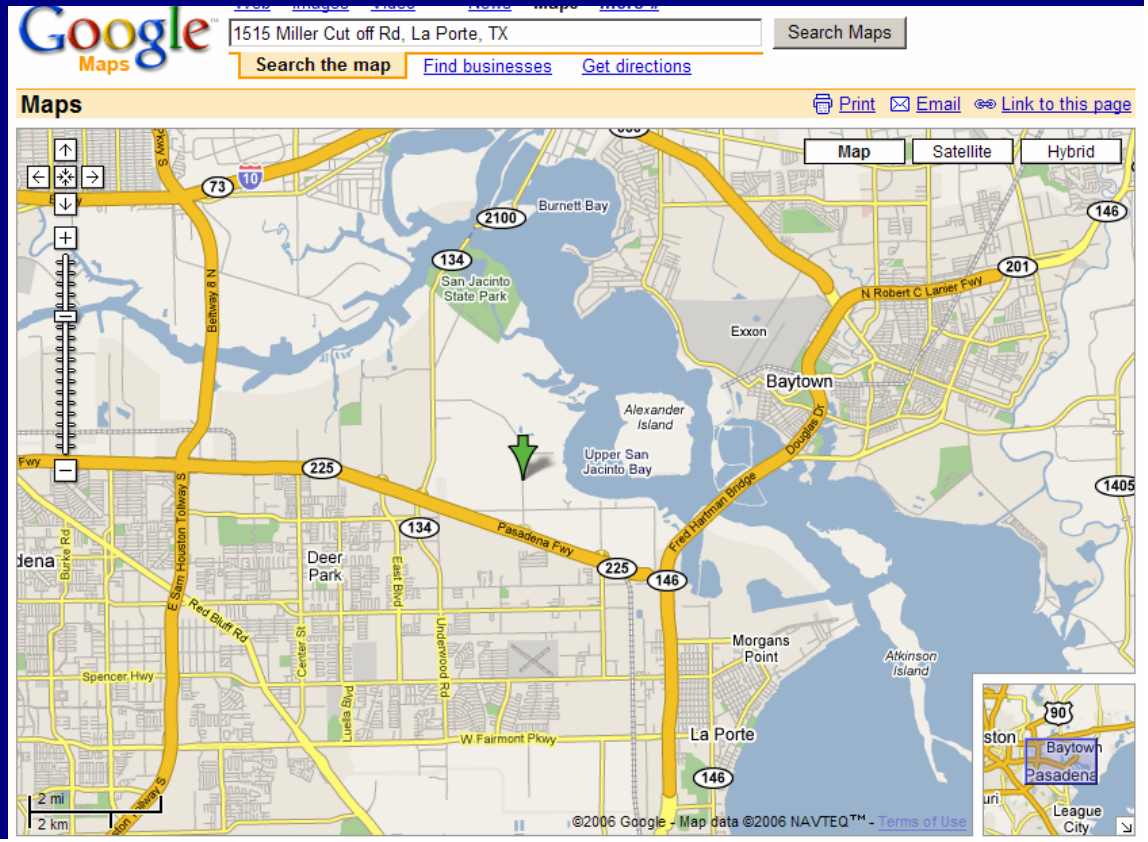
An Upset emissions case

TCEQ's Upset Emissions Report

http://www2.tnrcc.state.tx.us/eer/main/index.cfm?fuseaction=getDetails&target=81218

