1. Comparison CB-4 and SAPRC mechanisms
2. Improvement of Initial Condition
3. Improvement of meteorological simulations

Daewon W. Byun

S.T. Kim, B. Czader, F. Ngan, D. Lee, X. Li

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

1. CB-4 & SAPRC Comparison

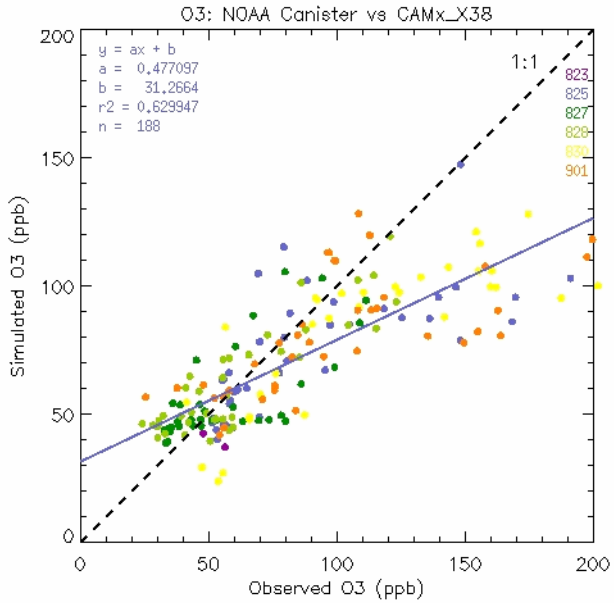
- 2000 TexAQS Episode with TEI2000/imputed HRVOC

- 2006 TexAQS-2 Sept 6-8 Episode with TEI2000/imputed HRVOC
- 2006 TexAQS-2 Sept 6-8 Episode with 2005 projected EI

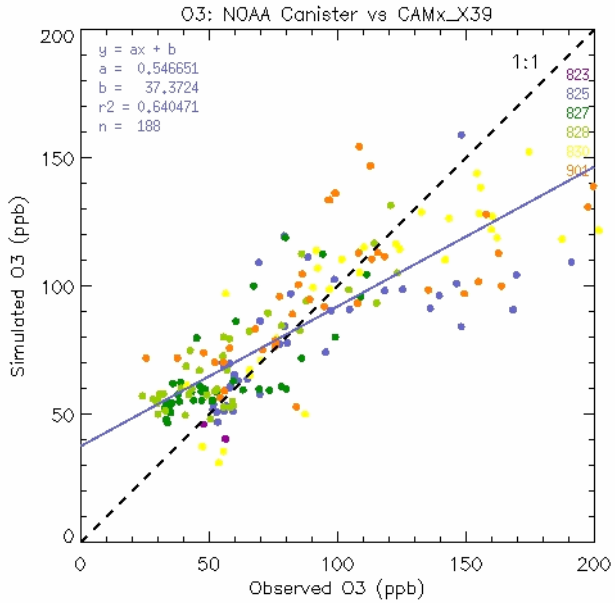
TexAQS 2000 Episode

NOAA Aircraft Canister

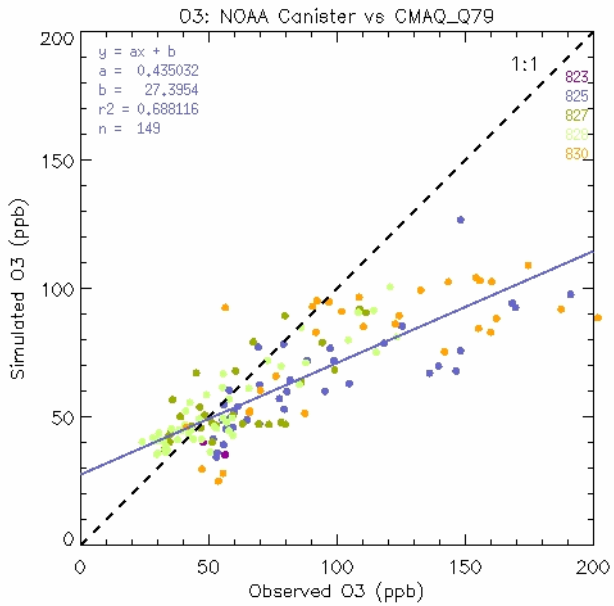
(a) CAMx CB-4



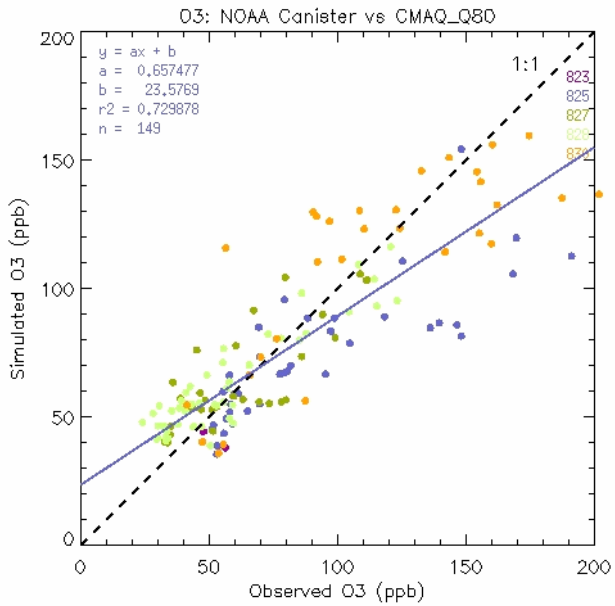
(b) CAMx SAPRC99



(c) CMAQ CB-4



(d) CMAQ SAPRC99



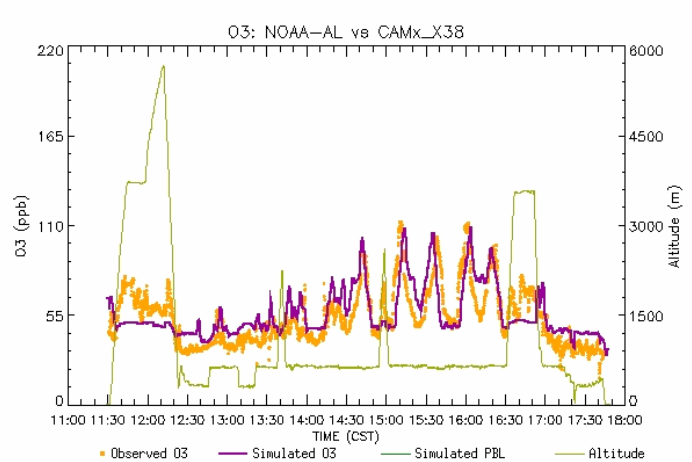
Improvement of high O3 predicted by SAPRC more pronounced with CMAQ

TexAQS 2000 Episode

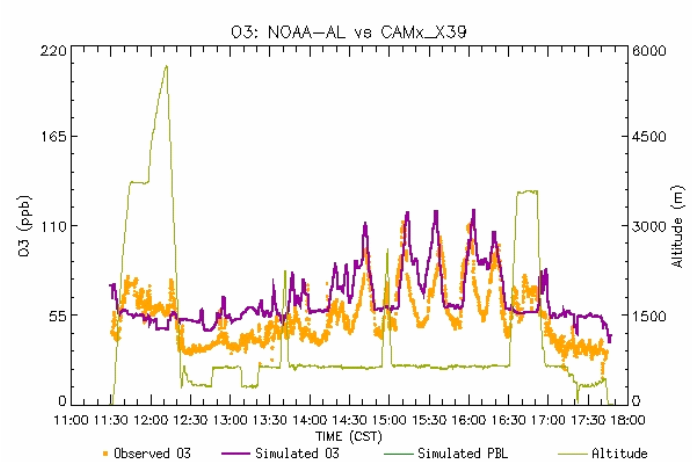
NOAA Aircraft

Ozone

(a) CAMx CB-4

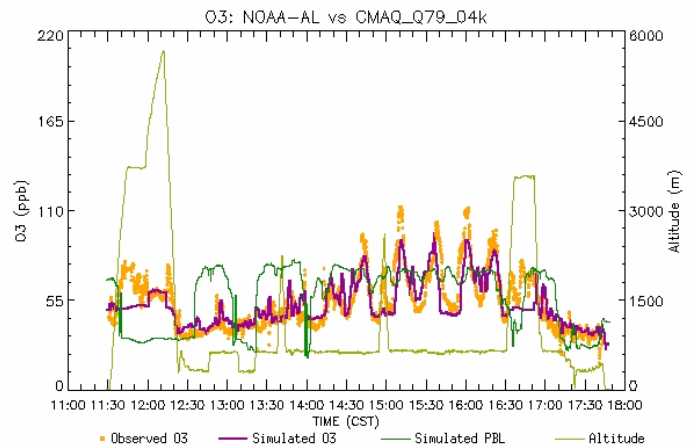


(b) CAMx SAPRC99

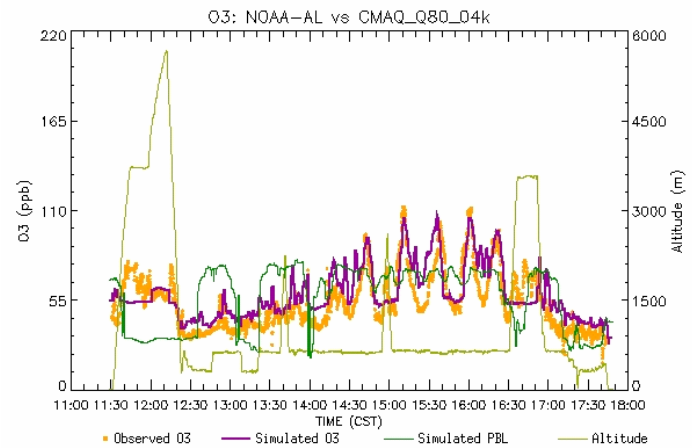


CAMx with CB-4 well simulated O3 peak but overpredicted with SAPRC

(c) CMAQ CB-4



(d) CMAQ SAPRC99



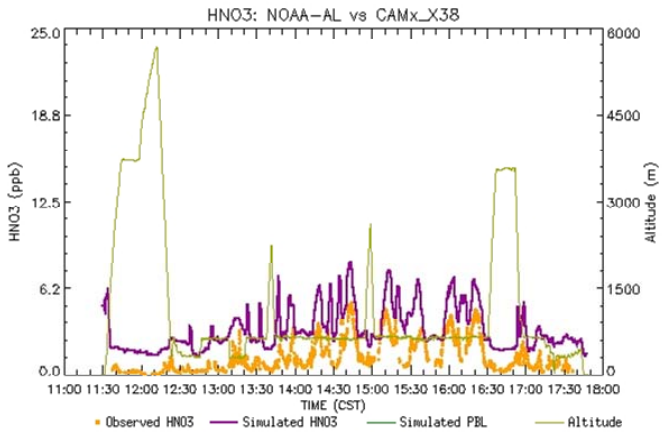
CMAQ with CB-4 underestimated O3 peak but well predicted with SAPRC

TexAQS 2000 Episode

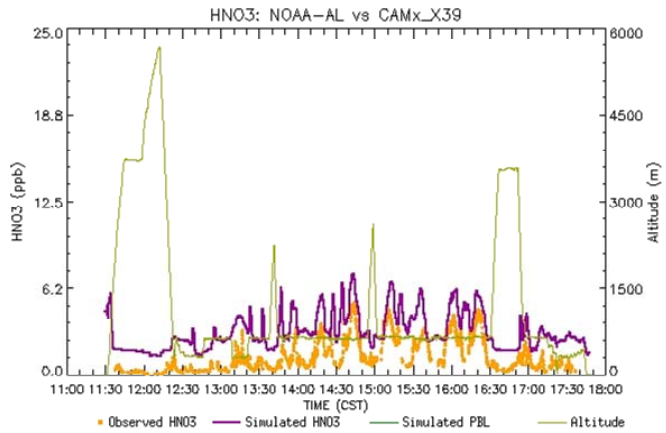
NOAA Aircraft

HNO3

(a) CAMx CB-4

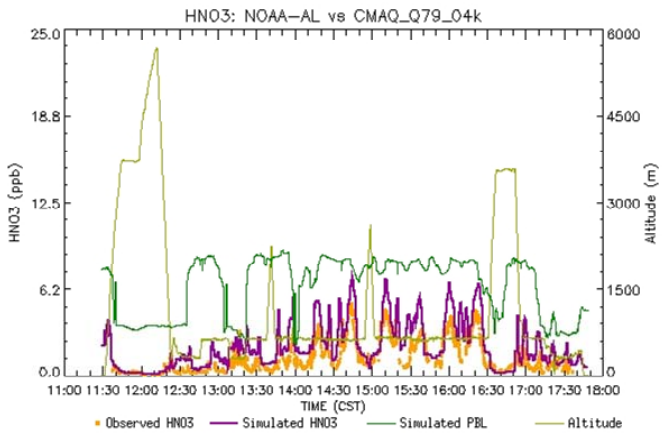


(b) CAMx SAPRC99

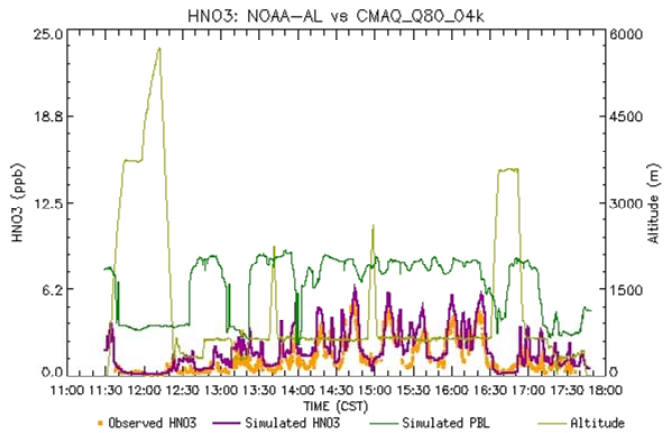


CAMx with CB-4 and SAPRC both overpredicted HNO3, including the background

(c) CMAQ CB-4



(d) CMAQ SAPRC99



CMAQ with CB-4 overpredicted HNO3 slightly, but SAPRC compared well with obs.

