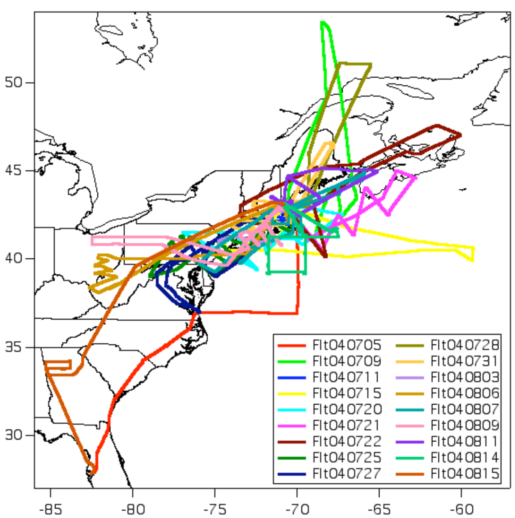
Comparison of WRF/Chem Photochemistry and PM2.5 Results with Aircraft Observations from Two Field Campaigns

Stu McKeen, Georg Grell, Steven Peckham and Si-Wan Kim
(CIRES/University of Colorado, NOAA/ESRL)

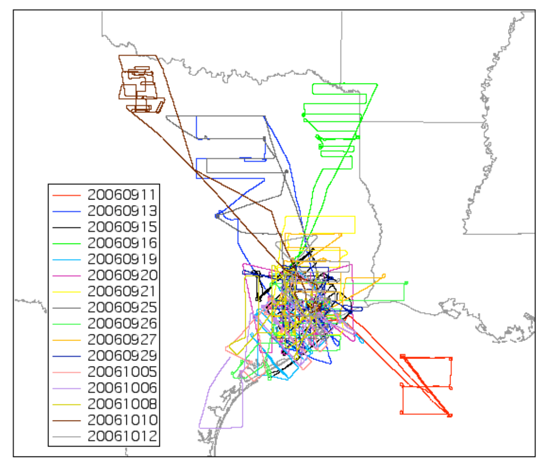
ICARTT/NEAQS - 2004, July-August:
- WRF/Chem relative to other models
- WRF/Chem historical progression
- New features in version 3

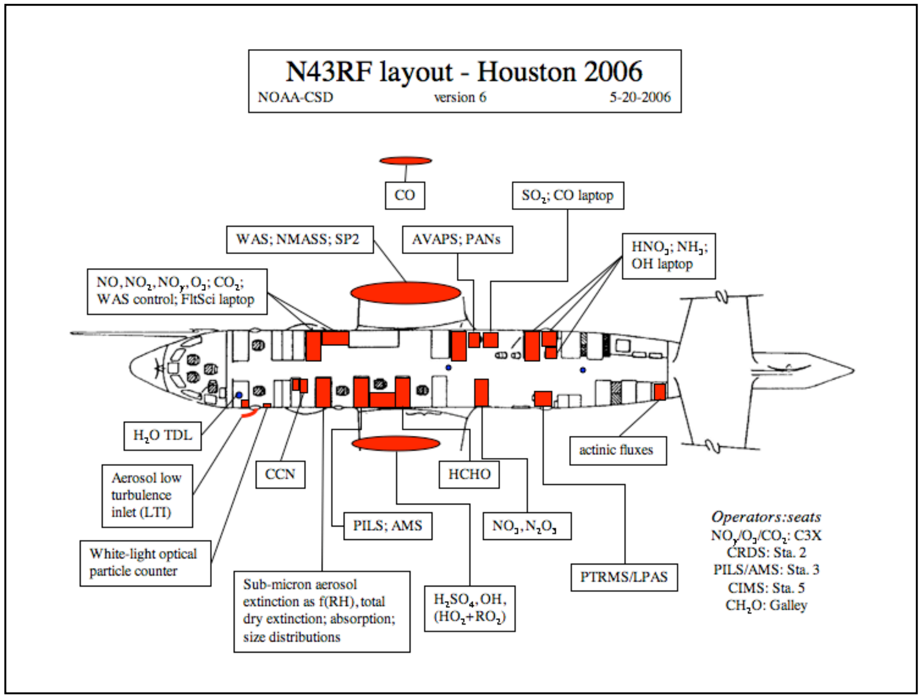
TexAQS - 2006, August-September:
- WRF/Chem relative to other models
- Evaluation of select options
- Emissions

