**Question I**

Why does the SAPRC chemical mechanism give different results than CB-IV?

Which replicates the actual chemistry better?

# Comparison of CB4 & SAPRC Mechanisms for Houston-Galveston Airshed

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*University of Houston*

# CB-4 & SAPRC Comparison

- 2000 TexAQS Episode with NEI99
- 2000 TexAQS Episode with TEI2000/imputed HRVOC

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- 2006 TexAQS-2 Sept 6-8 Episode with TEI2000/imputed HRVOC
- 2006 TexAQS-2 Sept 6-8 Episode with 2005 projected EI (SAPRC run not completed yet)

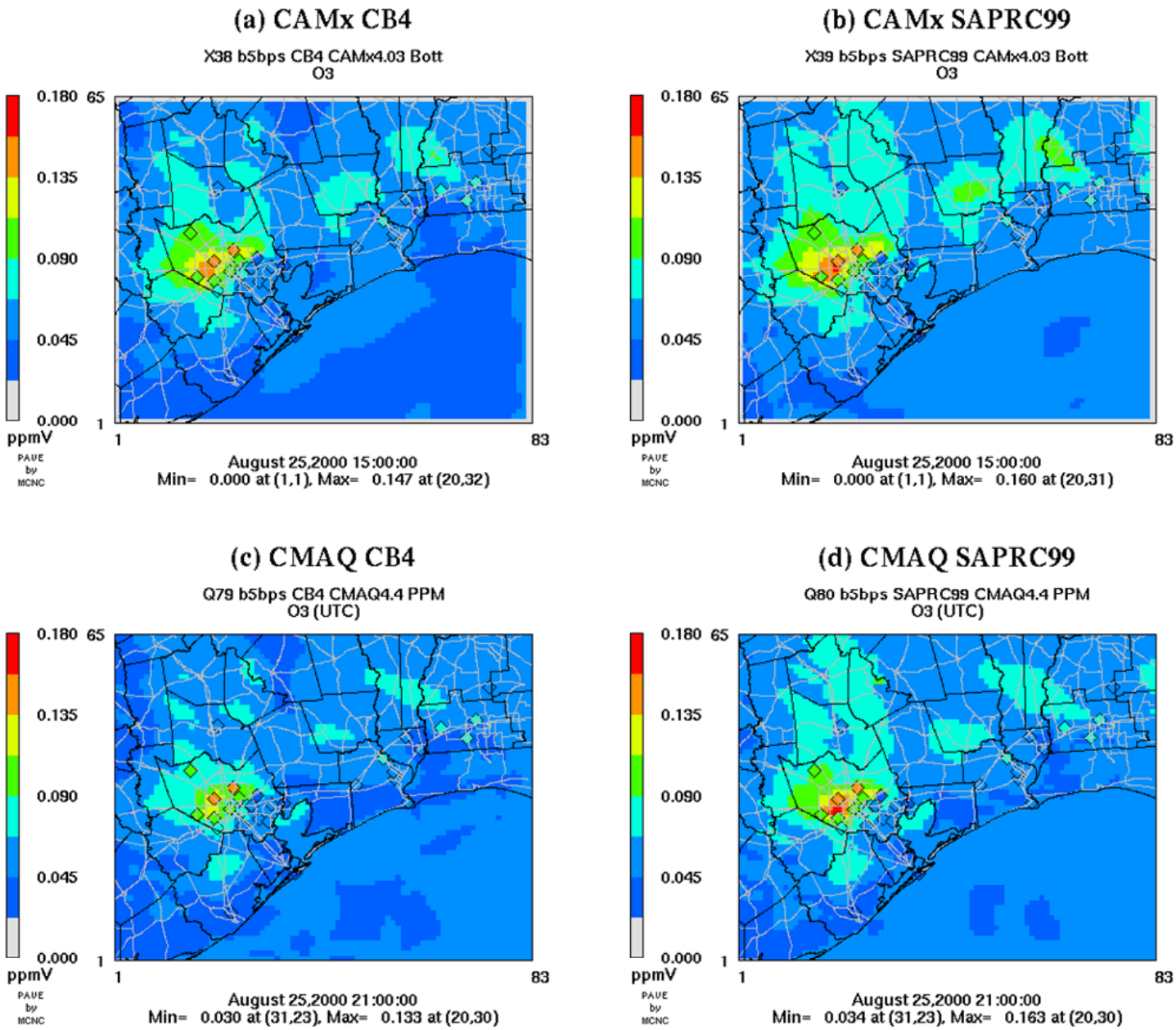
# *CAMx and CMAQ with CB-4 and SAPRC99*

## TexAQS 2000 Episode

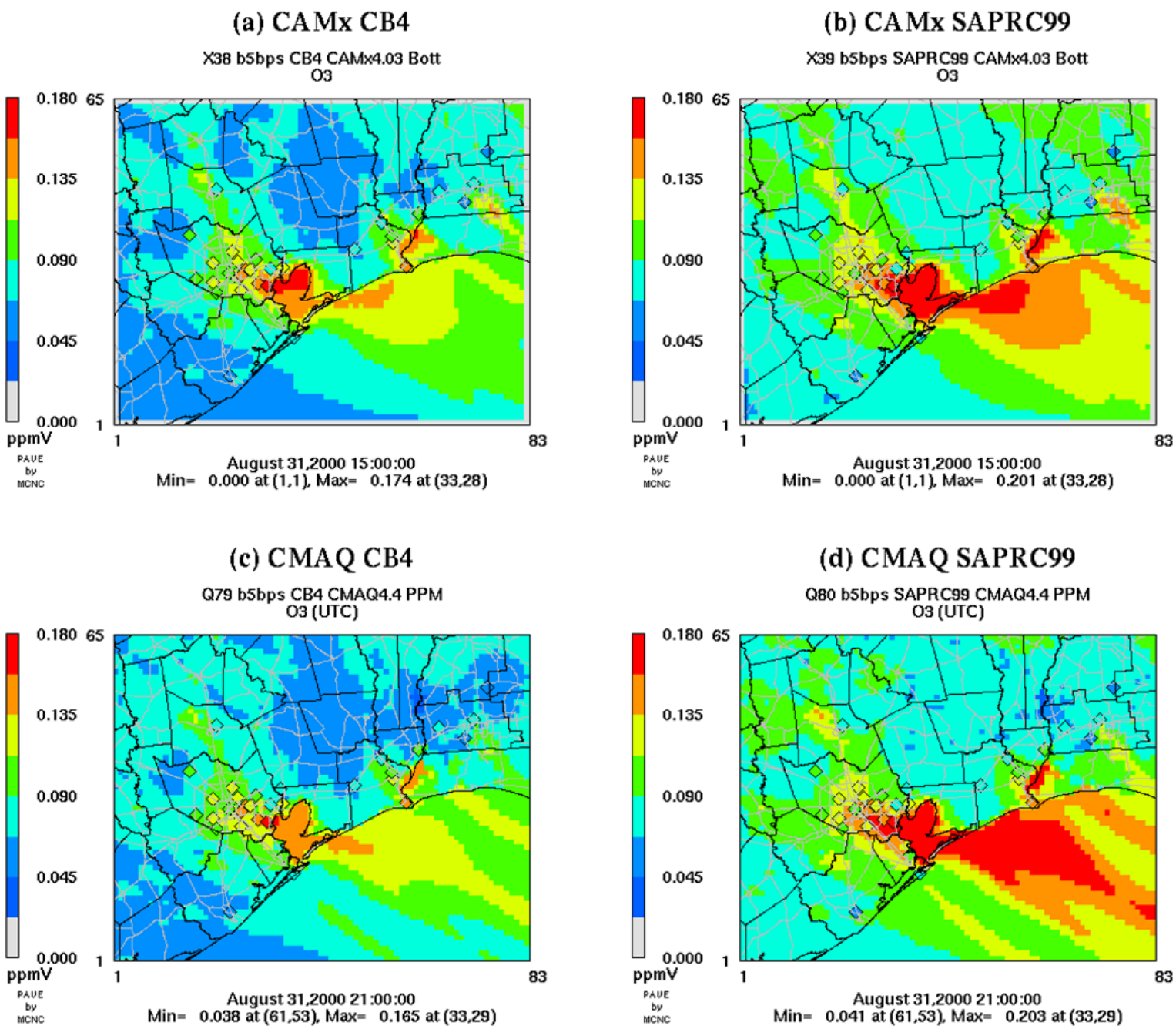
List of CAMx and CMAQ simulations for CB-4and SAPRC99

| Runs | X38 | X39 | Q79 | Q80 |
|---|---|---|---|---|
| Air Quality Model | CAMx 4.03 | CAMx 4.03 | CMAQ 4.4 | CMAQ 4.4 |
| Horizontal Advection | Bott | Bott | PPM | PPM |
| Chemical mechanism | **CB-4** | **SAPRC99** | **CB-4** | **SAPRC99** |
| Anthropogenic emissions | Base5b imputed, SMOKE-processed | | | |

August 25
2000
TEI2000
“imputed”



August 31
2000
TEI2000
“imputed”

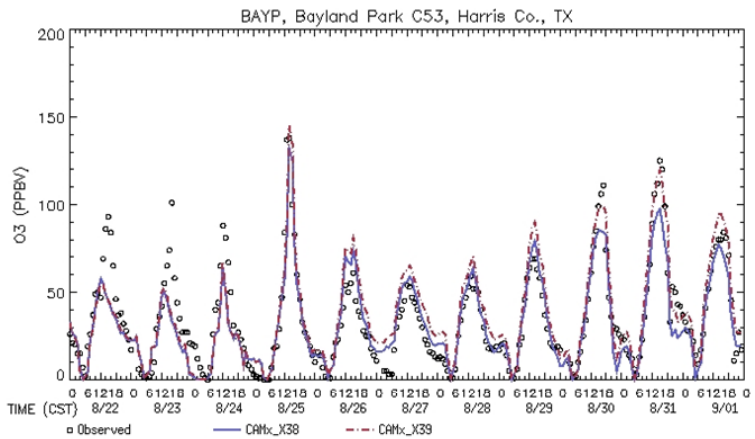


# CAMS Site Comparison: O3

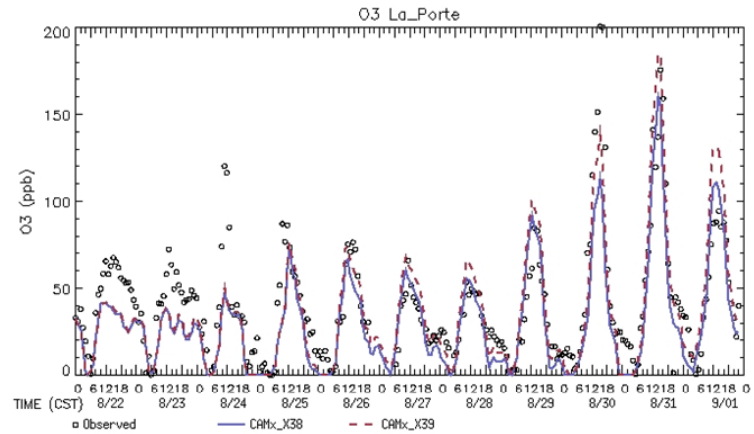
## X38=CB4, X39=SAPRC99, Q79=CB4, Q80=SAPRC99

Smaller difference between mechanism with CAMx

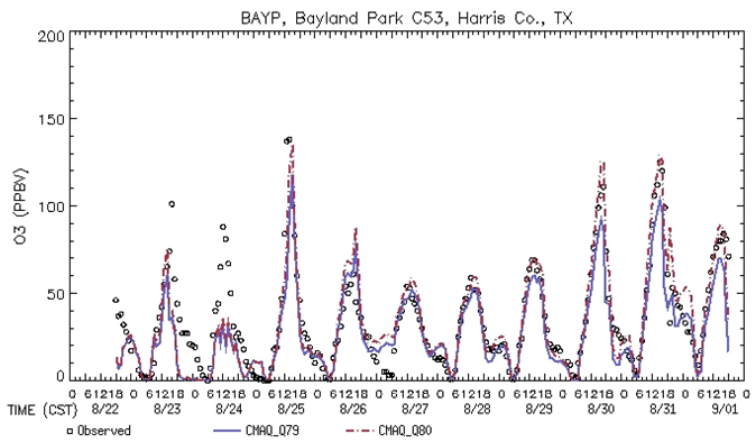
(a) CAMx (X38 & X39)




(c) CAMx (X38 & 39)

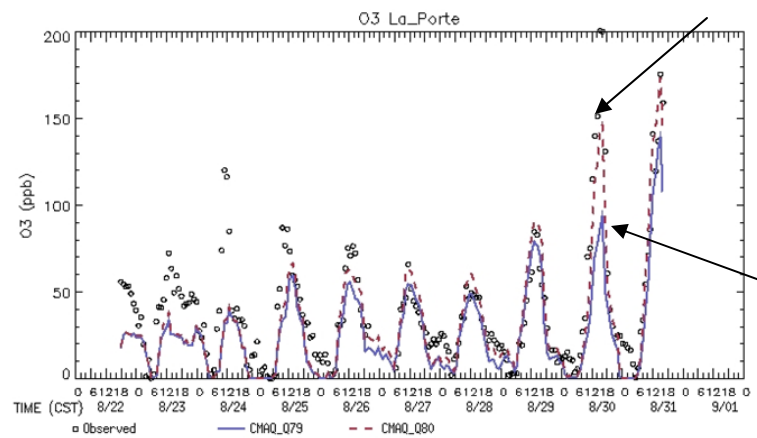



(b) CMAQ (Q79 & Q80)




(d) CMAQ (Q79 & Q80)

SAPRC




CB-4

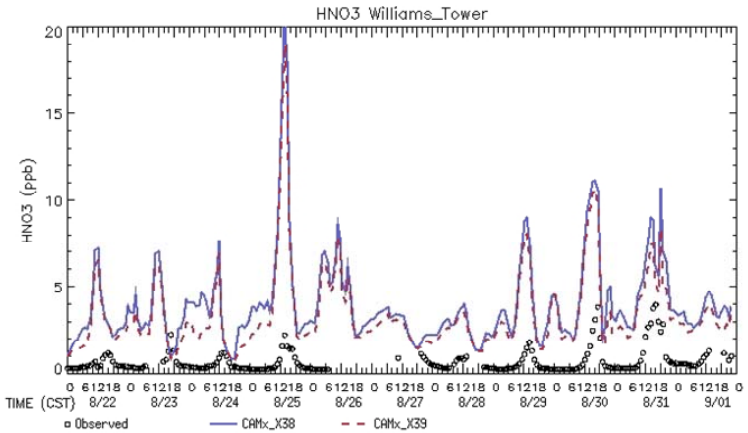
CMAQ at La Porte is very sensitive to the choice of mechanism

