East Texas Air Quality Forecasting Systems (ETAQ-F)

Evaluation of Summer 2006 Simulations for TexAQS II

Daewon W. Byun

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Institute for Multi-dimensional Air Quality Studies (IMAQS)

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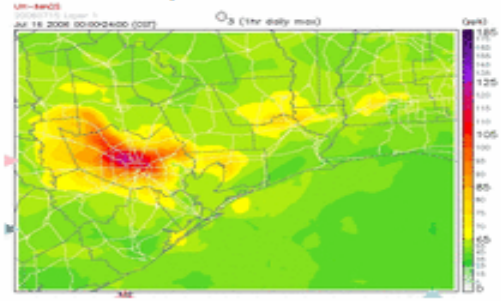
Welcome to the Institute for Multi-dimensional Air Quality Studies. We are a diverse group of researchers from fields of geosciences, math, computer science and chemistry committed to using premier scientific tools to model the complex issues of air quality and climate change. Our modeling efforts address 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

Review of June 1 2005 –May 30 2006

University of Houston Air Quality Forecasting Systems

Spatial Resolution

36 km : U.S. Continent

12 km : East Texas (2005) State of Texas, Louisiana (2006)

04 km : Houston and Galveston Area (05) & Dallas-Fort Worth area (06)

MM5 – with 43 layers

CMAQ – With 23 layers

Operation Period and Duration (May 2005 ~ Current)

Spin-up : 6 hrs

(0th day 18 CST – 0th day 23 CST)

Forecasting : 48 hrs

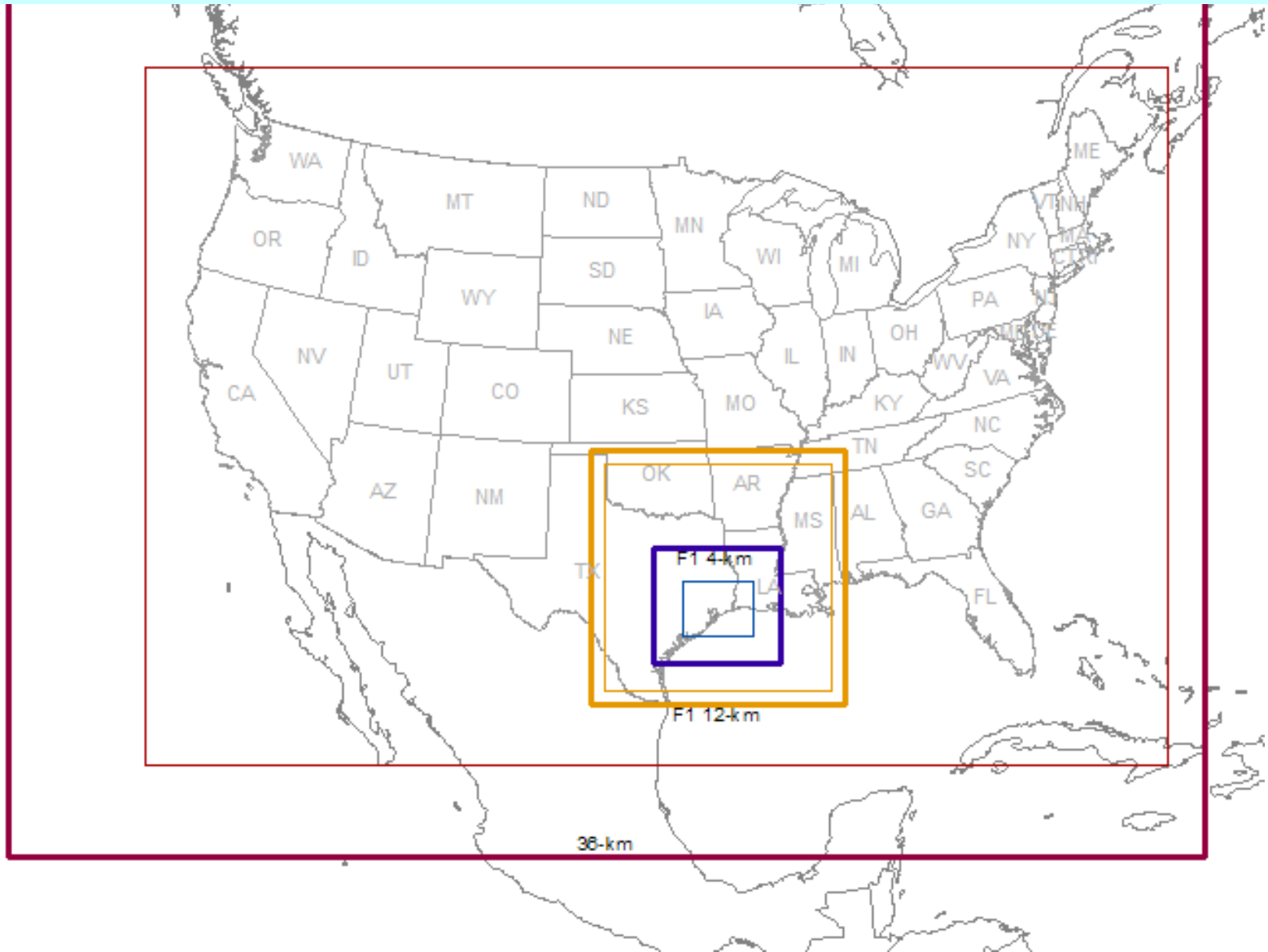
(1st day 00 CST – 2nd day 23 CST)

Two Different Air Quality Forecasting Systems

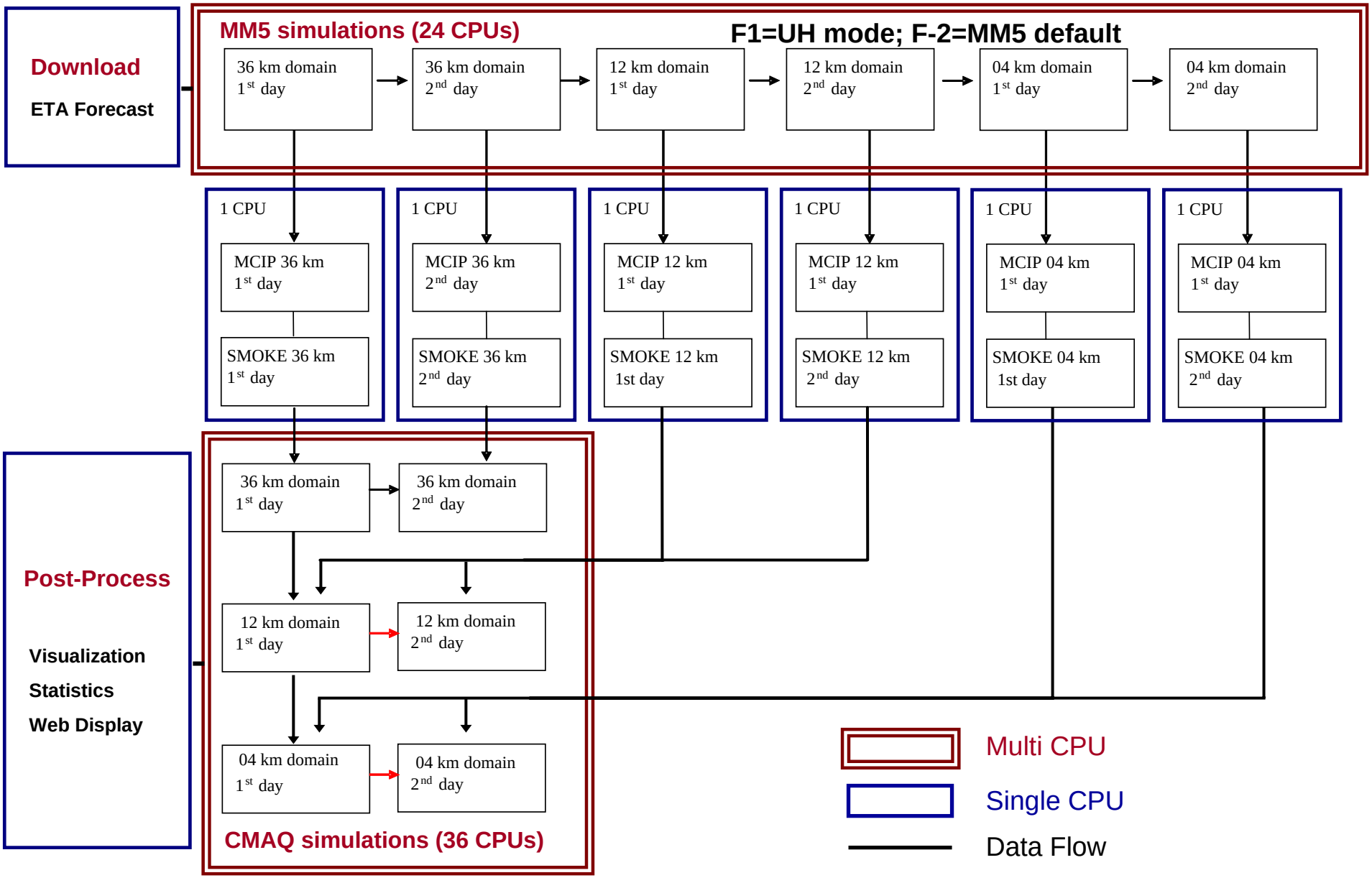
Forecasting 1 (F-1) : MM5 modified by UH + Emission + CMAQ v4.4

Forecasting 2 (F-2) : Default MM5 + Emission + CMAQ v4.4

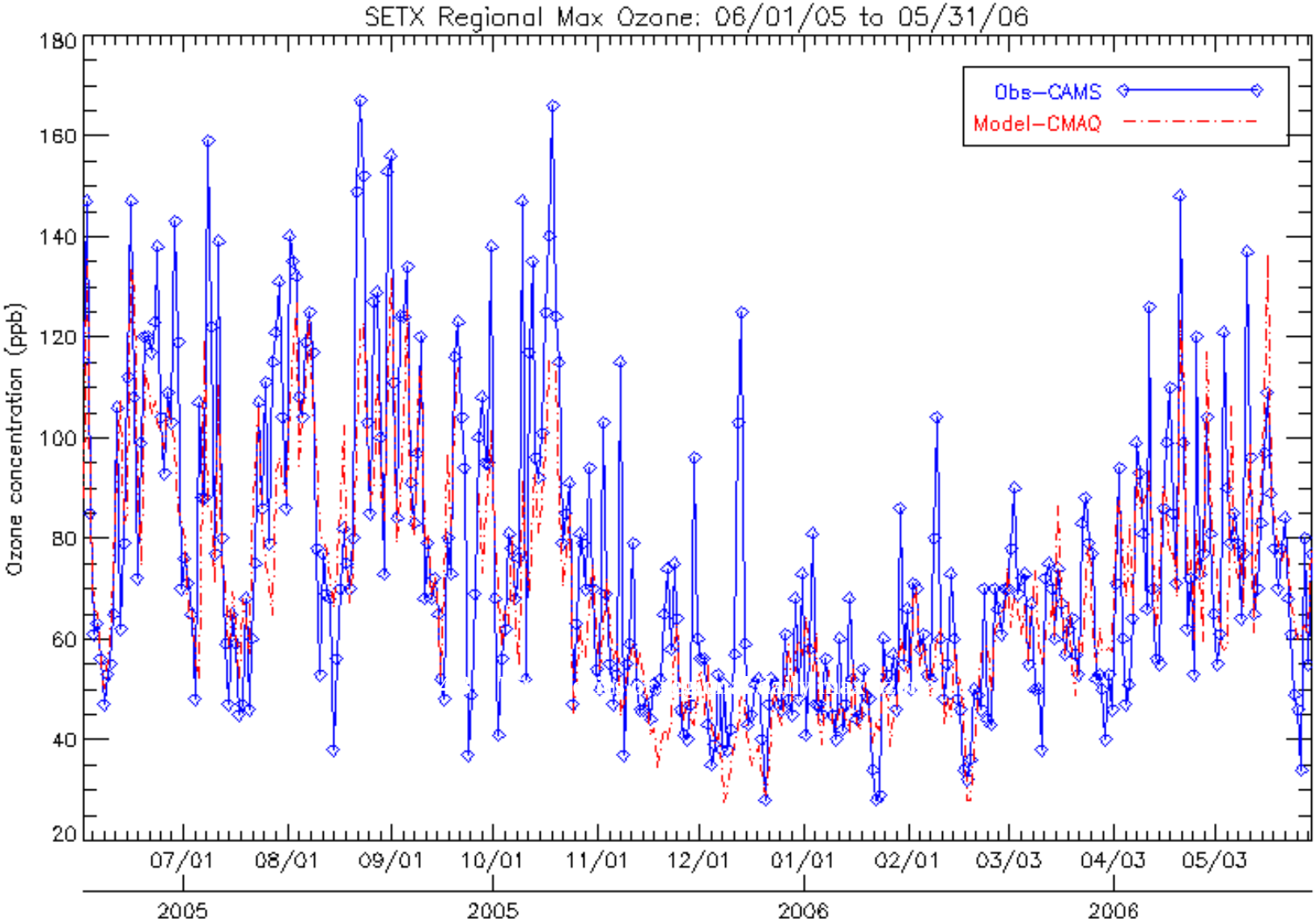
Modeling Domains – F1/F2 (June 2005 – May 2006)



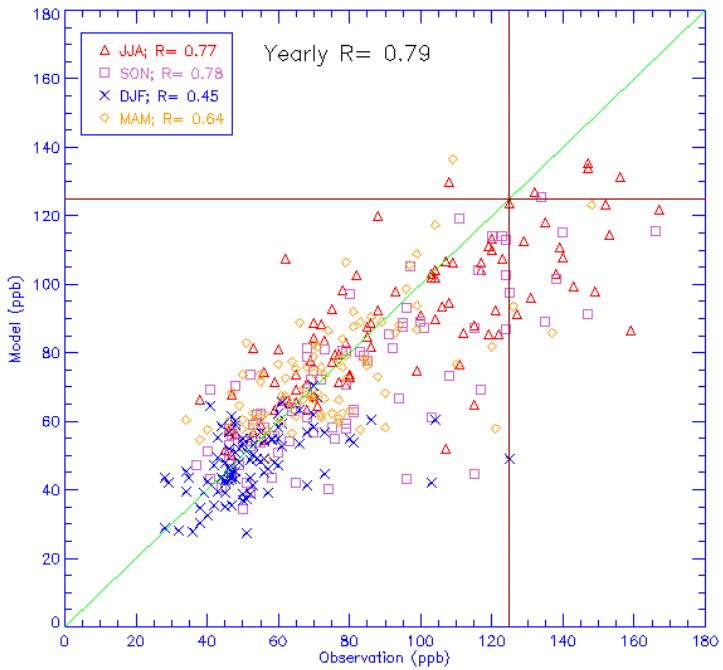
2005 UH AQF systems (F-1 & F-2)



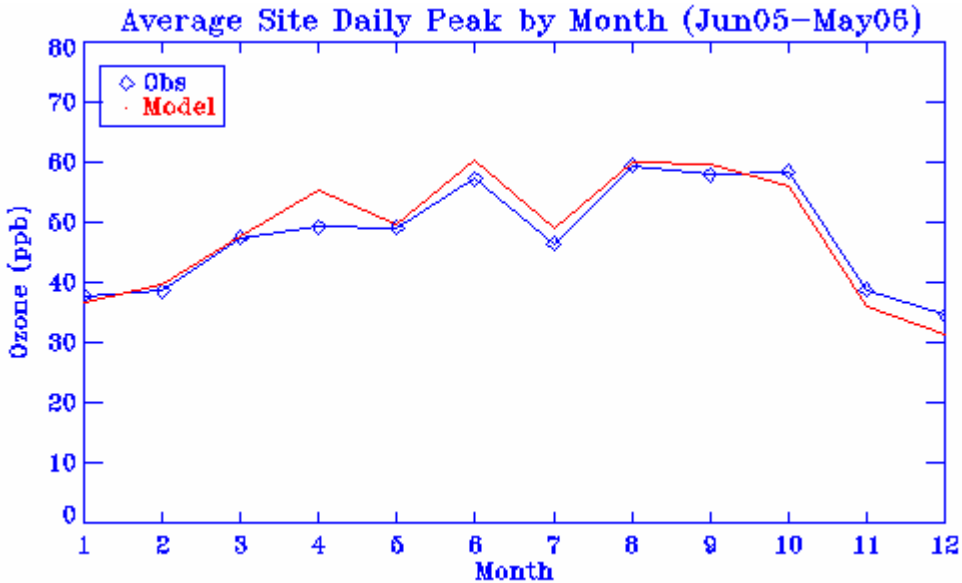
Time series of regional daily max ozone
June 2005 – May 2006