http://www.esrl.noaa.gov/csd/2006/modeleval/



NOAA WP-3D aircraft





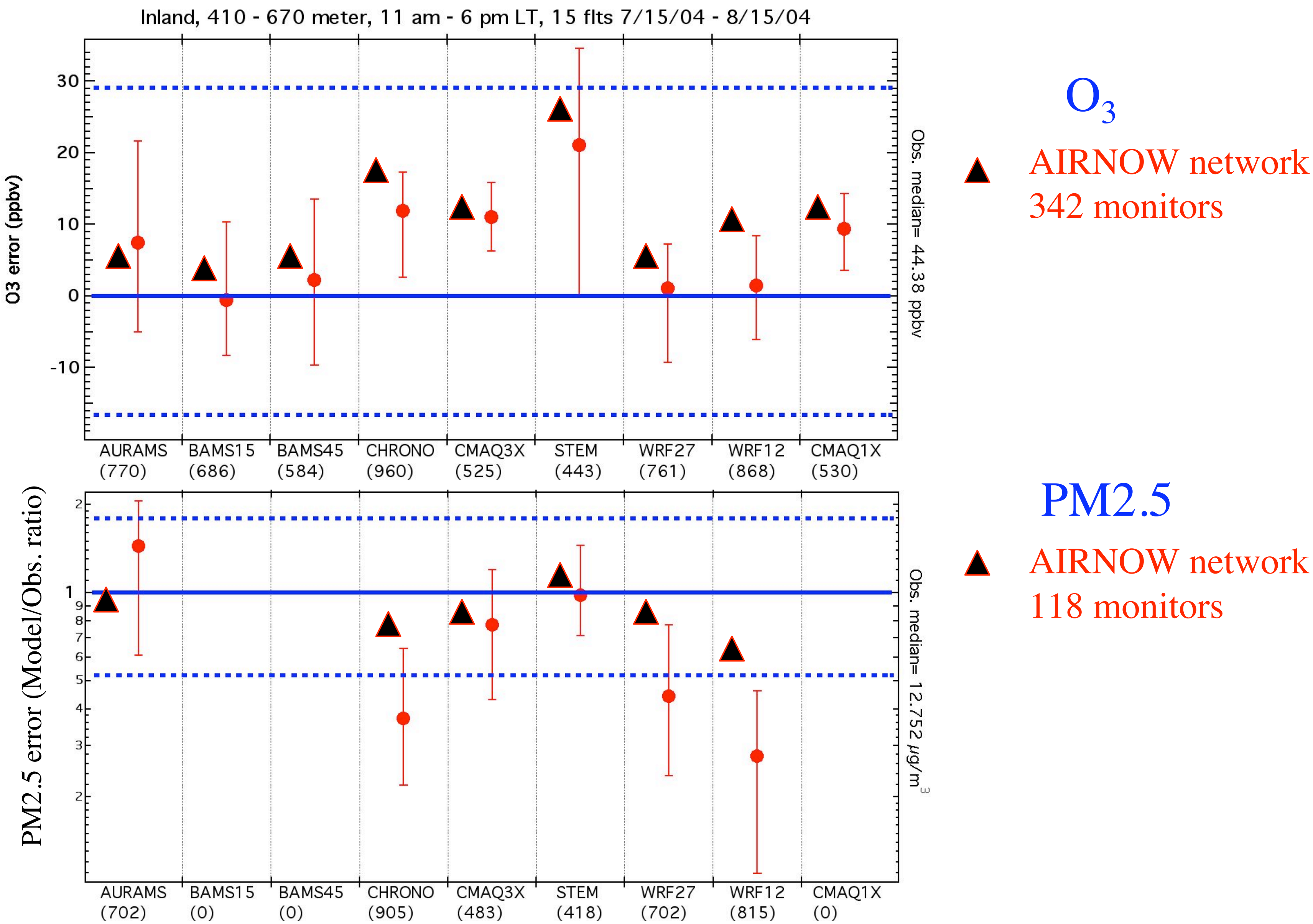
<u>Payload:</u>
- ~ 22 gas-phase at (1 to 10 sec res.)
- 6 PM2.5 constituents
- PM2.5 size distributions
- Actinic Flux and Radiation
- 1 second Meteorolgy variables

<u>Flight Patterns:</u>
- ~ 80% of time 300 and 600 m AGL
- 0 to 6 km vertical profiles
- ~ 70% of time from 10am to 4 pm LT
- Upwind/Downwind of Urban Plumes

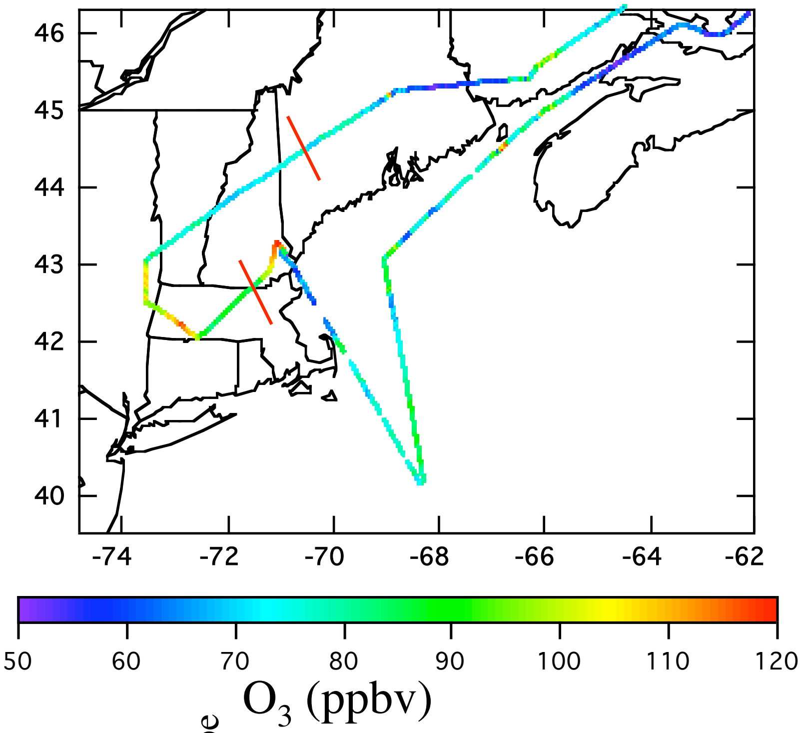
<u>Real-time Model Forecasts Collected by CSD:</u>
- 2 or 3 resolutions of online WRF/Chem (NOAA/GSD)
- offline CMAQ/ETA or CMAQ/WRF (NCEP or NOAA/ARL)
- offline Canadian CHRONOS model (GEMS)
- offline Canadian AURAMS model (GEMS)
- 3 resolutions of offline Baron AMS MAQSIP model (MM5)
- offline University of Iowa STEM model (MM5, WRF)