# HNO3 & PAN

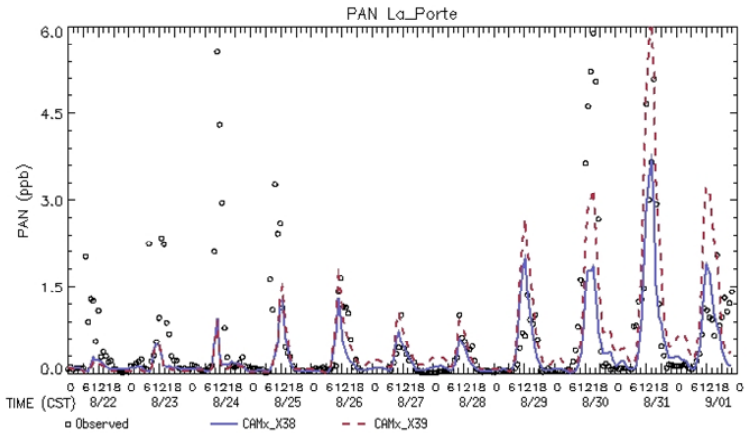
X38=CB4, X39=SAPRC99, Q79=CB4, Q80=SAPRC99

HNO3 CAMx PAN

(a) CAMx (X38 & 39)

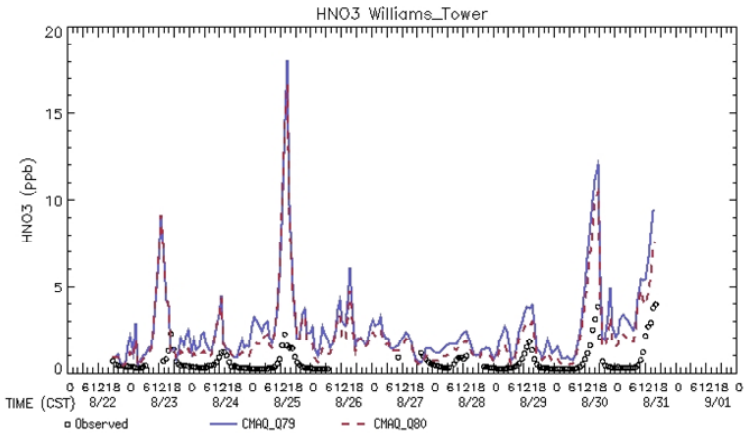



(a) CAMx (X38 & 39)

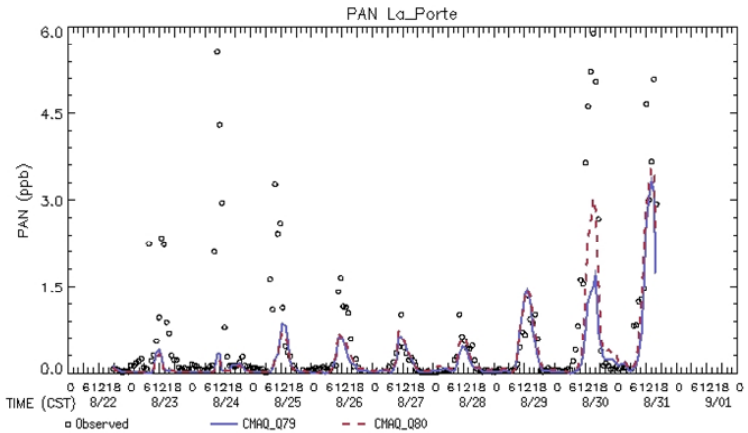



CMAQ

(b) CMAQ (Q79 & Q80)




(b) CMAQ (Q79 & Q80)




- Note: species definitions of PAN for CB-4 and SAPRC are not directly comparable
- SAPRC: HNO3↓ PAN↑