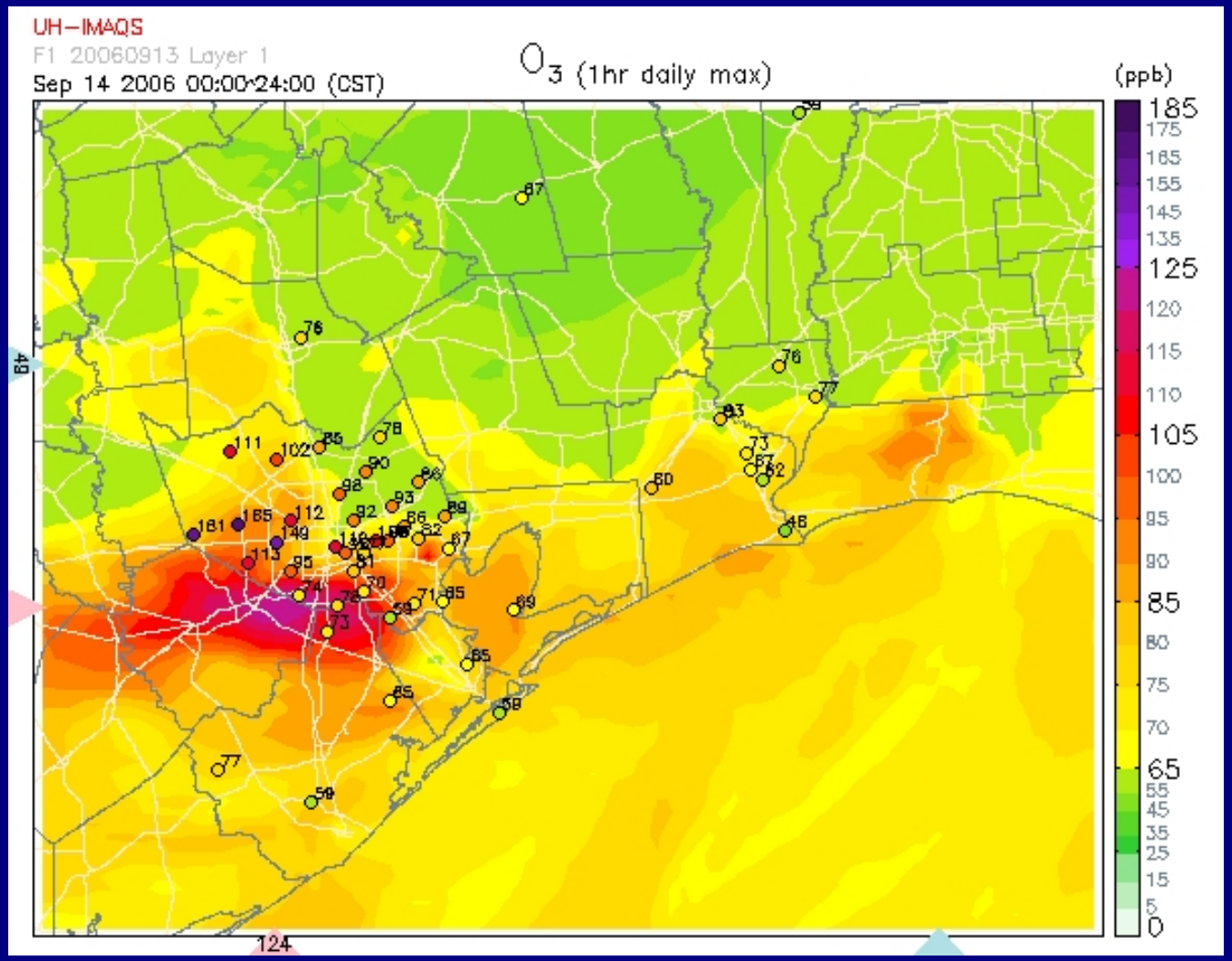
Amount Released; Ethlylene, 18,000 lbs (9 moles/sec)