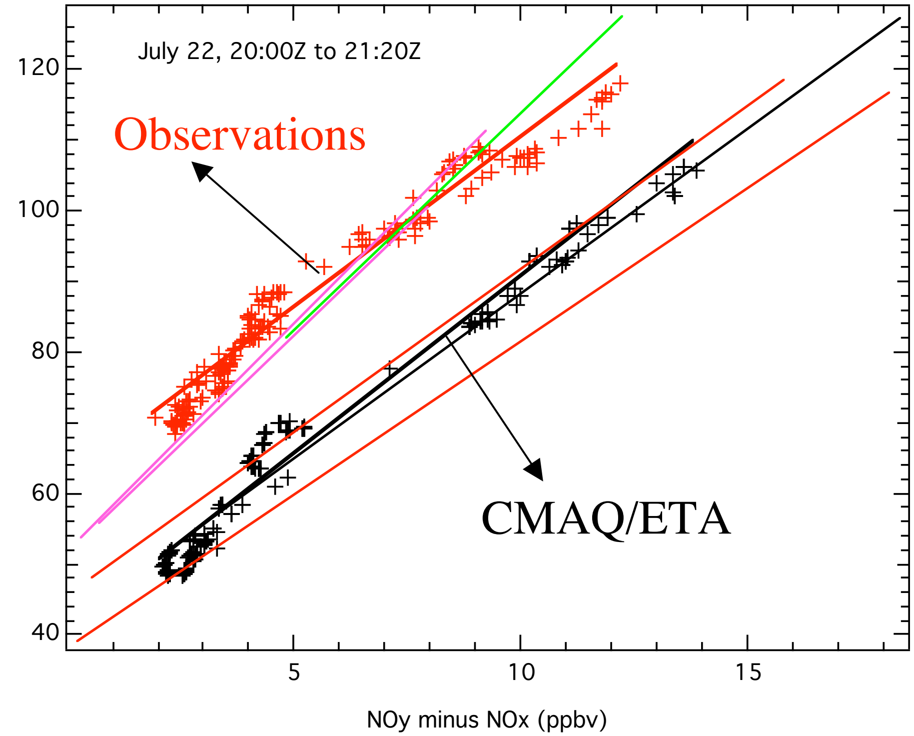
<u>Retrospective WRF/Chem Model Runs Collected by CSD:</u>
- ICARTT/NEAQ 2004 - 21
- TexAQS 2006 - 10

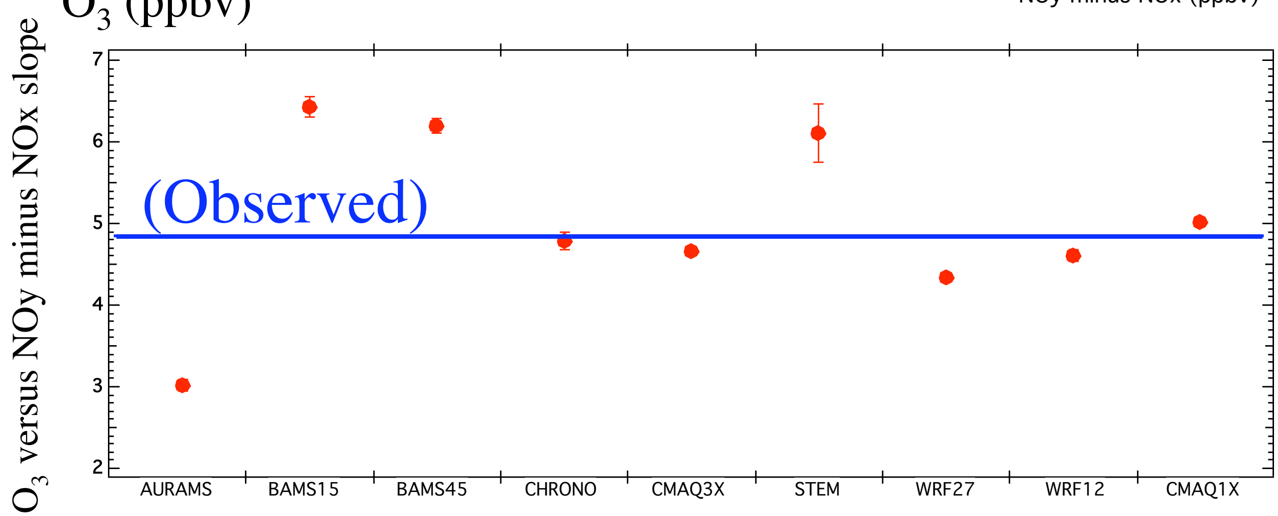
Summary statistics for ICARTT/NEAQS daytime, inland, 410-670m window