TexAQS 2000 Episode

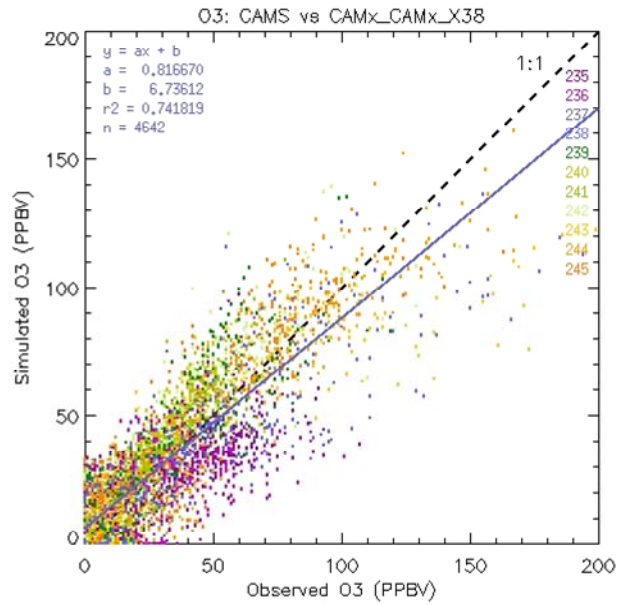
CAMS site

O3 from SAPRC > O3 from CB-4 for

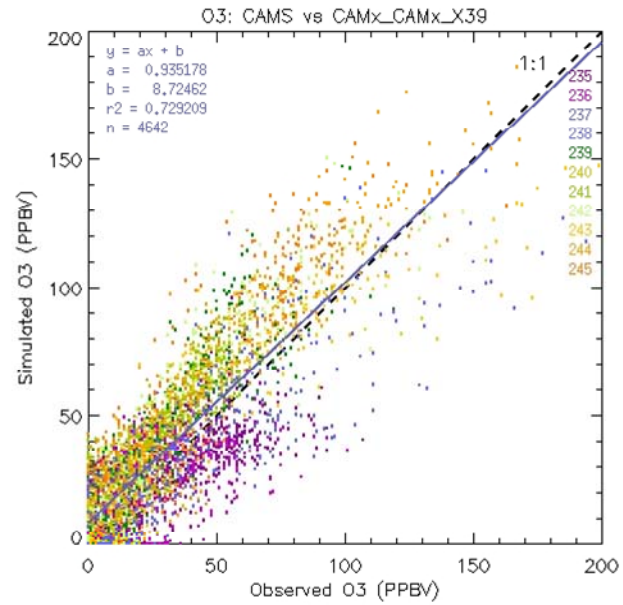
> 100 ppb

SAPRC has tendency of overestimating medium O3 range

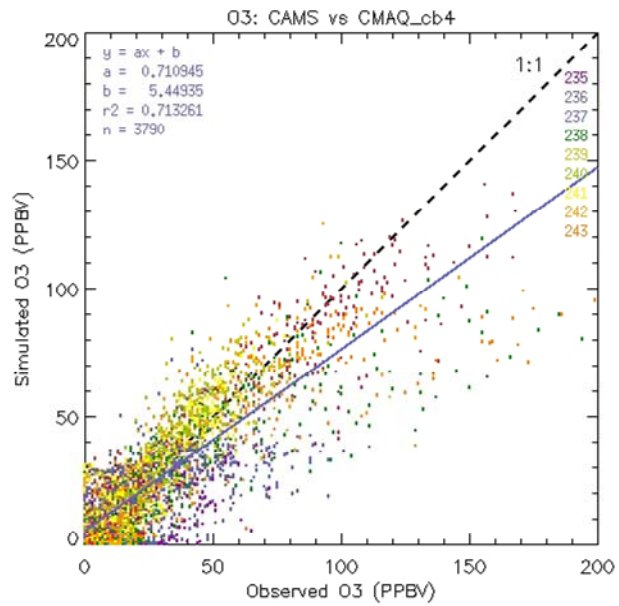
(a) CAMx CB-4



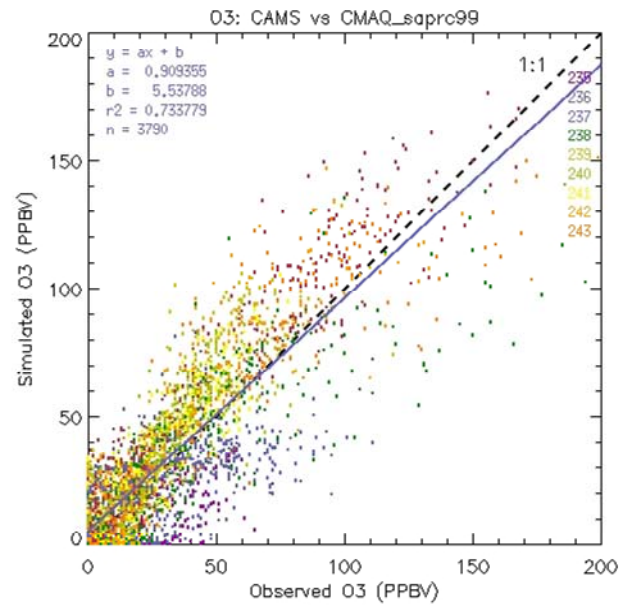

(b) CAMx SAPRC99




(c) CMAQ CB-4

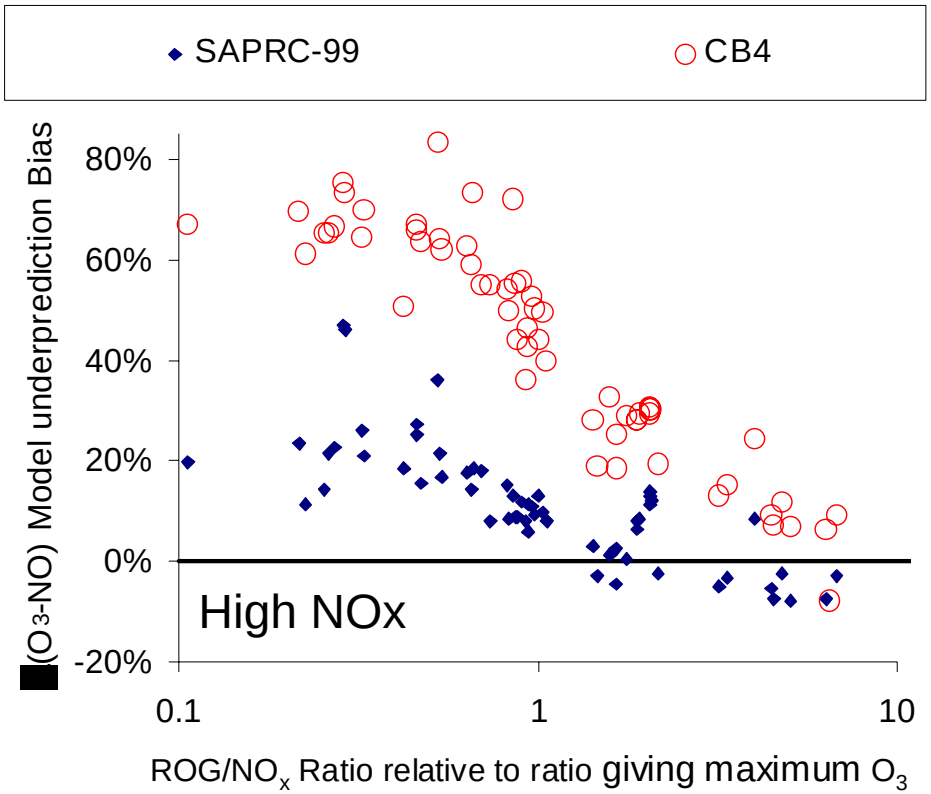



(d) CMAQ SAPRC99



# W.P.L Carter, Low NOx Mechanism Evaluation, Chamber Experiment Results

**COMPARISON OF CB4 AND SAPRC-99**
**MODEL ERRORS FOR UCR EPA SURROGATE RUNS**



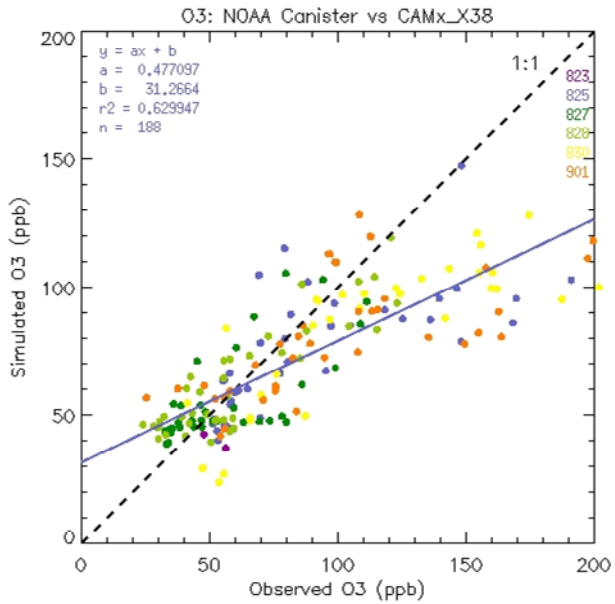

This includes more recent runs carried out for EPA OBM project

Low NOx – SAPRC shows slight overprediction

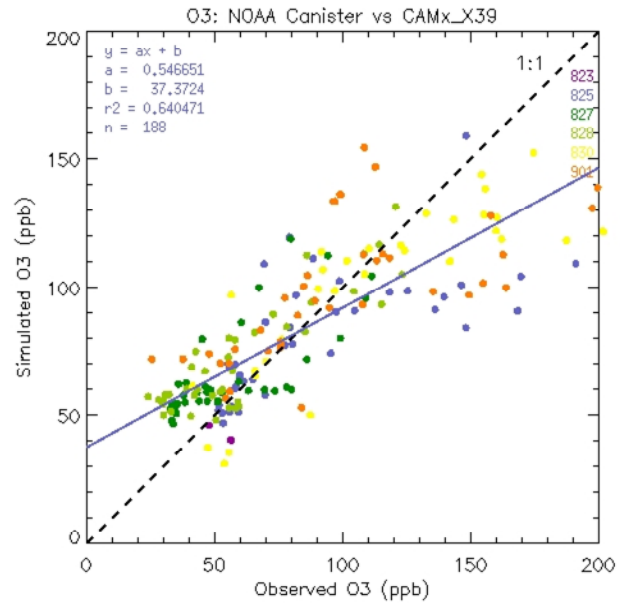
TexAQS 2000 Episode

NOAA Aircraft Canister

(a) CAMx CB-4

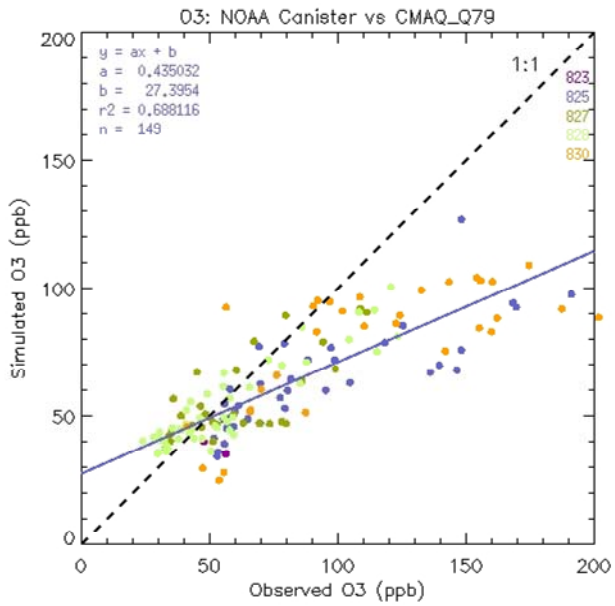



(b) CAMx SAPRC99

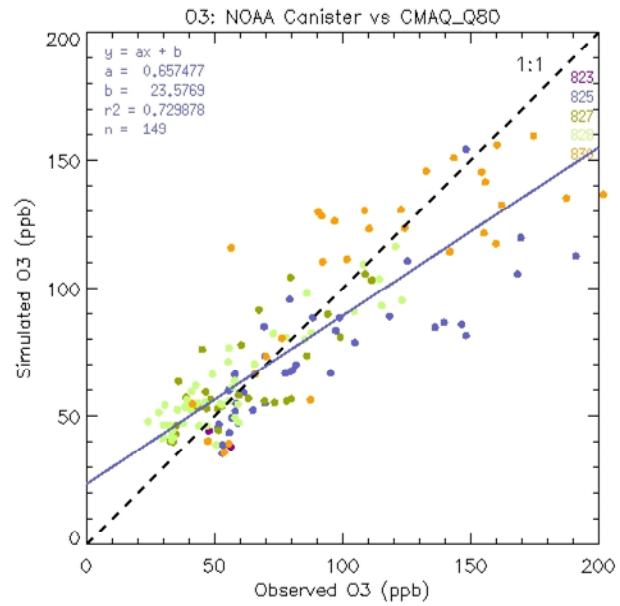



Improvement of high O3 predicted by SAPRC more pronounced with CMAQ

(c) CMAQ CB-4




(d) CMAQ SAPRC99

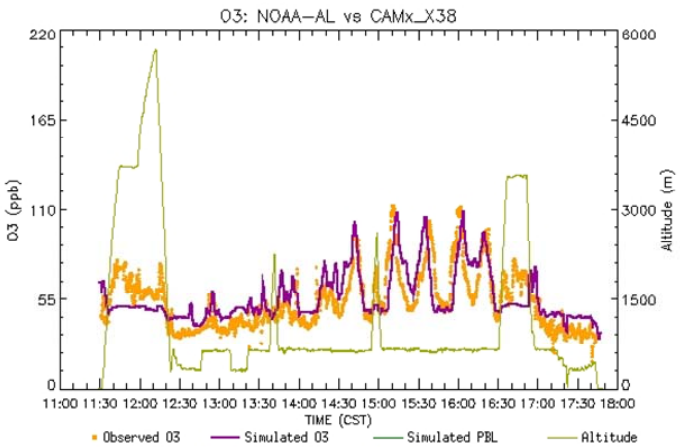


TexAQS 2000 Episode

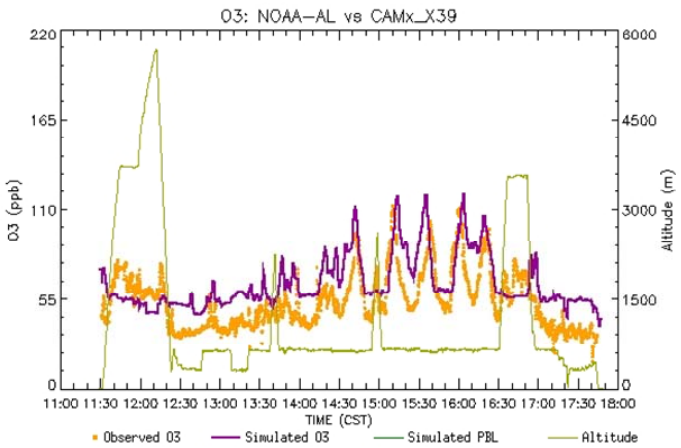
NOAA Aircraft

Ozone

(a) CAMx CB-4

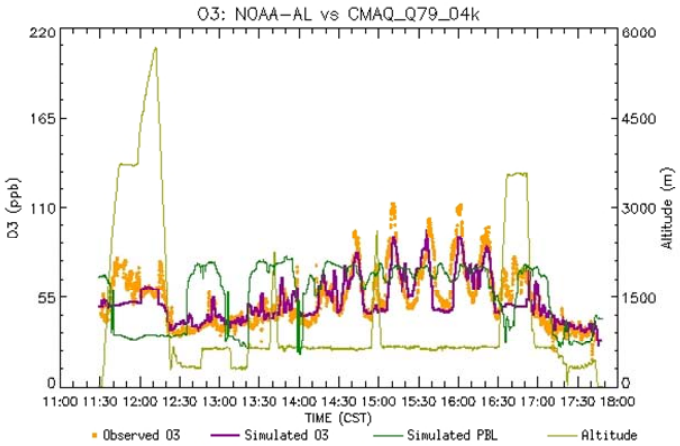



(b) CAMx SAPRC99

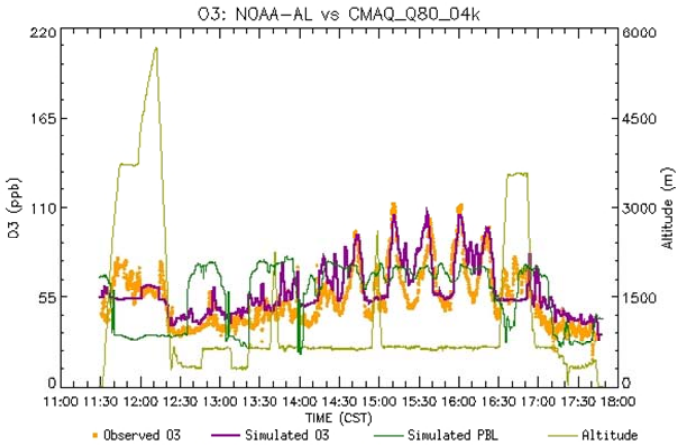



CAMx with CB-4 well simulated O3 peak but overpredicted with SAPRC

(c) CMAQ CB-4




(d) CMAQ SAPRC99



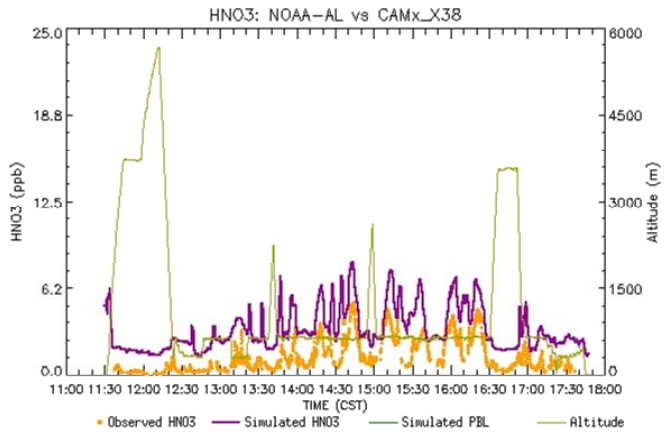

CMAQ with CB-4 underestimated O3 peak but well predicted with SAPRC

TexAQS 2000 Episode

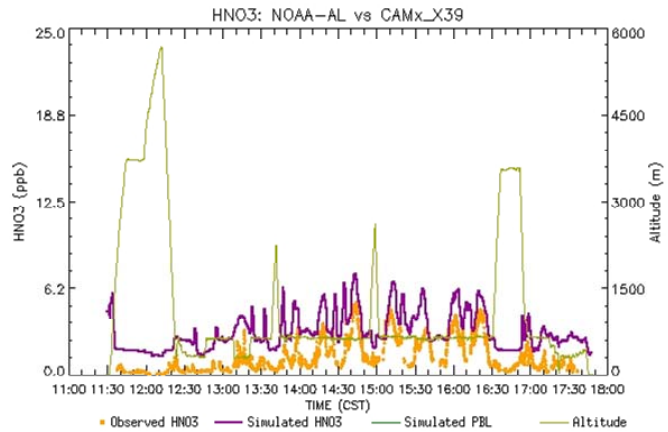
NOAA Aircraft

HNO3

(a) CAMx CB-4

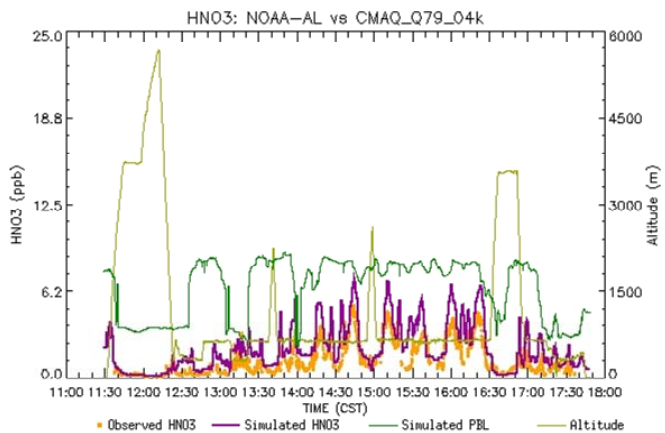



(b) CAMx SAPRC99

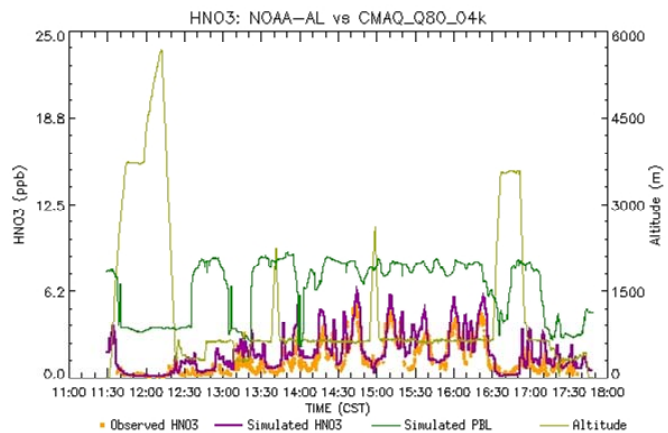



CAMx with CB-4 and SAPRC both overpredicted HNO3, including the background

(c) CMAQ CB-4

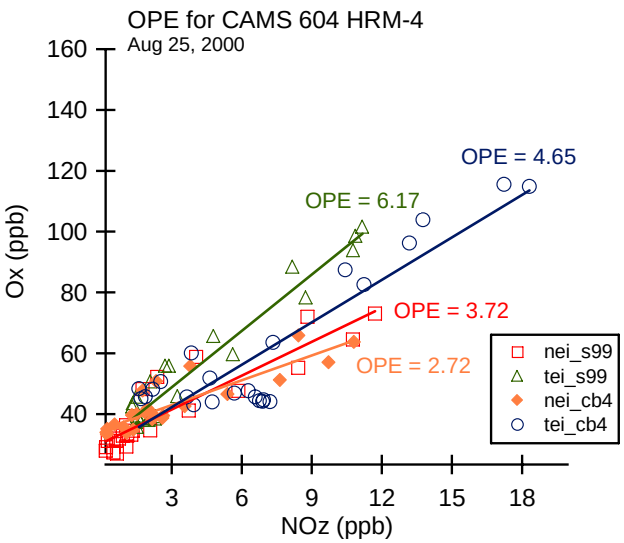


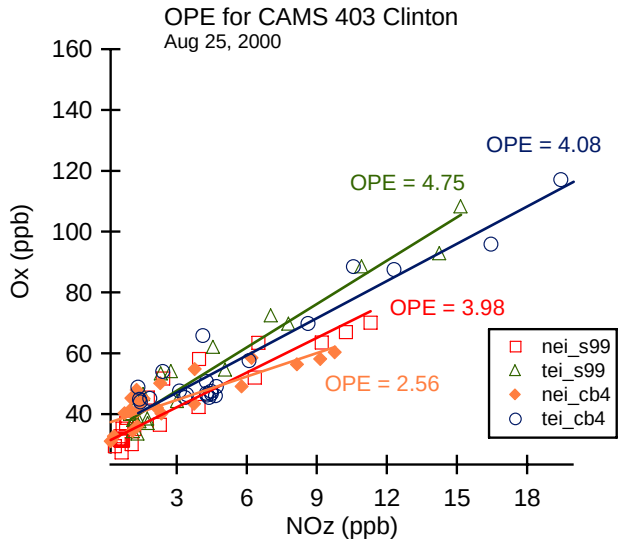

(d) CMAQ SAPRC99



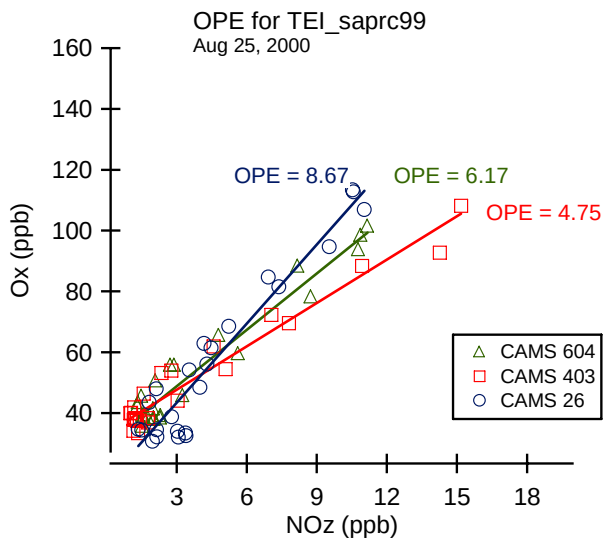

CMAQ with CB-4 overpredicted HNO3 slightly, but SAPRC compared well with obs.