O3: June 2005 – May 2006



Scatter plot of regional daily max ozone

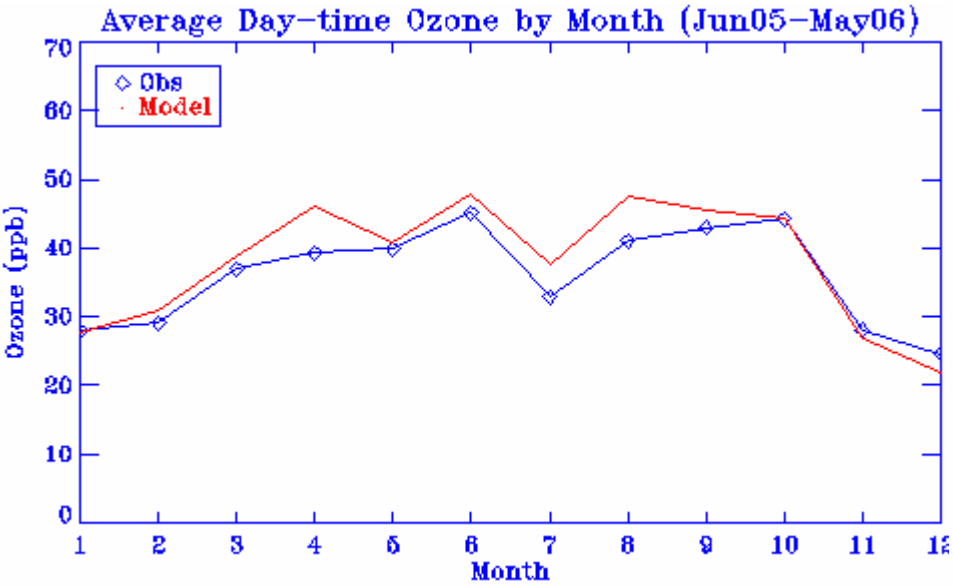


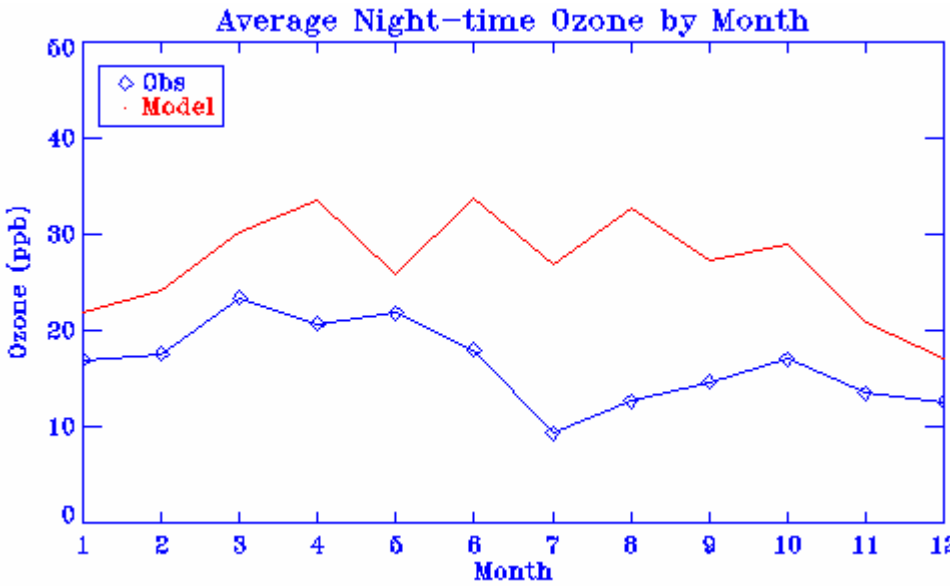
Average site daily peak by month

-Average site peak ozone is one of the best predicted ozone categories. The R is consistently high for all the months except for Jan and Nov

- However, the underprediction of regional max

O3: June 2005 – May 2006





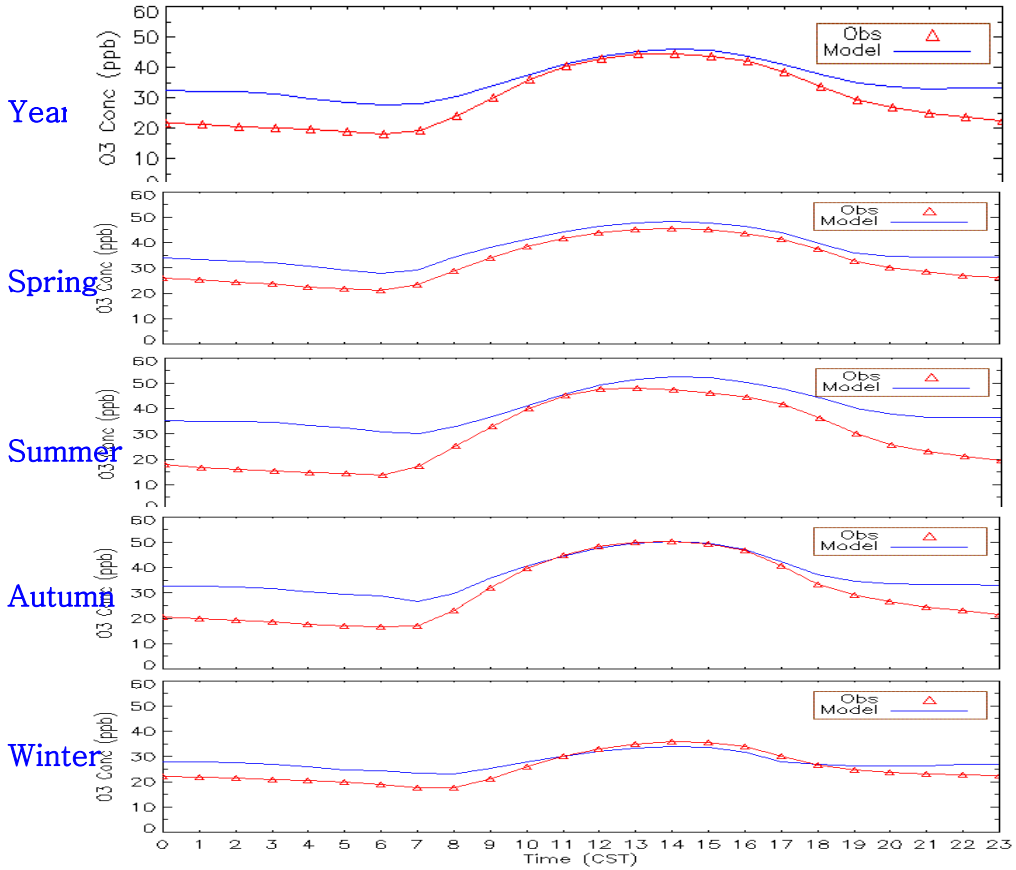
Average day-time ozone by month

Average night-time ozone by month

-Average site peak ozone in the daytime compares well with observed ozone. The R is consistently high for all the months except for Jan and Nov

- However, the model night time ozone considerably overestimated in the Summer.

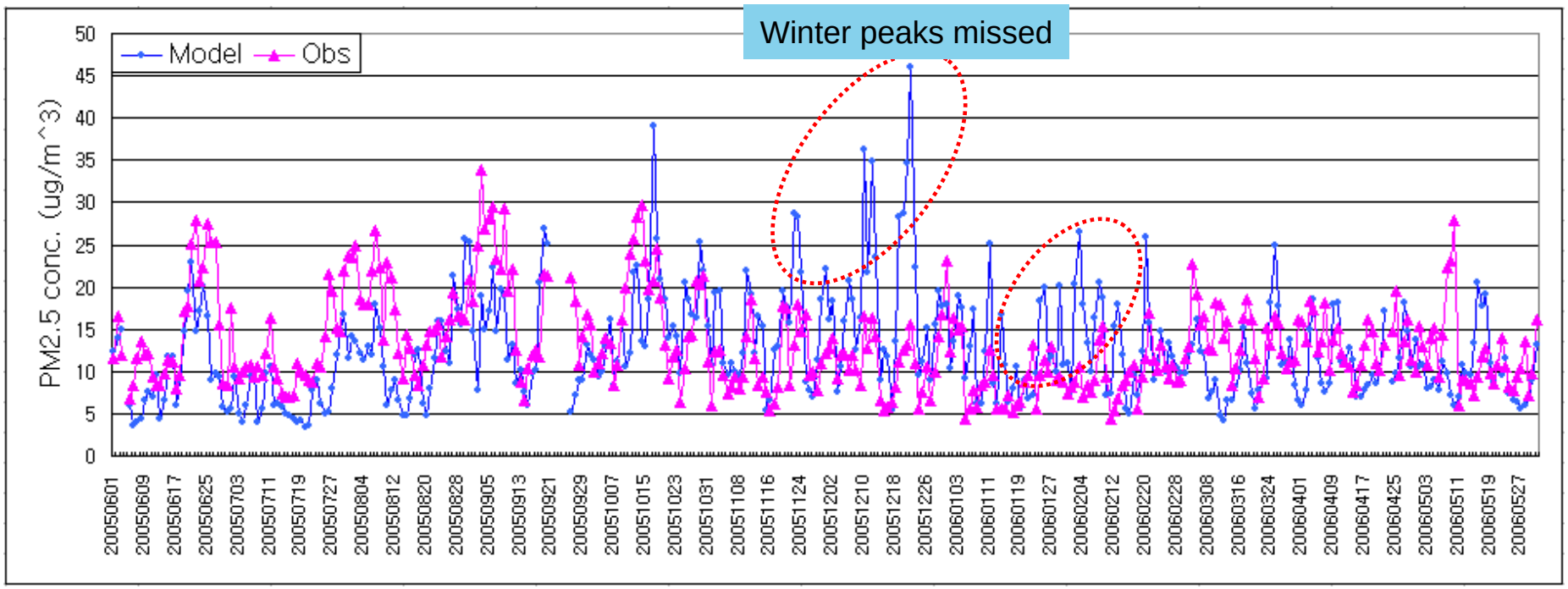
Summary of Hourly Ozone Forecasting Performance: 2005 June – 2006 May



PM2.5 TS plot for daily average

Yearly TS plot

Model highly over-predicted during Dec.



Number of days for over & under prediction

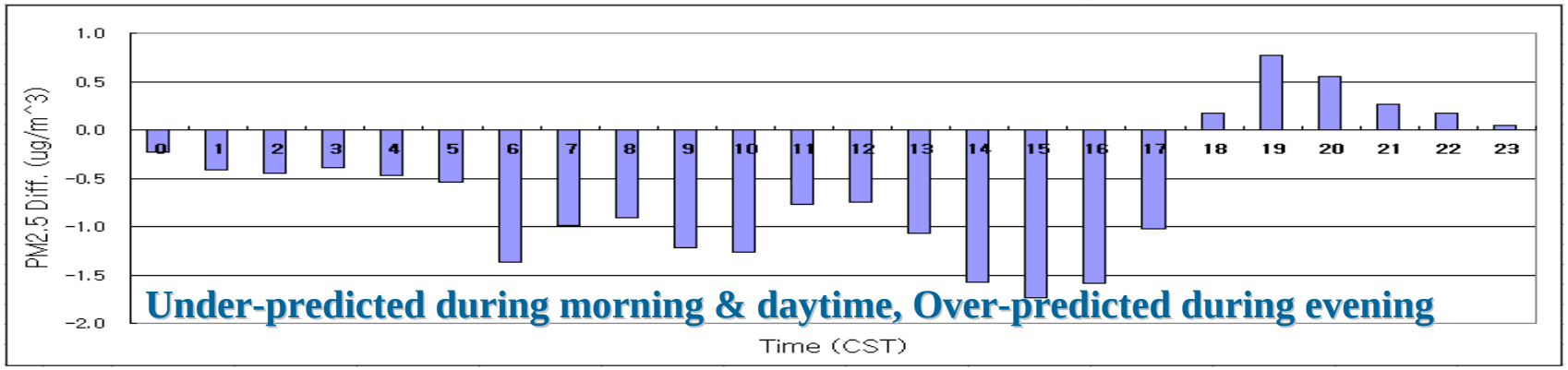
M-O > 0	M-O > 5	M-O > 10	M-O > 20	M-O < 0	M-O < -5	M-O < -10	M-O < -20
161	58	21	2	197	84	26	1

M-O : Model-Obs.
Unit : days

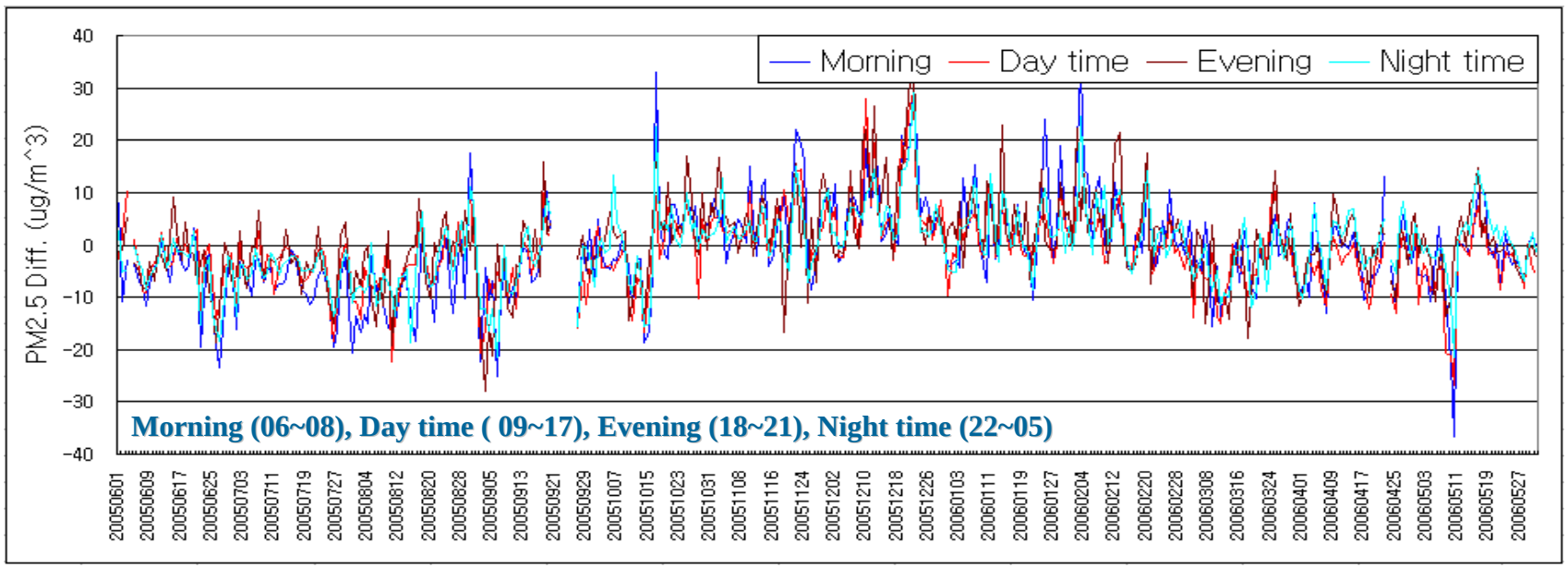
Overall, Model tends to slightly under-predict during the year

PM Model & Obs. Differences : [Model-Obs]

Model & Obs diff. for each hourly data



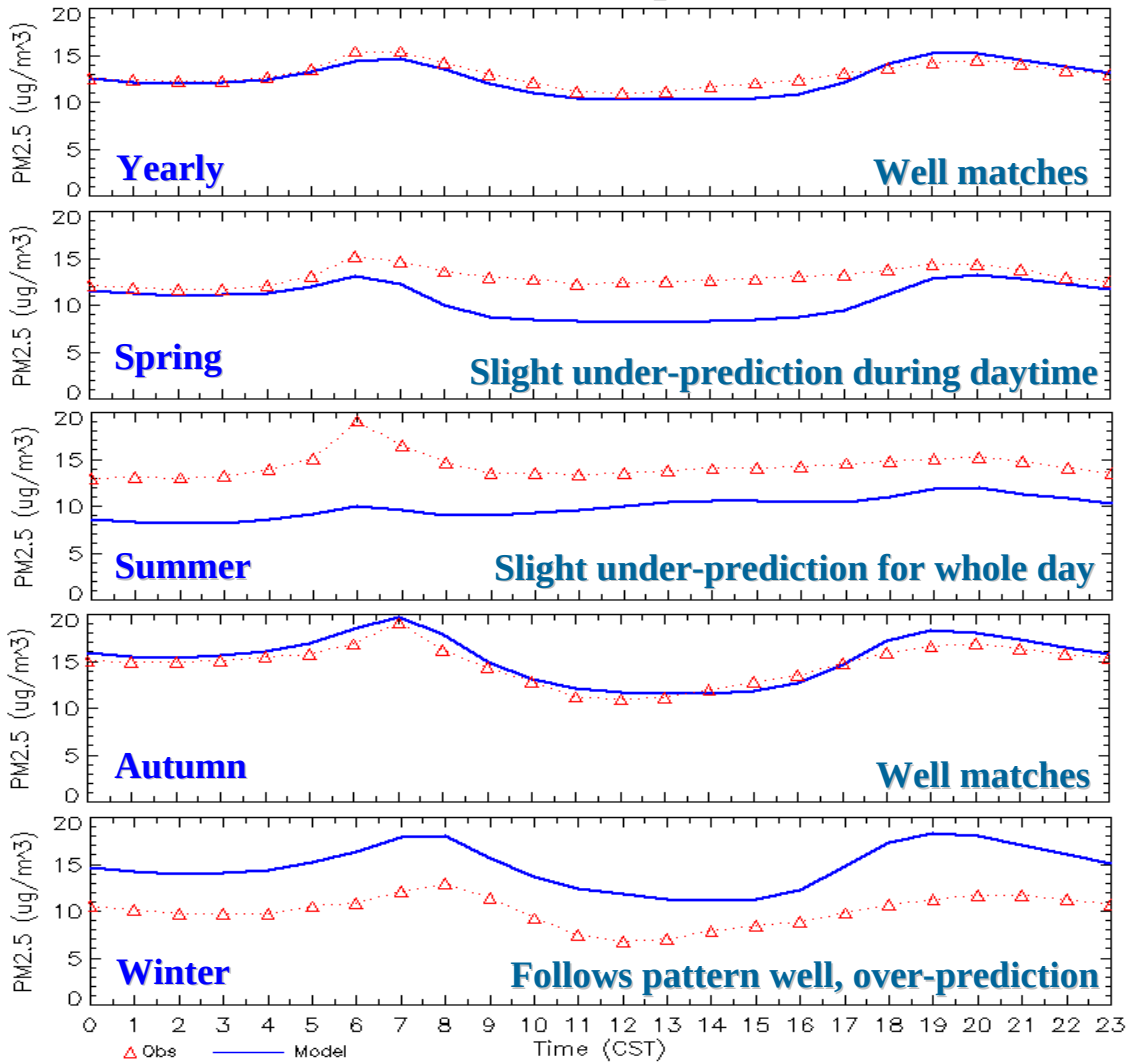
Model & Obs diff. for each day period



Model & Obs diff. doesn't show big differences among day period

Summary of Hourly PM2.5 Forecasting Performance: 2005 June – 2006 May

TS plot



2006 June – 2006 Oct (TexAQS-II)

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)