2006 simulations: AQF - F2, 4-km resolution

To compare CMAQ simulations between CB-4 and SAPRC99 for projected EI (lower NOx) at 2005 level

CMAQ4.4, CB4, Projected EI for 2005

CMAQ4.4, SAPRC, Projected EI for 2005

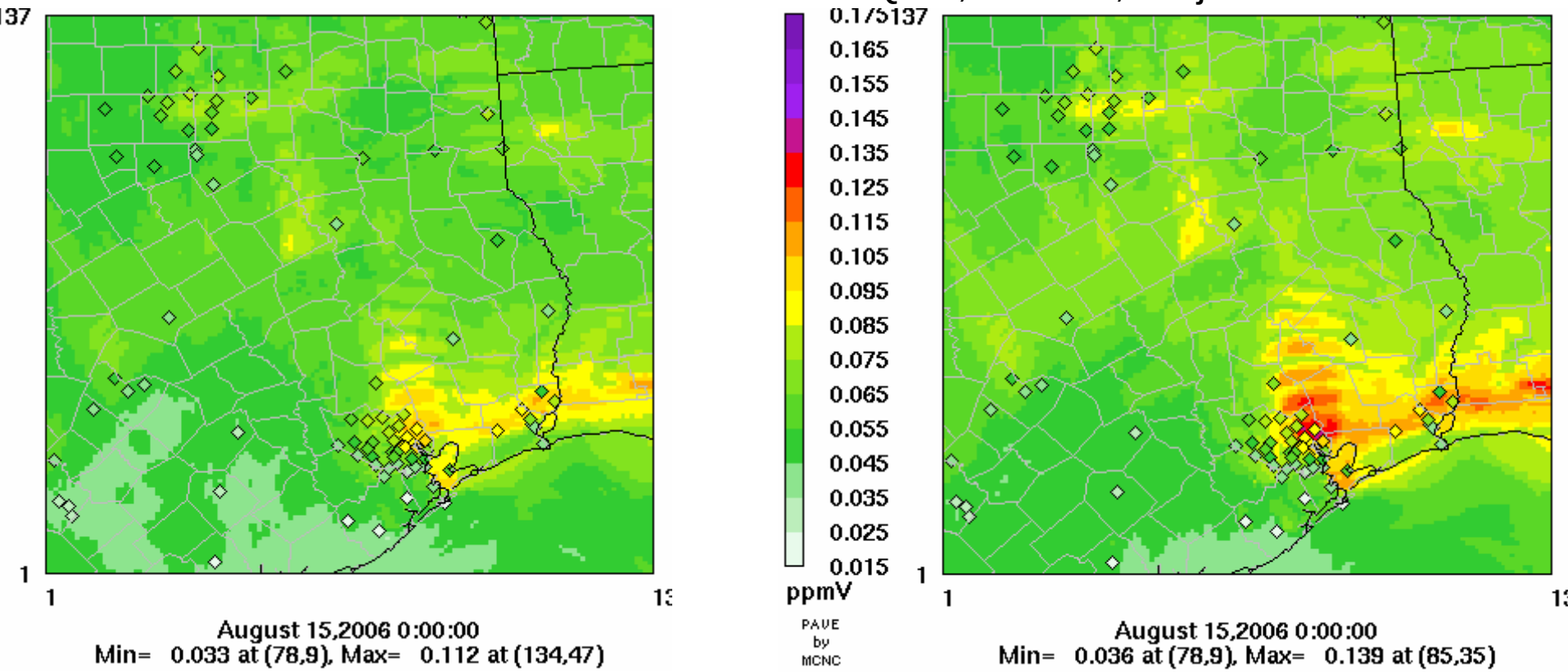


Figure. Spatial plots of daily maximum 1-hour ozone concentrations with (a) CB4 and (b) SAPRC99 chemical mechanisms for August 15th, 2006.

2006 simulations: AQF - F2, 4-km resolution

To compare CMAQ simulations between CB-4 and SAPRC99 for projected EI (lower NOx) at 2005 level

CMAQ4.4, CB4, Projected EI for 2005

CMAQ4.4, SAPRC, Projected EI for 2005

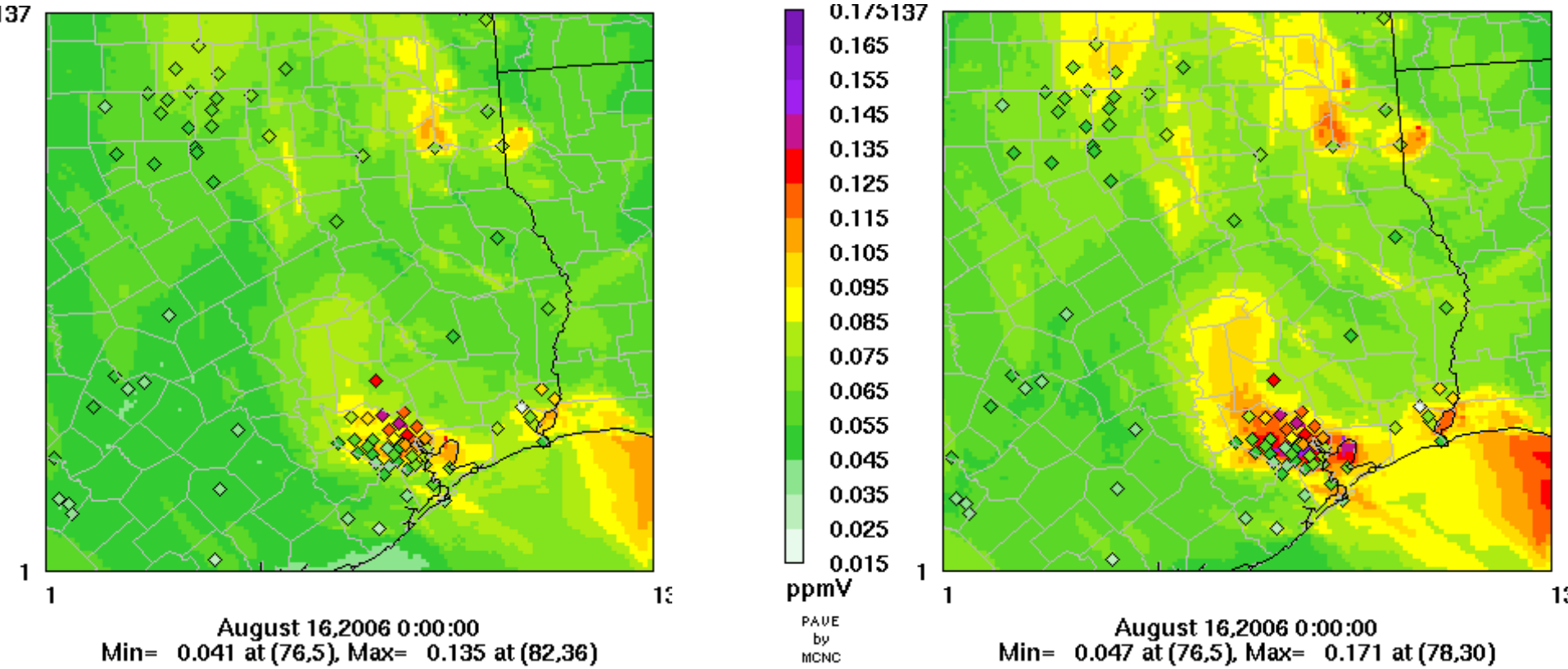


Figure. Spatial plots of daily maximum 1-hour ozone concentrations with (a) CB4 and (b) SAPRC99 chemical mechanisms for August 16th, 2006.

2006 simulations: AQF - F2, 4-km resolution

To compare CMAQ simulations between CB-4 and SAPRC99 for projected EI (lower NOx) at 2005 level

CMAQ4.4, CB4, Projected EI for 2005

CMAQ4.4, SAPRC, Projected EI for 2005

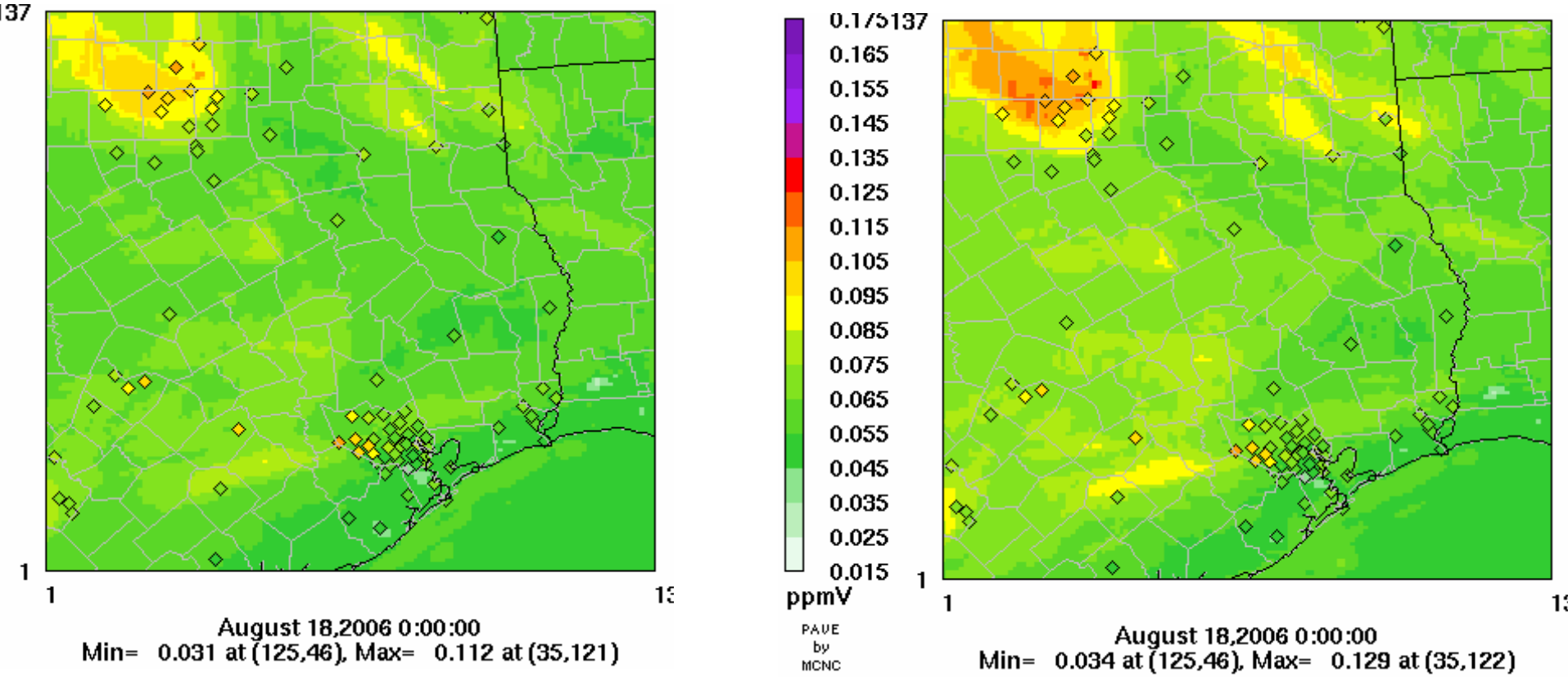


Figure. Spatial plots of daily maximum 1-hour ozone concentrations with (a) CB4 and (b) SAPRC99 chemical mechanisms for August 18th, 2006.

2006 simulations: AQF - F2, 4-km resolution

To compare CMAQ simulations between CB-4 and SAPRC99 for projected EI (lower NOx) at 2005 level

CMAQ4.4, CB4, Projected EI for 2005

CMAQ4.4, SAPRC, Projected EI for 2005

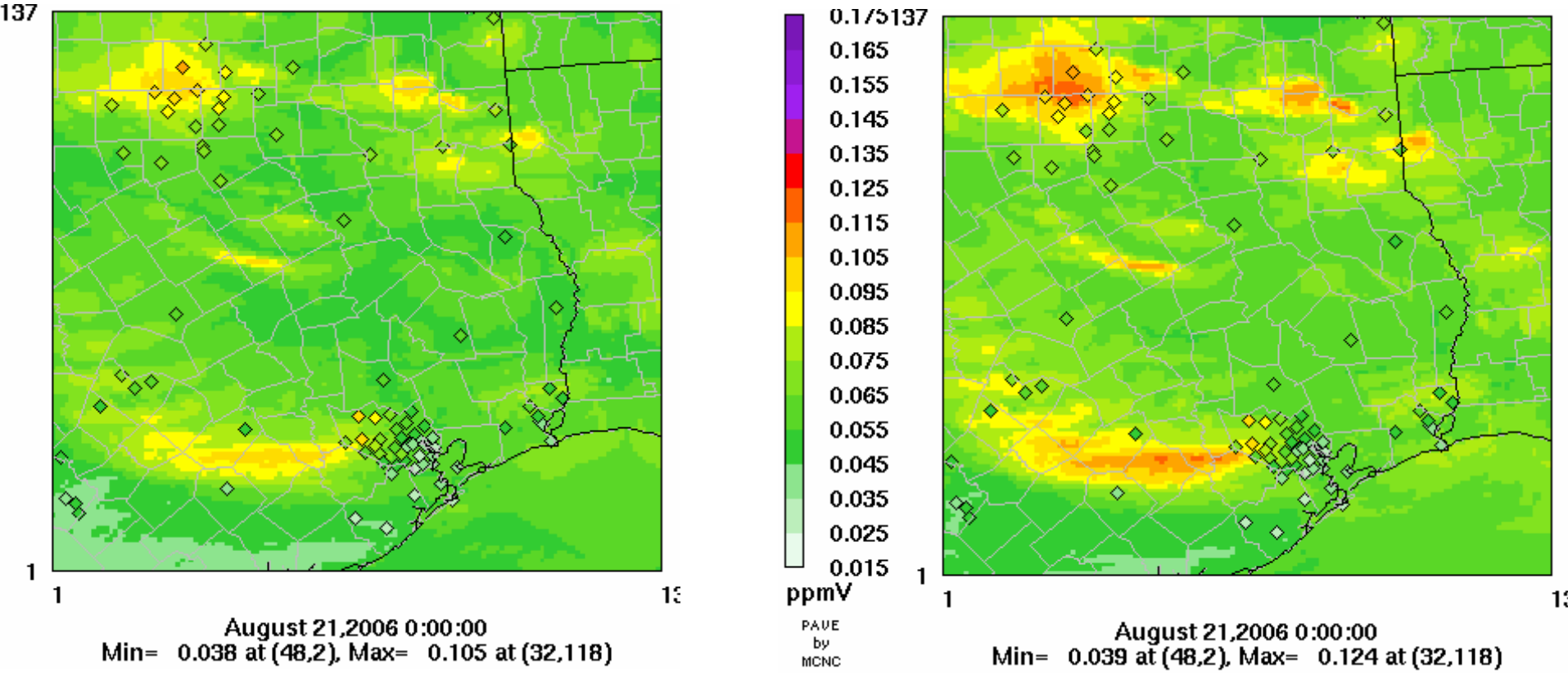
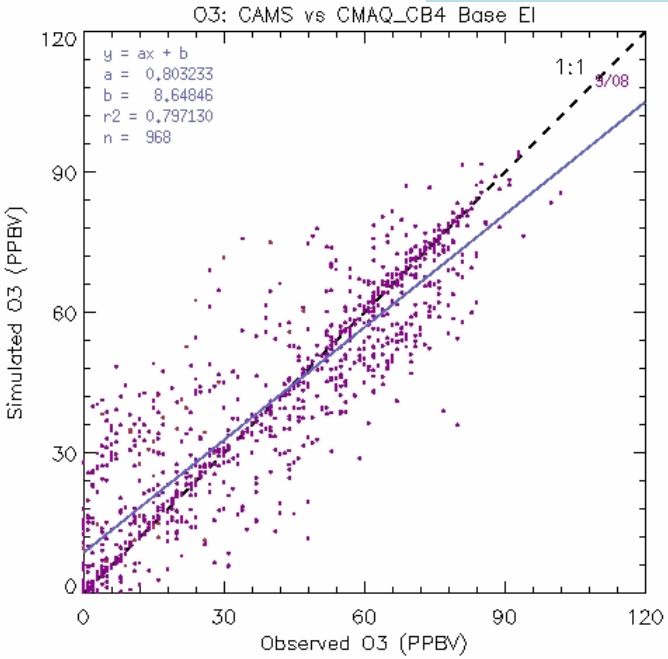


Figure. Spatial plots of daily maximum 1-hour ozone concentrations with (a) CB4 and (b) SAPRC99 chemical mechanisms for August 21st, 2006.