# Ozone production efficiency for Aug. 25, 2000




CMAQ with NEI99, TEI 4a emissions



# 2006 simulations

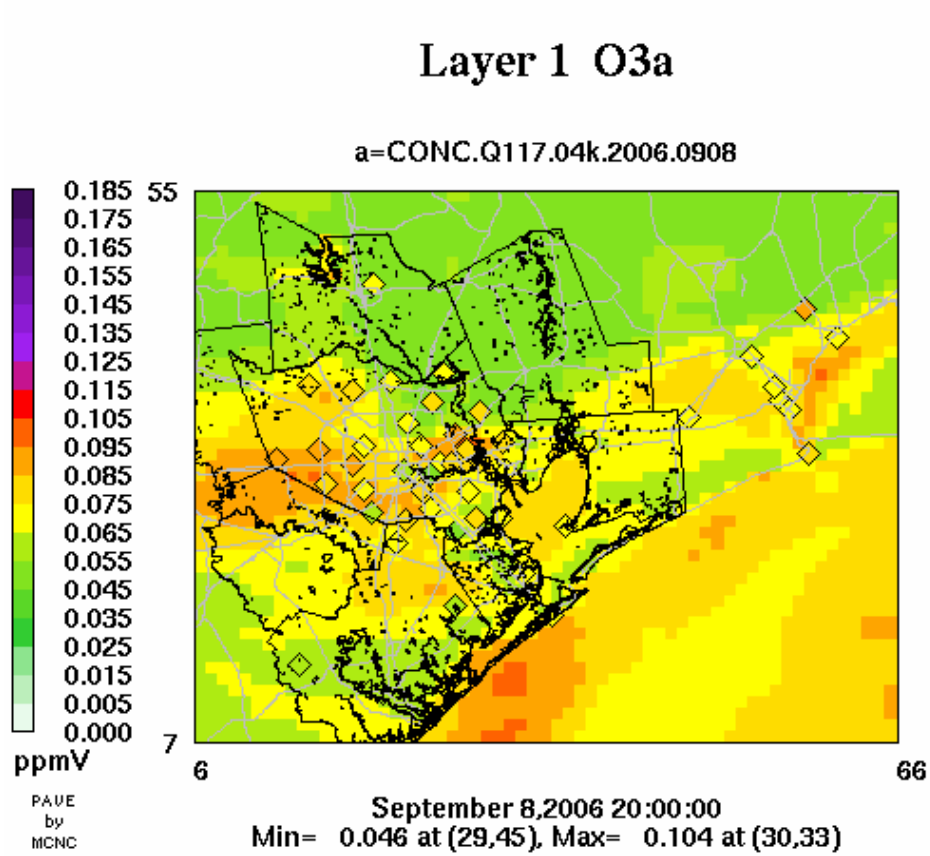
Purpose 1: To compare CMAQ simulations for CB4 and SAPRC99

Purpose 2: To compare CMAQ simulations for base year EI and projected EI (lower NOx) for 2005

CB4_B (Q117): CMAQ4.4, CB4, Base year EI (2000)
S99_B (Q118): CMAQ4.4, SAPRC99, Base year EI (2000)
CB4_P (Q119): CMAQ4.4, CB4, Projected EI for 2005

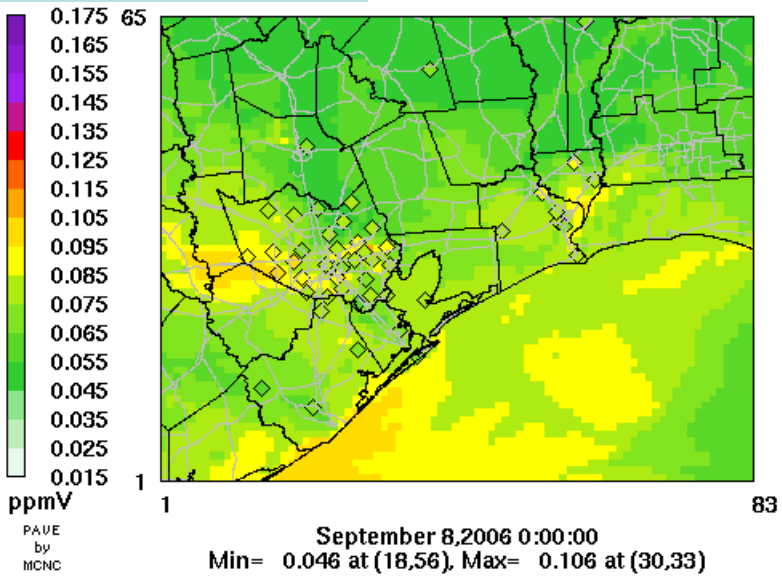
AQF: F1

- Dates: September 6th ~ 9th, 2006
- Domain: HGBPA 4-km domain
- MCIP: AQF F1 MCIP