MM5 – 43 layers, CMAQ-23 layers

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)

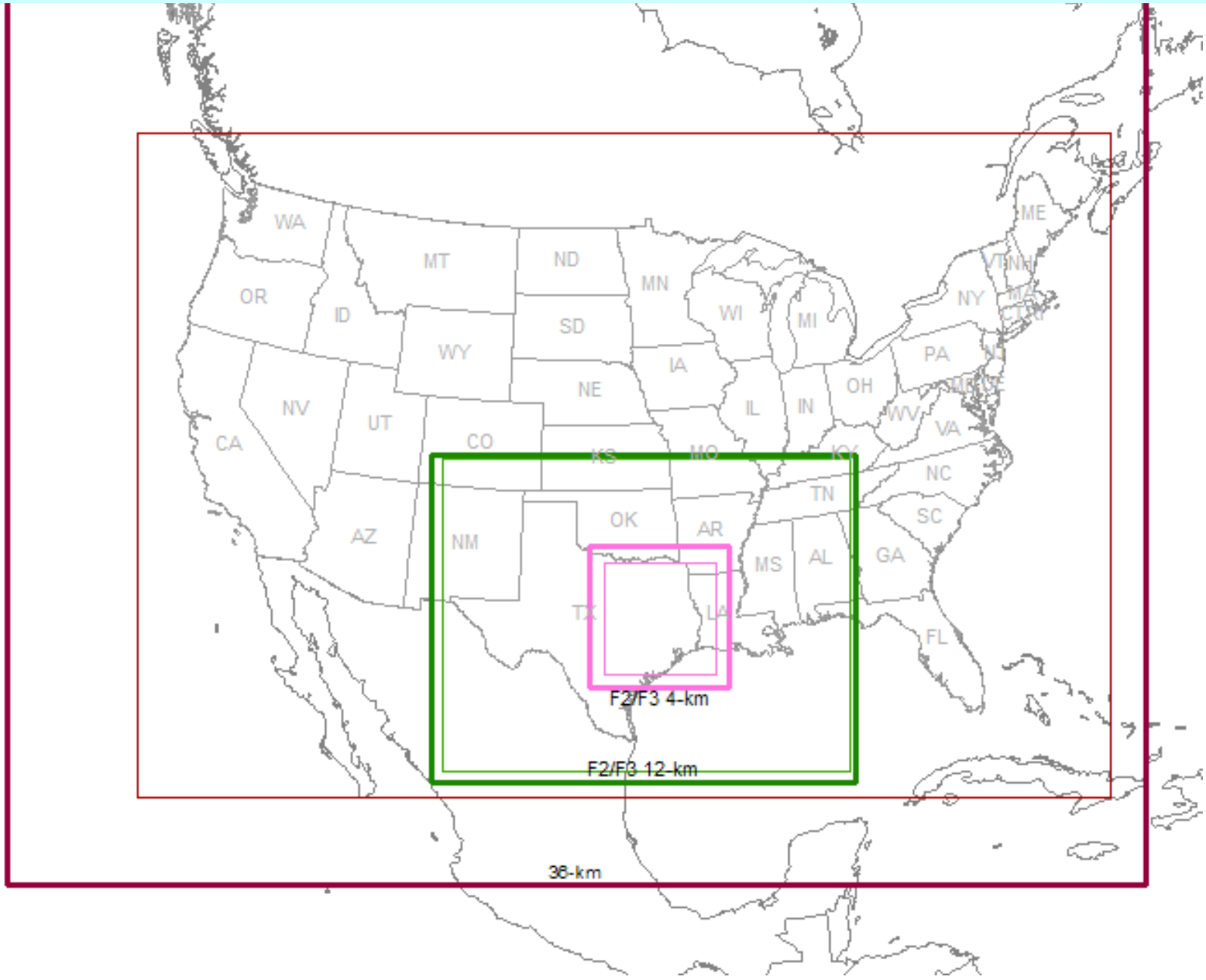
Different Air Quality Forecasting Systems

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 v4.4

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

Modeling Domains – F2/F3, TexAQS-II



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

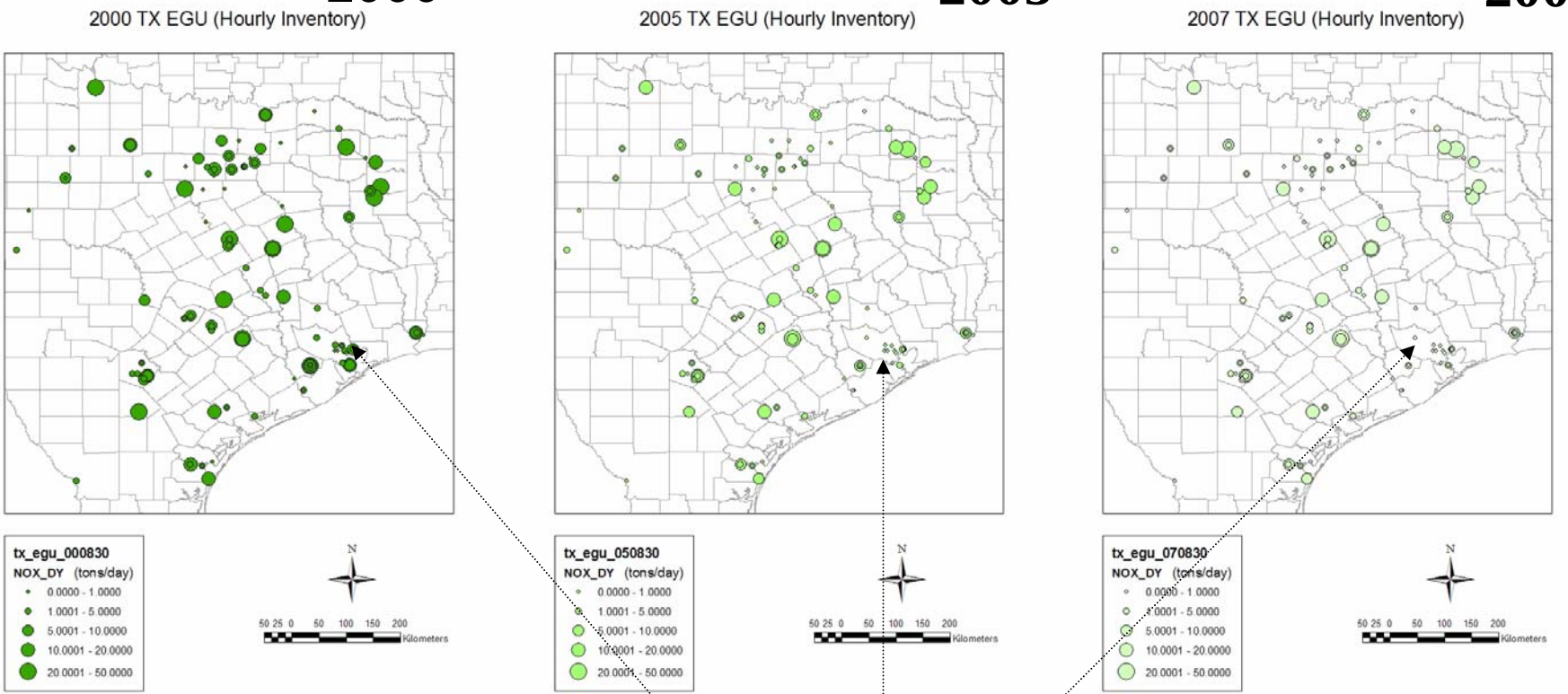
- NEI99 (Final version 3)
  - CONUS 36-km domain
  - Particulate matters and precursors (NH3, SO2)

- 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)

2000 **2005** **2007**



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

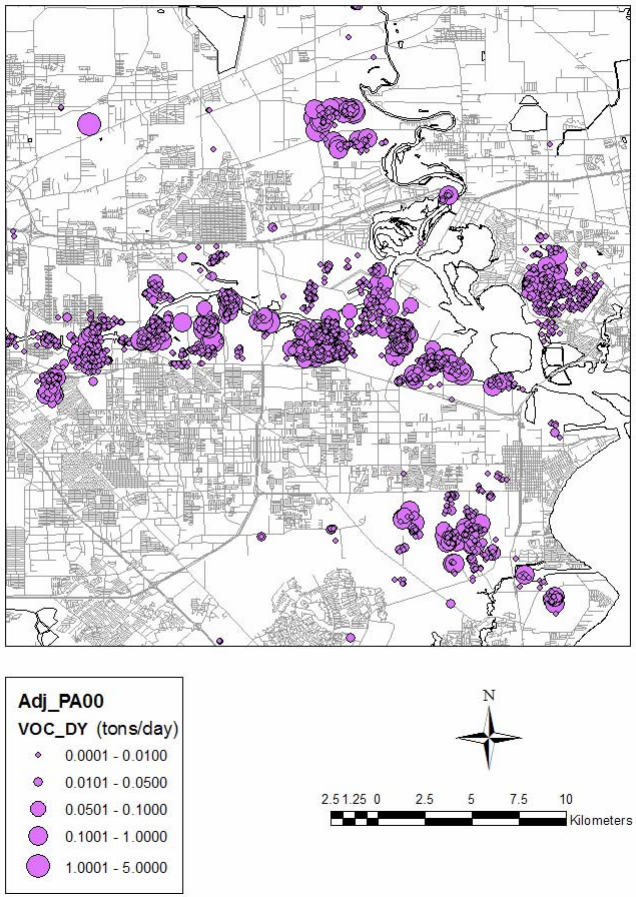
✓ For HG NOx emissions for 2005, a factor of 1.747 was applied on 2007 EI based on the 2005/2007 MECT (Mass Emission Cap and Trade) allowances.

Anthropogenic Emissions: for F2/F3 (2006)

VOC emissions for imputation after SIP

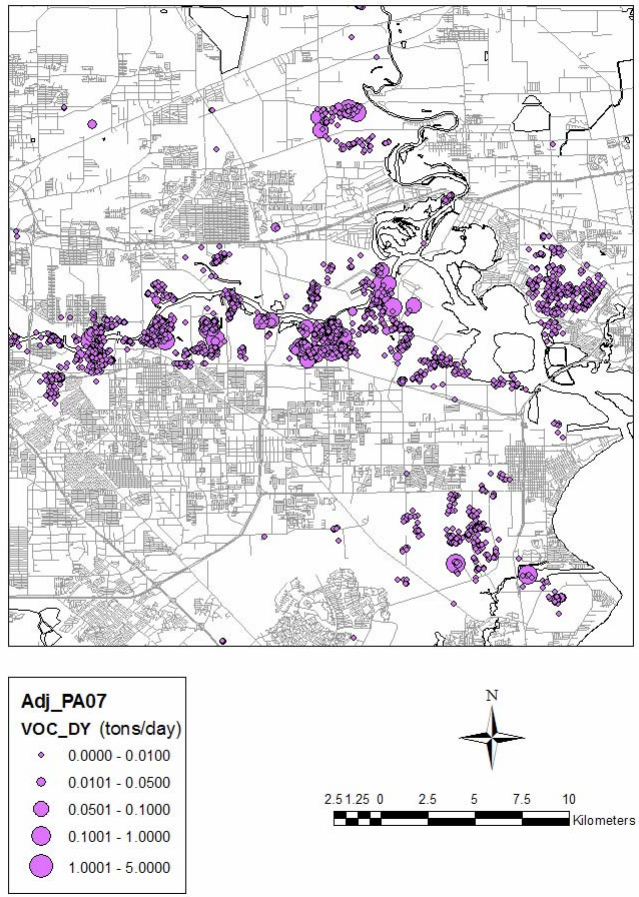
2000

2000 Additonal VOC (Daily Inventory)



2007

2007 Additonal VOC (Daily Inventory)

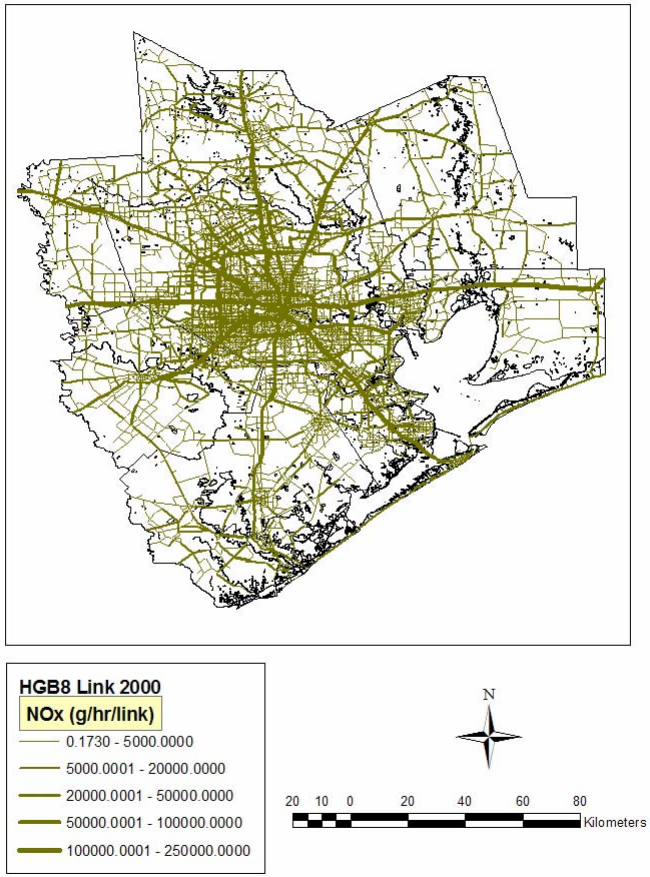


✓ UH AQF system uses additional VOC emissions at the 2007 level.

MOBILE6 NOx emissions for 2000 and 2007

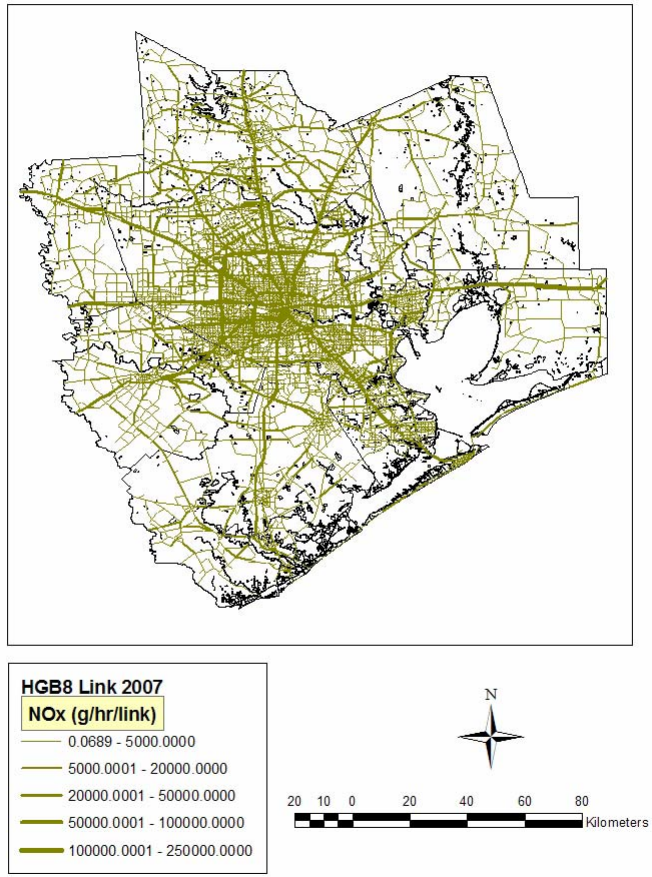
2000

HGB Links for MOBILE6 emissions



2007

HGB Links for MOBILE6 emissions



✓ 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)