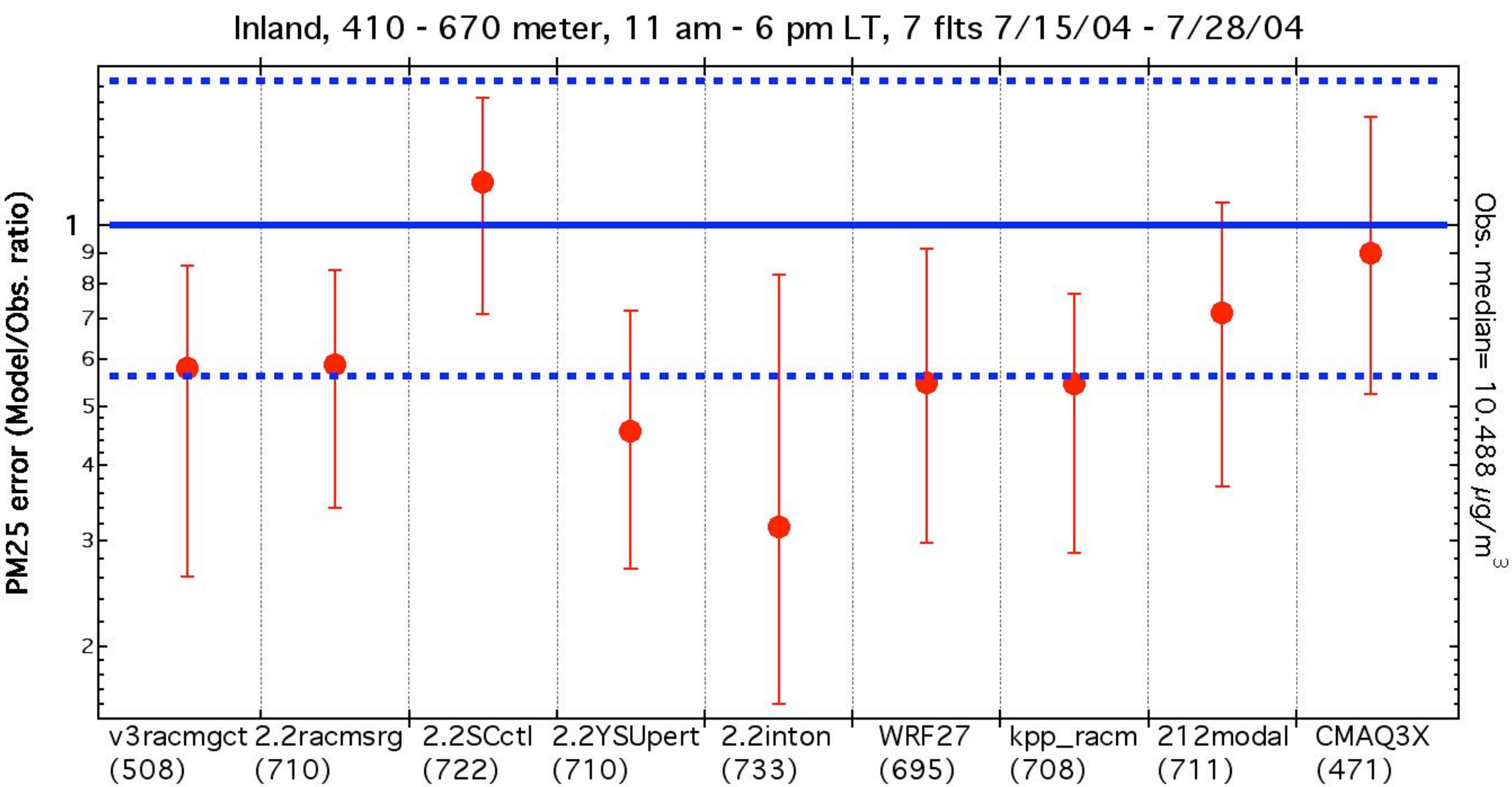
O_3 photochemistry tests: 7/22/04 20:00Z to 21:20Z, O_3 versus NOy minus NOx







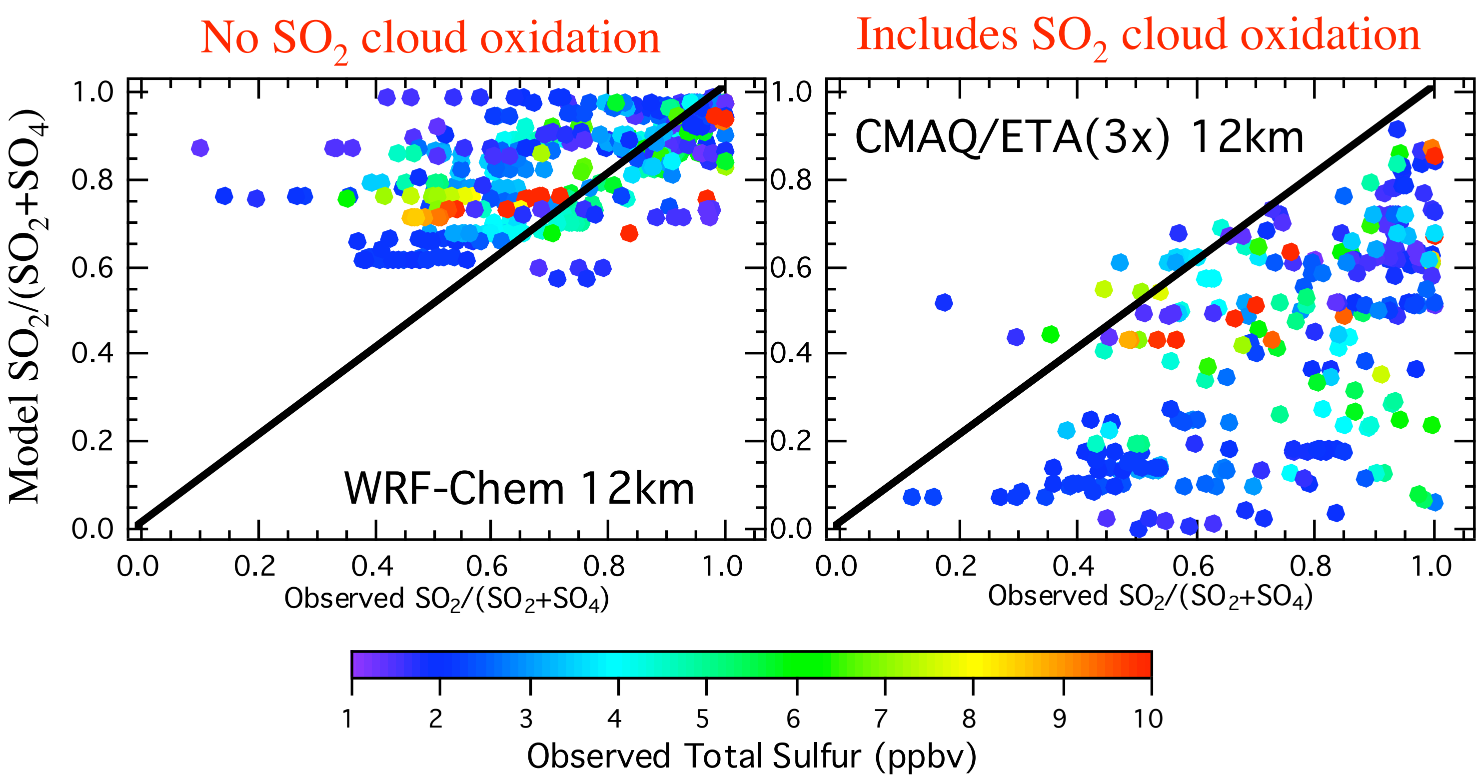
WRF/Chem intercomparisons - same emissions, domain, 27km resolution