September 8, 2006

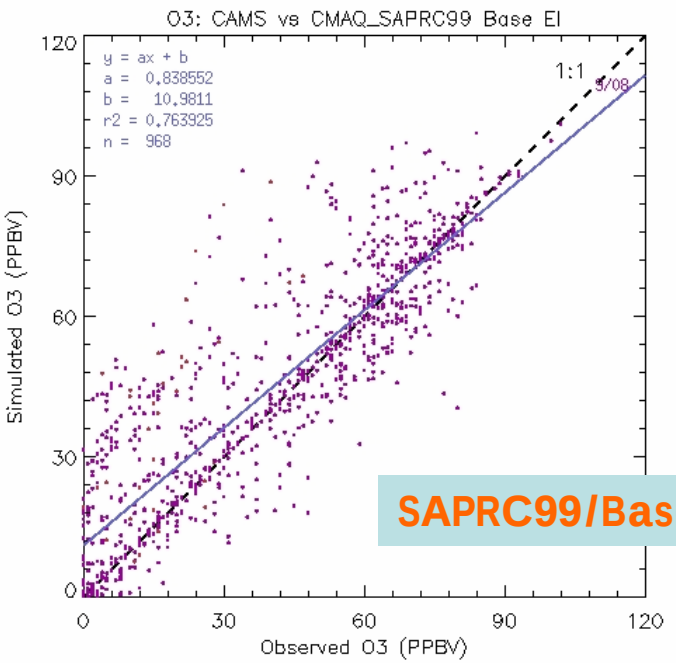
CB4/Base year EI



1-hr O3

HGA

1 hr



SAPRC99/Base year EI

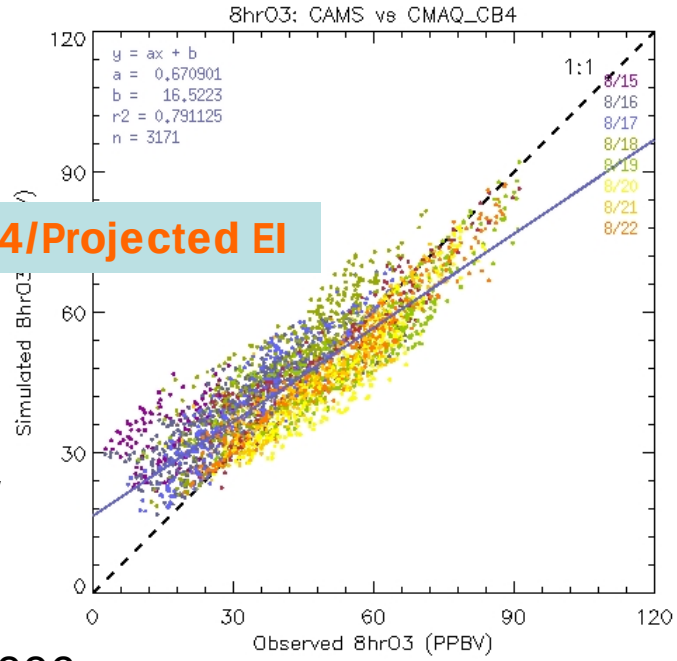
8-hr O3

8 hr

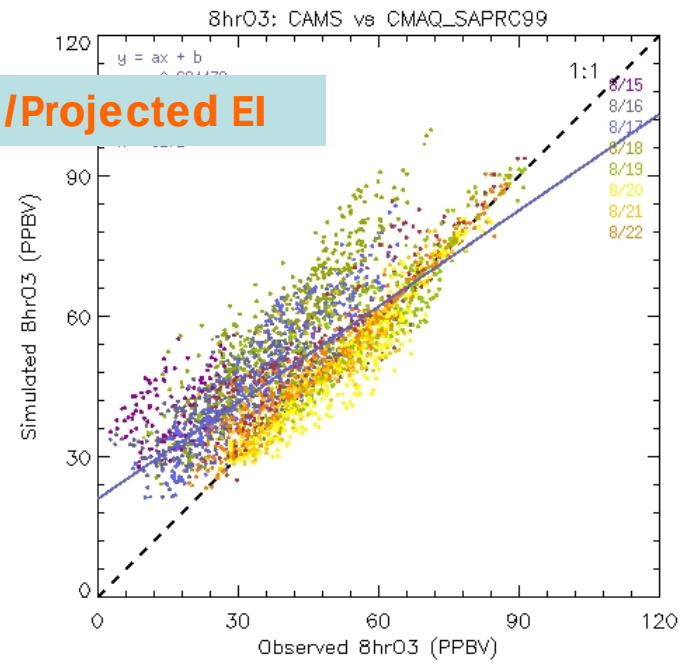
DFW

8/15-22, 2006

CB4/Projected EI

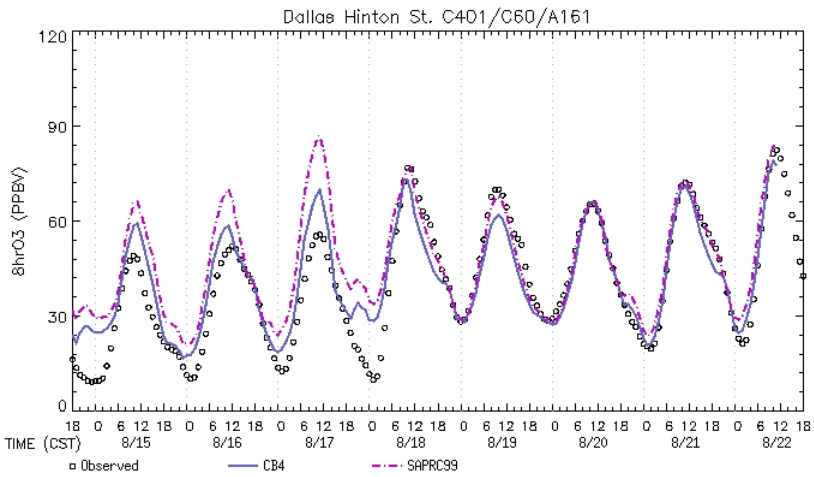


SAPRC99/Projected EI

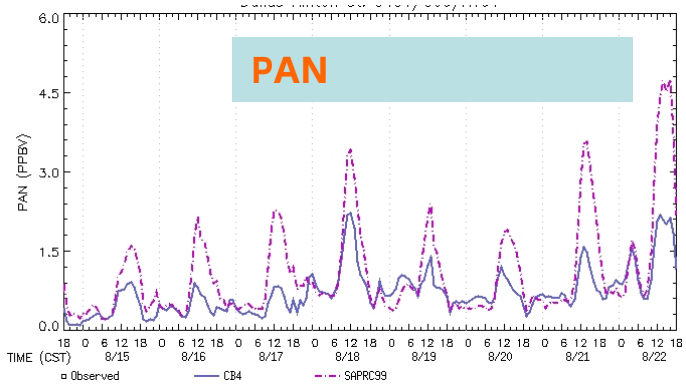


Dallas area – ozone

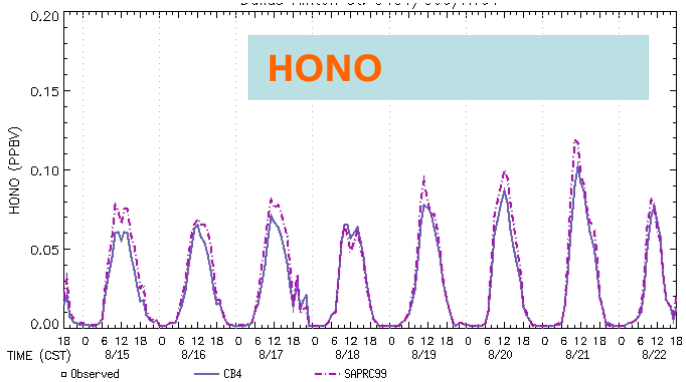
Dallas Hinton, O3



PAN

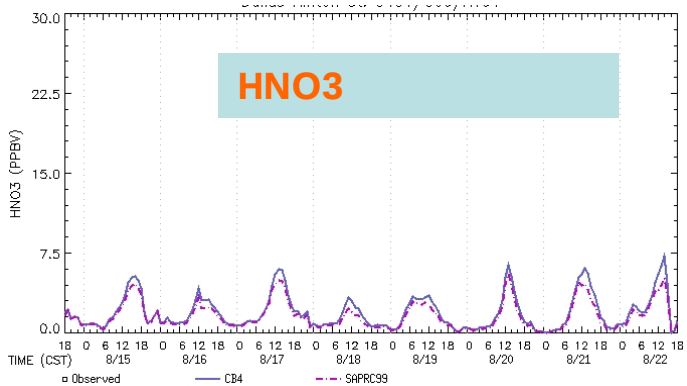


HONO

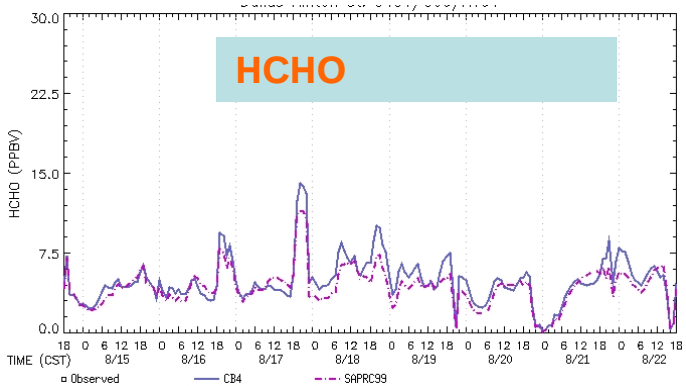


In general, SAPRC99 produces higher PAN, HONO, but lower HNO3, HCHO

HNO3



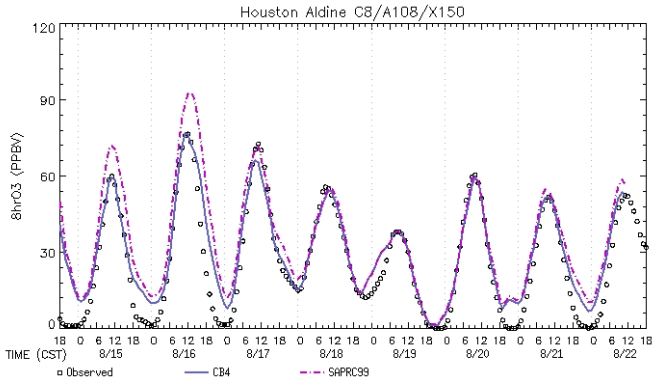
HCHO



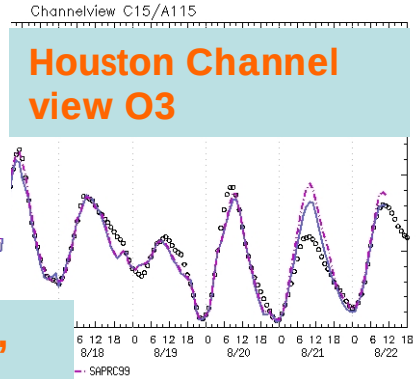
Houston area – ozone

In general, SAPRC99 produces higher PAN, HONO, but lower HNO3, HCHO

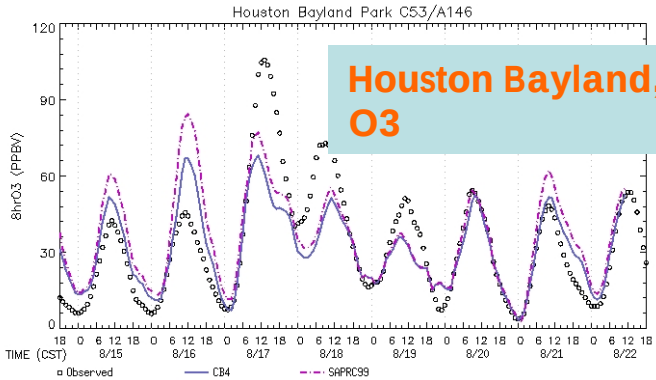
Houston Aldine, O3



Houston Channel view O3