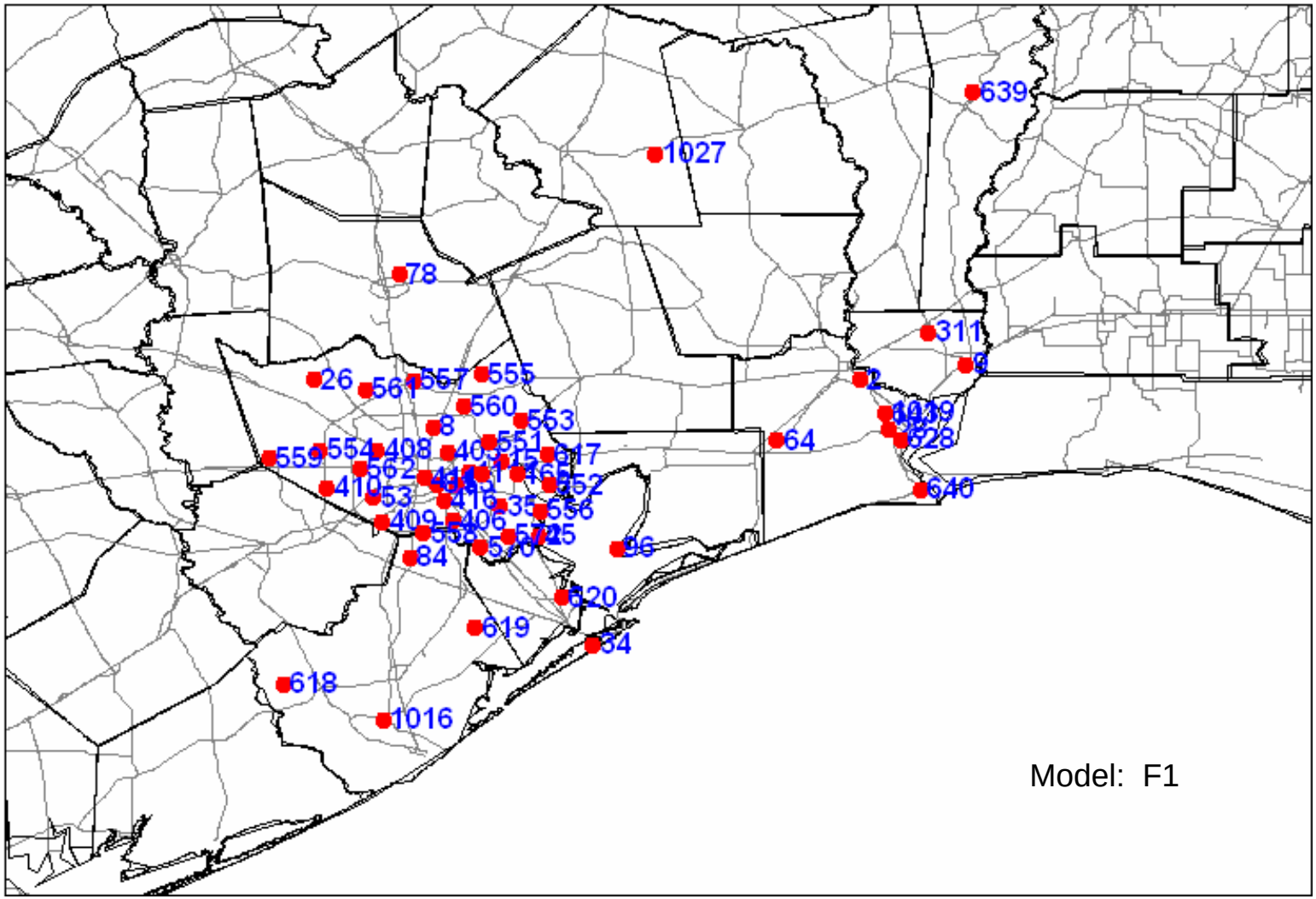
CMAQ (F1 = HGB 4-km vs. F2 = F3 = Extended 4-km (HGB + DFW)

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

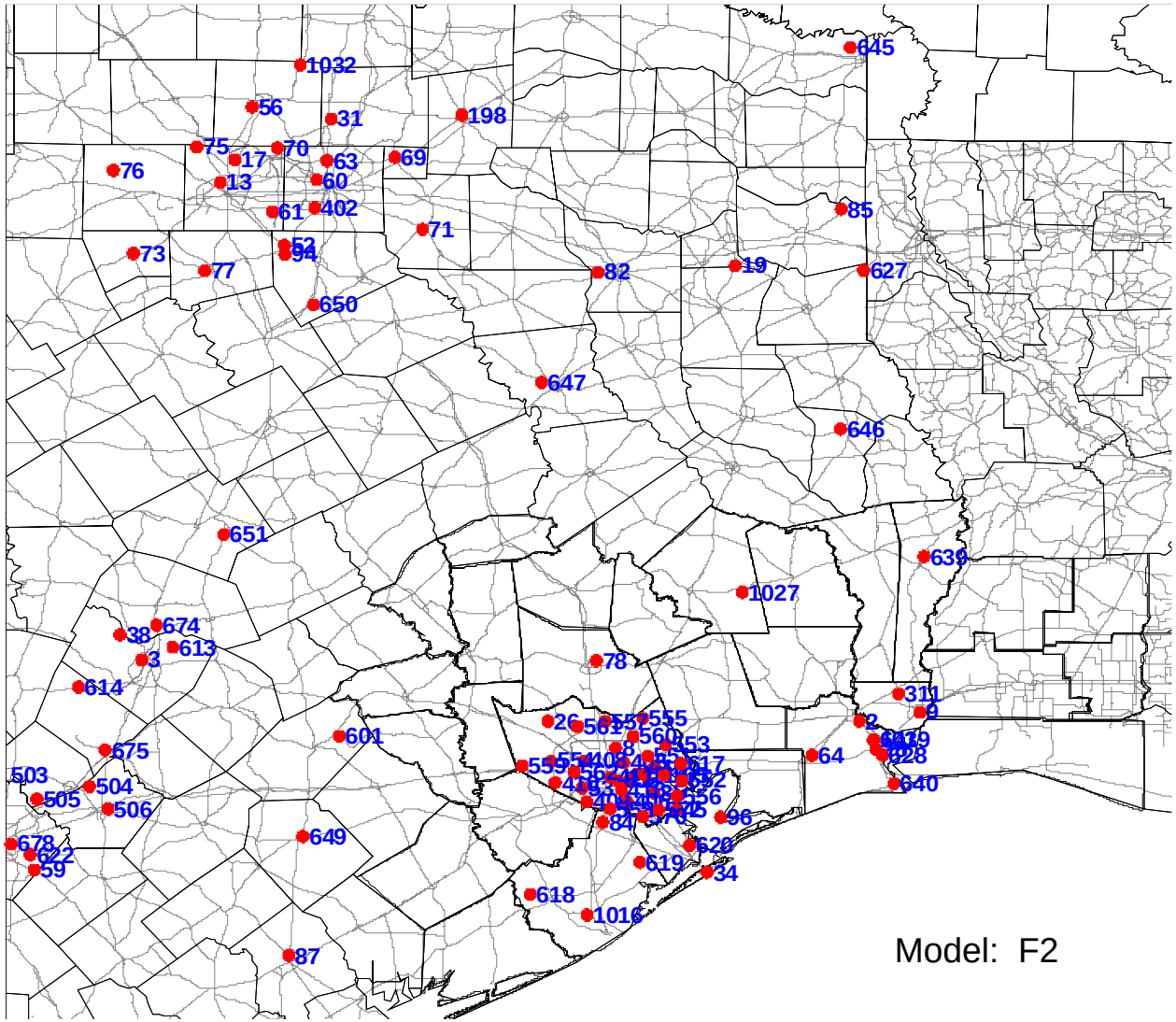
Performance Analysis of 2006 AQF

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

Monitoring site on Houston-Galveston domain F1

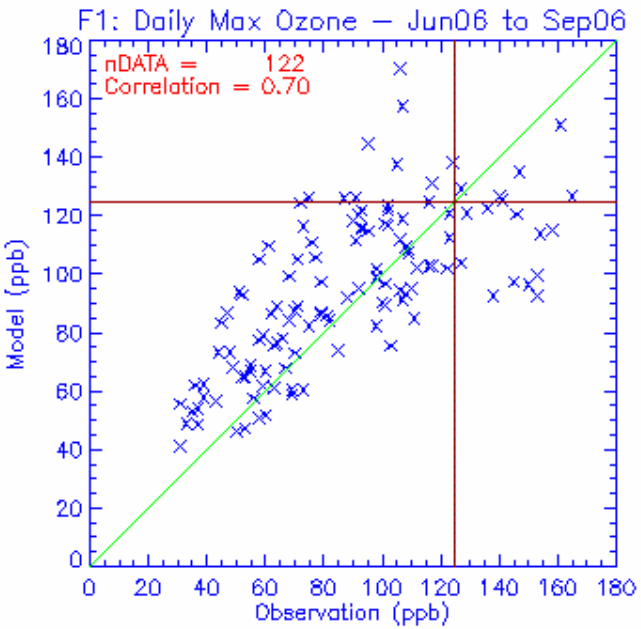


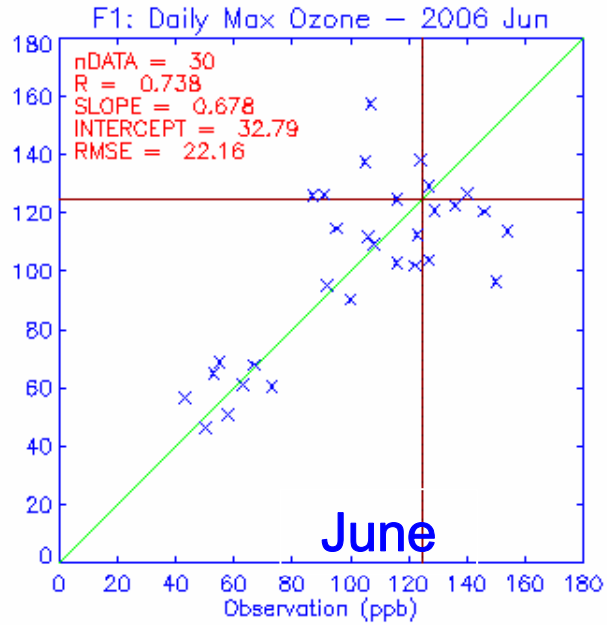
Monitoring sites for Dallas & Houston domain F2

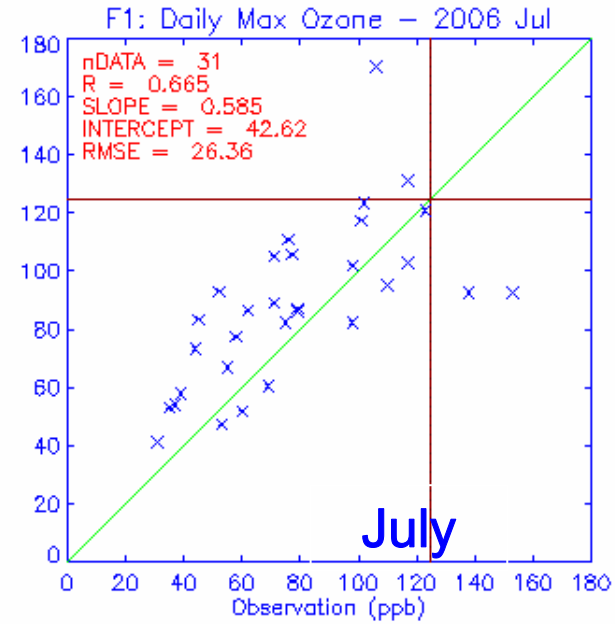


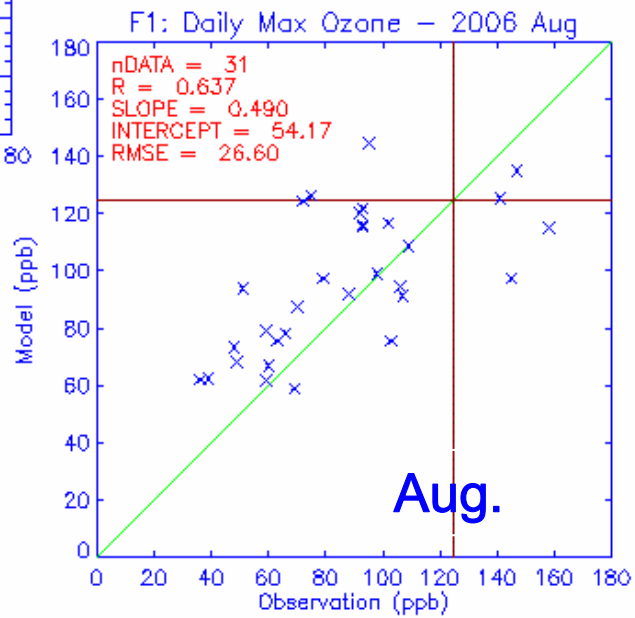
Model: F2

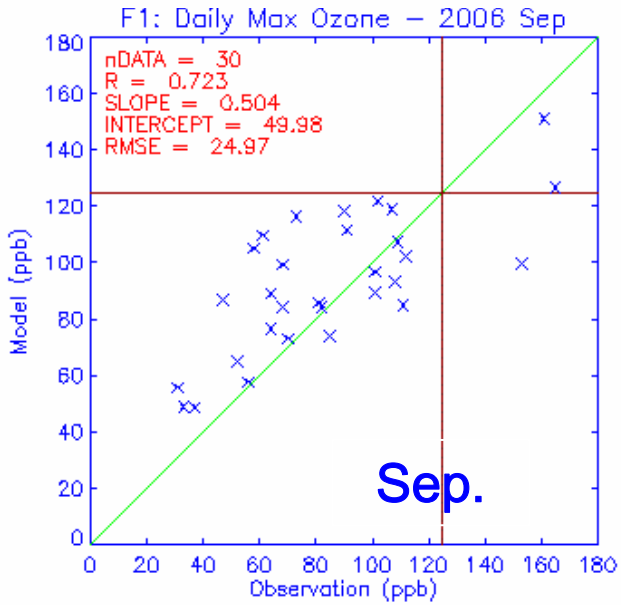
O3 Scatter plot for F1 (daily max)