V3	V2.2	V2.2	V2.2	V2.2	V2.03	V2.12	V2.12
RACM	RACM	CBM-Z	RADM	RADM	RADM	RACM	RADM
GoCart	Sorgam	MOSAIC	Sorgam	Sorgam	Sorgam	Sorgam	Sorgam
YSU	YSU	YSU	YSU	MYJ	YSU	YSU	YSU
							(No convection)

Comparing SO_2 oxidation rates, Models versus Obs.

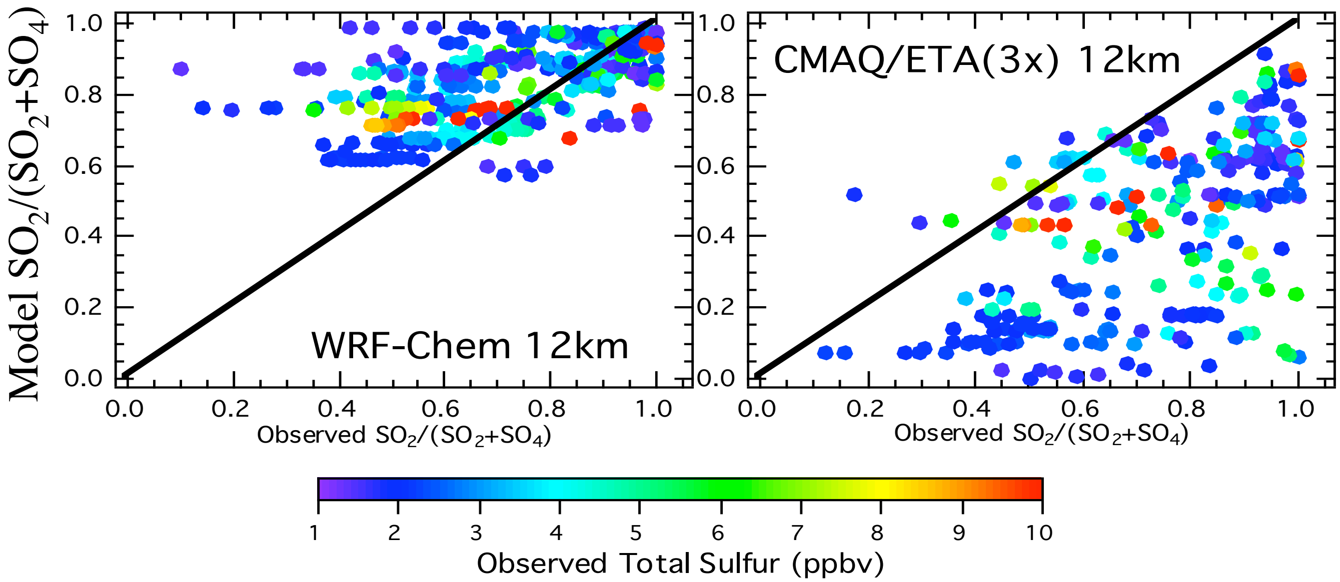
(Inland, 410 - 670 meter, 11:00 am to 4:00 pm LT,7 flights 7/15/04 - 7/28/04)