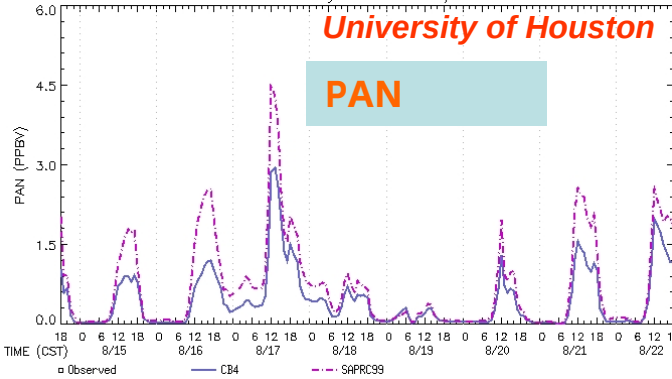


Houston Bayland, O3



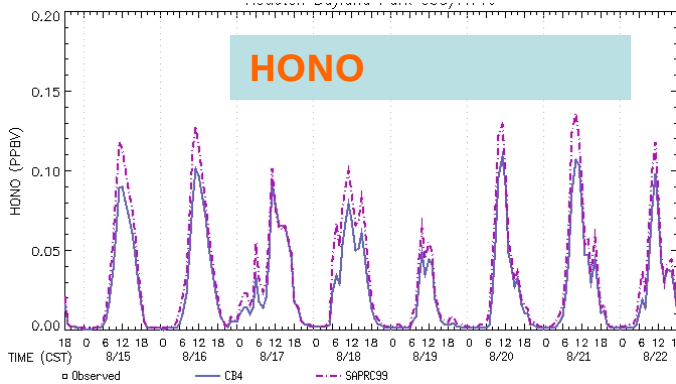
University of Houston

PAN

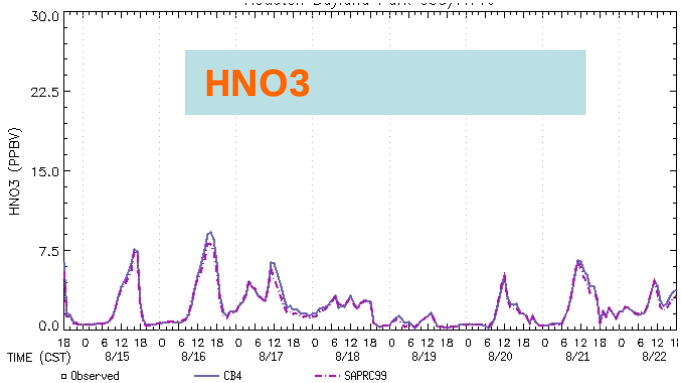


Houston Bayland

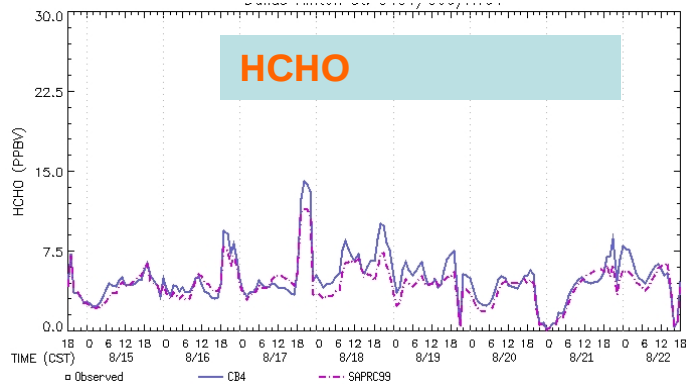
HONO



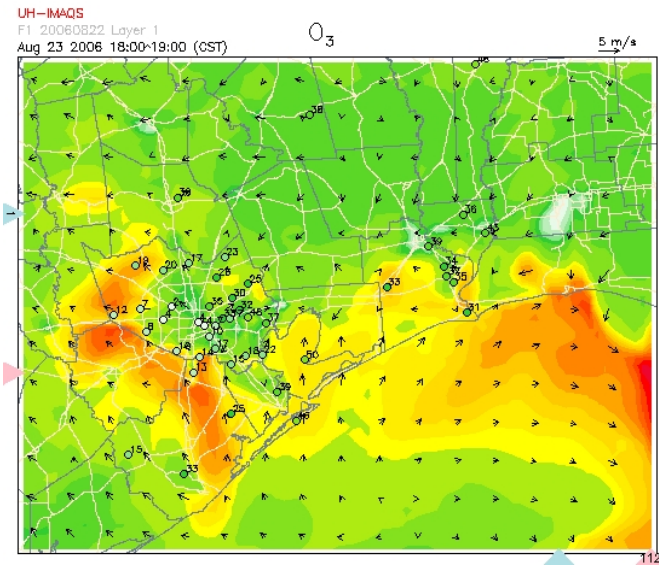
HNO3



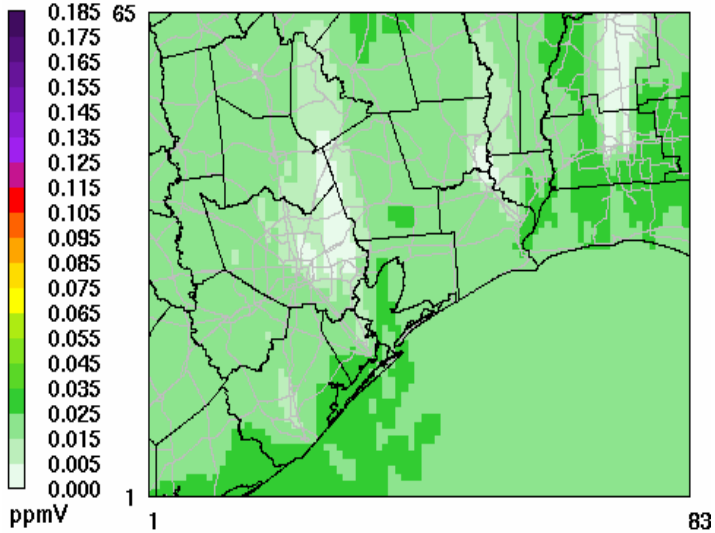
HCHO



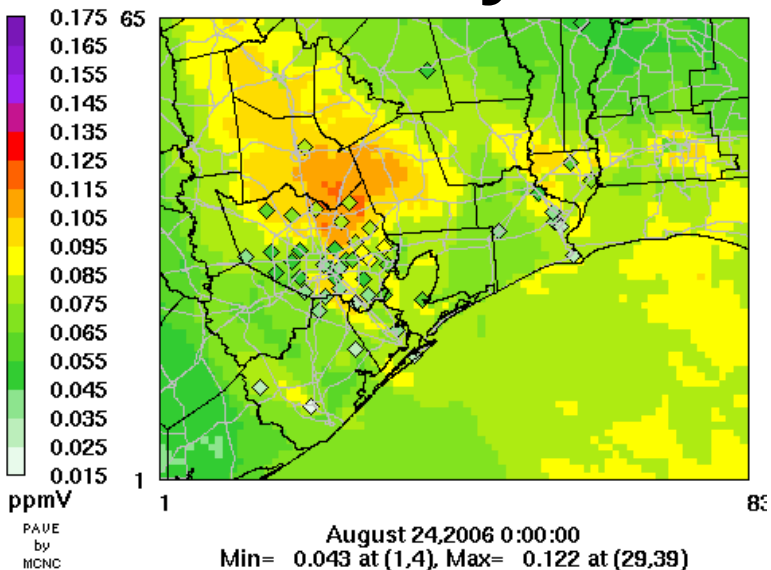
2. Sensitivity to initial condition

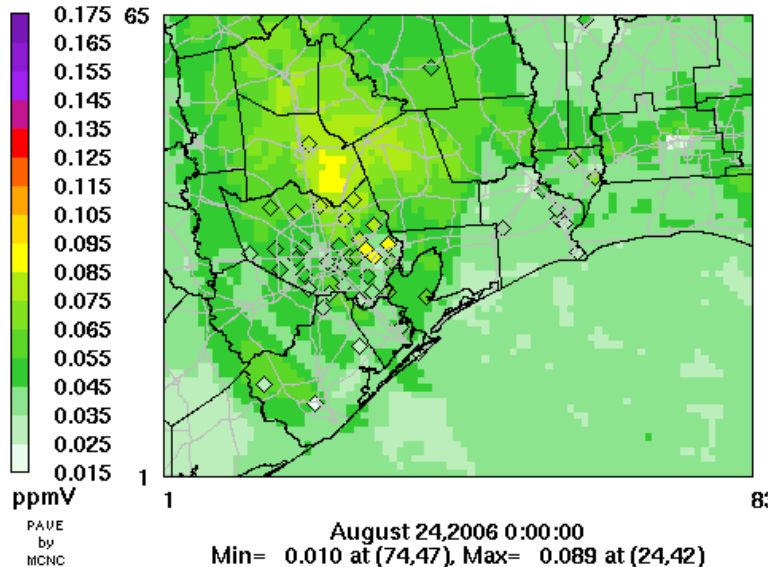


Clean conditions

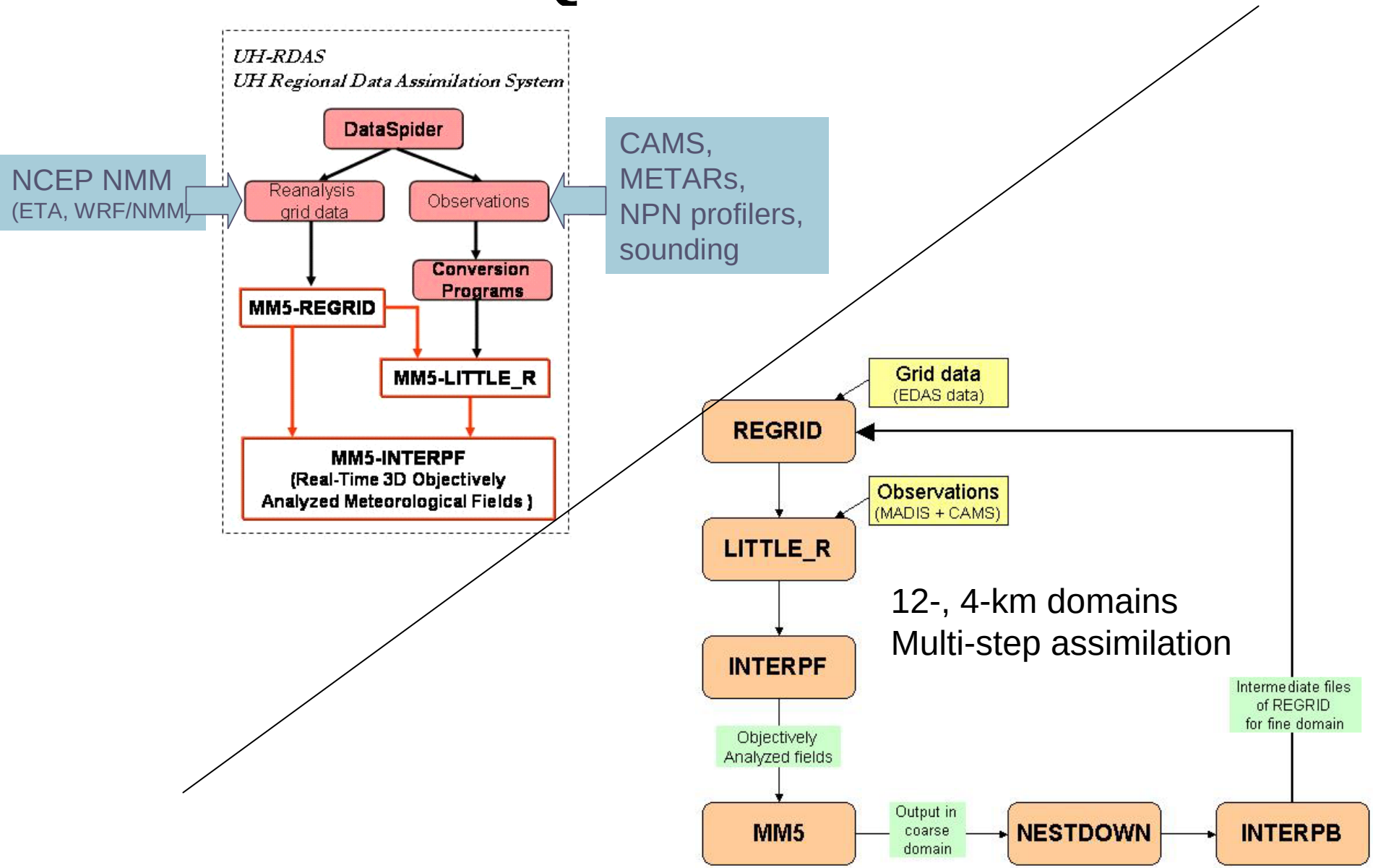


Daily maximum resulted



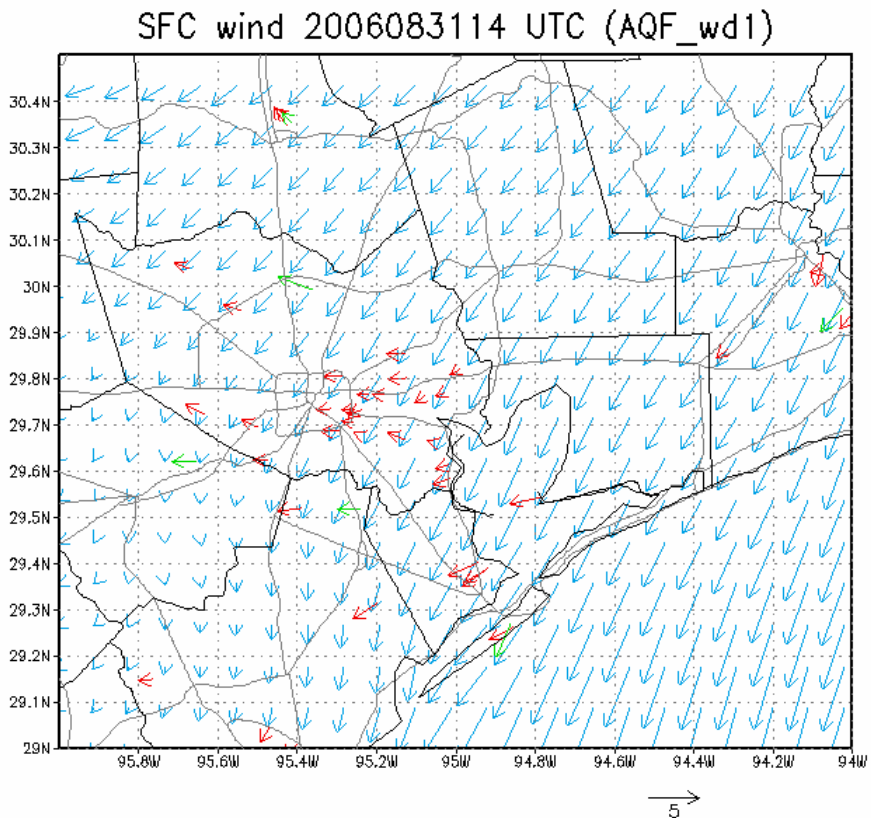


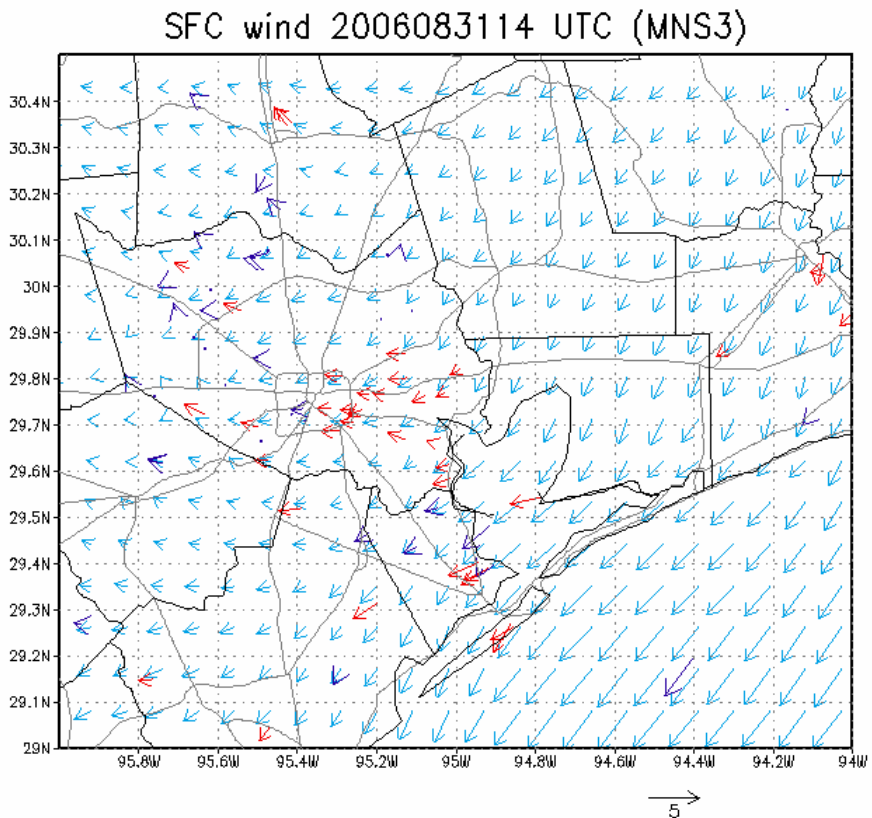
3. MM5 AQF vs. Assimilation



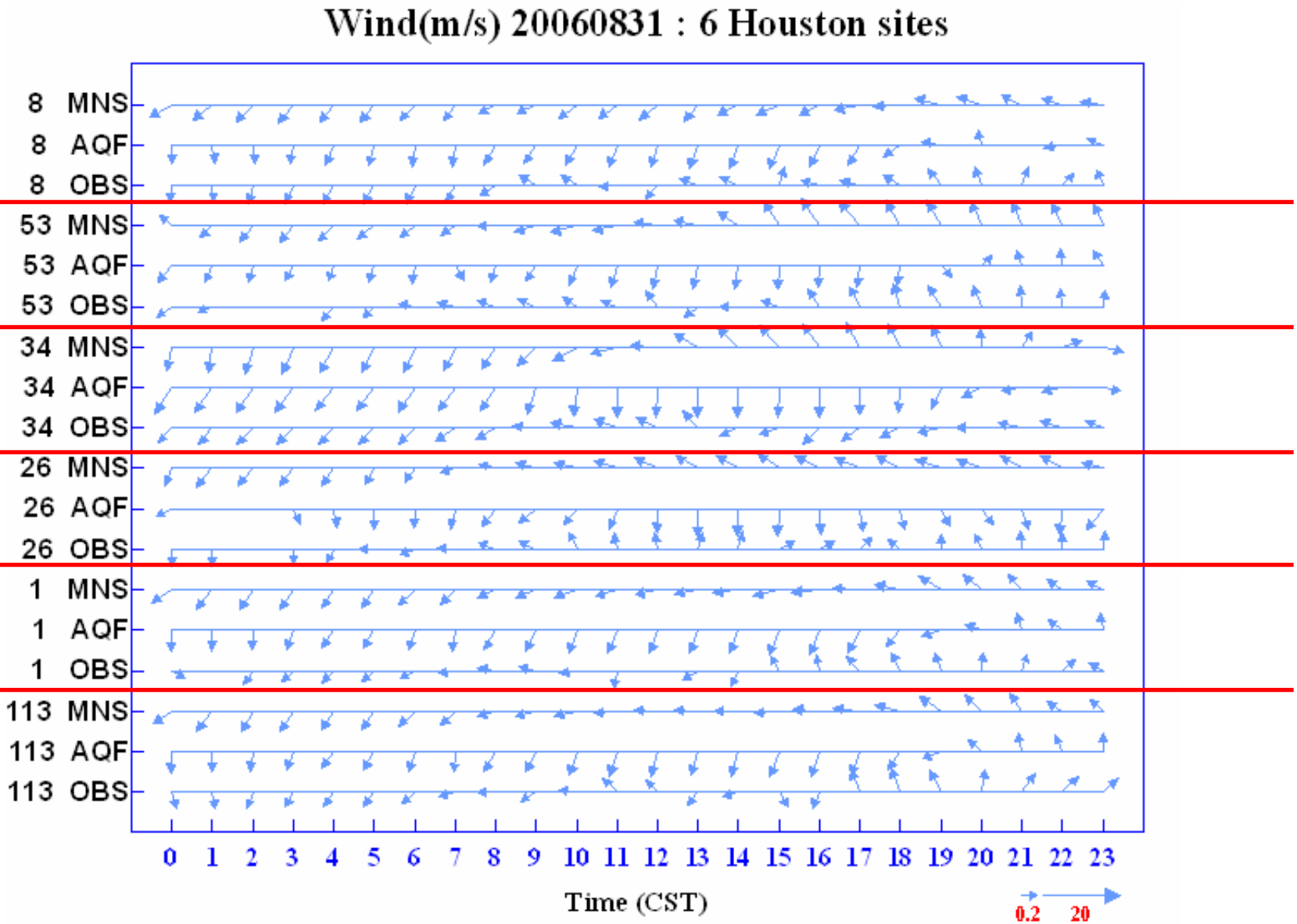
Statistical summary *(provided by Dr. XiangShang Li)*

		Corr	IOA	RMSE	MAE	MB
AQF	**U**	0.3	0.55	1.5	1.2	-0.6
	V	0.56	0.63	2.3	1.9	-1.4
MNS3	**U**	0.57	0.64	1.5	1.2	-1
	V	0.78	0.83	1.2	1	-0.6