Event began:	09/13/2006 7:10PM
Event ended:	09/14/2006 5:10AM

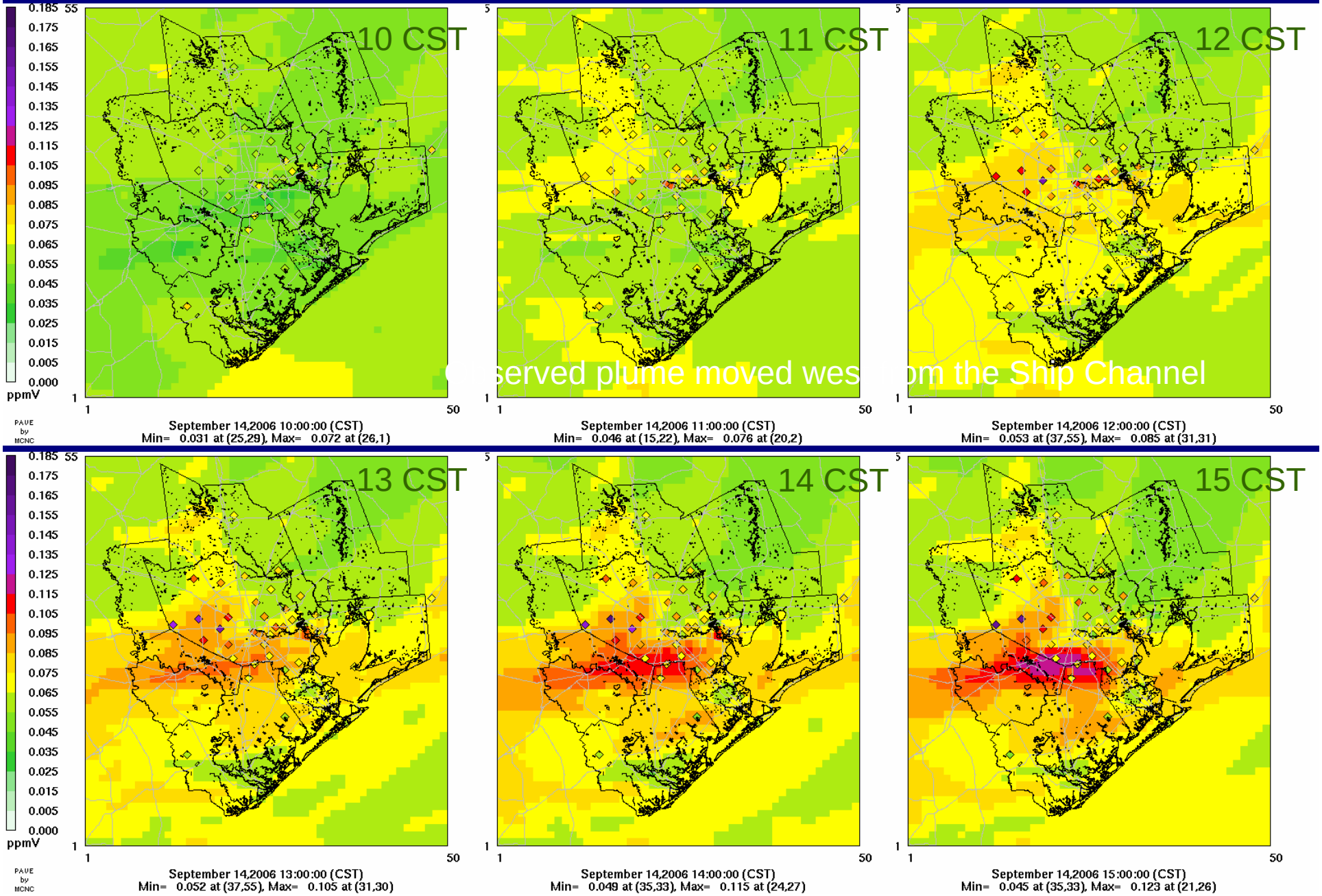


Daily maximum 1-hr O3 for September 14th, 2006: F1

High ozone was observed to the west of Houston downtown while predicted high ozone was south west. Difference in daily maximum 1-hr ozone concentrations observed and predicted was larger than 40 ppb.

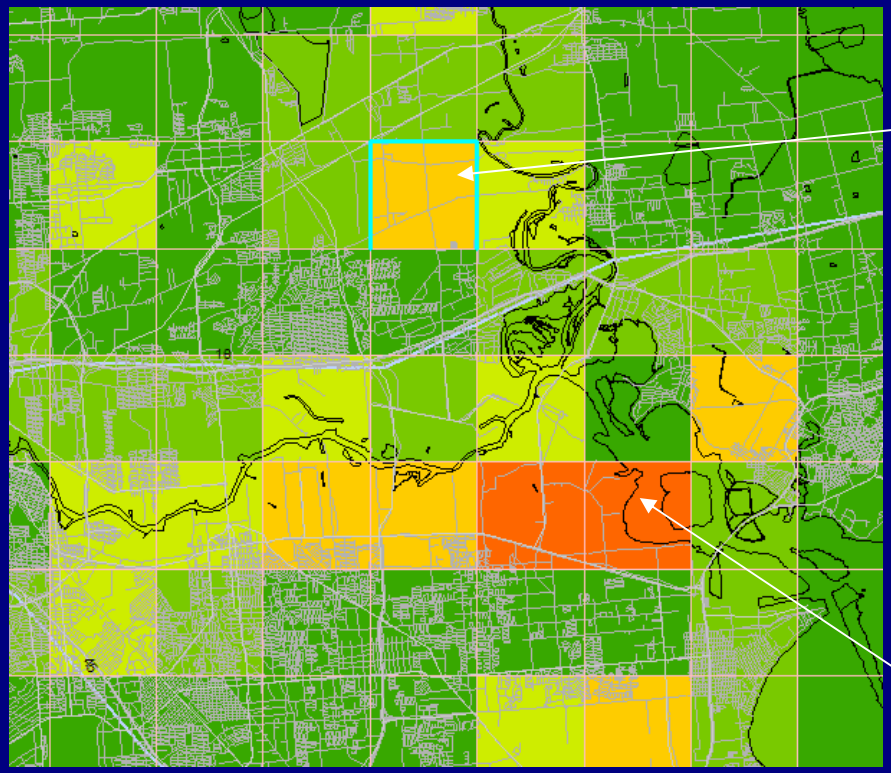


1-hr O3 for September 14th, 2006: F1



Sensitivity run

- Imputed cell: (29, 33) – The dominant wind simulated was northeasterly while observation was easterly. The source cell was alternated to allow the imputed emissions to move over the observed high ozone plume area.
- Amounts: 9 moles/s of ETH as reported, but x10 times used (to compensate coarse model resolution)
- Imputation time: Sept. 13th, 2006 19 CST ~ Sept. 14th, 8 CST (+3 hr reported)
- Layer: 1st layer