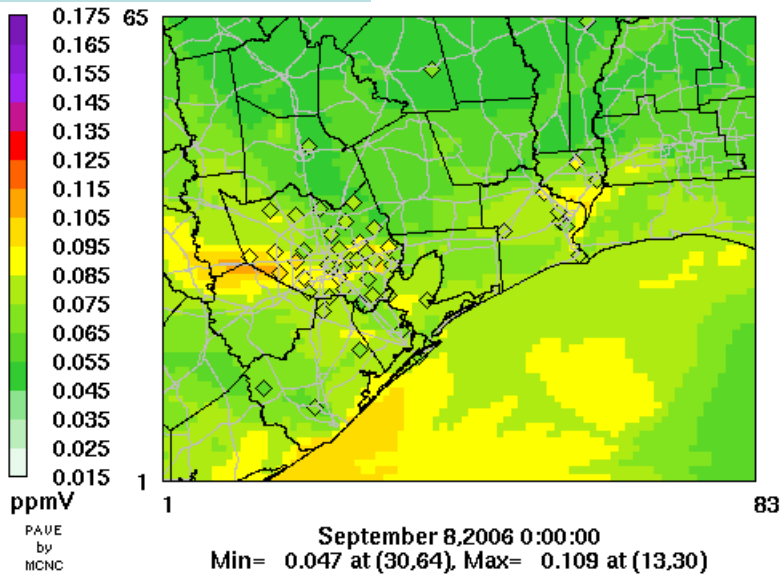


# Daily max 1-hr O3 for September 8th, 2006

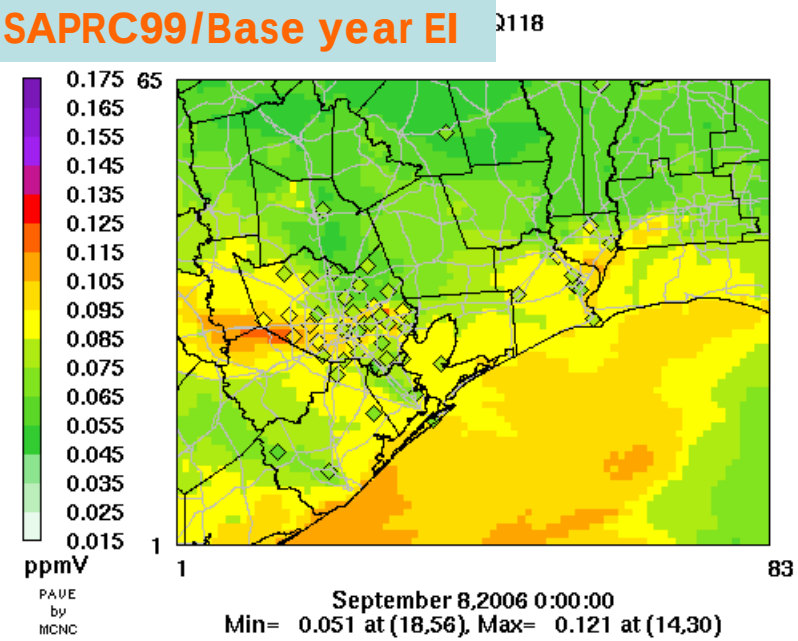
**CB4/Base year EI**




**CB4/Projected EI**



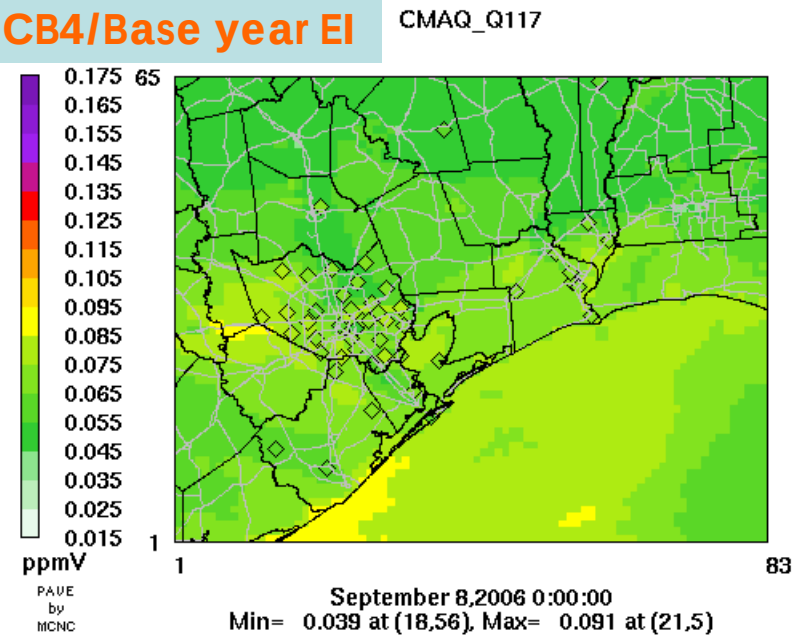

**SAPRC99/Base year EI**



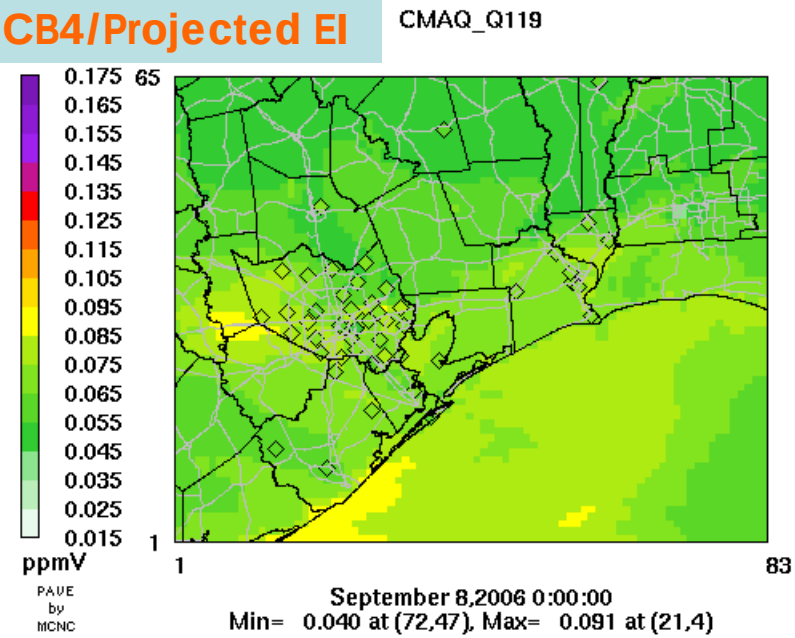

- CB4_B: 106 ppb
- SAPRC99_B: 121 ppb
- CB4_P: 109 ppb

# Daily max 8-hr O3 for September 8th, 2006

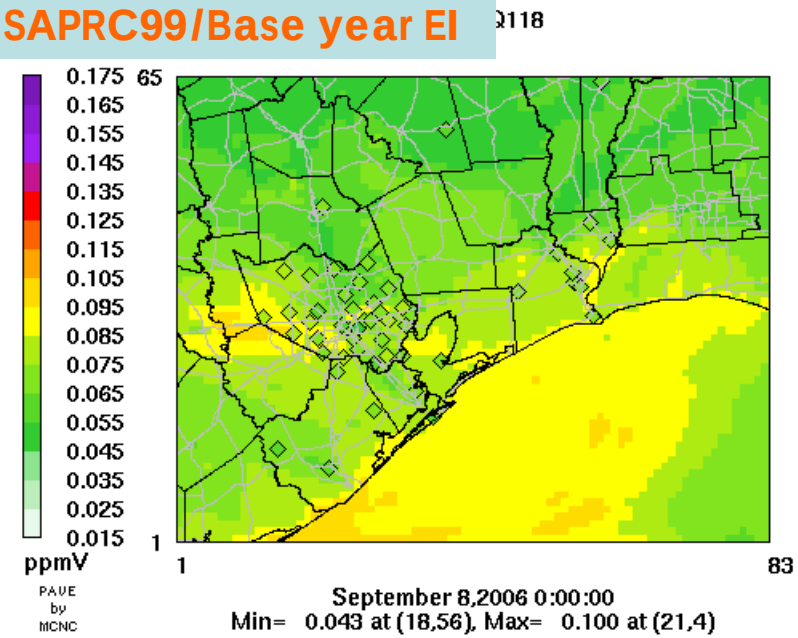
**CB4/Base year EI**




**CB4/Projected EI**



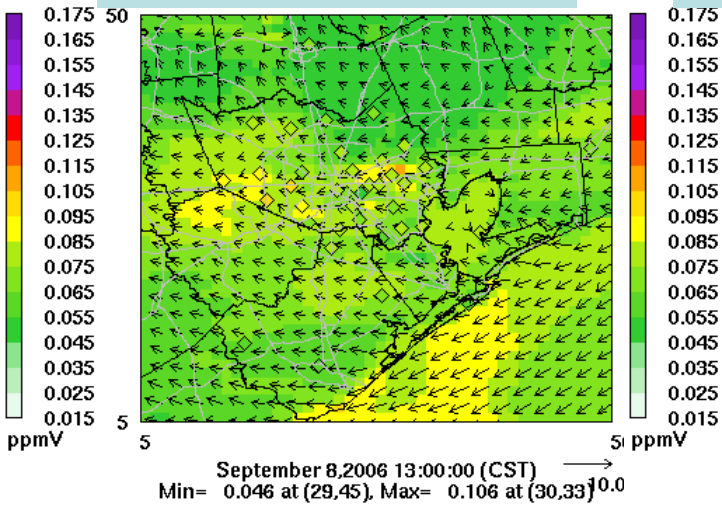

**SAPRC99/Base year EI**



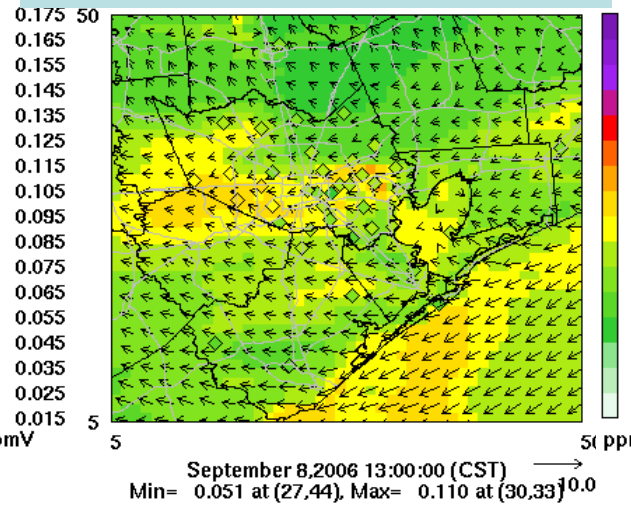

- CB4_B: 91 ppb
- SAPRC99_B: 100 ppb
- CB4_P: 91 ppb

# 1-hr O3 for September 8th, 2006 at 13 CST

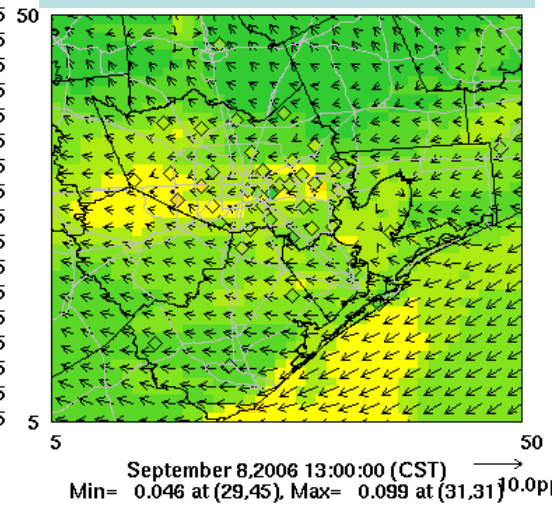
**(a) CB4/Base year EI**




**(b) SAPRC99/Base year EI**



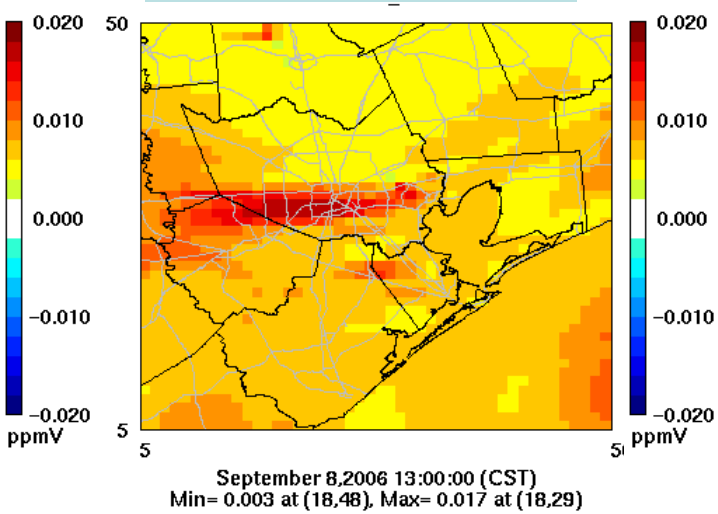

**(c) CB4/Projected EI**



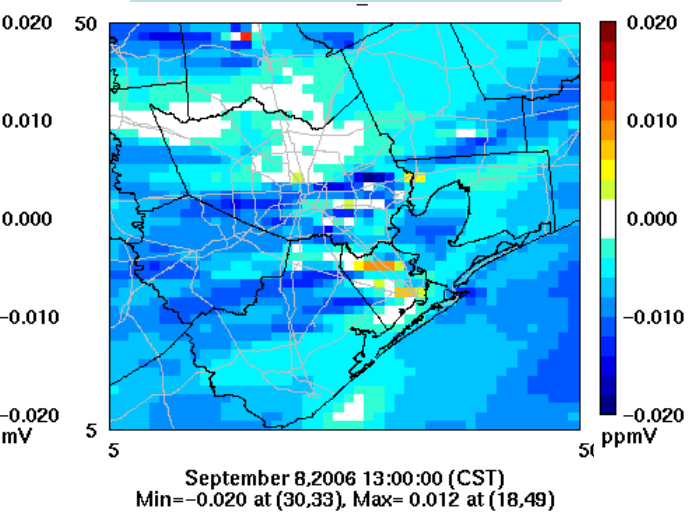

SAPRC99 predicted ~ 10 ppb higher O3 over downtown Houston.

Reduced NOx emissions from point sources.

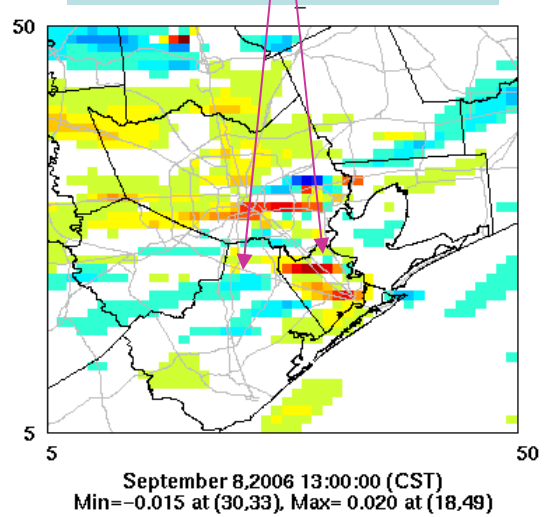
**Difference (b) - (a)**




**Difference (c) – (b)**



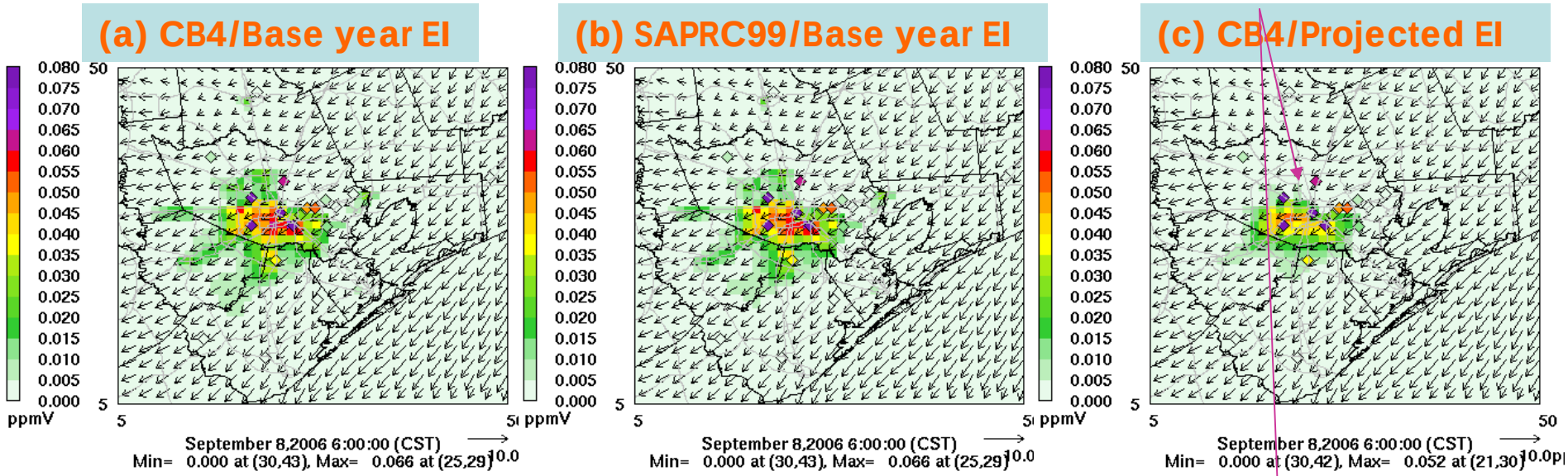

**Difference (c) – (a)**



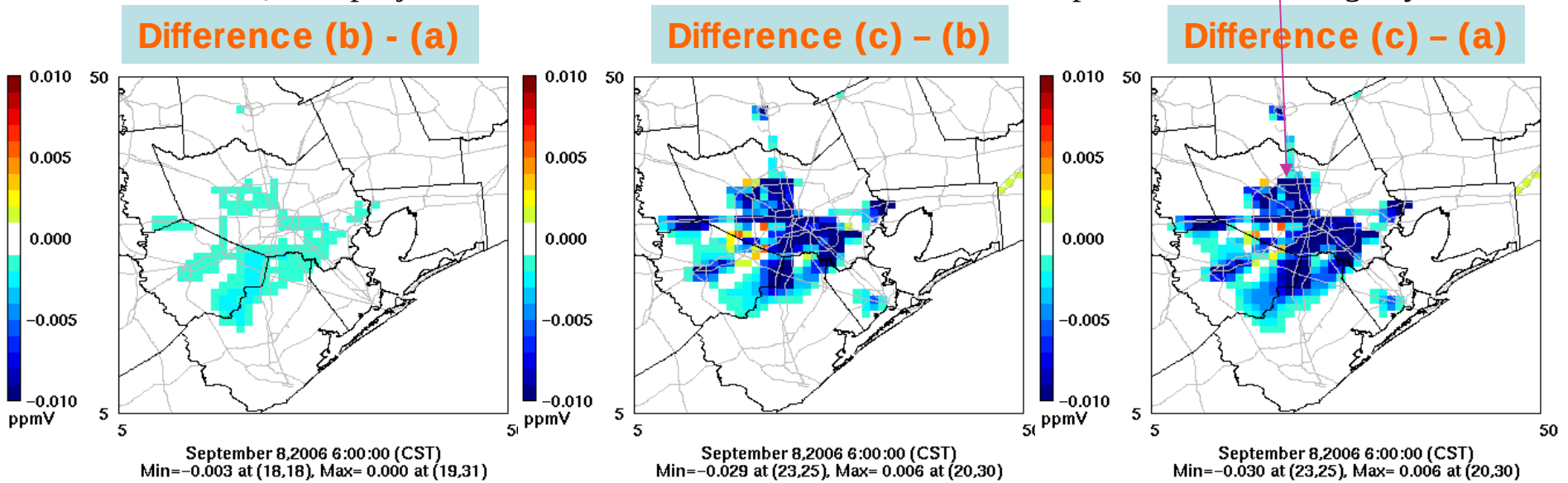
# 1-hr NO for September 8th, 2006 at 06 CST

In early morning, mobile source is dominant.

Lower NO concentrations predicted w/ projected EI.

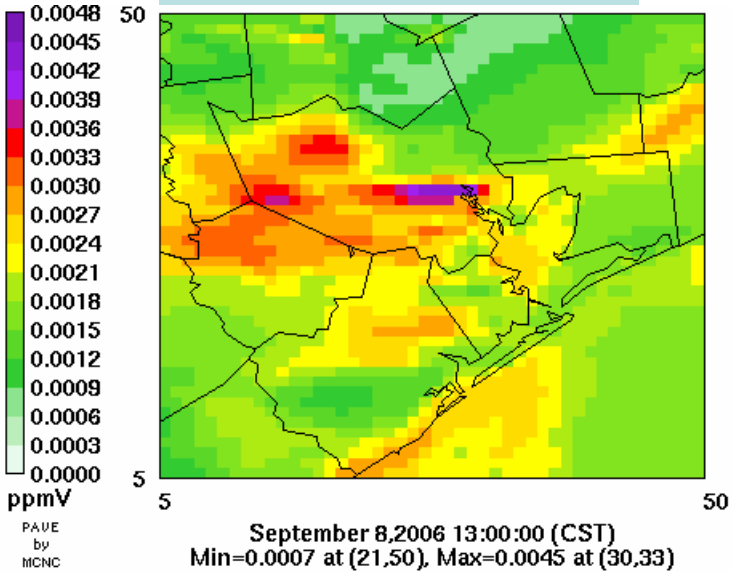



CMAQ with projected EI shows lower NO concentrations from point sources during daytime.