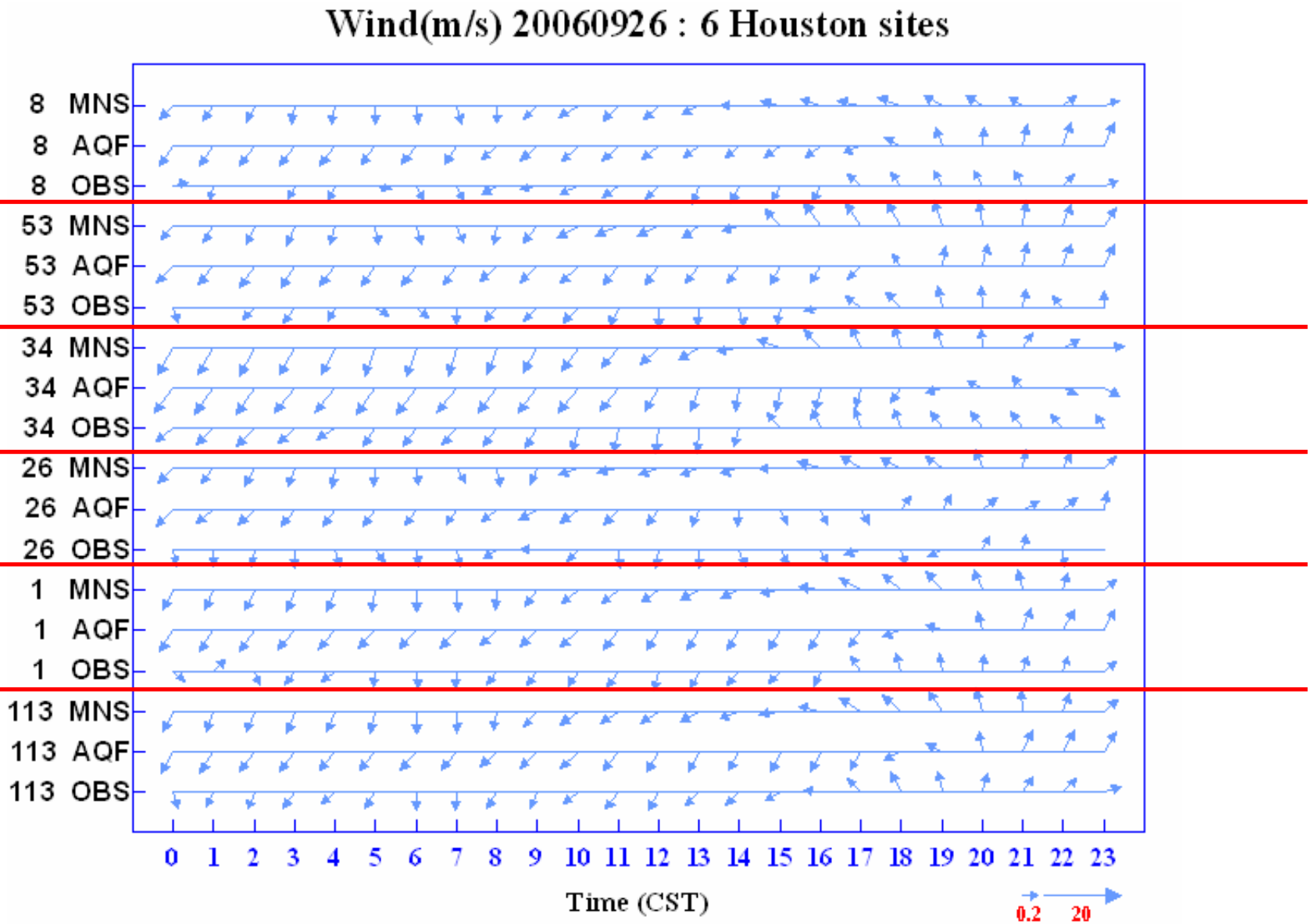




Comparison of Wind



Comparison of Wind

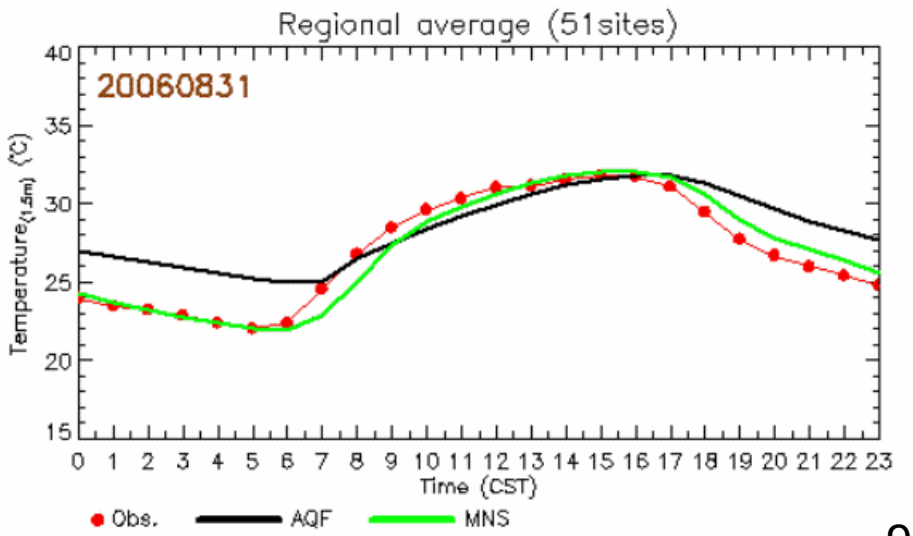


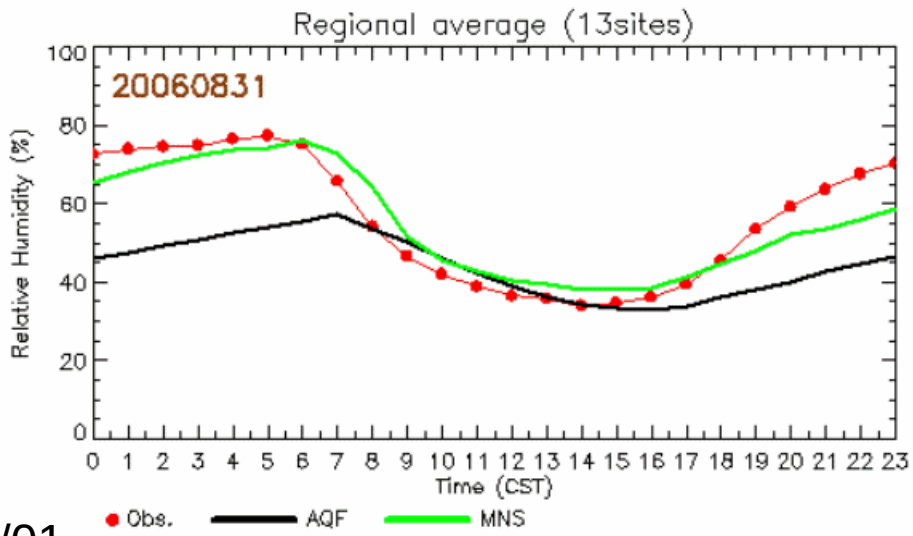
MM5 MS-FDDA Assimilation Results

Temperature

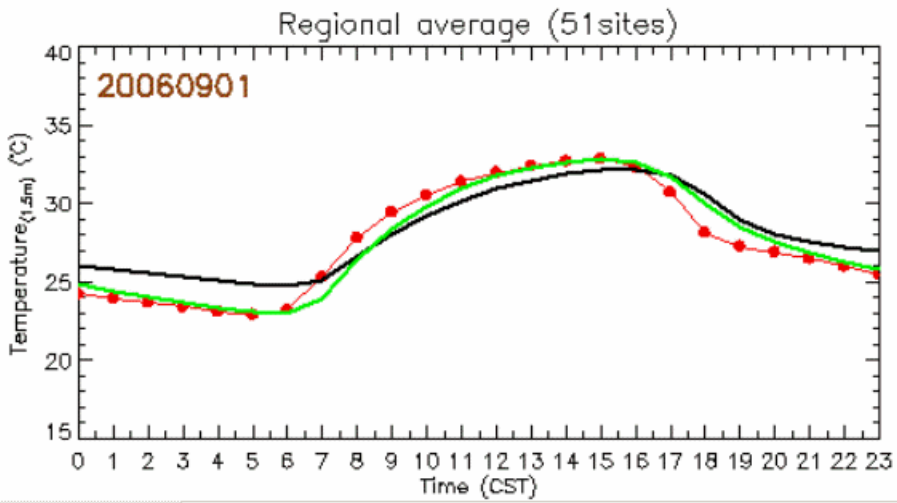
8/31

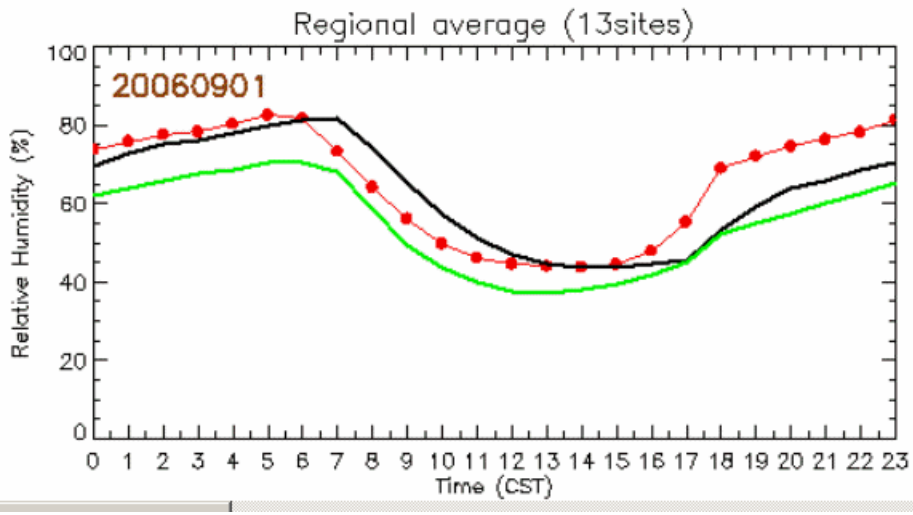
Humidity





9/01



