Comparison of air quality forecast model predictions with WP3 data during TexAQS II

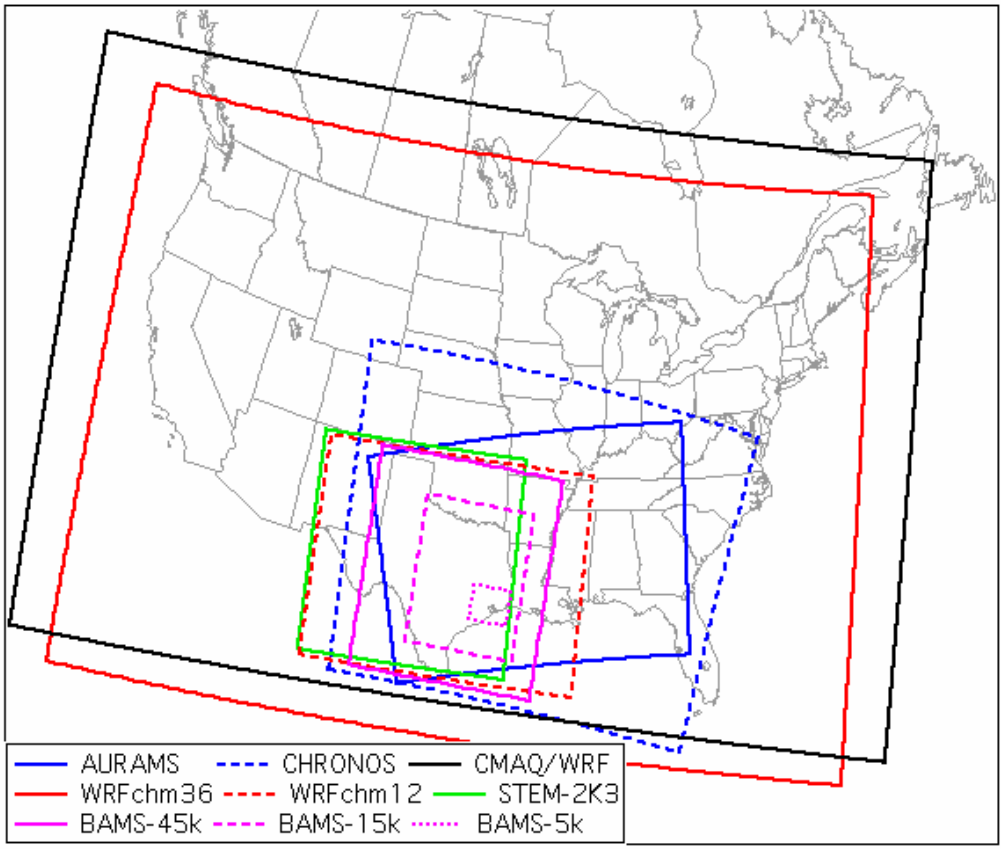
Stu McKeen NOAA /ESRL/CSD and CIRES

Georg Grell, Steven Peckham (NOAA/ESRL/GSD) -WRF/Chem
Jeff McQueen and Pius Lee (NOAA/NWS) - CMAQ/WRF
Youhua Tang (NOAA/NWS) and Greg Carmichael (U of Iowa) - STEM
John McHenry, Carley Coats (Baron AMS) - BAMS
Wanmin Gong, Veronique Bouchet (Env. Canada) - AURAMS,CHRONOS

TexAQS II Forecast Model Science Objectives (RSST - Question J):

- Background of models
- Evaluation web-site
- Preliminary comparisons related to O_3

Real-time Forecast Models Operational During the Summer of 2006



Model:	Emission Inventory:
→ AURAMS - 28km CHRONOS - 21km	Canadian National Inv.
→ CMAQ/WRF(5x) - 12km	National 2001 inv., grown to 2006
BAMS - 45km → BAMS - 15km BAMS - 5km	
→ WRF/CHEM - 36km(*) → WRF/CHEM - 12km(*)	NEI-99, NOAA/ESRL/CSD 2004 CEMS
→ STEM(2K3) - 12 km	