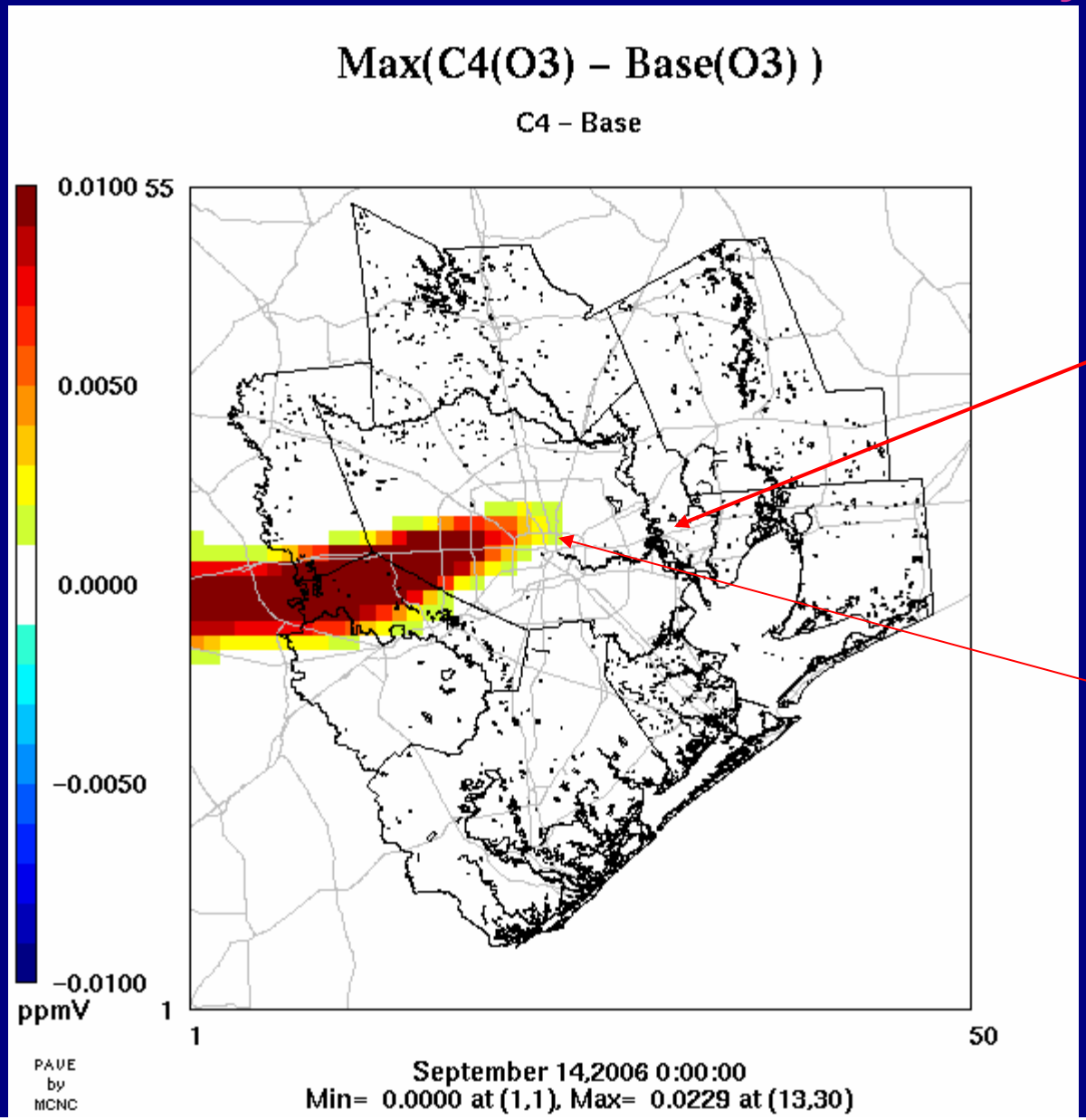


New imputation cell to have the effect on observed high plume area.

10 times higher, 3hrs longer than the reported emissions

Original imputation cell

Difference in daily maximum 1-hr O3 between the sensitivity & Base



The imputed cell

Predicted ozone concentrations increased by ~ 23 ppb, replicating high ozone plume observed.

Summary of Forecasting Difficulties

1. Need to evaluate performance of MM5 with new NCEP/NAM

2. Improve stable PBL characterization
   - Wind speed
   - PBL height

3. Evaluate predictability of precipitation events

4. Need to set up a smart re-initialization strategy (short term)

5. Need to use realistic regional BCs (how to obtain)

6. AQF requires to develop a real-time data assimilation system (long-term)