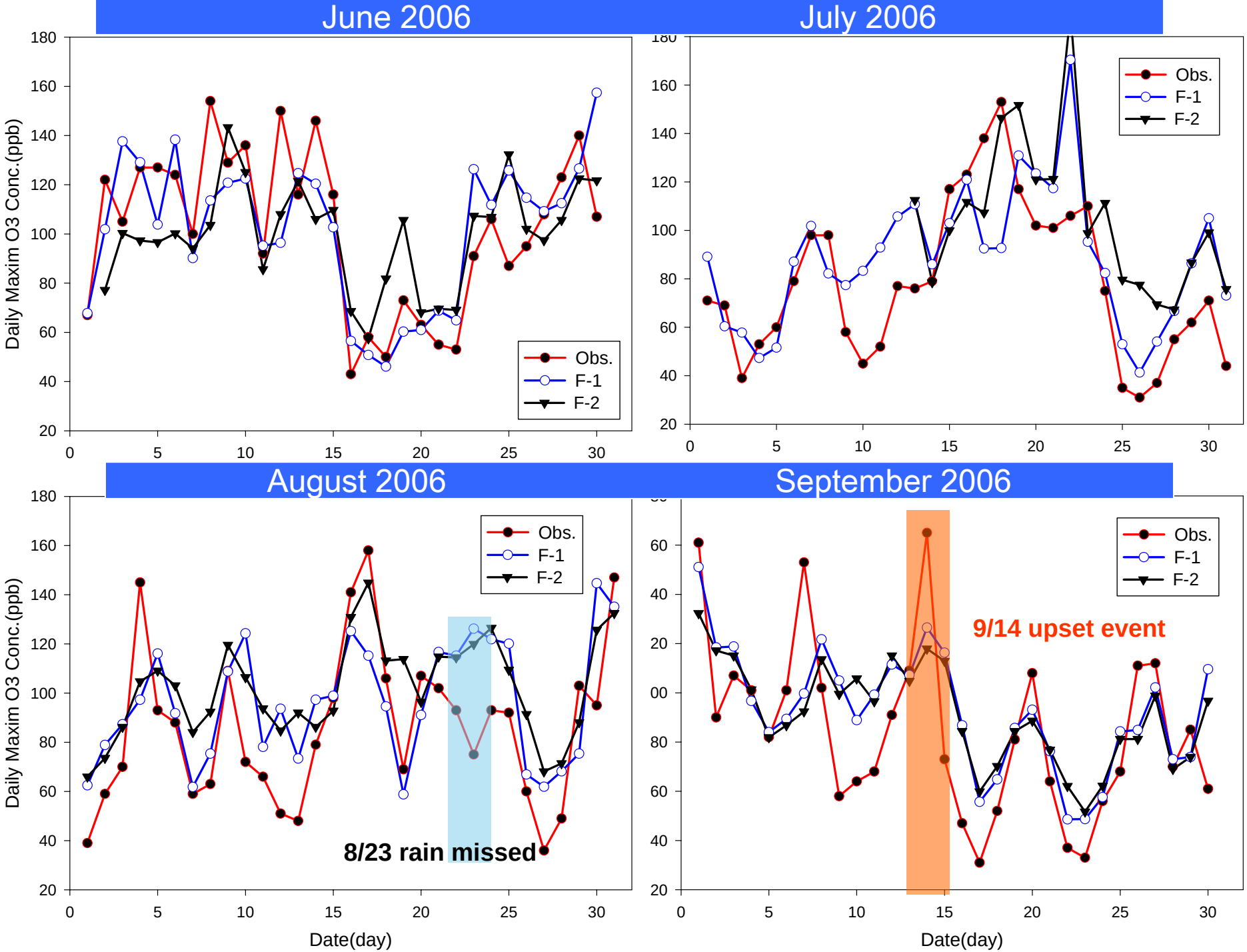




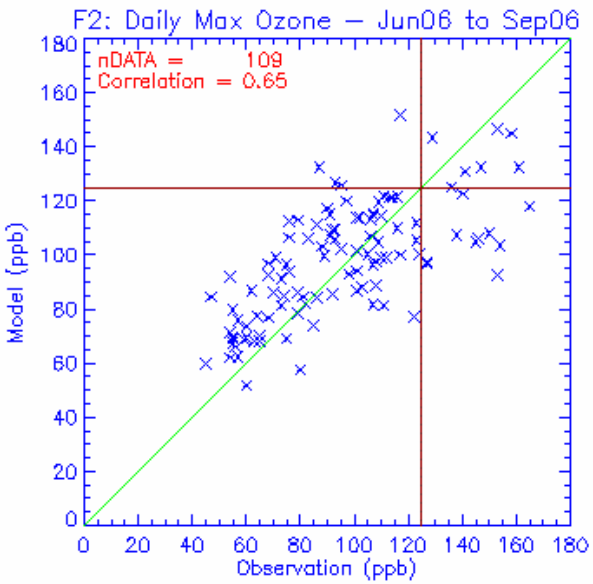


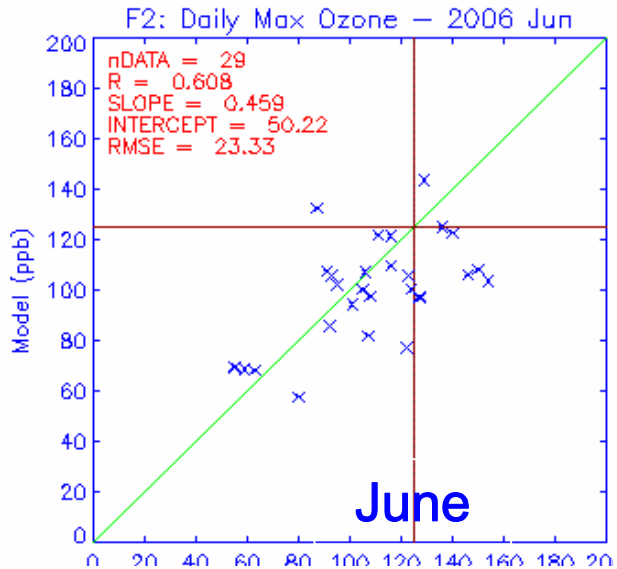


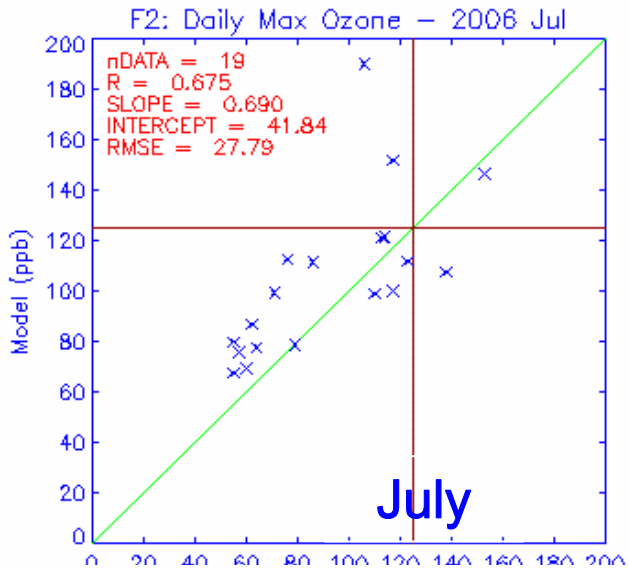


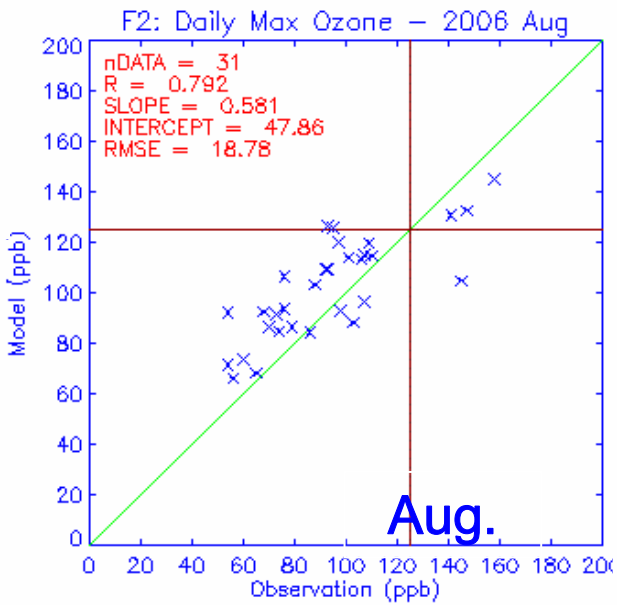

June 2006
July 2006
August 2006
September 2006
Daily Maxim O3 Conc.(ppb)
Date(day)
Obs.
F-1
F-2
8/23 rain missed
9/14 upset event

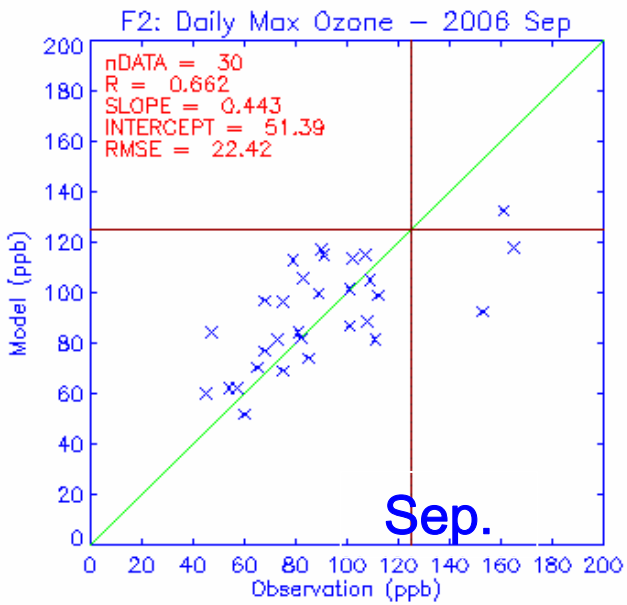
O3 Scatter plot for F2 (daily max)





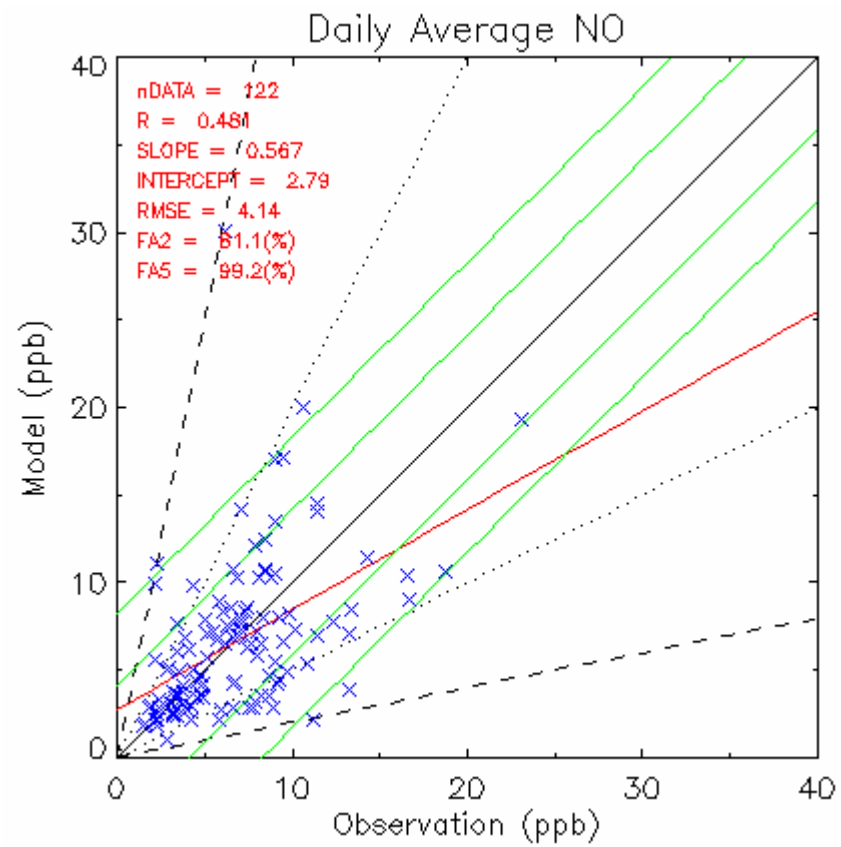




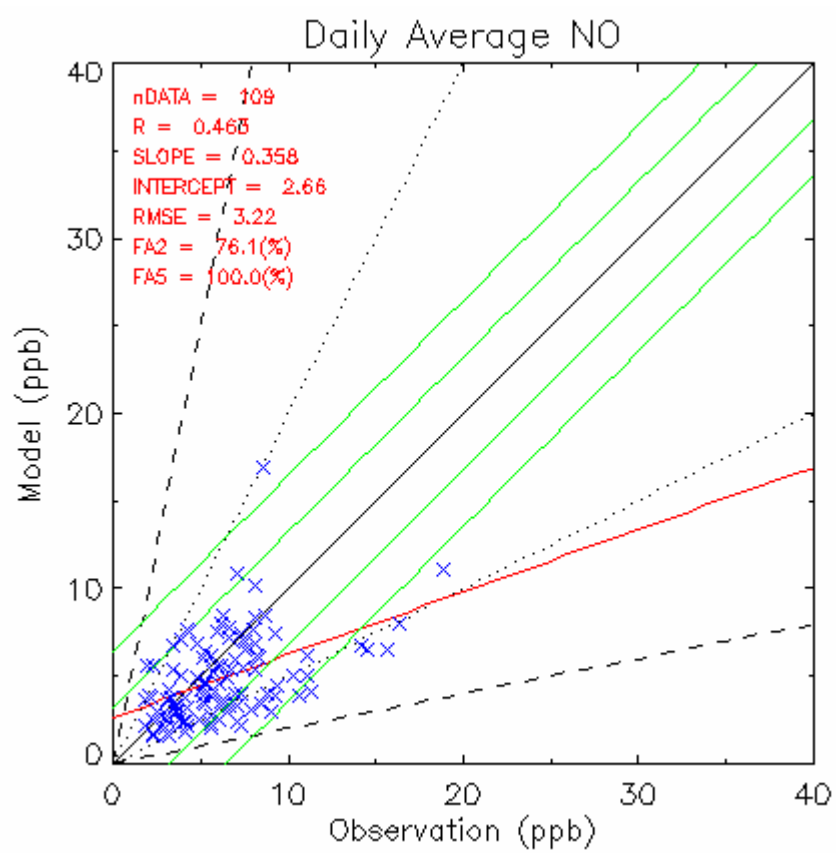


NO concentration differences

F-1



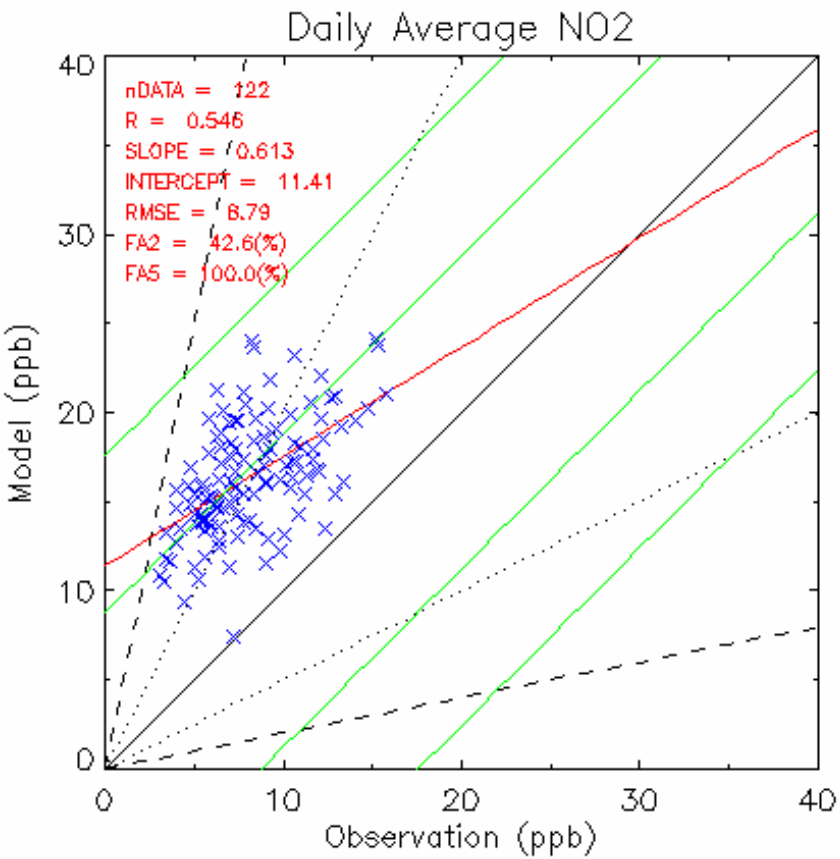
F-2



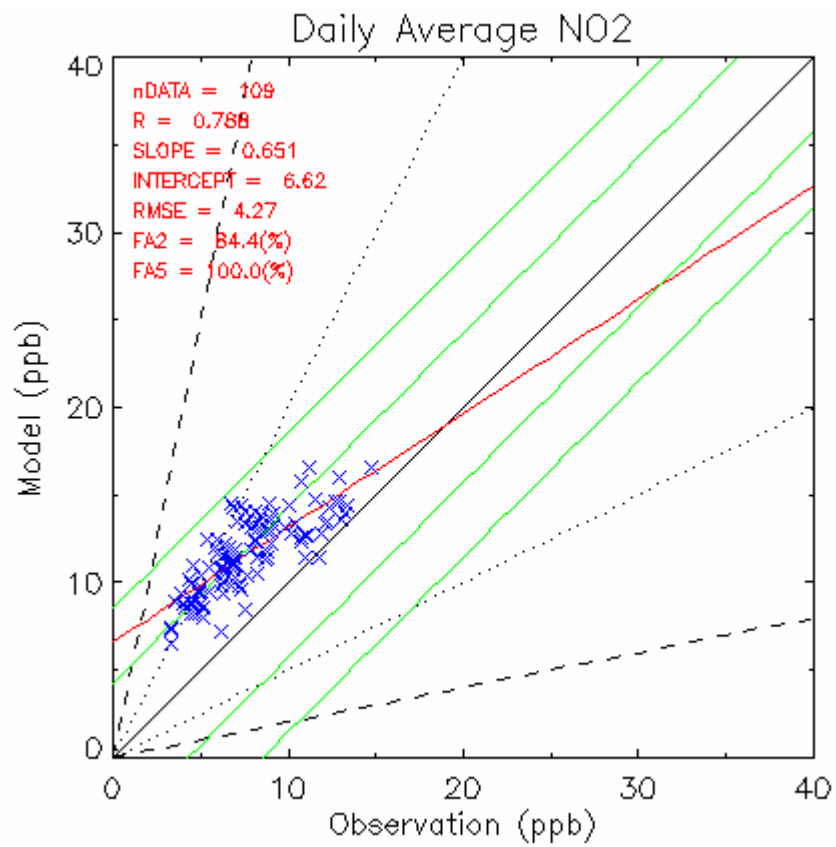
Note: Consider domain differences between F1 & F2