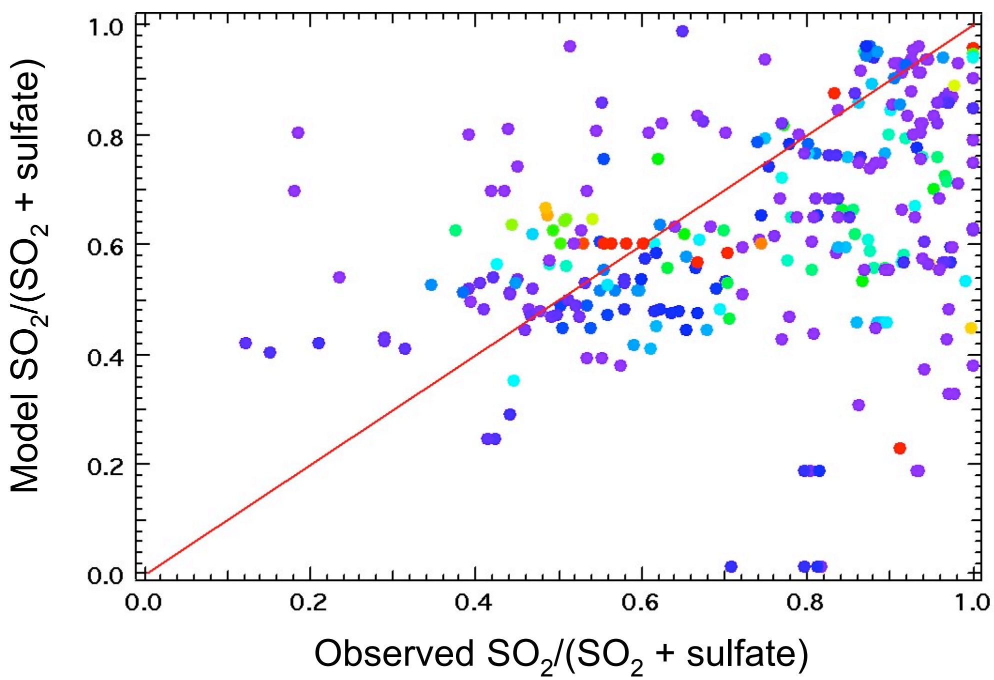


Models without cloud oxidation under-predict SO_4 and SO_2 oxidation

Models with cloud oxidation over-predict SO_4 and SO_2 oxidation

WRF/Chem version 3.0 GOcart aerosol - aqueous phase SO_2 oxidation

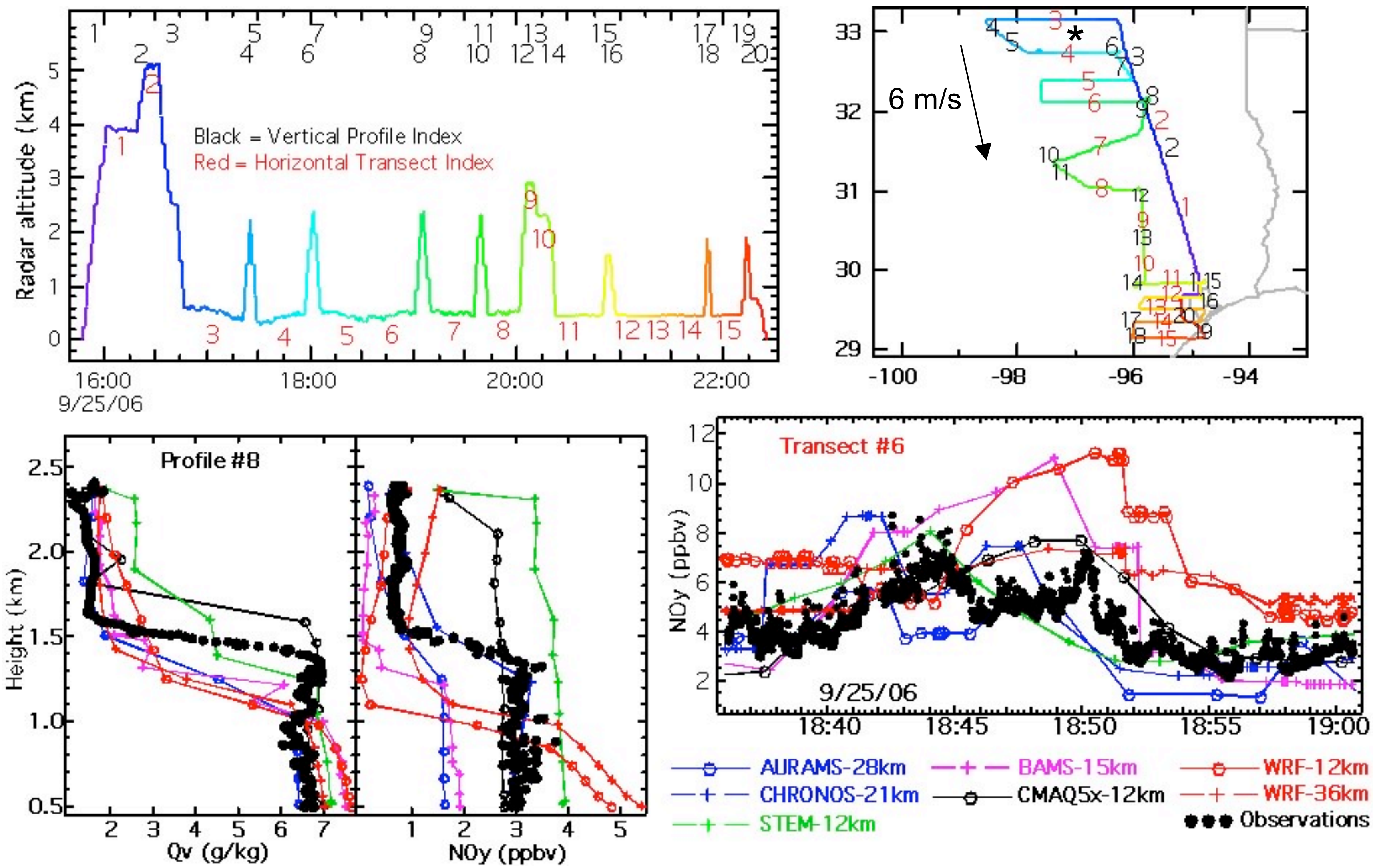




WRF/Chem version 3.0
RACM-GOcart

Simple (instantaneous) Cloud Oxidation of SO_2 with H_2O_2

TexAQS-2006, Upwind and Downwind Sampling of Houston and Dallas
(Example of 9/25/06 flight, transect 80 km downwind of Dallas)



Fluxes upwind and downwind of sources (300 to 670 m AGL horizontal transects)

1) Upwind mixing ratio or concentration (lowest 1/8 of sorted distribution, X_{upwind}) - track uncertainty (min. to lowest 1/4)

2) $\vec{v} \bullet \vec{n}$ (where $\vec{n}$ is normal vector <u>perpendicular to aircraft heading</u>)