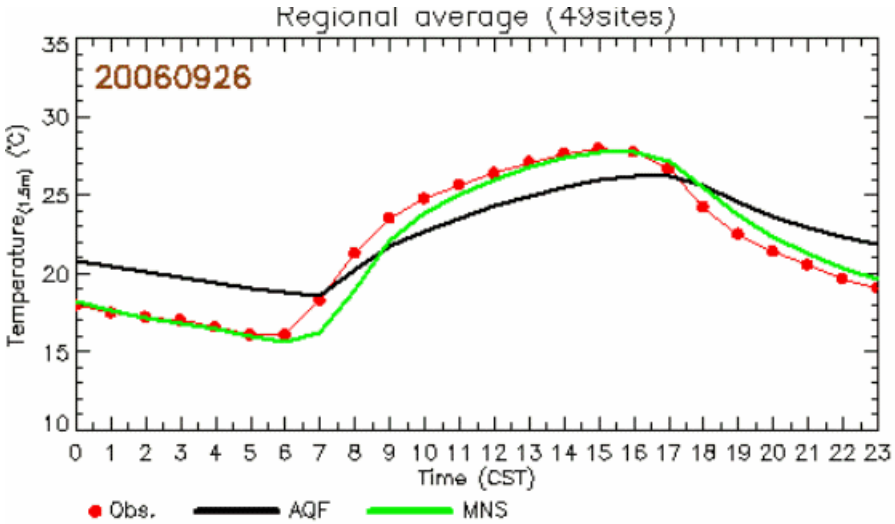


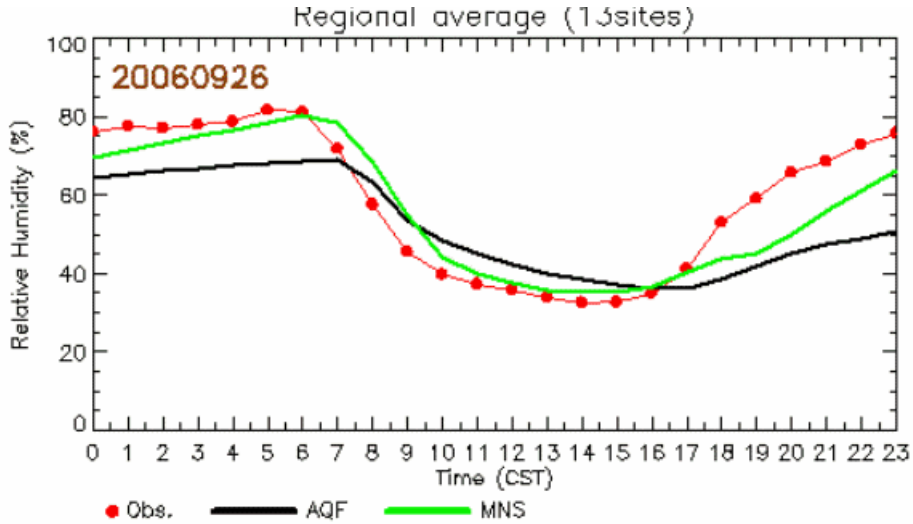
MM5 MS-FDDA Assimilation Results

Temperature

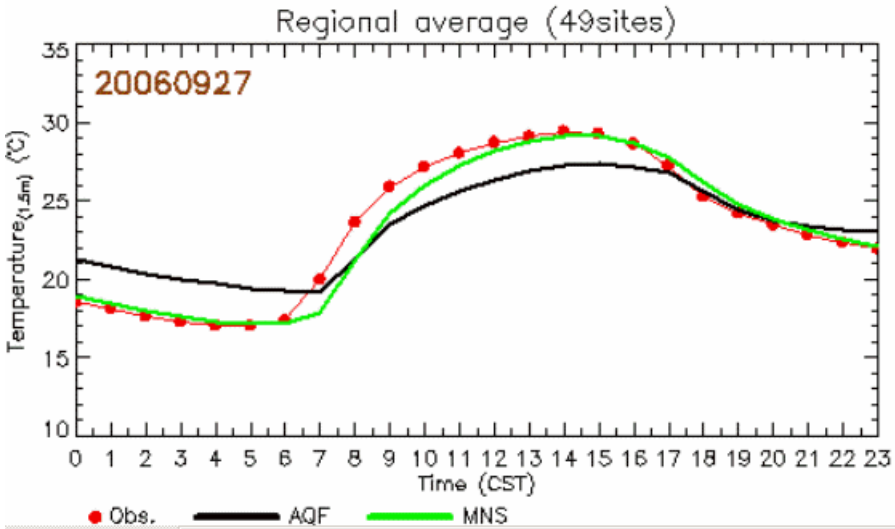
9/26

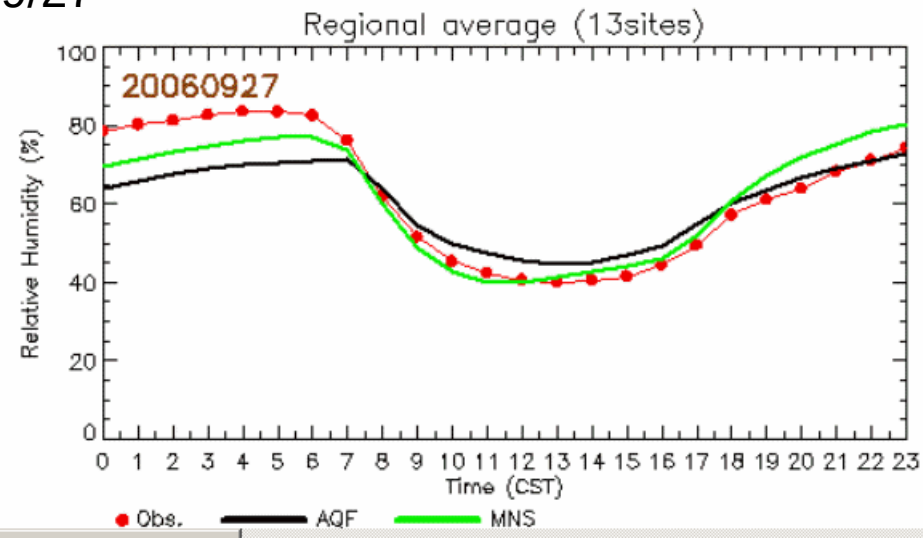
Humidity





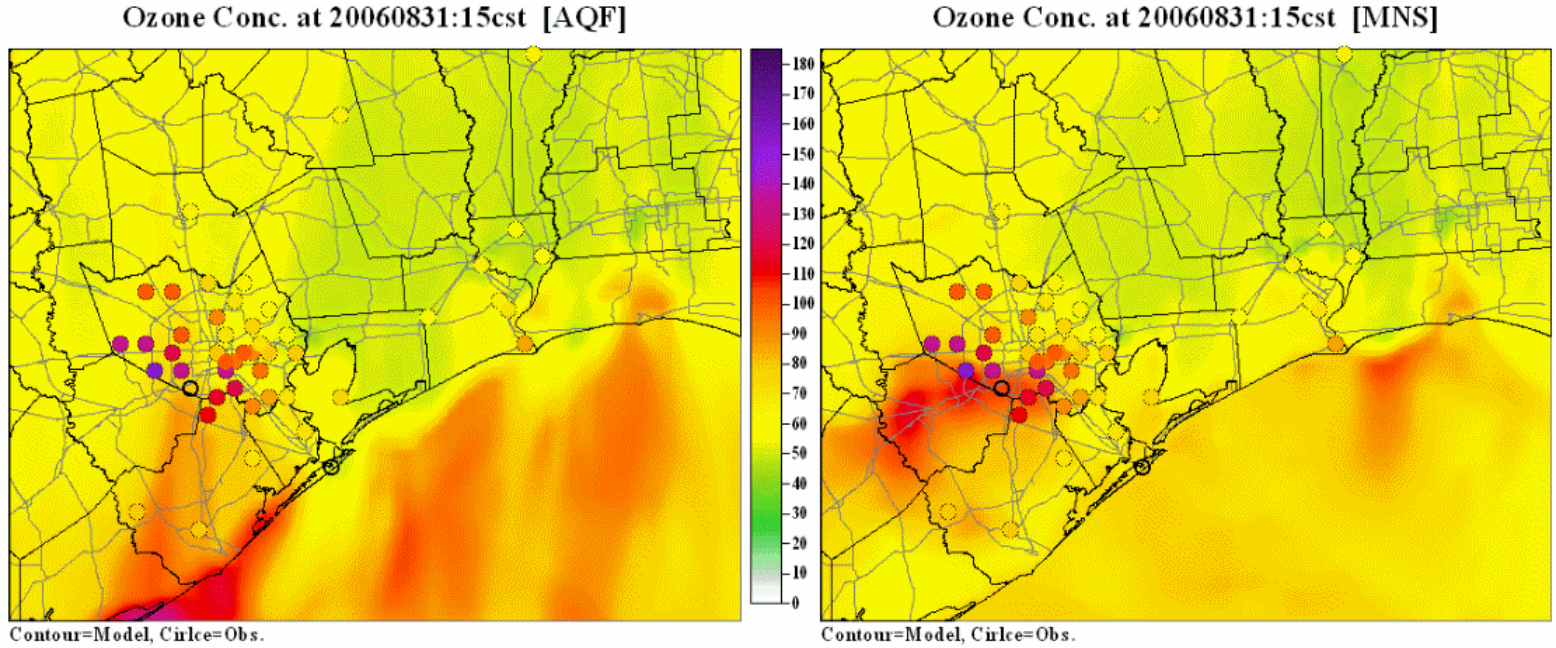
9/27



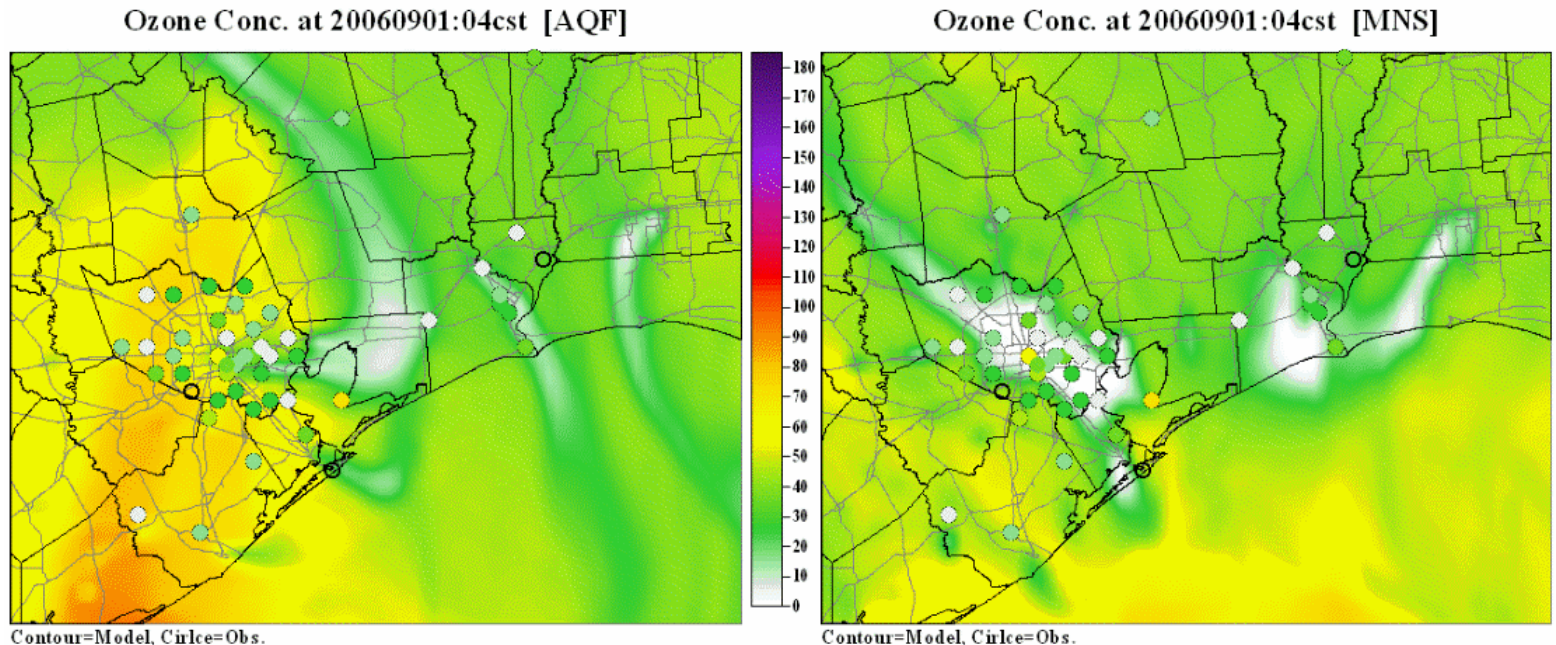


O3 comparison