as well as reductions in NOx emissions in F2

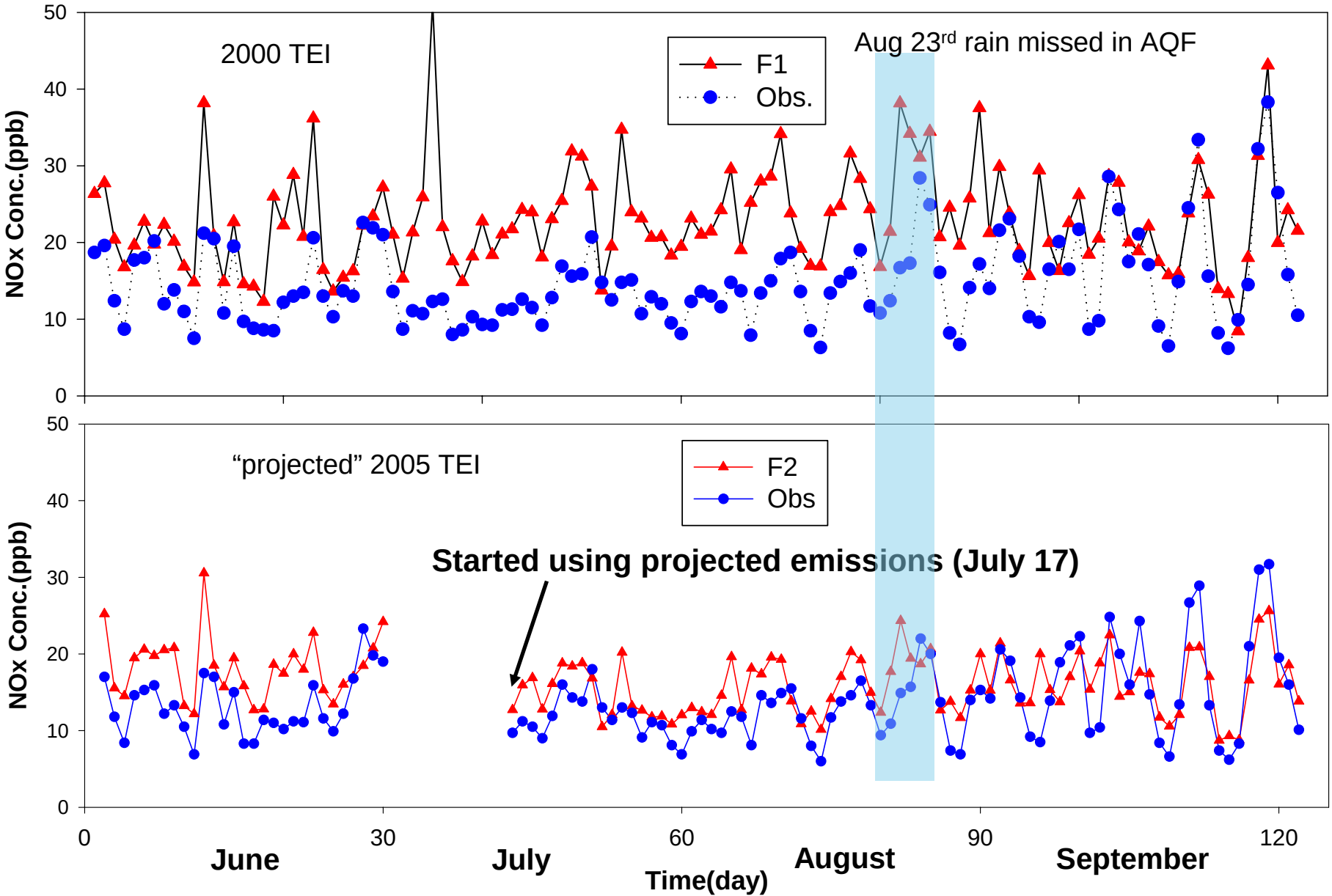
F-1


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

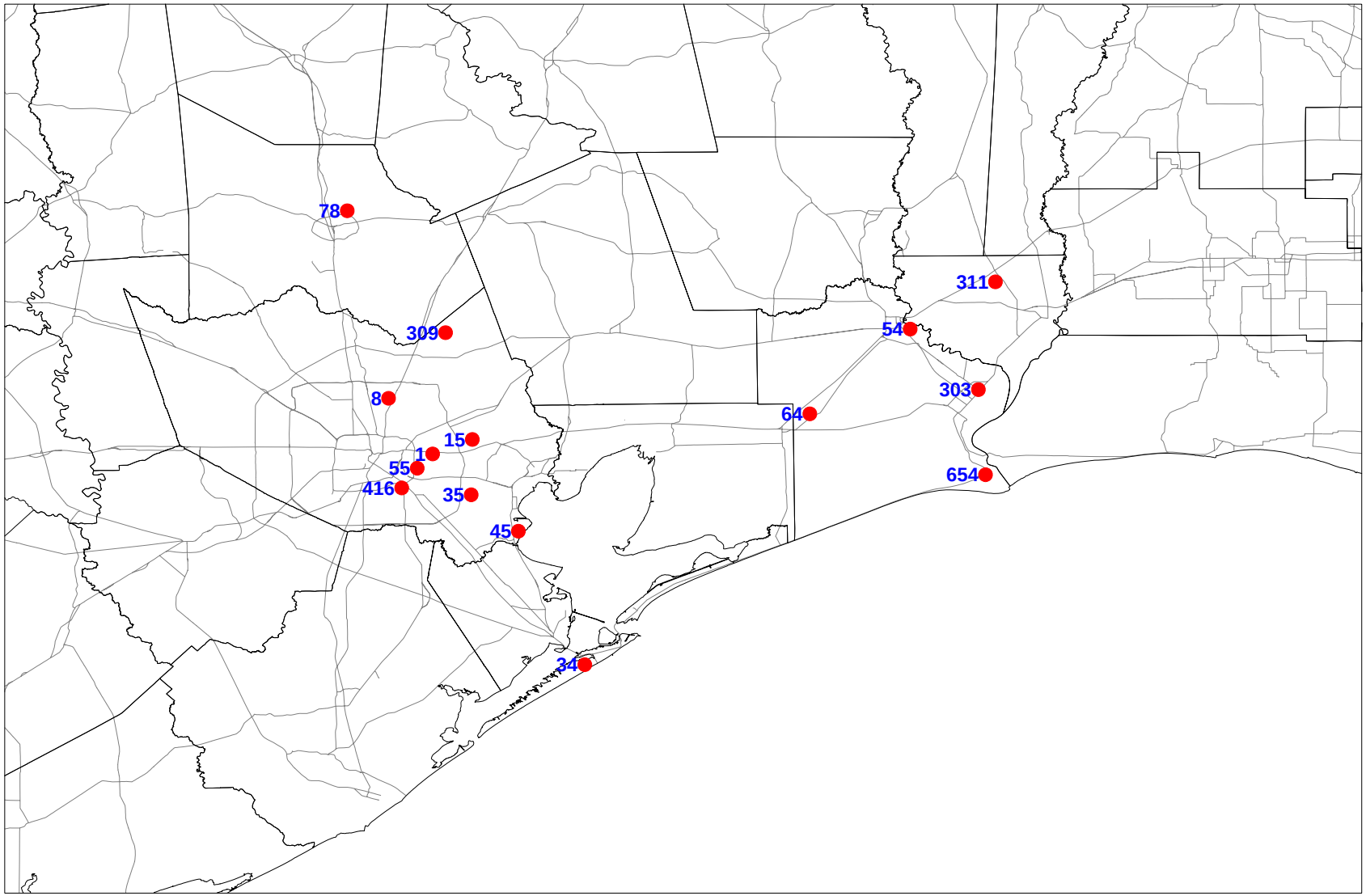

Daily Average NO2
nDATA = 109
R = 0.788
SLOPE = 0.651
INTERCEPT = 6.62
RMSE = 4.27
FA2 = 84.4(%)
FA5 = 100.0(%)
Model (ppb)
Observation (ppb)
0
10
20
30
40

NOx daily mean time series for F1 & F2



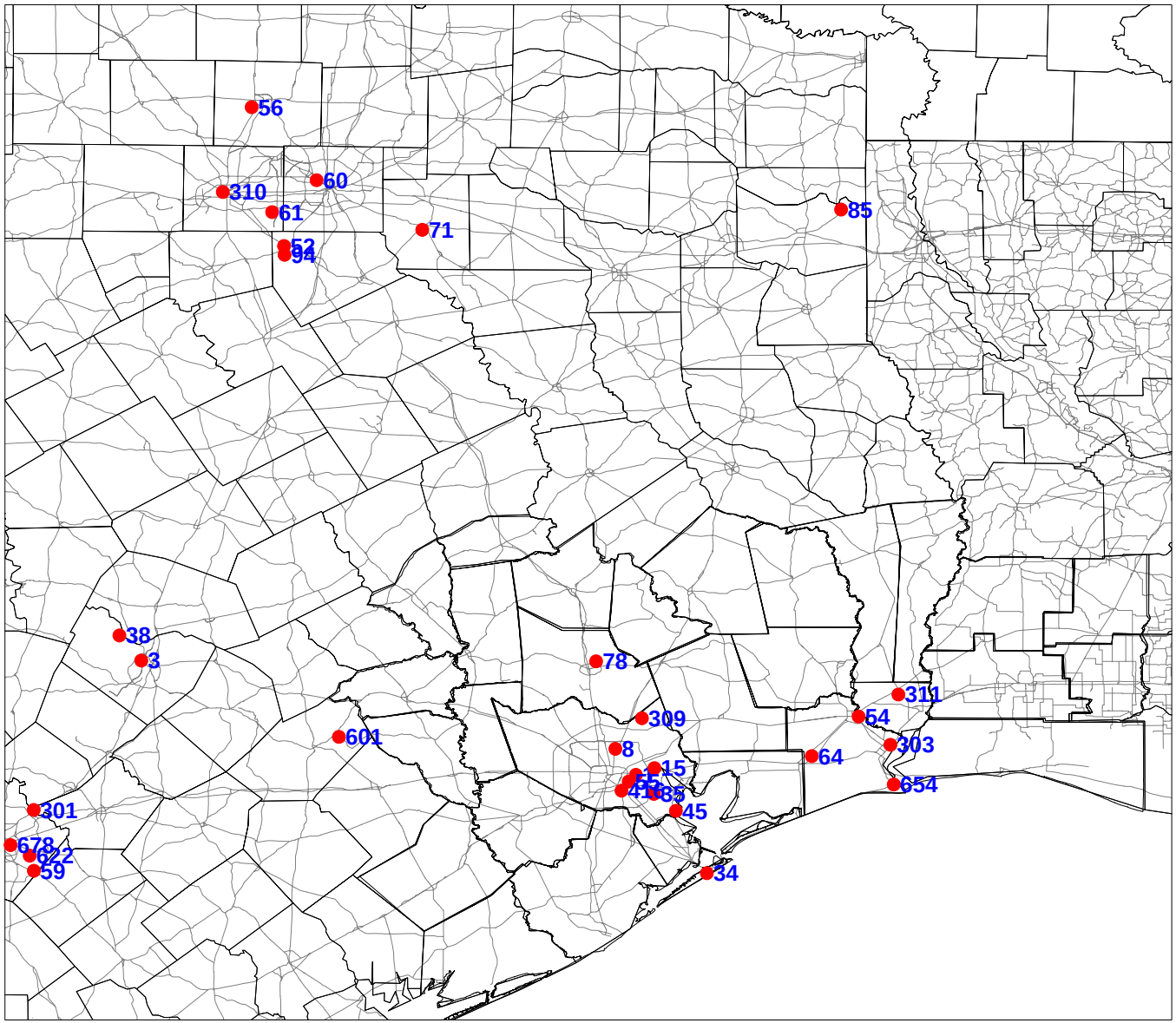
PM2.5 CAMS site location

F-1 : 15 sites

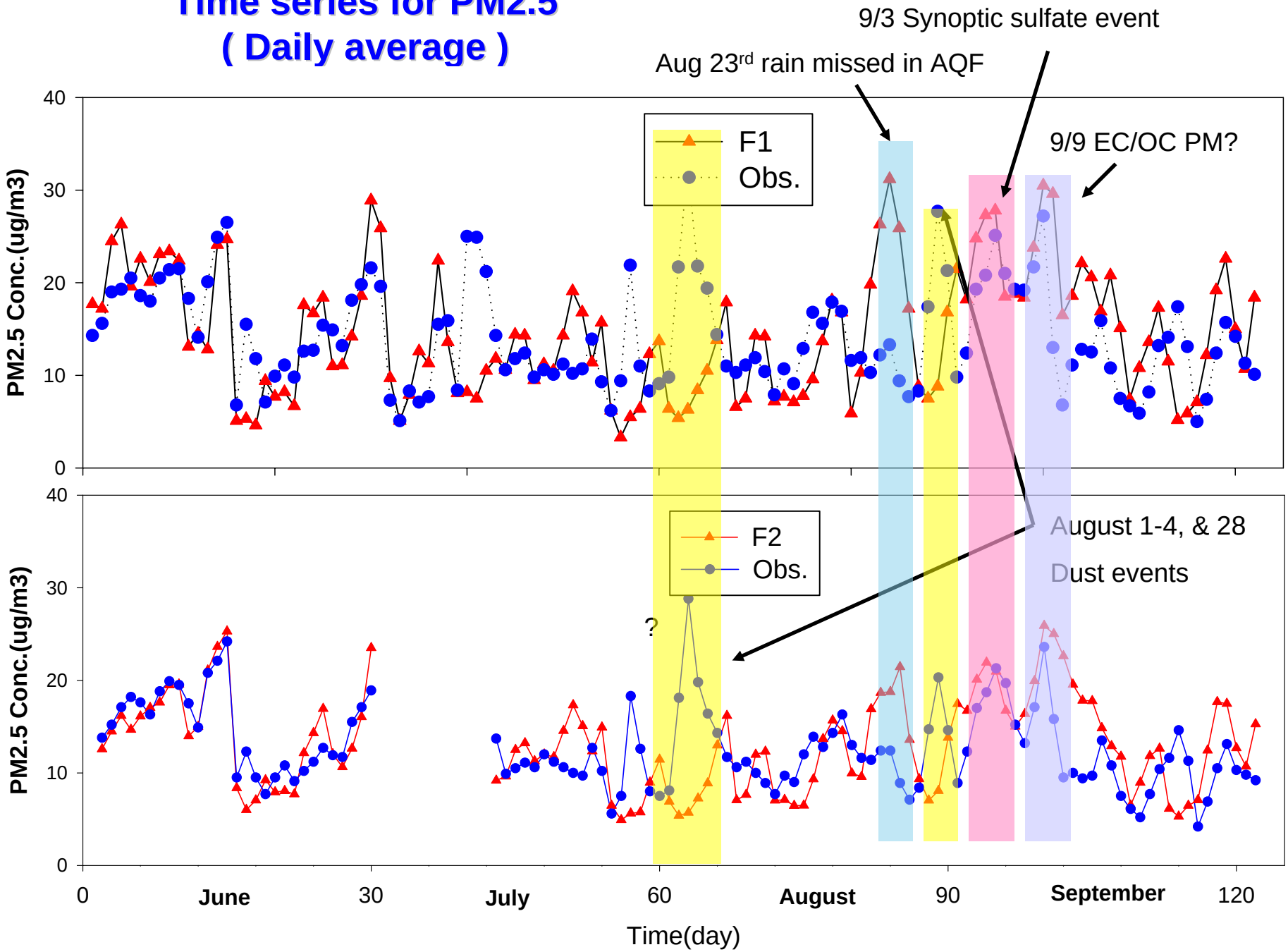


PM2.5 CAMS site location

F-2 : 30 sites

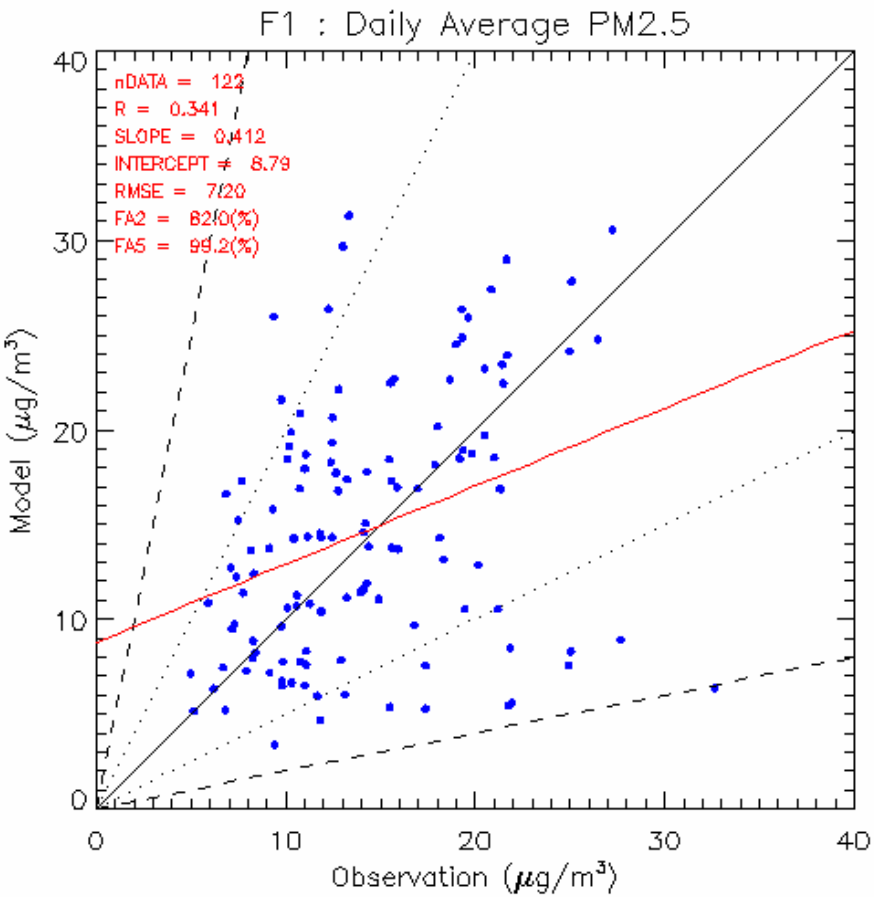


Time series for PM2.5
(Daily average)

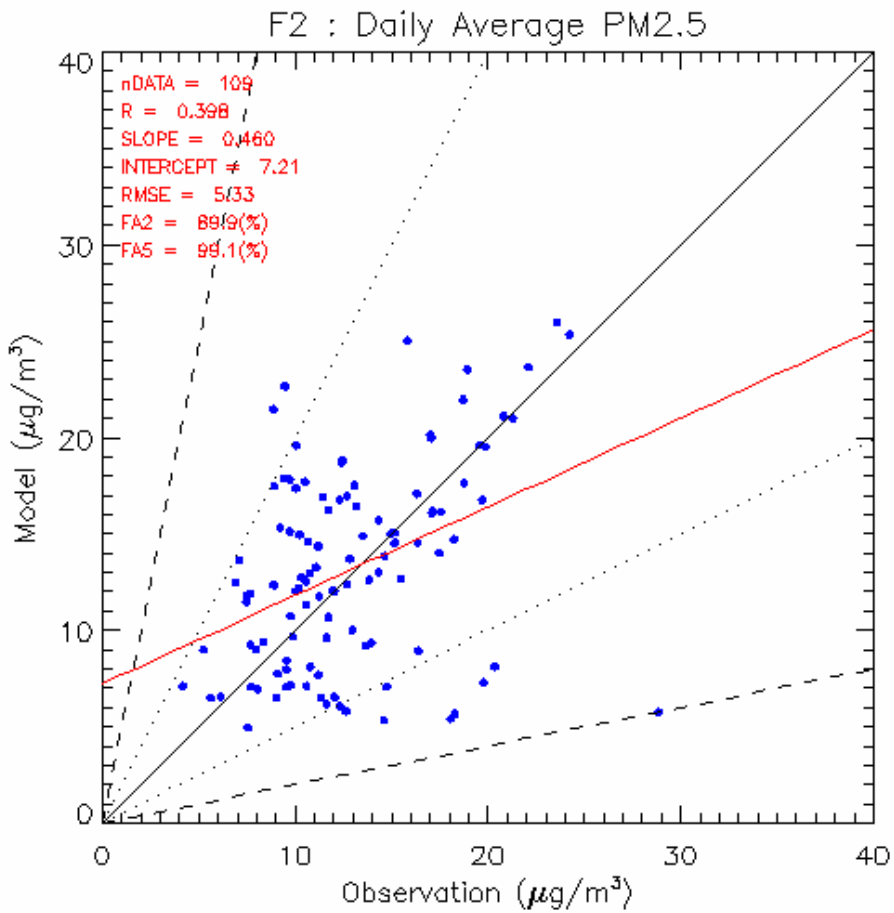


Scatter diagram for PM2.5
(Daily average)