3) Average concentration above background (lowest quartile)

$$\sum(X_i - X_{upwind})/n$$

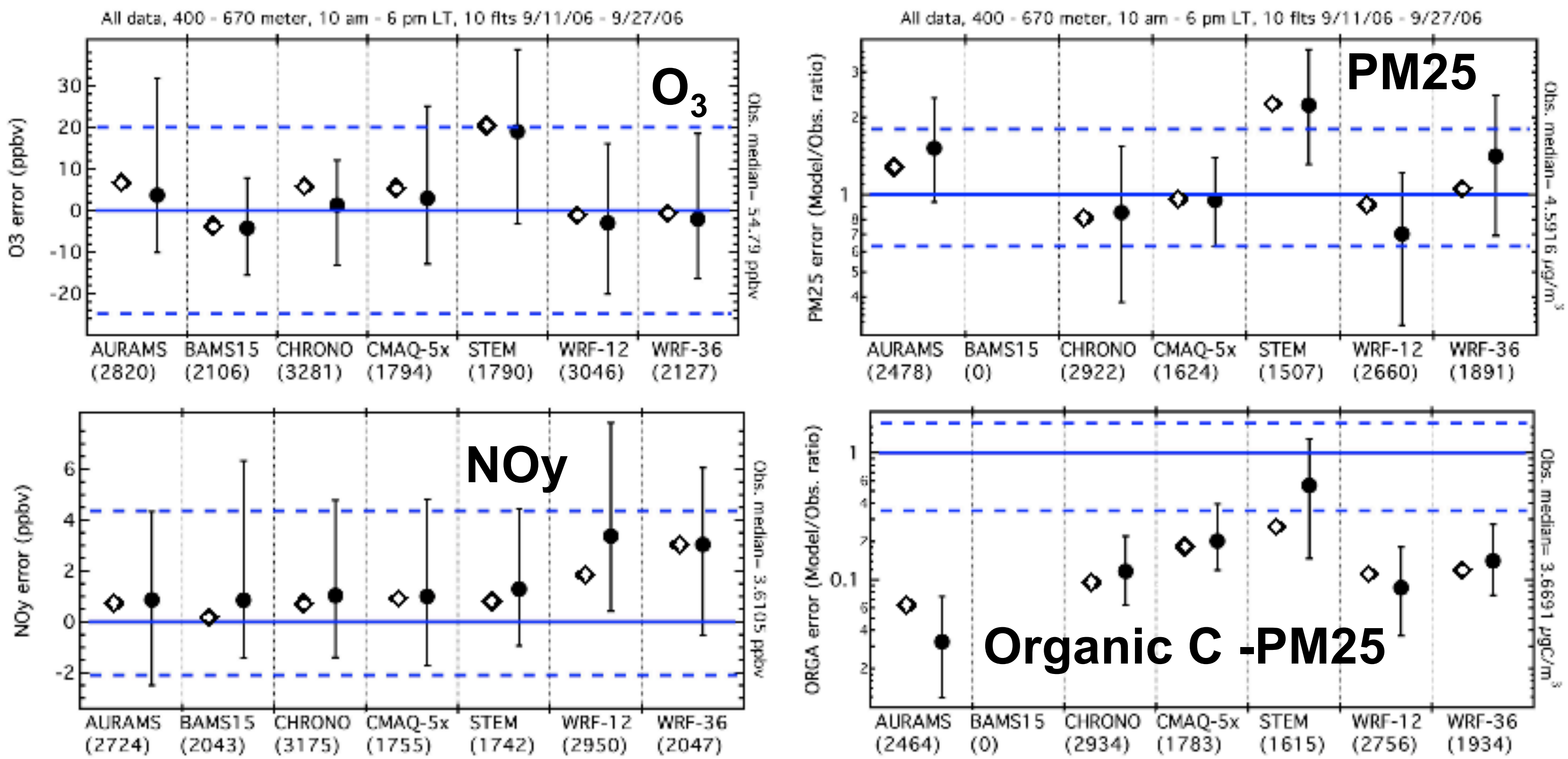
$$[\text{if } X_i > X_{upwind}, \text{ otherwise } 0]$$

4) Total flux (above background) through the plane defined by the aircraft heading

Applied identically to observations and models

TexAQS-2006 Bias statistics

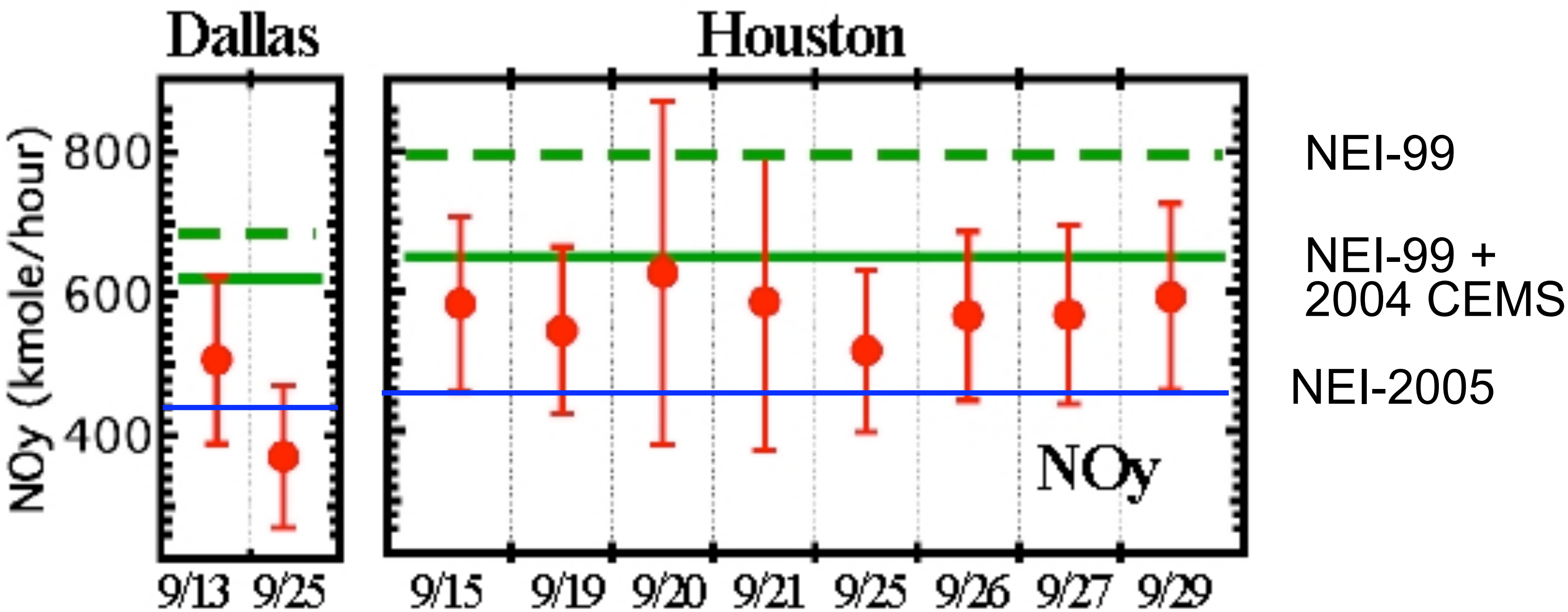
(410 - 670 meter, 11:00 am to 4:00 pm LT,10 flights 9/15/06 - 9/27/06)