(*) Indicates a retrospective run

→ Indicates models in today's talk

Web-page for NOAA-P3/AQ model comparisons: http://majaji.esrl.noaa.gov/csd/~stu

Three graphical products for analysis/comparisons

- Individual horizontal transects and vertical profiles (~11000 plots)

  Fly the aircraft through the model results
  Store/display grid values - no interpolation

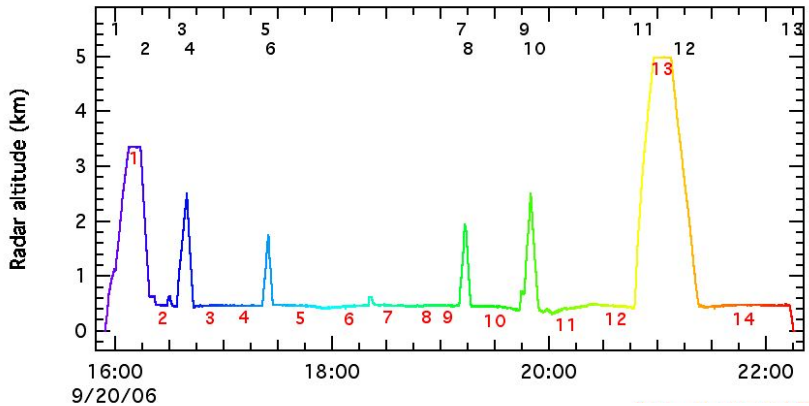
- Upwind and Downwind Fluxes along horizontal transects (~200 plots)

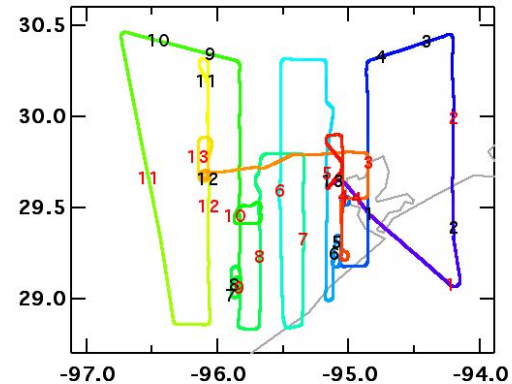
  350 meter to 650 meter (AGL) P3 horizontal transects
  (Houston, Dallas, East Texas Power Plants)
  Inflow condition
  Flux of gas/aerosol in excess of inflow condition

- Downwind Flux ratios (~200 plots)