F-1



F-2



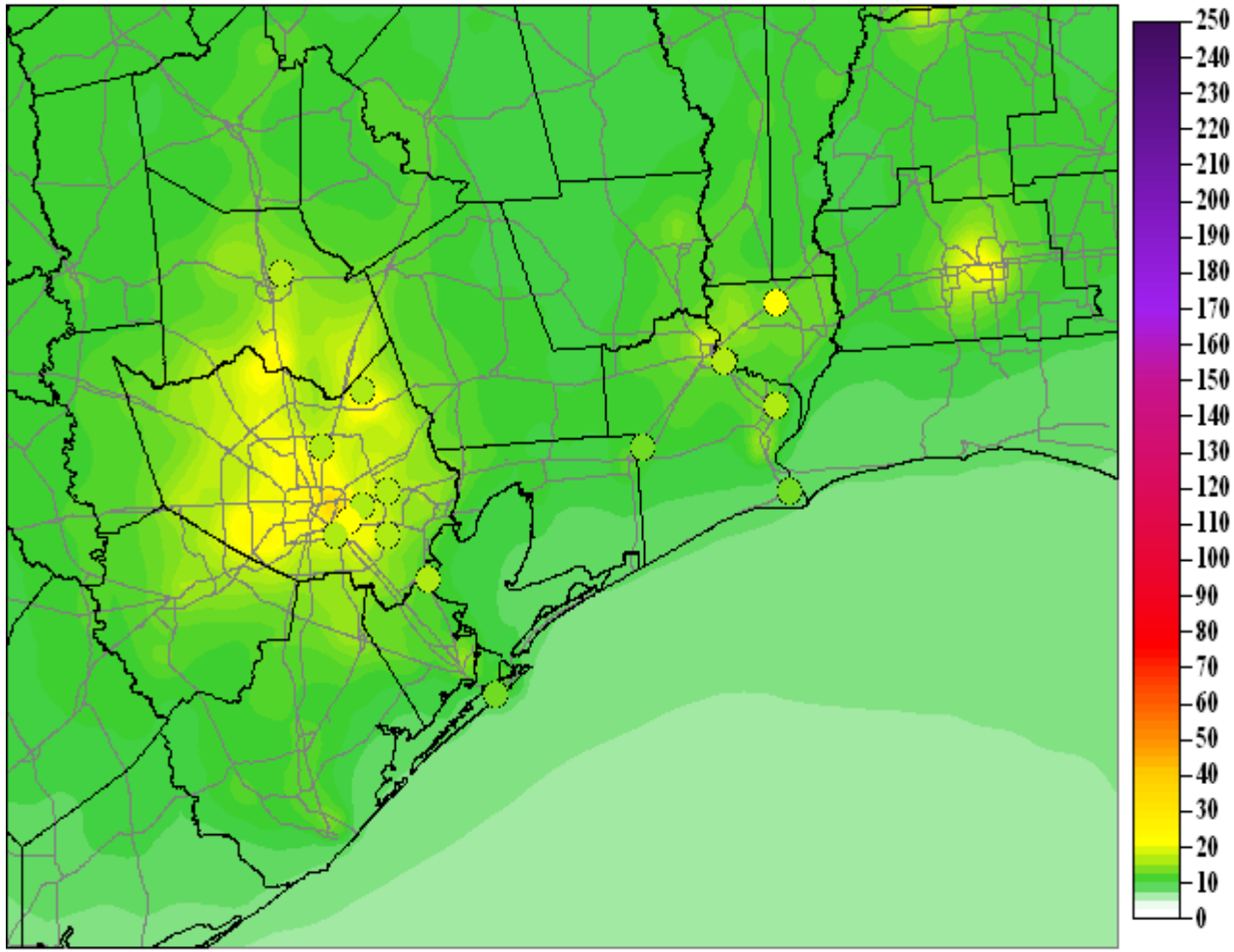
Detailed daily average analysis

F1 Forecasting Results

(Analysis of F2 on-going)

Overall performance of F1: Spatial distribution

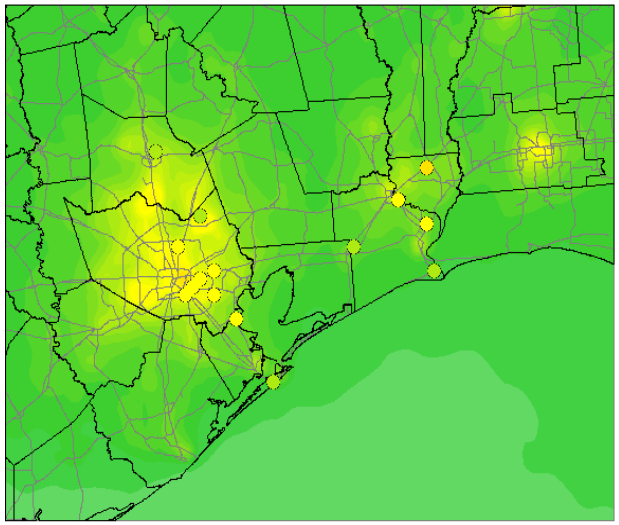
PM2.5 Conc. during TexAQS2



Contour=Model, Cirlce=Obs.

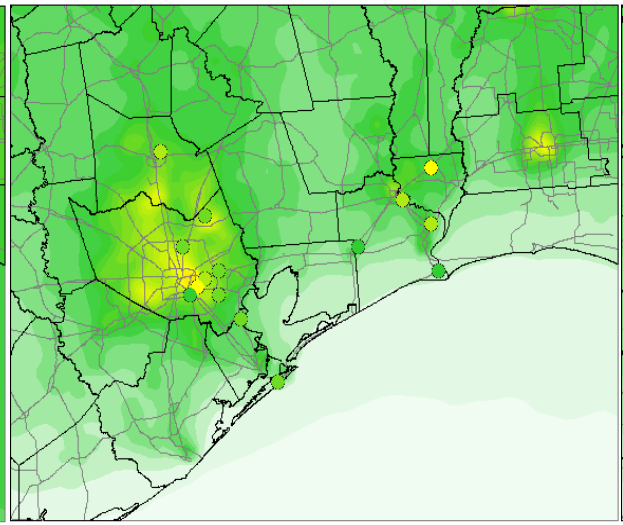
Overall performance of F1 : Spatial distribution

PM2.5 Conc. for Jun.



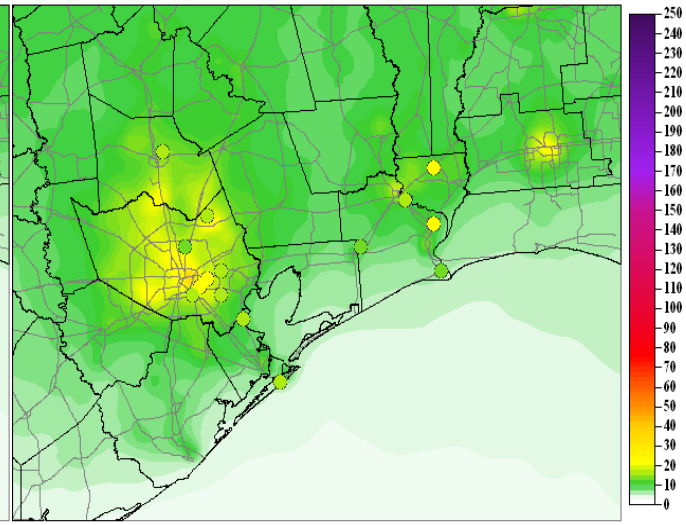
Contour=Model, Cirlce=Obs.

PM2.5 Conc. for Jul.



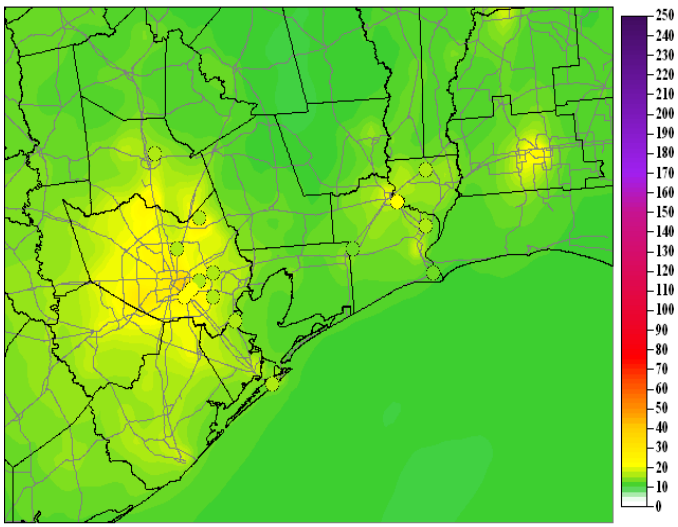
Contour=Model, Cirlce=Obs.

PM2.5 Conc. for Aug.



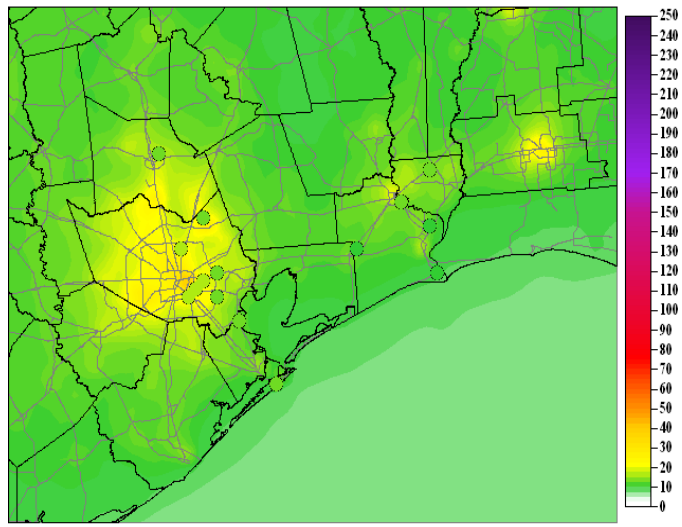
Contour=Model, Cirlce=Obs.

PM2.5 Conc. for Sep.



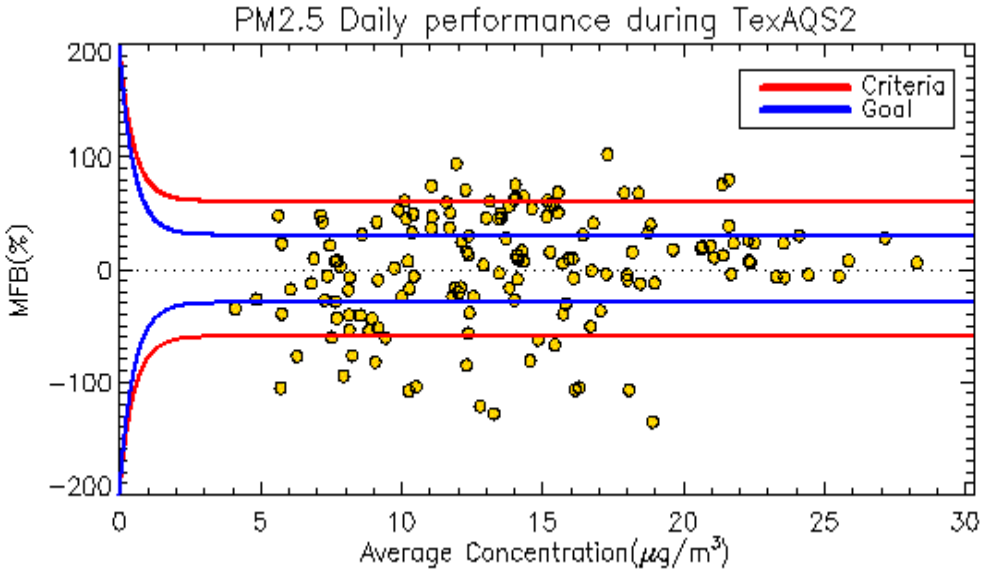
Contour=Model, Cirlce=Obs.

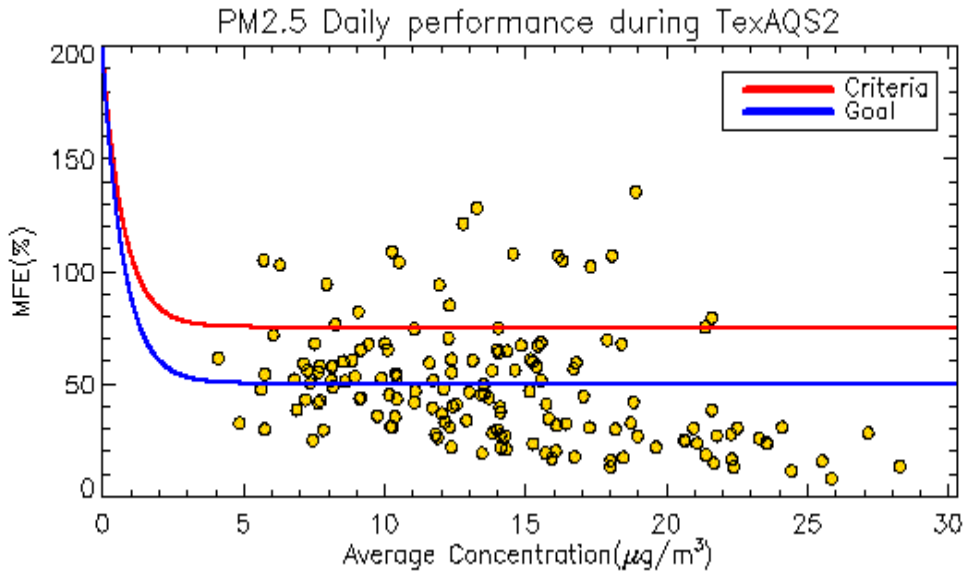
PM2.5 Conc. for Oct.



Contour=Model, Cirlce=Obs.