8/31 15 CST

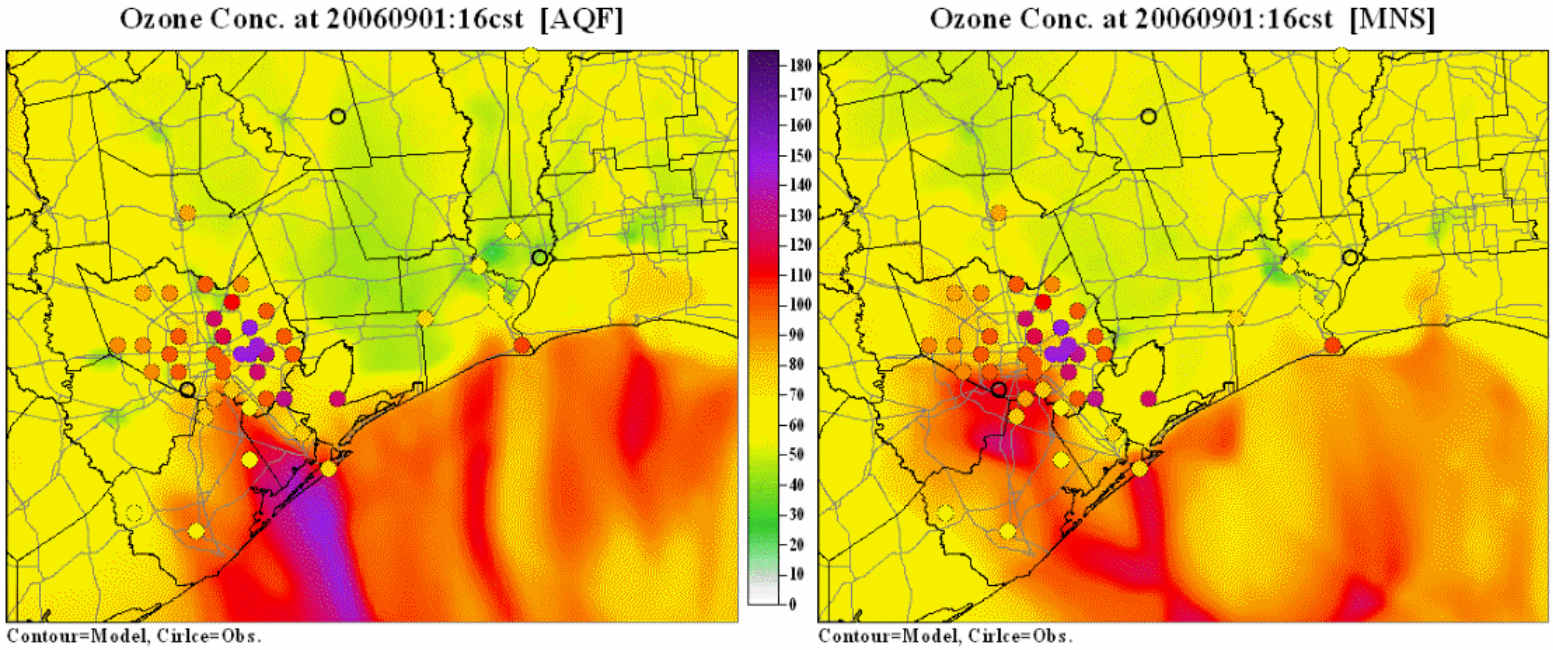


9/01 04 CST

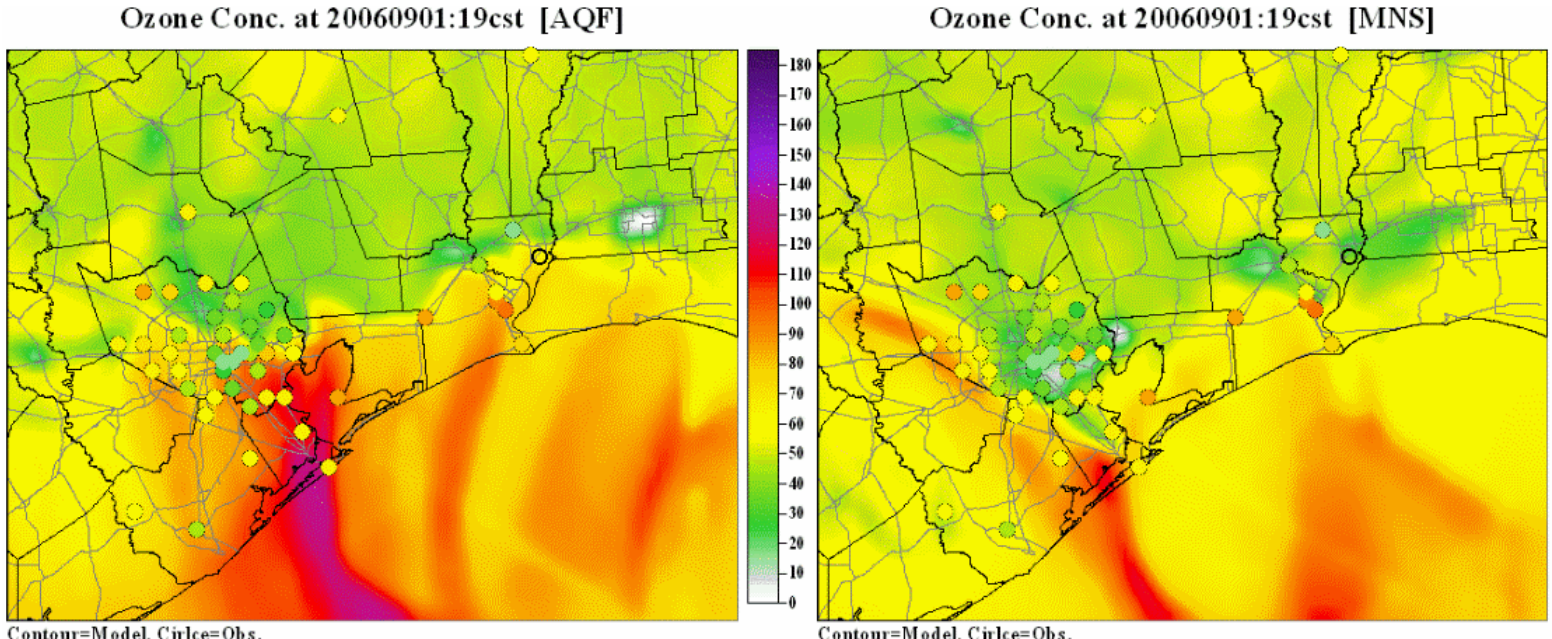


O3 comparison

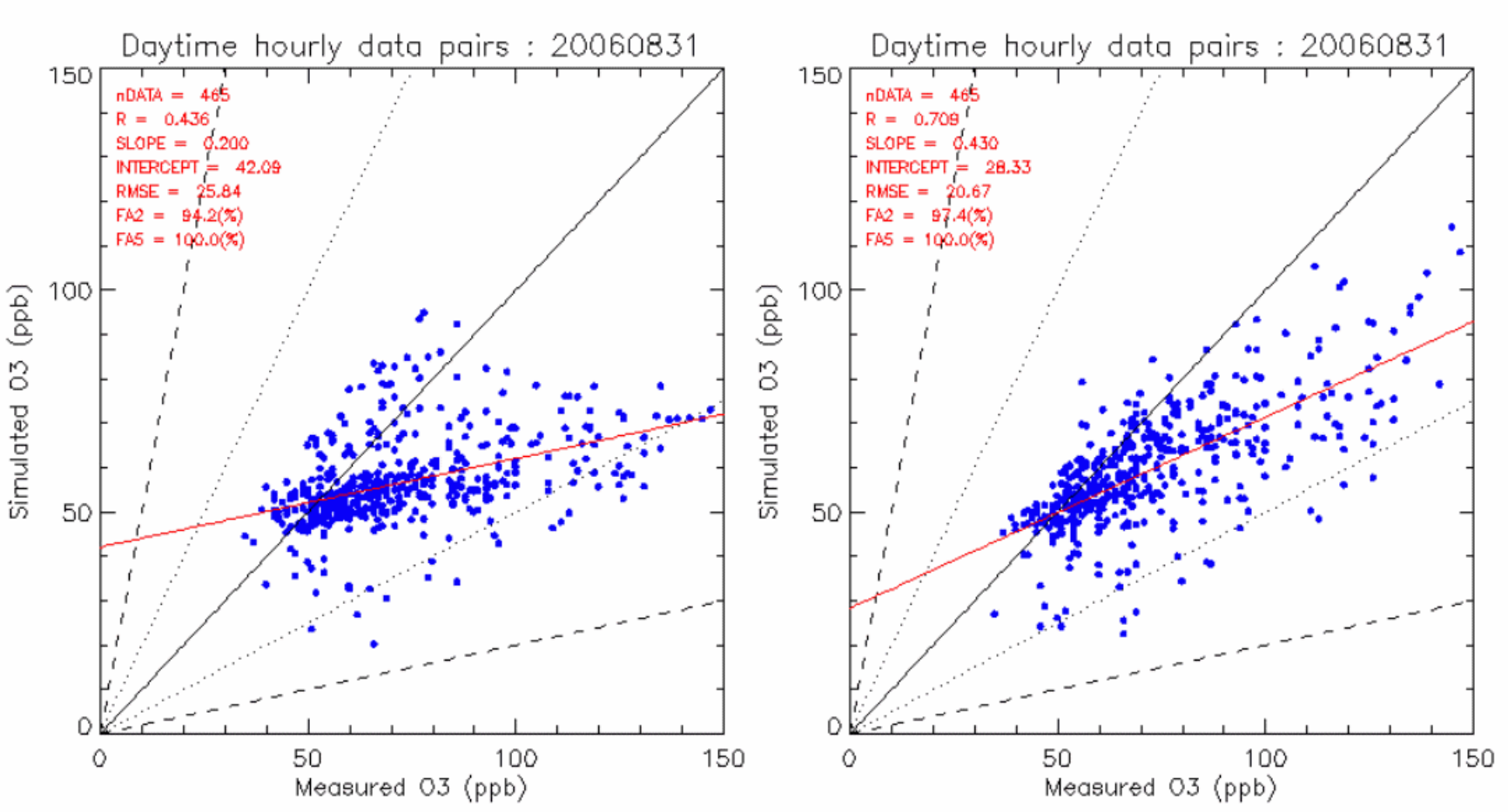
9/01 16 CST



9/01 19 CST

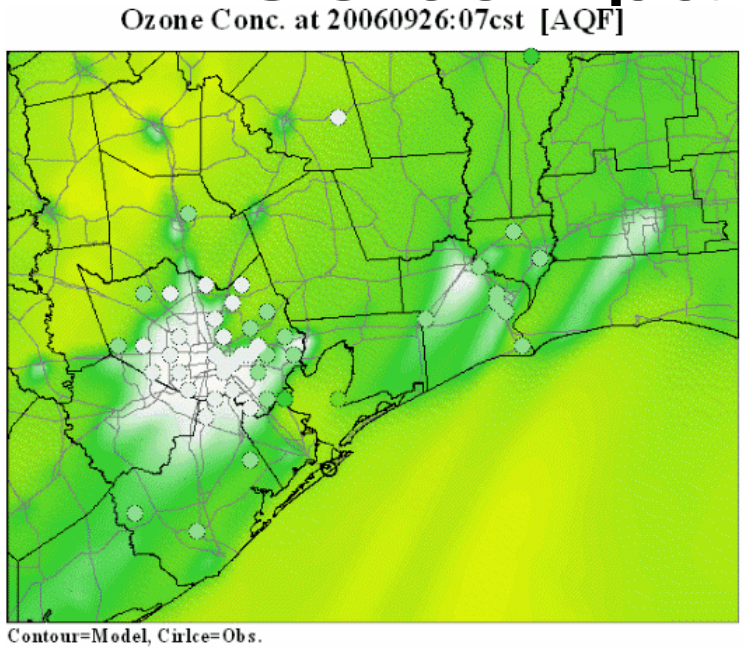


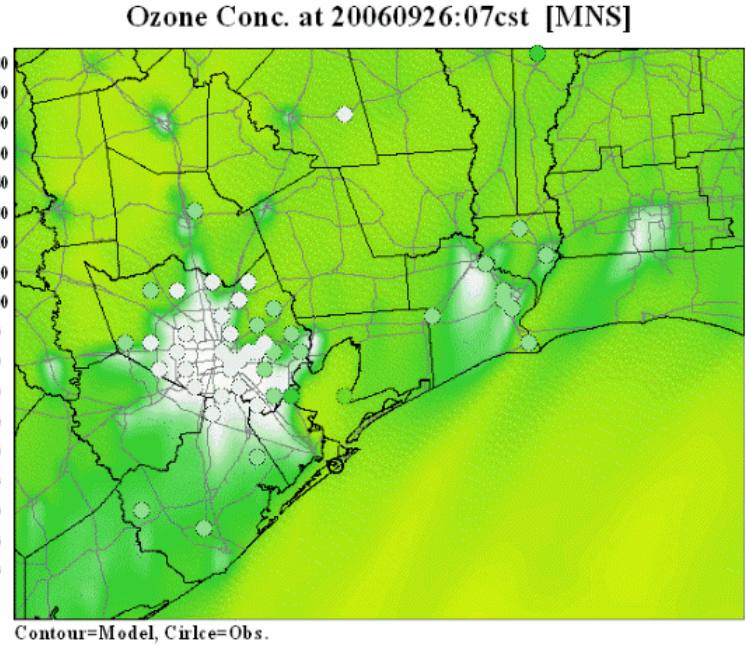
AQF vs MS-FDDA Met.
O3 comparison (Daytime 8/31/06)