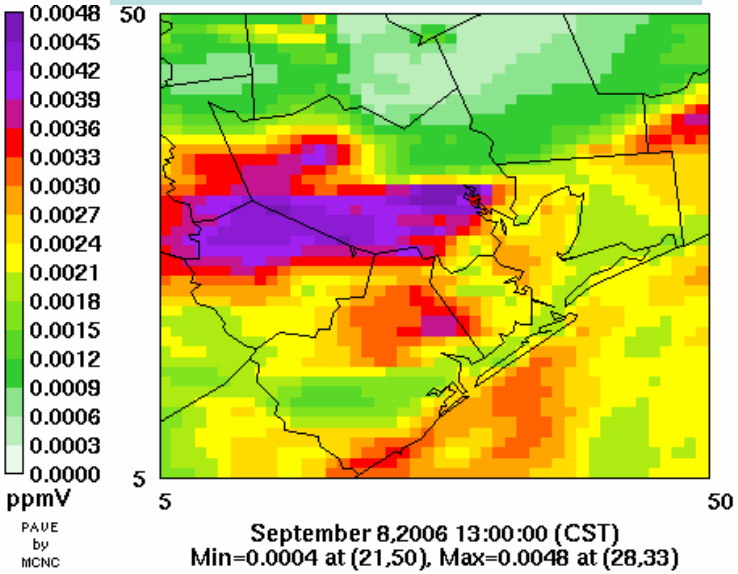


# 1-hr PAN for September 8th, 2006 at 13 CST

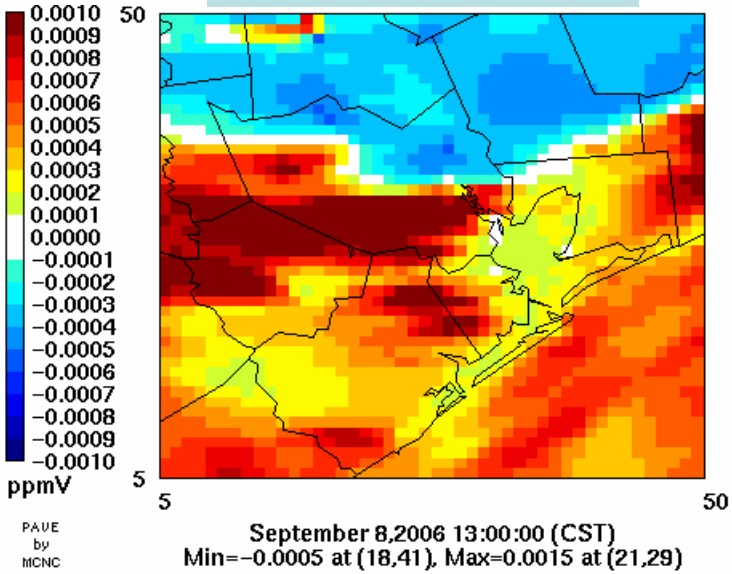
**(a) CB4/Base year EI**




**(b) SAPRC99/Base year EI**



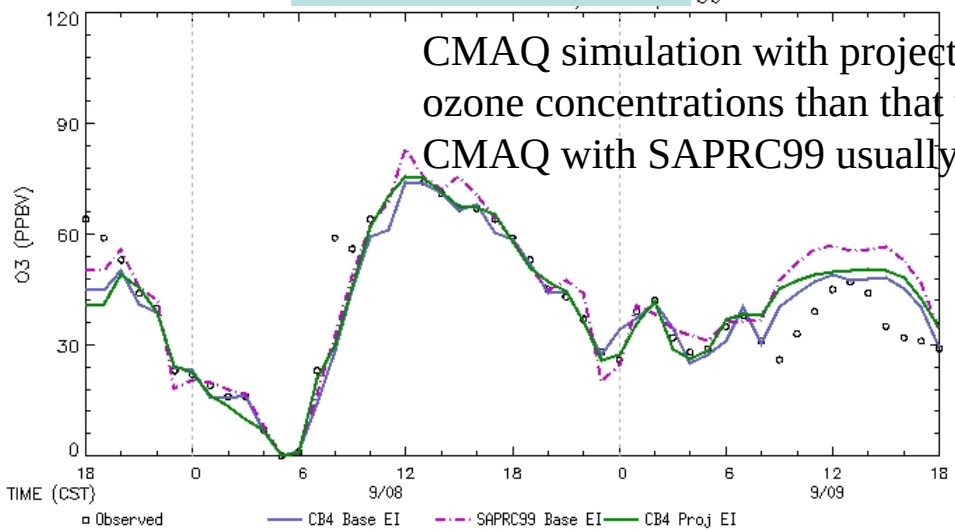

**Difference (b) - (a)**



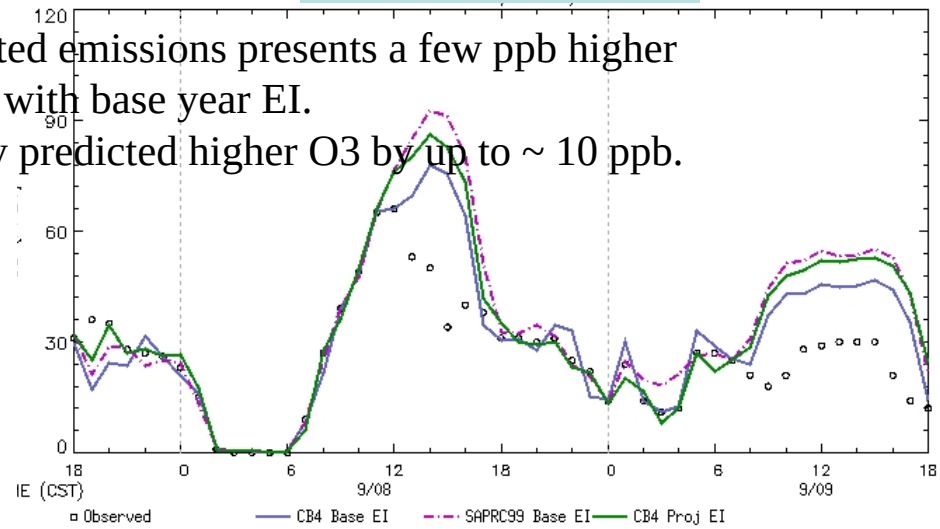
# Ozone concentrations at CAMS sites

CMAQ simulation with projected emissions presents a few ppb higher ozone concentrations than that with base year EI.
CMAQ with SAPRC99 usually predicted higher O3 by up to ~ 10 ppb.

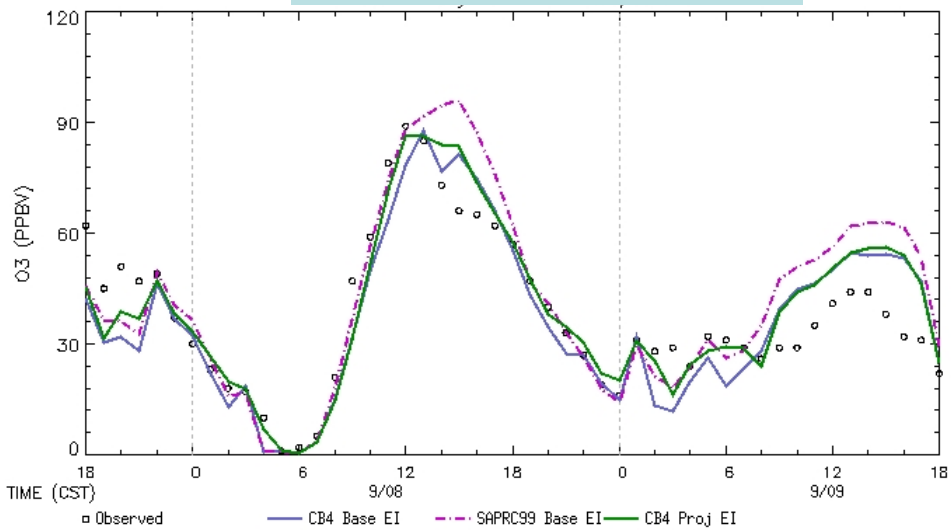
**Deer Park C35**



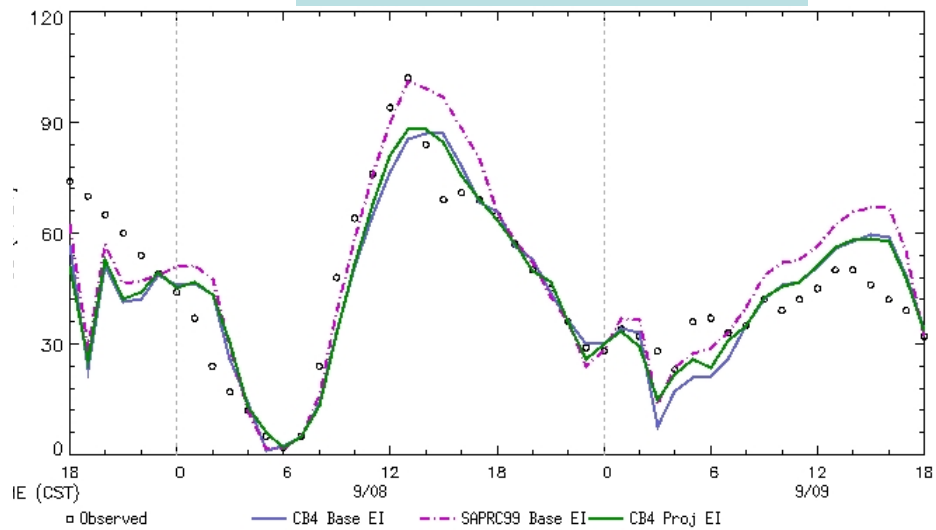

**Clinton C403**




**Bayland Park C53**



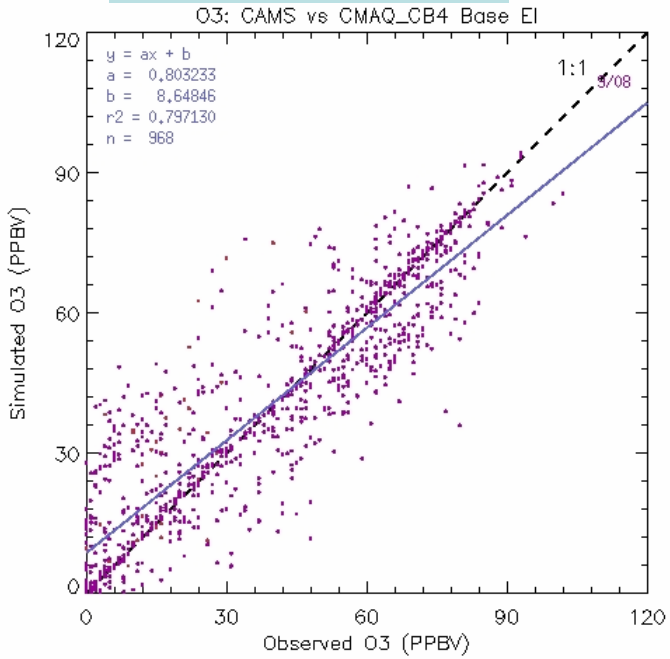

**Westhollow C410**



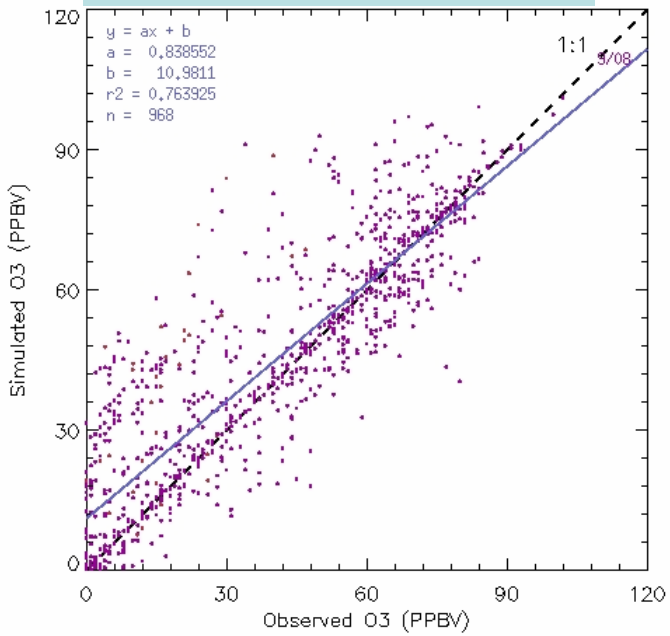
# 1-hr O3 Concentrations

September 8, 2006

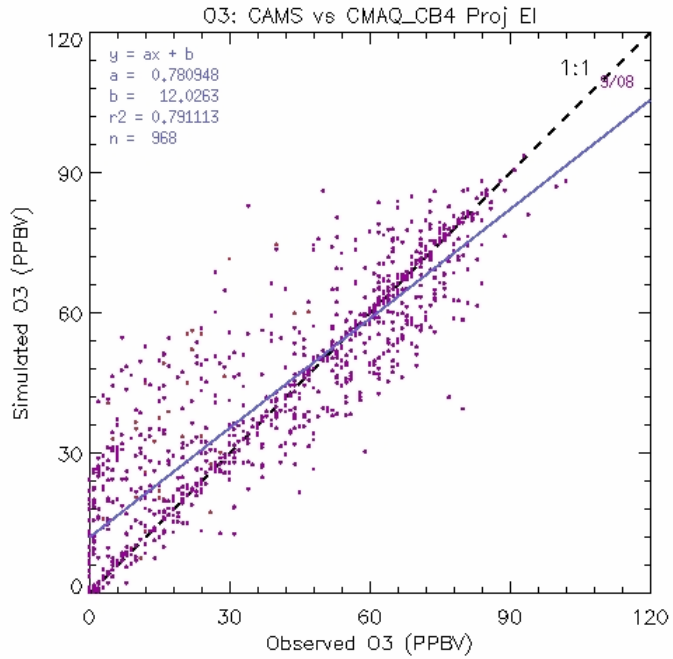
**CB4/Base year EI**




**SAPRC99/Base year EI**




**CB4/Projected EI**

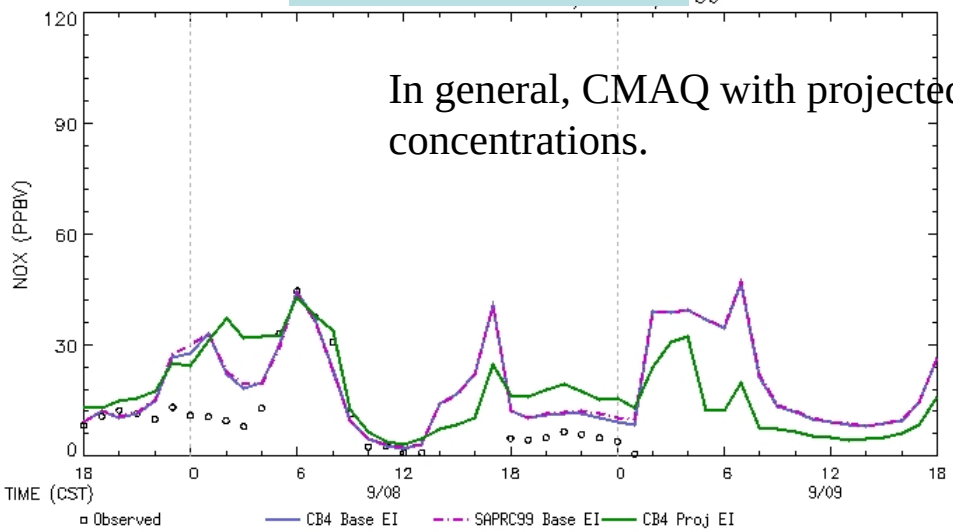



- CB4_B: $R^2$=0.797, Slope=0.80
- SAPRC99_B: R2=0.764, Slope=0.84
- CB4_P: R2=0.781, Slope=0.79

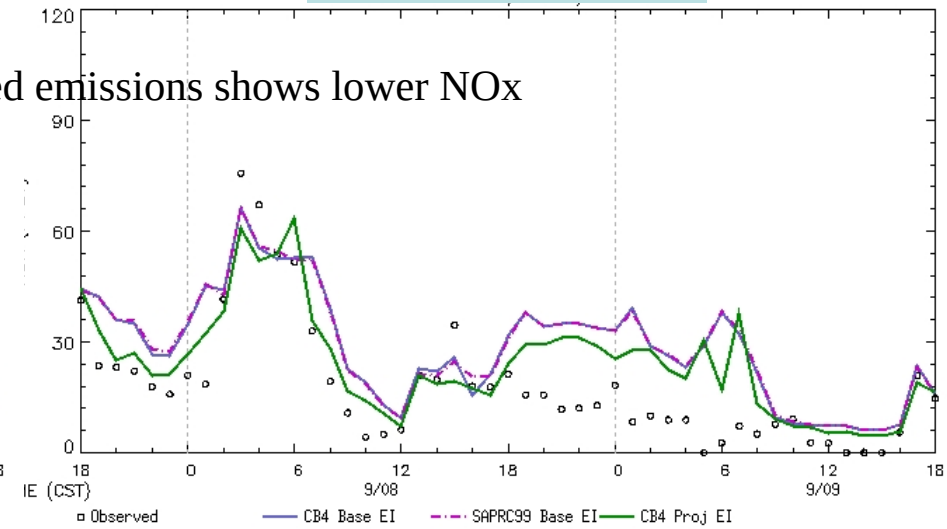
# NOx concentrations at CAMS sites

In general, CMAQ with projected emissions shows lower NOx concentrations.