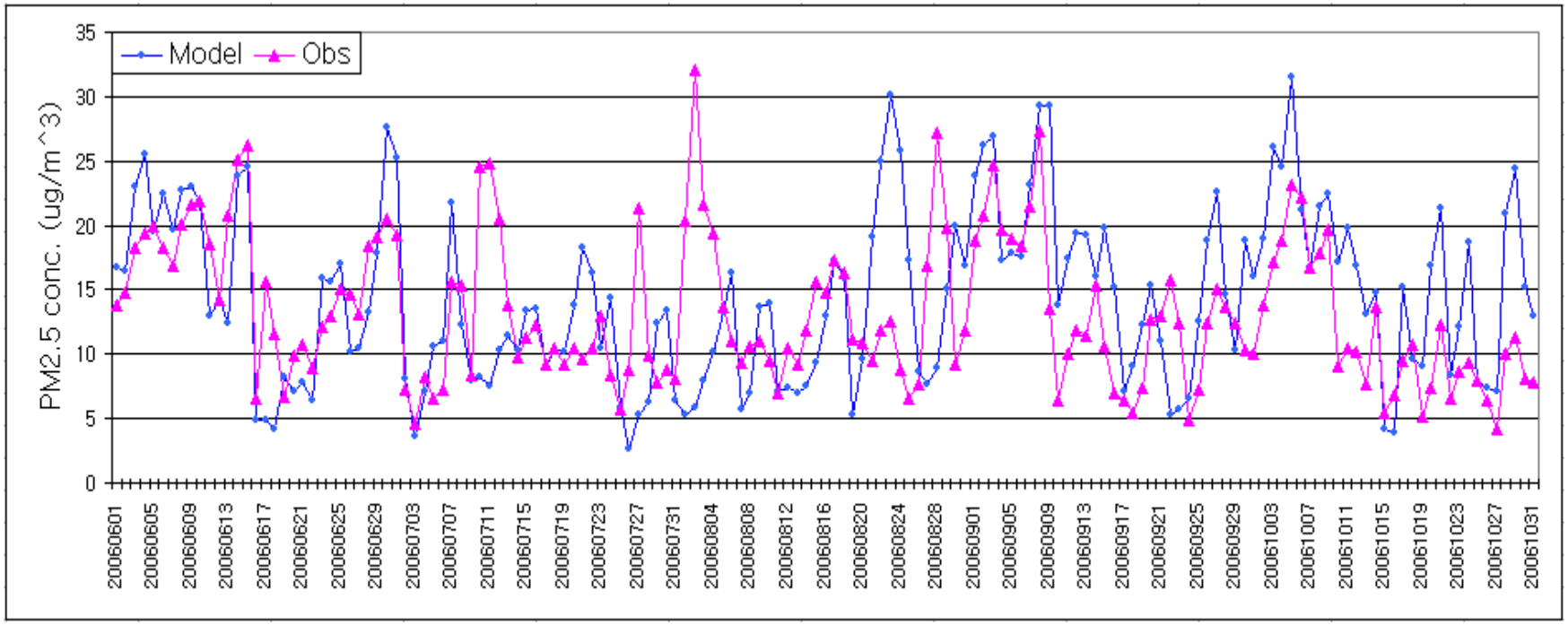
Bugle plot for all daily avg. data





TS plot for daily average data for F1

TS plot for Jun.~Oct. 2006



Number of days for over & under prediction

M-O > 0	M-O > 5	M-O > 10	M-O > 20	M-O < 0	M-O < -5	M-O < -10	M-O < -20
92	44	8	0	61	20	10	1

M-O : Model-Obs.
Unit : days

Daily average analysis for each site: F1

Statistics for daily average of each sites: F1

Statistics for Jun.~Oct. 2006

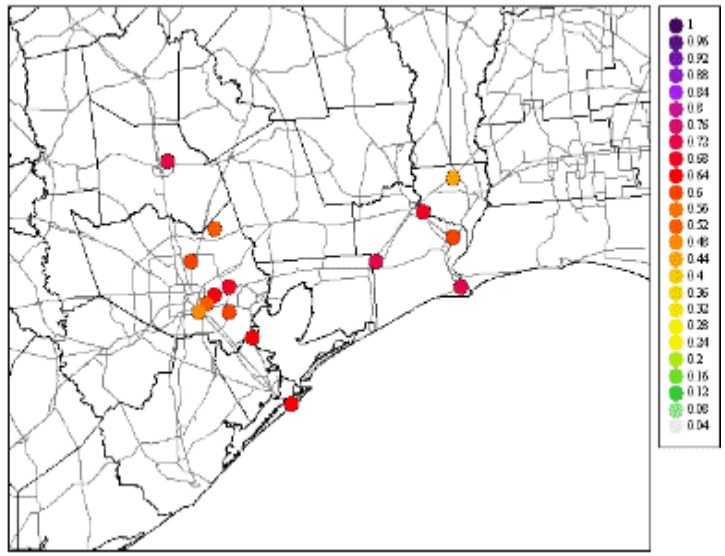
Site ID	nData	Meam_M	Mean_O	Stdev_M	Stdev_O	MB	ME	IOA	R	R^2
78	139	15.25	13.00	6.76	5.91	2.26	5.12	0.69	0.50	0.25
8	120	19.32	13.44	7.78	6.21	5.87	7.26	0.58	0.48	0.23
654	153	7.88	10.35	6.24	6.26	-2.48	4.91	0.69	0.47	0.22
15	152	16.49	13.54	7.32	5.99	2.95	5.89	0.65	0.46	0.21
64	153	10.32	10.35	6.85	6.26	-0.03	4.86	0.70	0.45	0.21
1	150	18.40	14.48	7.95	6.08	3.91	6.90	0.61	0.41	0.17
35	147	17.68	12.92	8.36	6.13	4.76	7.74	0.59	0.41	0.16
54	152	12.43	14.51	6.93	5.90	-2.08	5.39	0.65	0.40	0.16
34	153	9.54	11.28	6.87	5.87	-1.74	5.23	0.63	0.36	0.13
309	153	19.18	12.48	7.96	5.41	6.70	8.10	0.49	0.36	0.13
45	134	10.91	12.24	6.44	6.43	-1.33	5.30	0.63	0.35	0.12
311	135	12.12	16.95	6.19	14.87	-4.84	8.84	0.43	0.30	0.09
303	120	11.17	14.08	6.42	6.53	-2.91	5.76	0.58	0.30	0.09
55	153	19.08	17.24	8.65	6.59	1.84	7.44	0.52	0.22	0.05
416	46	18.36	13.90	8.94	6.87	4.46	7.59	0.46	0.15	0.02
Avg.	-	**14.54**	**13.38**	**7.31**	**6.75**	**1.16**	**6.42**	**0.59**	**0.37**	**0.15**

<Sorted by R>

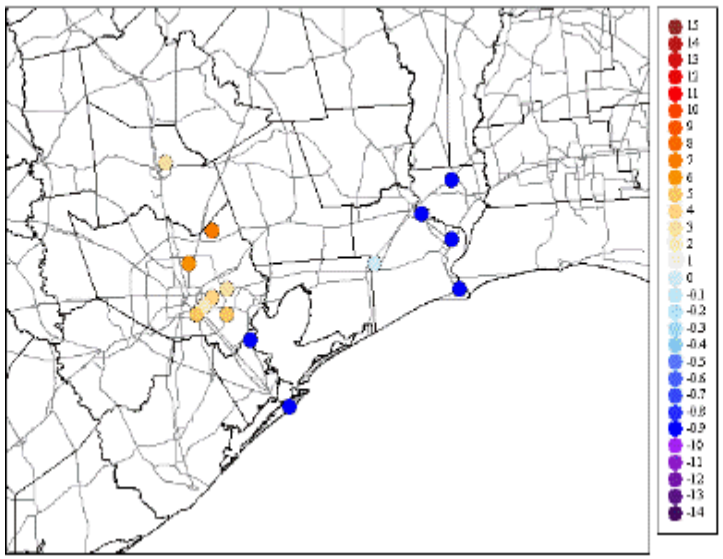
Spatial distribution of stats. Index during TexAQS-II: F1

Correlation Coefficient(R) during TexAQS2

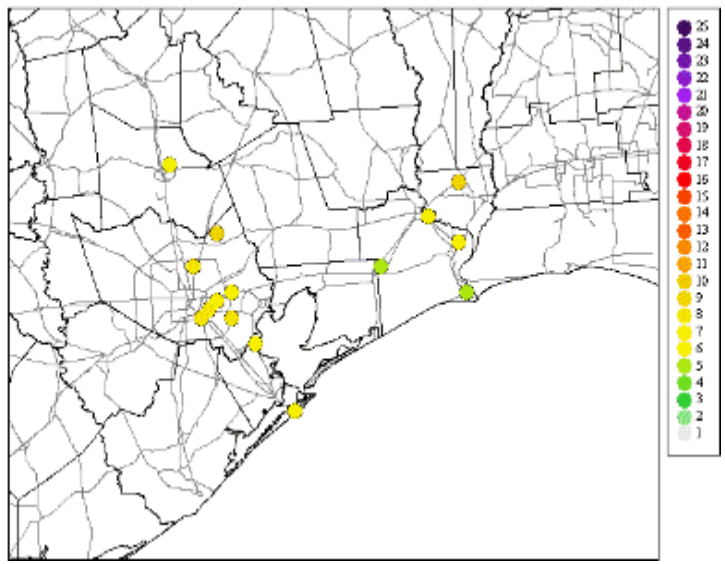
Index of Agreement(IOA) during TexAQS2



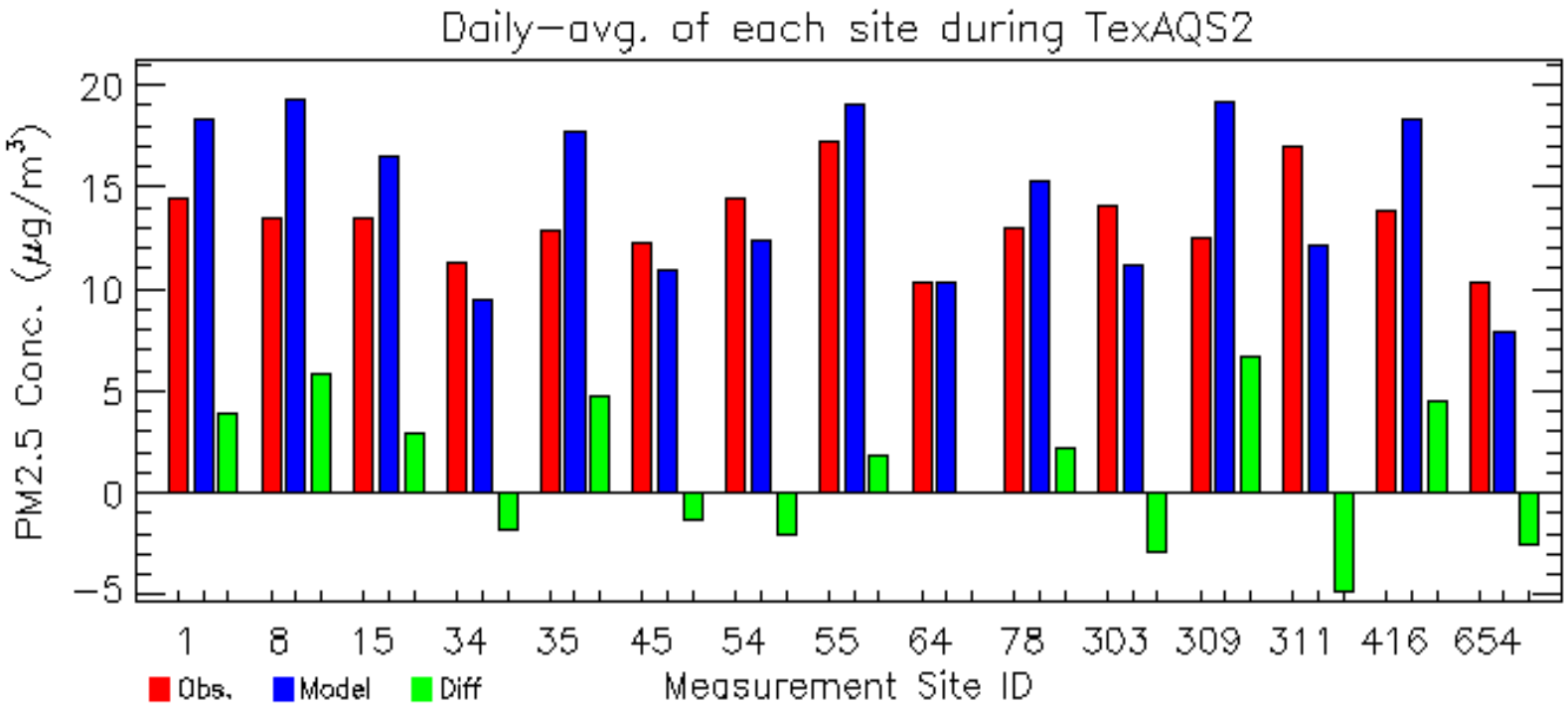
Mean Bias(MB) during TexAQS2



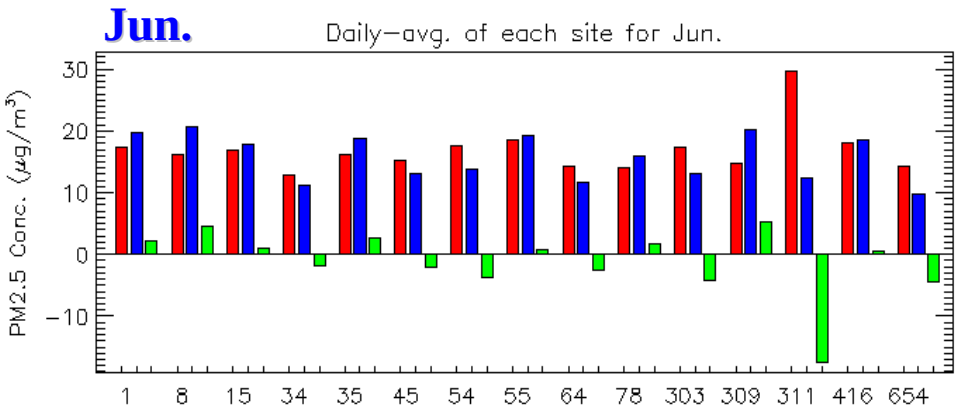
Mean Error(ME) during TexAQS2

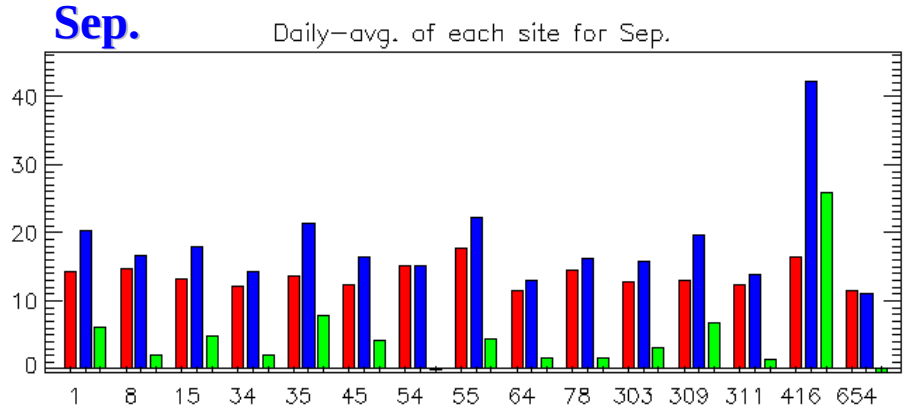


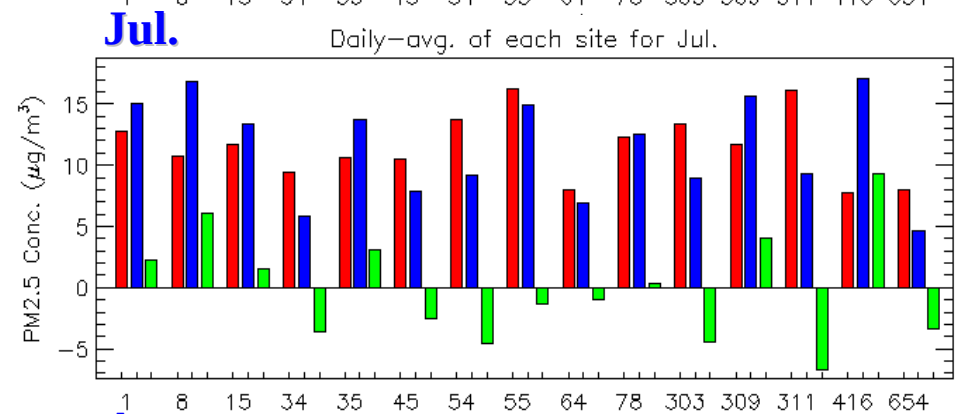
Bar chart for daily average of each sites: F1

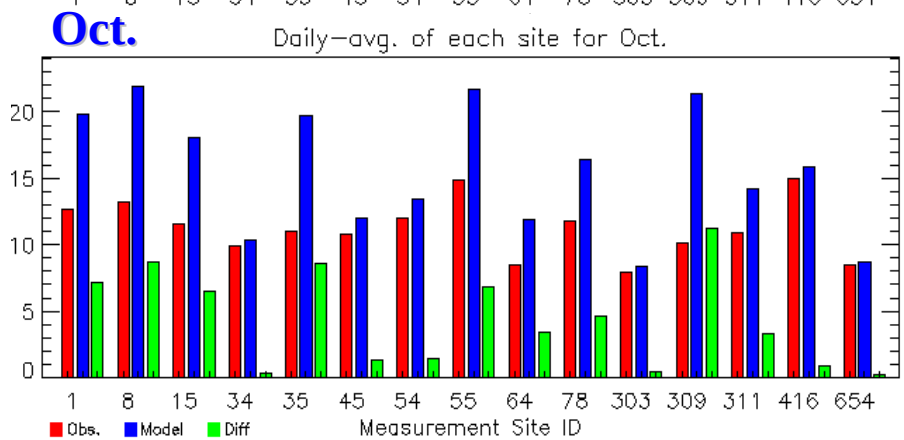


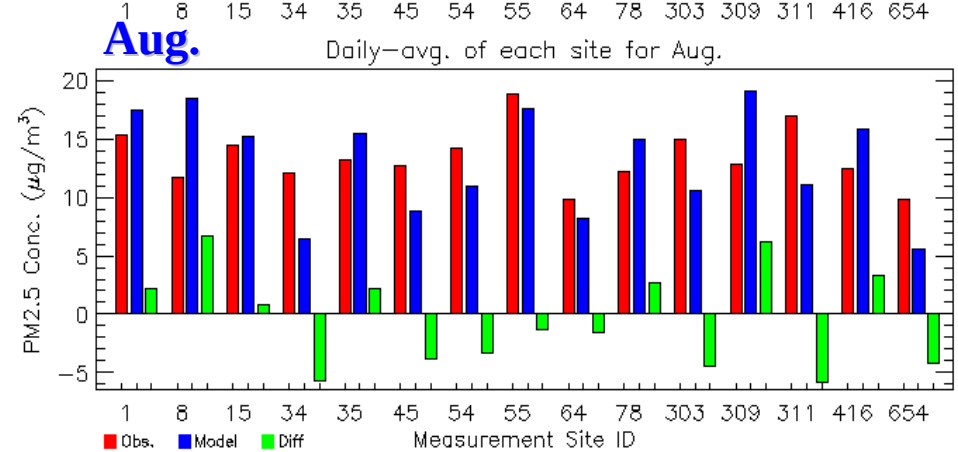
Bar chart for daily average of each sites: F1











Summary of Forecasting Difficulties

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

2. Improve meteorological characterizations
   - Wind speed (seasonal and day & night bias?)
   - PBL height (seasonal and day & night bias?)

3. Must evaluate predictability of precipitation (met.) and upset emissions event, as well as long-range transport cases!

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

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

6. Need to evaluate/improve PM precursor emissions

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