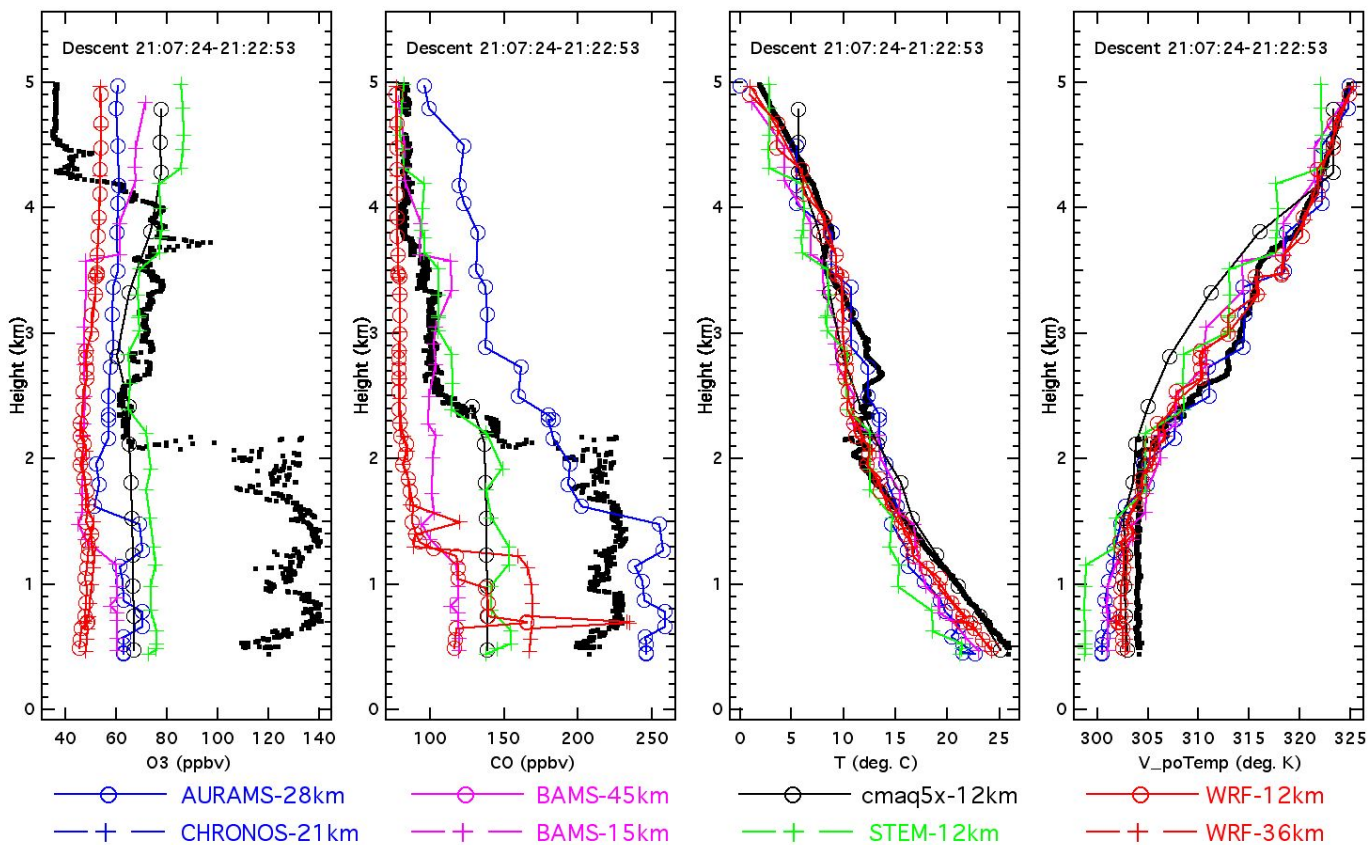
  Ratios of excess gas/aerosol flux downwind of sources