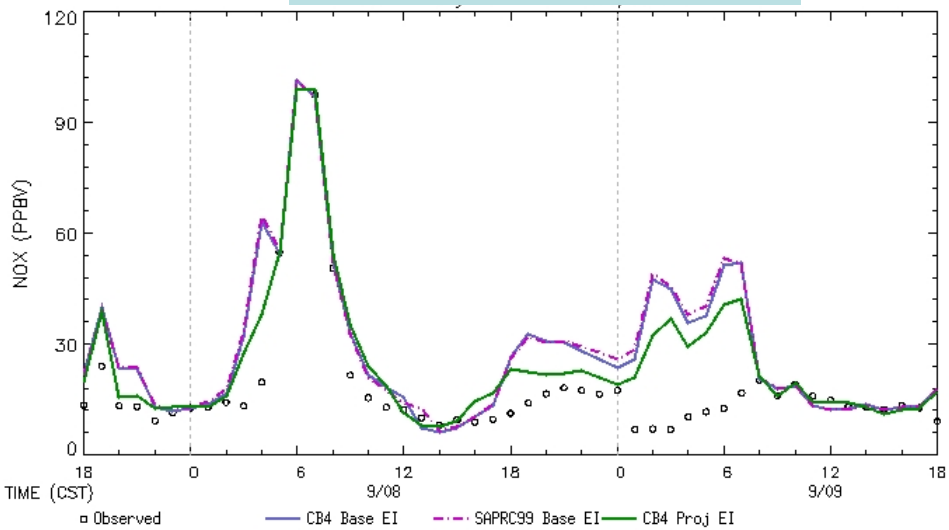
**Deer Park C35**



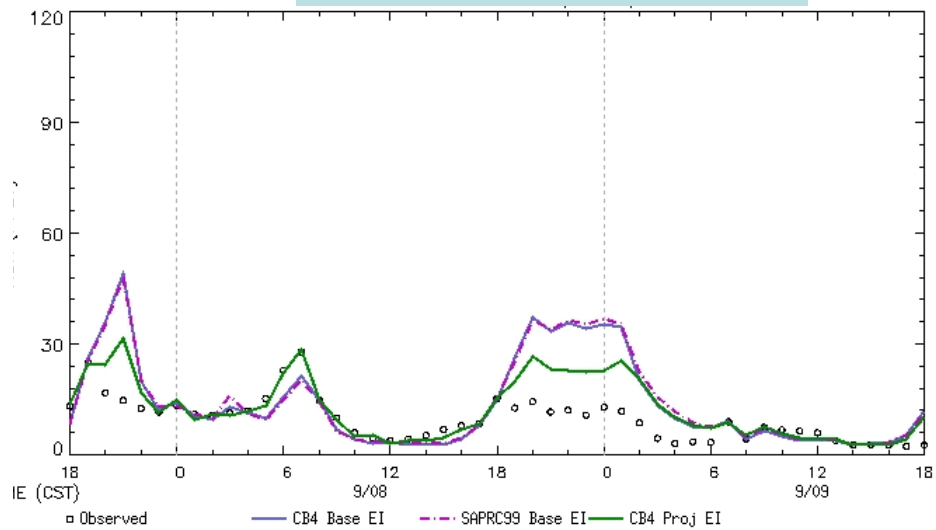

**Clinton C403**




**Bayland Park C53**

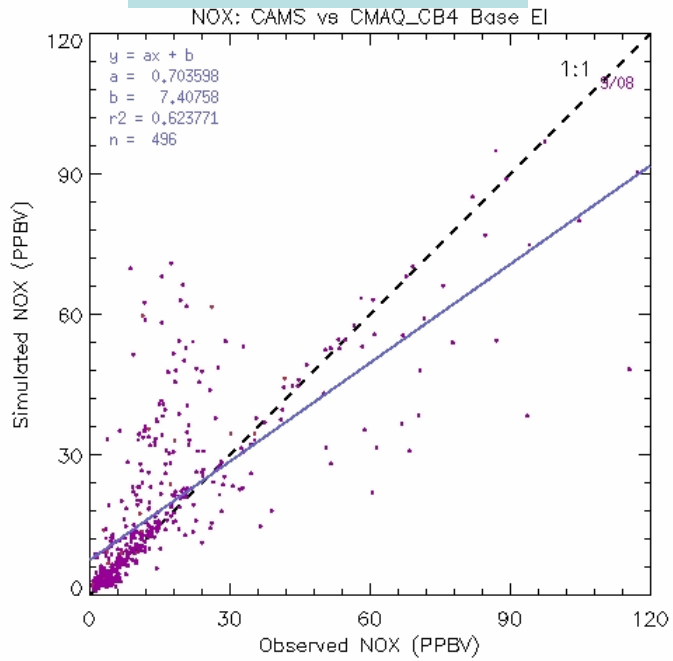



**Northwest Harris C26**

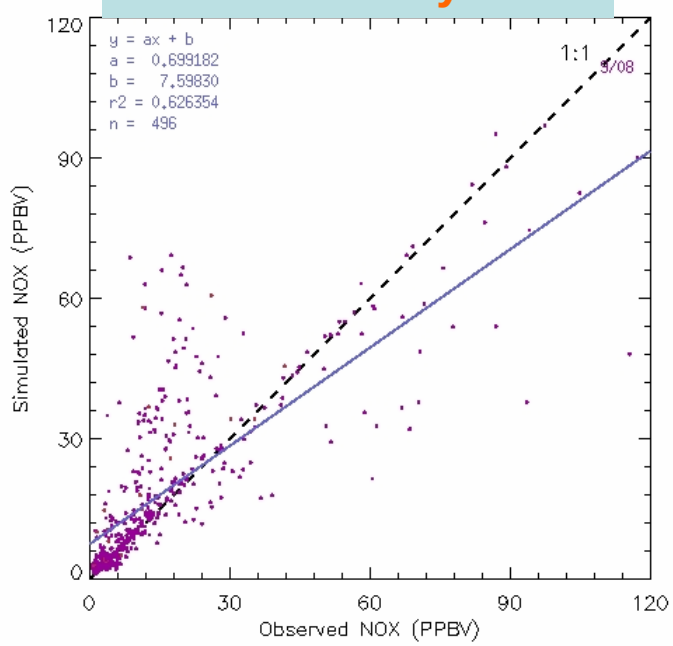


# 1-hr NOx Concentrations

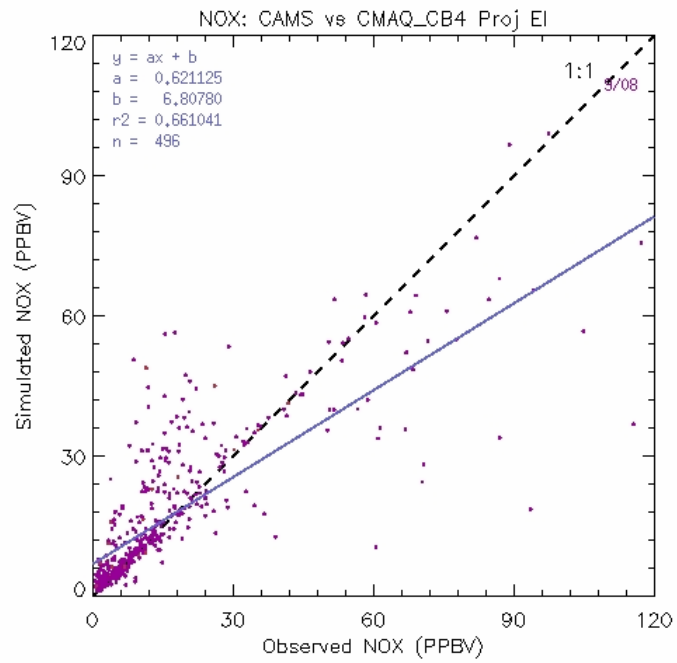
**CB4/Base year EI**




**SAPRC99/Base year EI**




**CB4/Projected EI**




1. CB4 and SAPRC99 simulations with base year EI doesn't show appreciable difference in NOx concentrations predicted.

2. Simulation with projected EI presents reduced high NOx bias

# Summary (Houston)

- 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

- 2006 results with SAPRC with projected inventory not yet available.

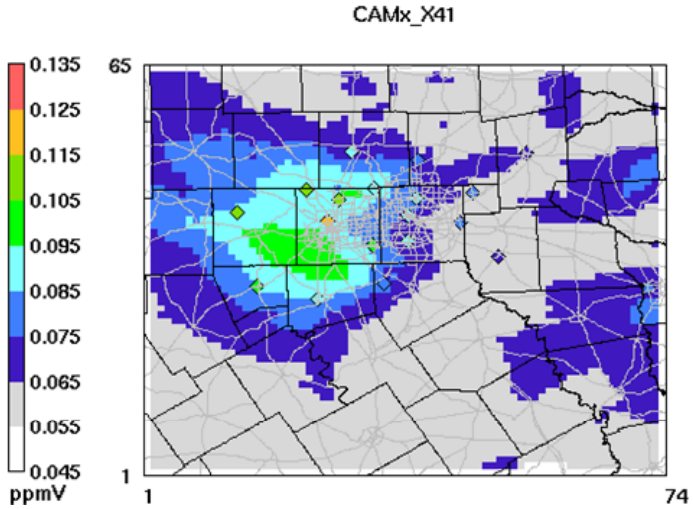
# Dallas 2005 (preliminary)

**Table** CAMx and CMAQ base simulations for 2005

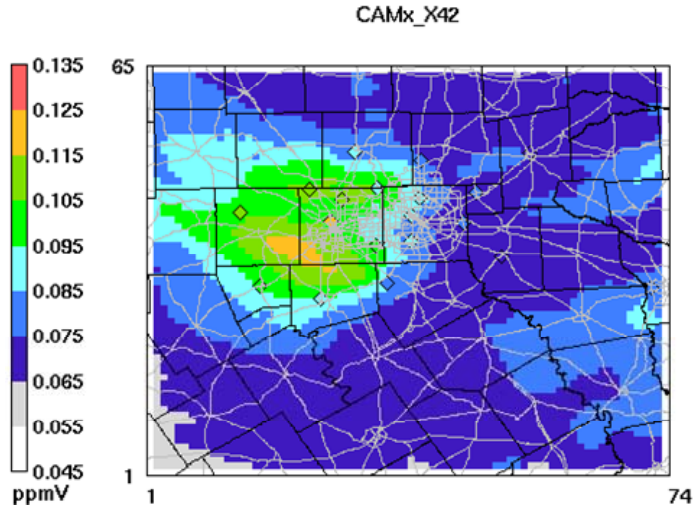
| Run | Description |
|---|---|
| X41 | CAMx 4.31, CB4, TAMU MM5, June 18 ~ June 23, 2005 |
| X42 | CAMx 4.31, SAPRC99, TAMU MM5, June 18 ~ June 23, 2005 |
| X43 | CAMx 4.31, CB4, TAMU MM5, August 30 ~ September 9 2005 |
| X44 | CAMx 4.31, SAPRC99, TAMU MM5, August 30 ~ September 9 2005 |
| Q84 | CMAQ 4.4, CB4, TAMU MM5, June 19 ~ June 23, 2005 |
| Q85 | CMAQ 4.4, SAPRC99, TAMU MM5, June 19 ~ June 23, 2005 |
| Q86 | CMAQ 4.4, CB4, TAMU MM5, August 31 ~ September 9 2005 |
| Q87 | CMAQ 4.4, SAPRC99, TAMU MM5, August 31 ~ September 9 2005 |

June 21, 2005

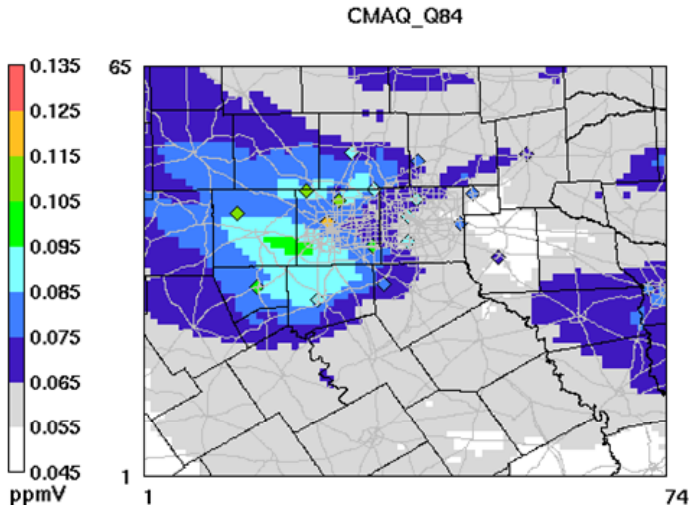
(a) CAMx CB4




(b) CAMx SAPRC99




(c) CMAQ CB4




(d) CMAQ SARPC99

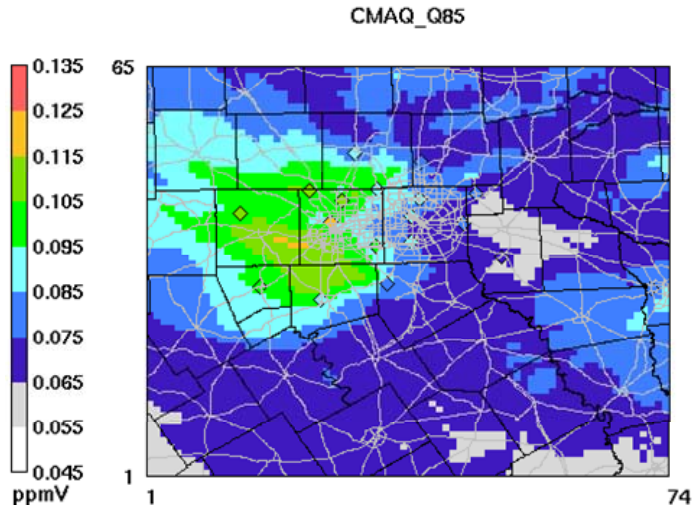
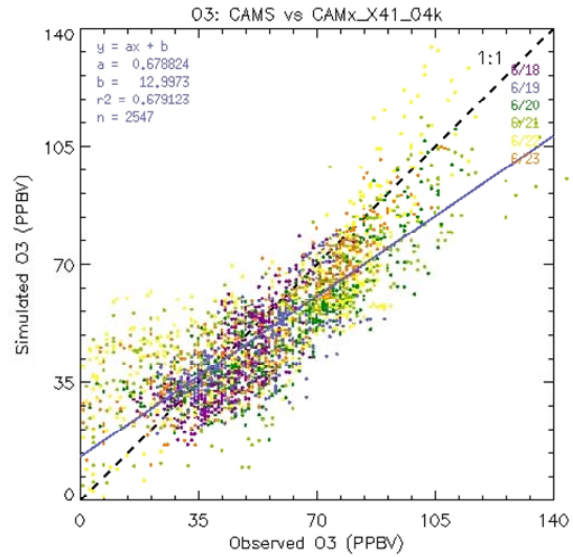


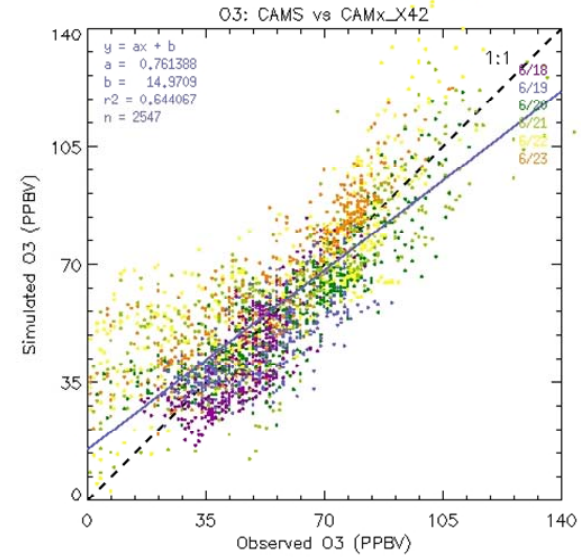

**Figure** Daily maximum 8-hr $O_3$ concentrations predicted by (a) CAMx CB4, (b) CAMx SAPRC99, (c) CMAQ CB4, and (d) CMAQ SAPRC99 for June 21$^{st}$, 2005.