Solid circles: All data

Hollow diamonds: Upwind Transects Only (~ 10% of all data)

NOy 11:00 am LT emissions from Houston and Dallas
Derived from upwind/downwind transects, and emission inventories

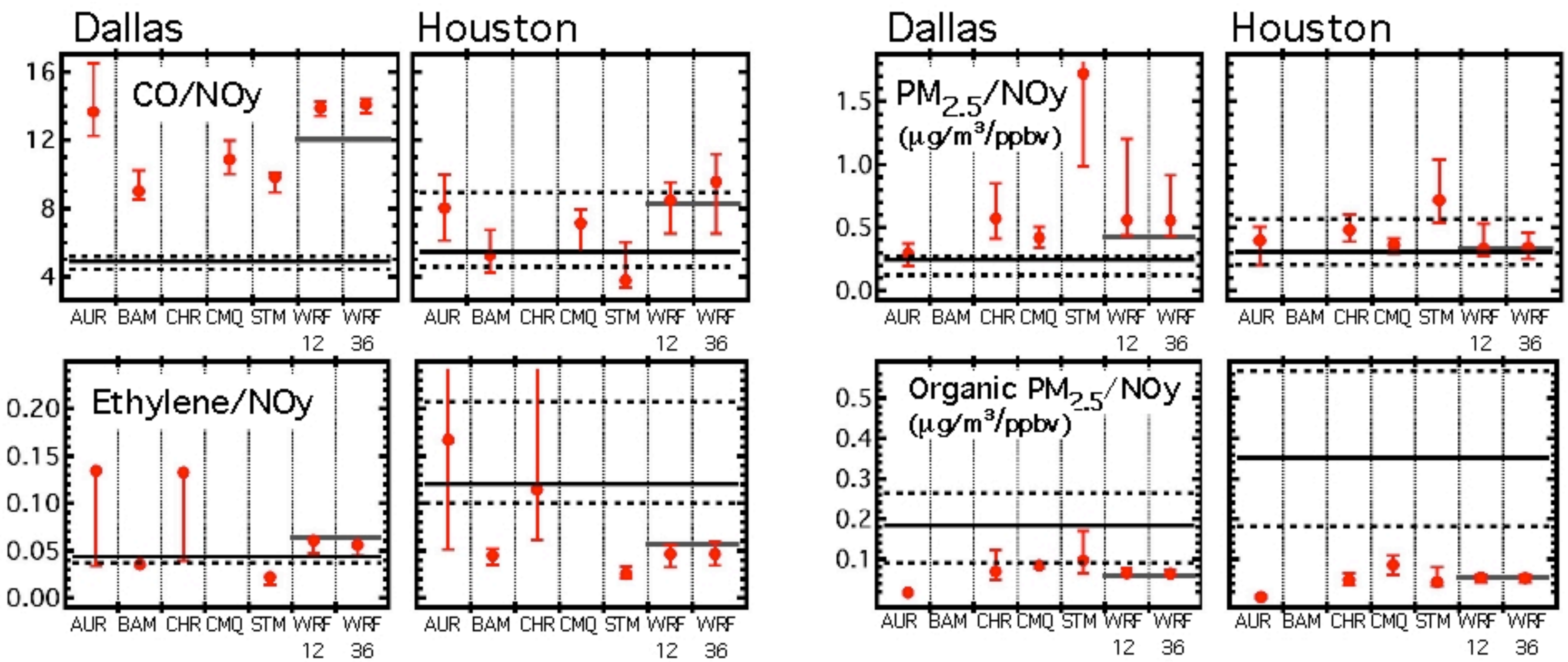


Uncertainty limits in observations include PBL and background uncertainties

Emission inventory from 11:00am to noon, LT (representative of daylight average)

over pre-determined ~1000 km^2 domains

Model and Observed concentration difference ratios (and NEI-99 emission ratios) downwind (< 50 km) of Houston and Dallas



Red circles: Model median ratios (whiskers - central 2/3 of sorted distributions)

Black lines: Observed medians (dashed lines - central 2/3 of sorted distributions)

Gray lines over WRF/Chem models - From NEI-99 (used in WRF/Chem runs)

Summary and Conclusions

WRF/Chem O_3 photochemistry conforms to available observations
(RACM, CBM-Z slightly hotter than RADM2)

WRF/Chem PM2.5 less reliable - sensitive to several processes

GOcart Aerosol Option in Version 3 has benefits

Chemistry biases very sensitive to PBL scheme

Emissions (both from inventories and satellite data) are changing rapidly
Work on 2005 NEI with 2006 CEMS underway - CO2 + more

Found a way to accurately relate raw model output to emission ratios