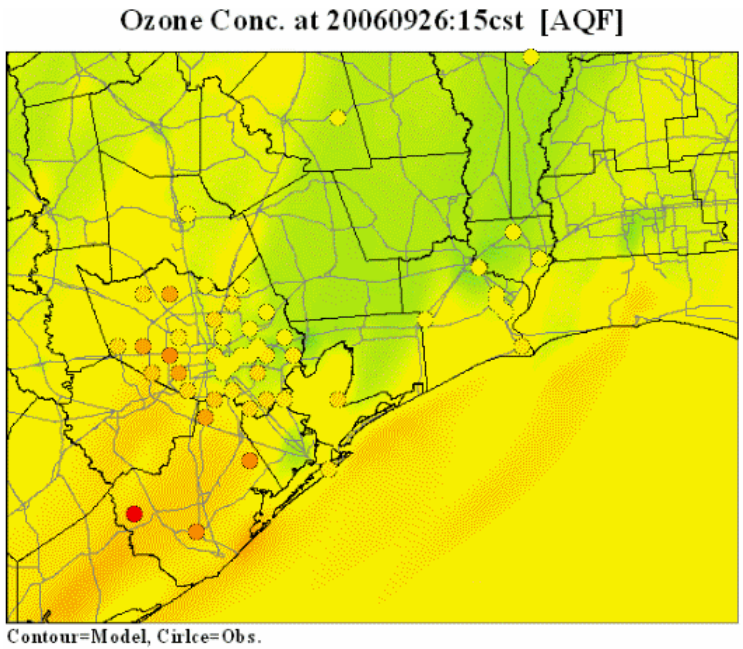
O3 comparison

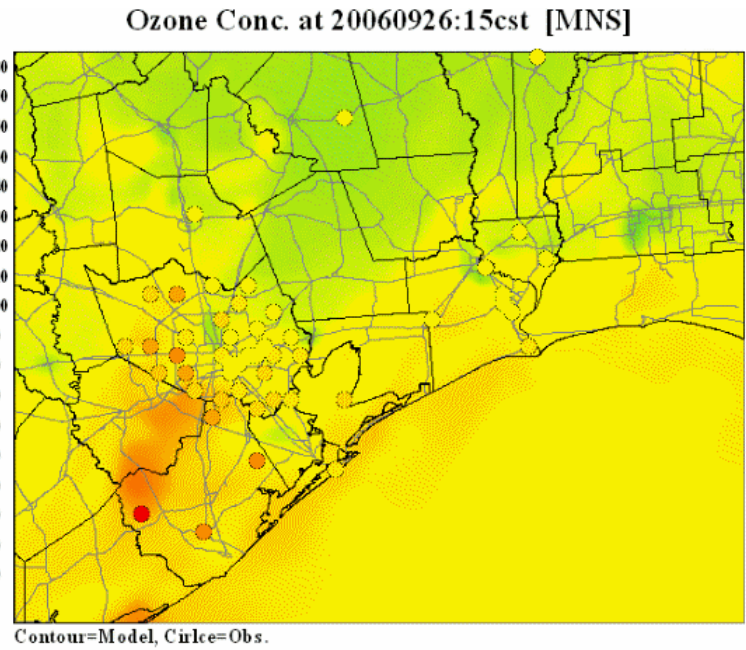
9/26 07 CST





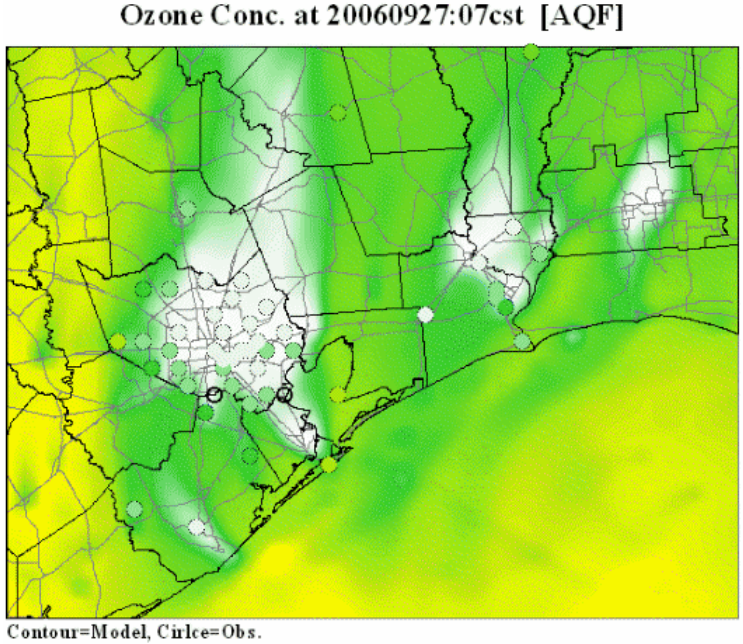
9/26 15 CST

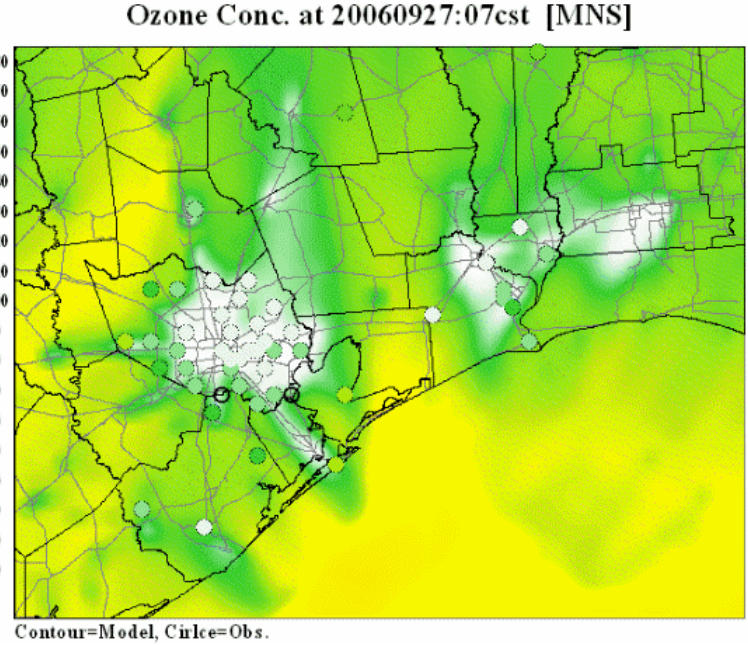




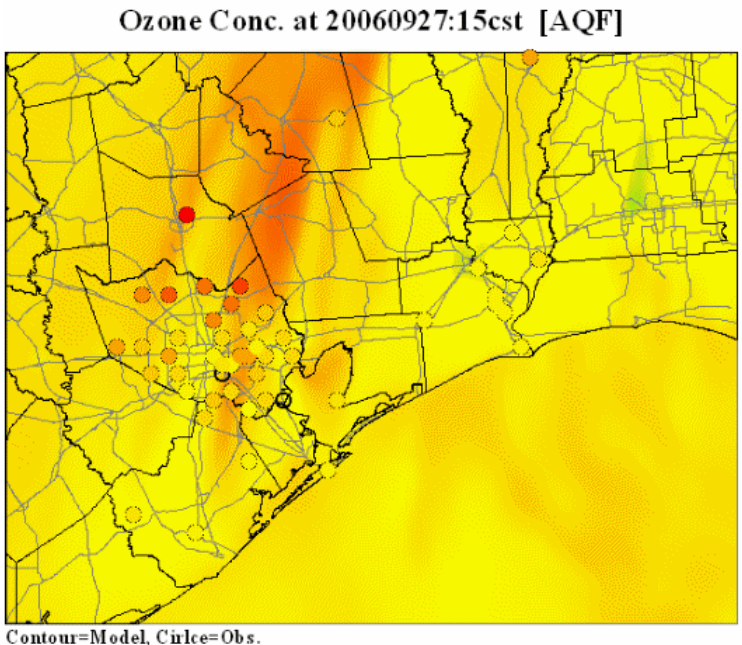
O3 comparison

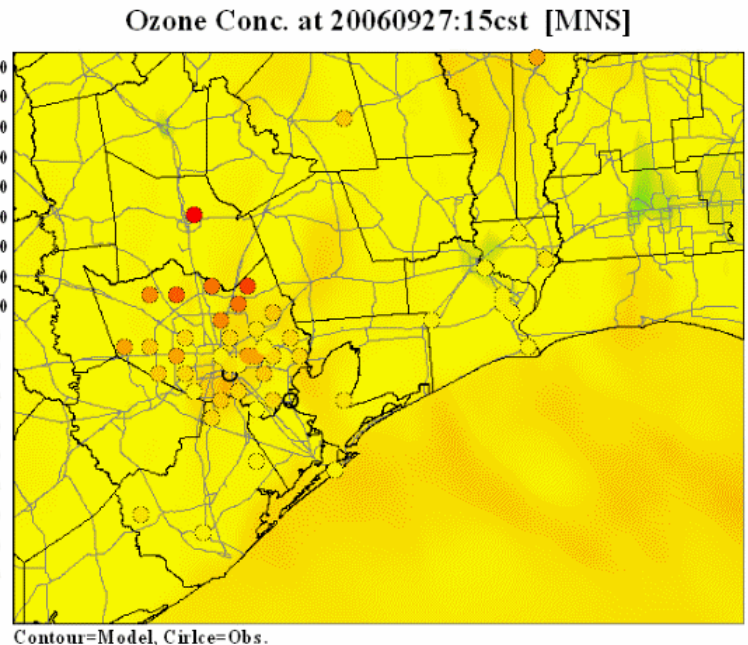
9/27 07 CST



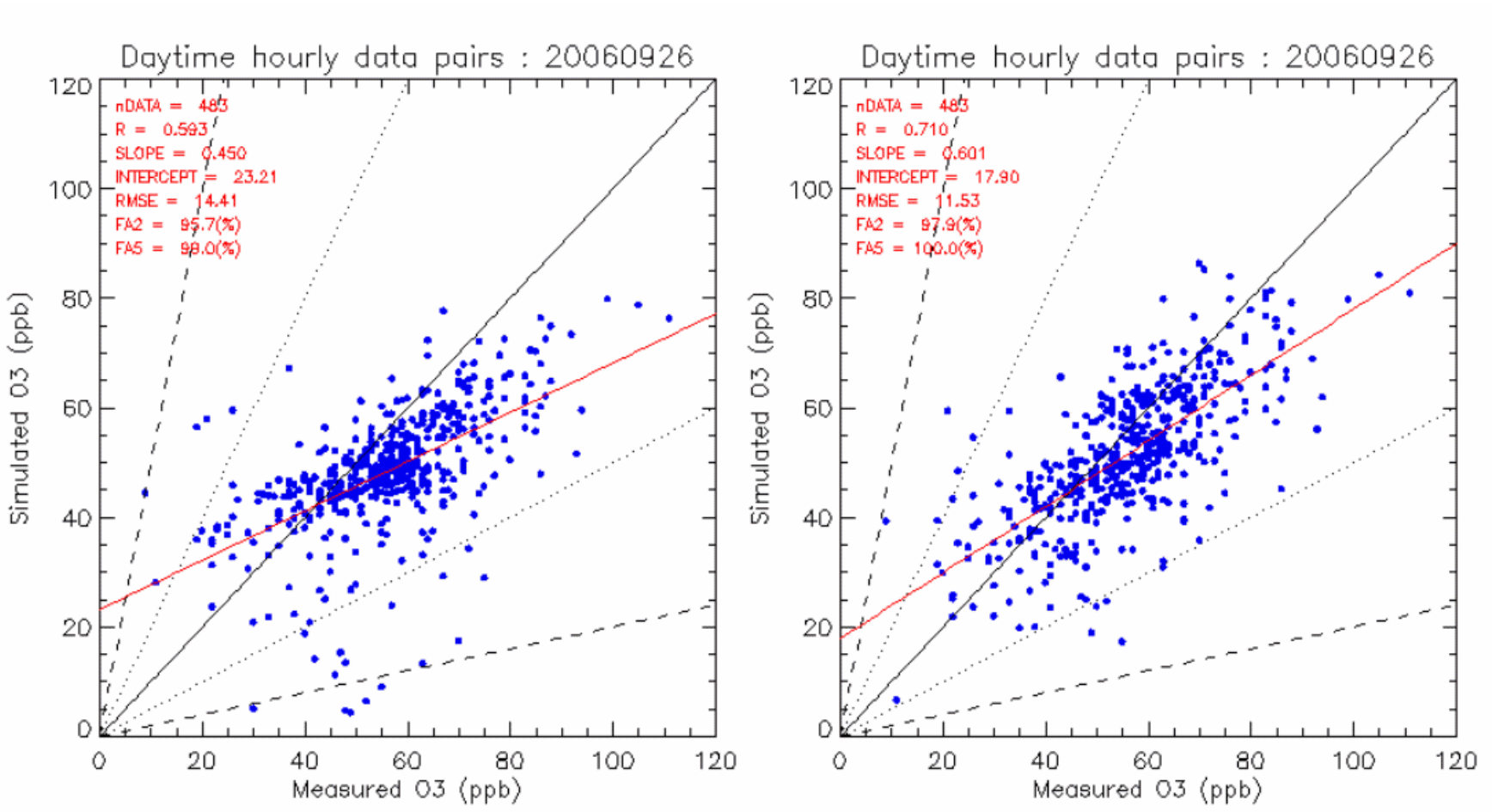


9/27 15 CST





AQF vs MS-FDDA Met.
O3 comparison (Daytime, 9/26/06)



Conclusive Remarks

CB4 vs. SAPRC

- For 2000, CMAQ with SAPRC performed well both O3, HNO3
- CB4 generated more HNO3 less PAN
- SAPRC generated less HNO3 more PAN, thus higher O3 productivity at O3 > 90 ppb
- SAPRC overpredcted medium range O3 a few ppb

- For 2006, CB-4 with 2000 EI and projected 2005 (actually 2003 NOx) compared: show small difference in O3.
- With SAPRC, high O3 enhancement area coinicides with the downwind area of high HRVOC emissions.
- SAPRC with 2000 EI overpredicted observation at 60 ppb range, but compared well with O3 > 90 ppb.

MS-FDDA

MM5 multi-stage 4D data assimilation runs are promising, but need to be evaluated and improved further