Dallas
June 18-23, 2005

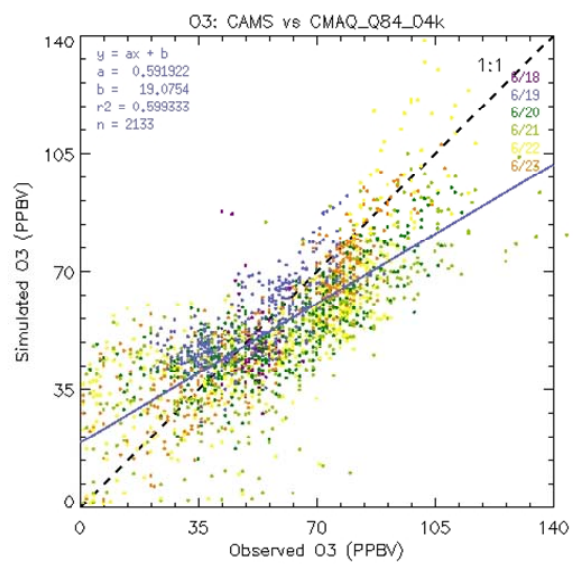
(a) CAMx CB4




(b) CAMx SAPRC99




(c) CMAQ CB4




(d) CMAQ SAPRC99

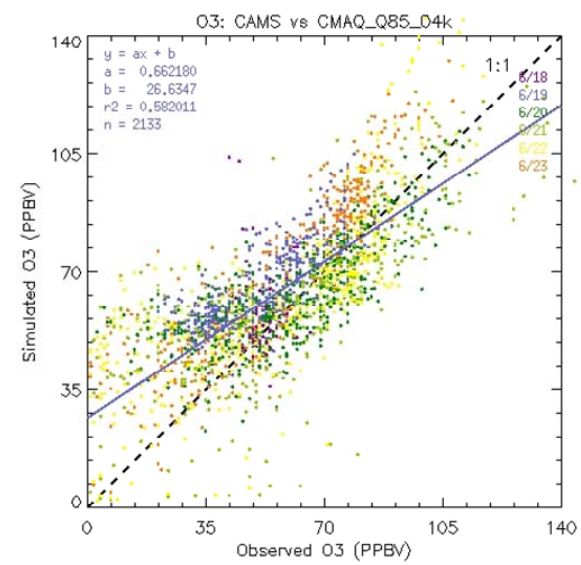
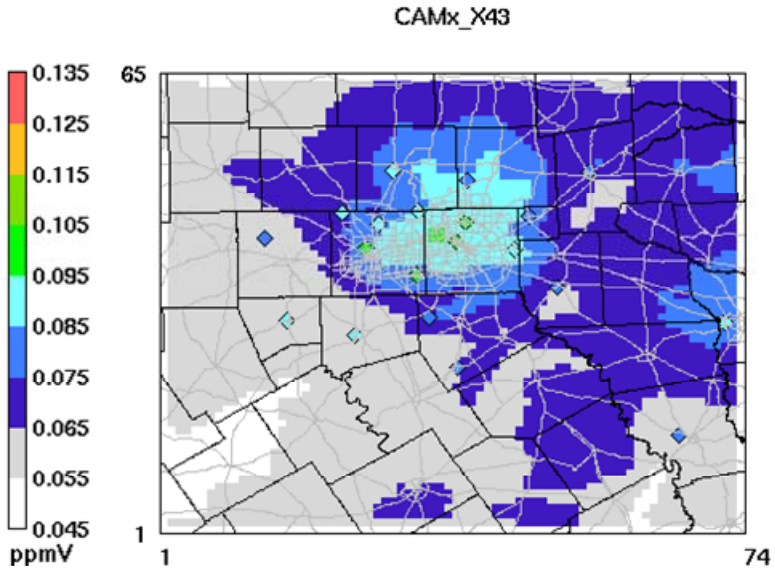


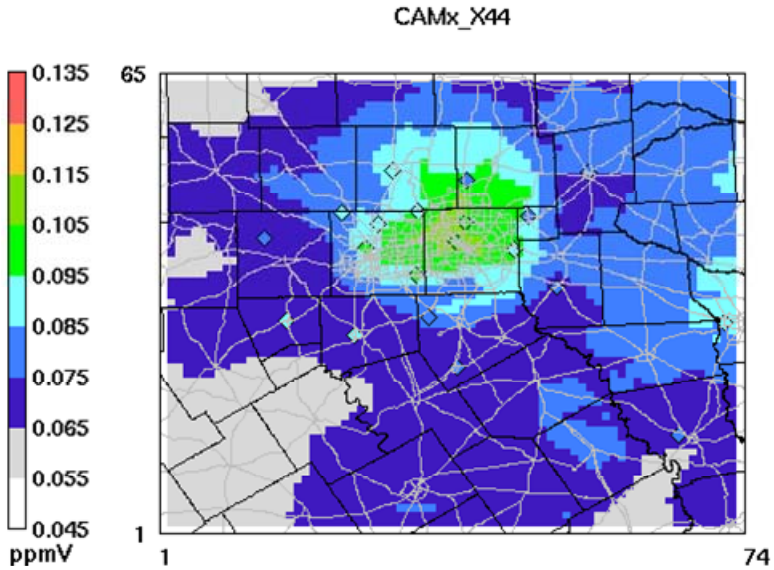

**Figure** Scatter diagrams of (a) CAMx CB4, (b) CAMx SAPRC99, (c) CMAQ CB4, and (d) CMAQ SAPRC99 compared to CAMS measurements for the period of June 18$^{th}$ ~ 23$^{rd}$, 2005.

Sept 1, 2005

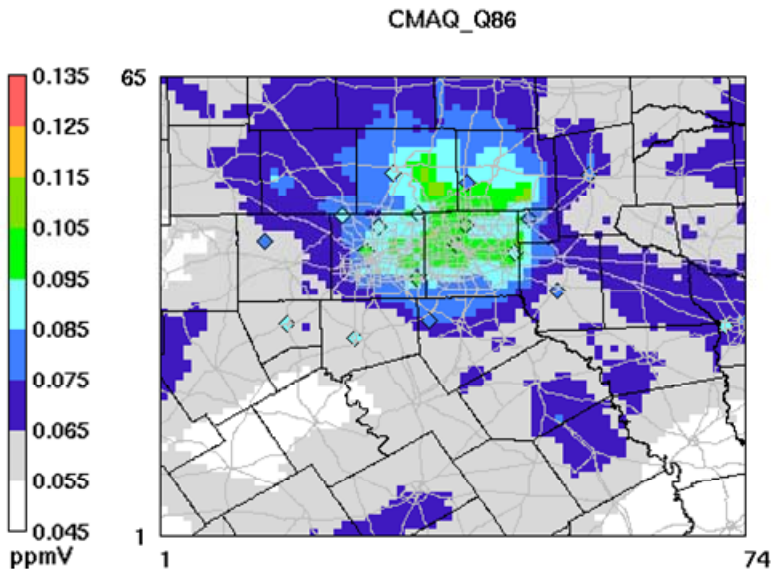
(a) CAMx CB4



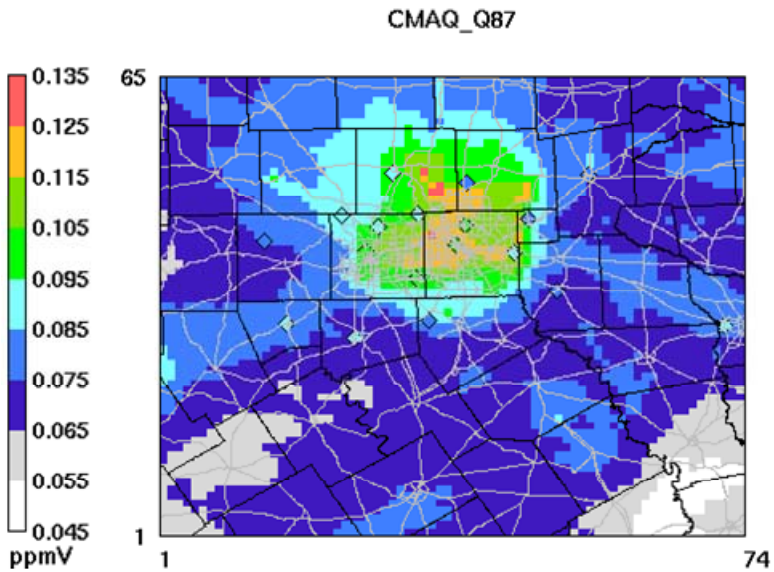

(b) CAMx SAPRC99




(c) CMAQ CB4

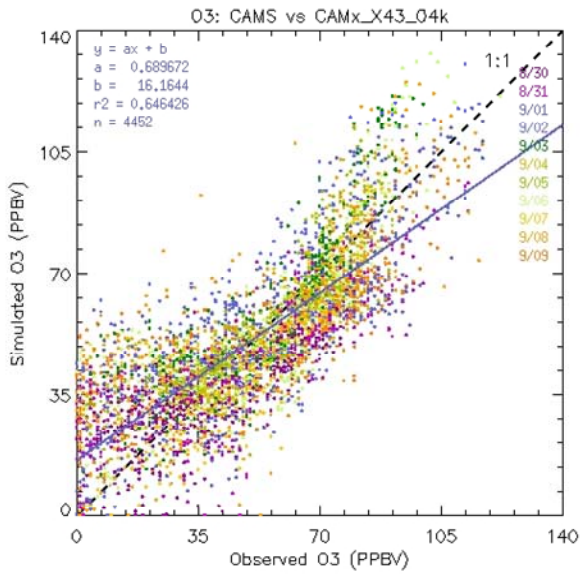



(d) CMAQ SARPC99

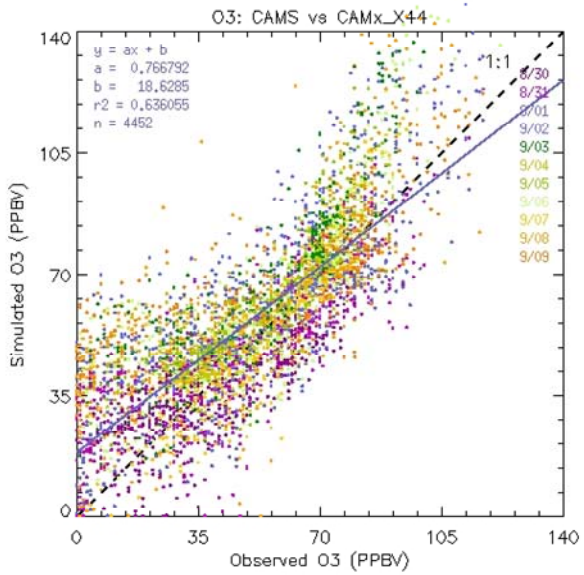


Dallas
8/30-9/9, 2005

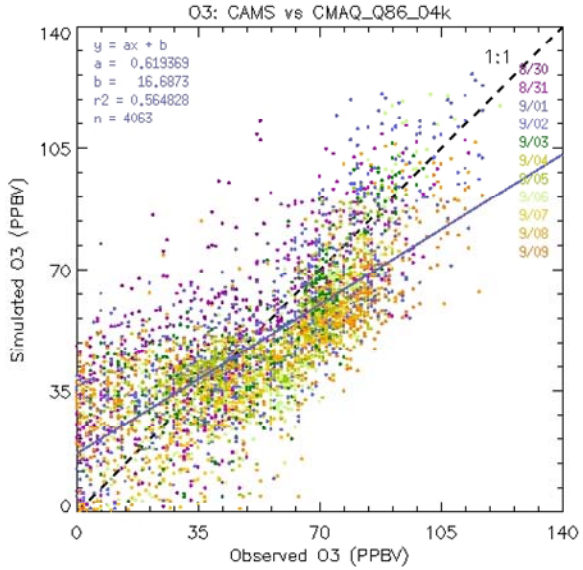
(a) CAMx CB4




(b) CAMx SAPRC99




(c) CMAQ CB4




(d) CMAQ SAPRC99

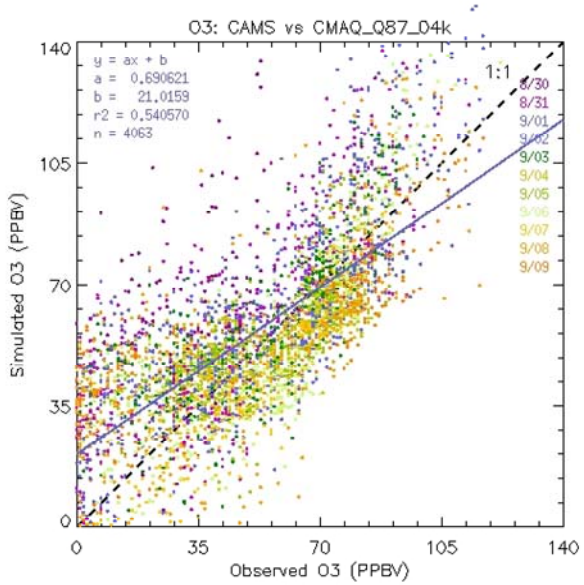



**Figure** Scatter diagrams of (a) CAMx CB4, (b) CAMx SAPRC99, (c) CMAQ CB4, and (d) CMAQ SAPRC99 compared to CAMS measurements for the period of August 30$^{th}$ ~ September 9$^{th}$, 2005.