Example of Vertical Profiles for 9/20/06

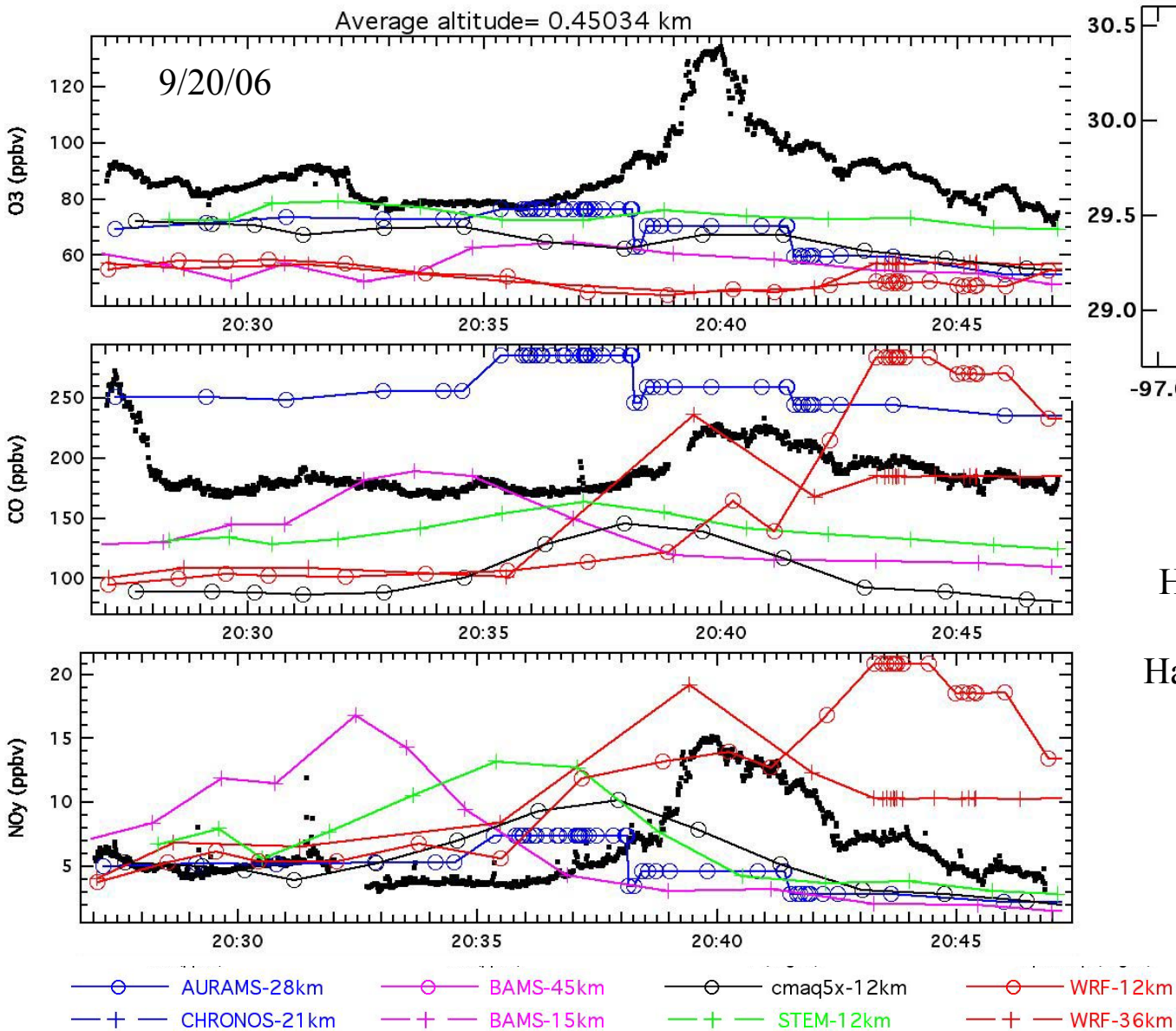


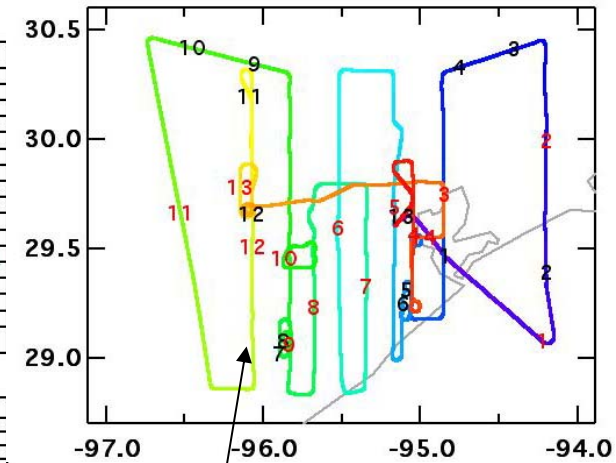


Vertical Profile #12



Example of Horizontal Transect for 9/20/06





Horizontal Transect #12
70 km downwind of
Harris County Courthouse

Model variables available for Comparison with NOAA Aircraft data

gas phase chemistry

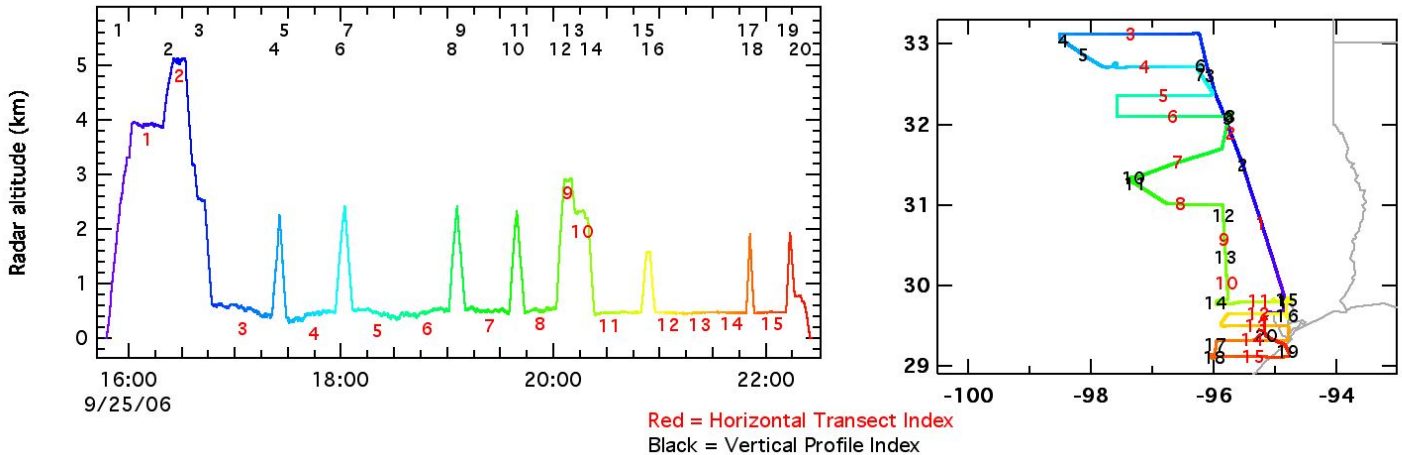
	AURAMS	BAMS	CMAQ(5x)	WRF-2
O_3	√	√	√	√
CO	√	√	√	√
NO	√	√	√	√
NOx	√	√	√	√
NOy	√	√	√	√
PAN	√	√	√	√
Isoprene	√	√		√
SO_2	√	√	√	√
NO_3	√	√	√	√
N_2O_5	√	√	√	√
CH_3CHO	√		√	√
Toluene	√	√		√
Ethylene	√	√		√
NH_3	√		√	√

aerosols, radiation, meteorology

	AURAMS	BAMS	CMAQ(5x)	WRF-2
PM2.5	√		√	√
Asol SO_4	√		√	√
Asol NH_4	√		√	√
Asol OC	√		√	√
Asol EC	√		√	√
Asol NO_3	√		√	√
JNO_2				√
T	√	√	√	√
P	√	√	√	√
H_2O	√	√	√	√
winds	√	√	√	√
SST	√		√	√
Radiation				√
CH_2O	√	√	√	√

http://majaji.esrl.noaa.gov/csd~stu

Horizontal Transects (300 to 700 m AGL)
Both Upwind and Downwind of Sources in September



	Sept. 13, Dallas	5.0 m/s	northerly
	Sept. 15, Houston	4.5 m/s	southeasterly
	Sept. 16, East TX stacks	6.0 m/s	southerly
	Sept. 19, Houston	7.5 m/s	northeasterly
	Sept. 20, Houston	5.0 m/s	easterly
→	Sept. 21, Houston	9.5 m/s	southerly
	Sept. 25, Dallas	3.0 m/s	northerly
	Sept. 25, Houston	6.0 m/s	northerly
	Sept. 26, Houston	3.0 m/s	northeasterly
→	Sept. 27, Houston	5.5 m/s	southerly
	Sept. 29, Houston	3.5 m/s	southerly

Fluxes upwind and downwind of sources
(300 to 700 m AGL horizontal transects)

1) Upwind mixing ratio or concentration (average, X_{upwind})

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

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

$$\sum (X_i - X_{upwind})(\vec{v_i} \bullet \vec{n})$$

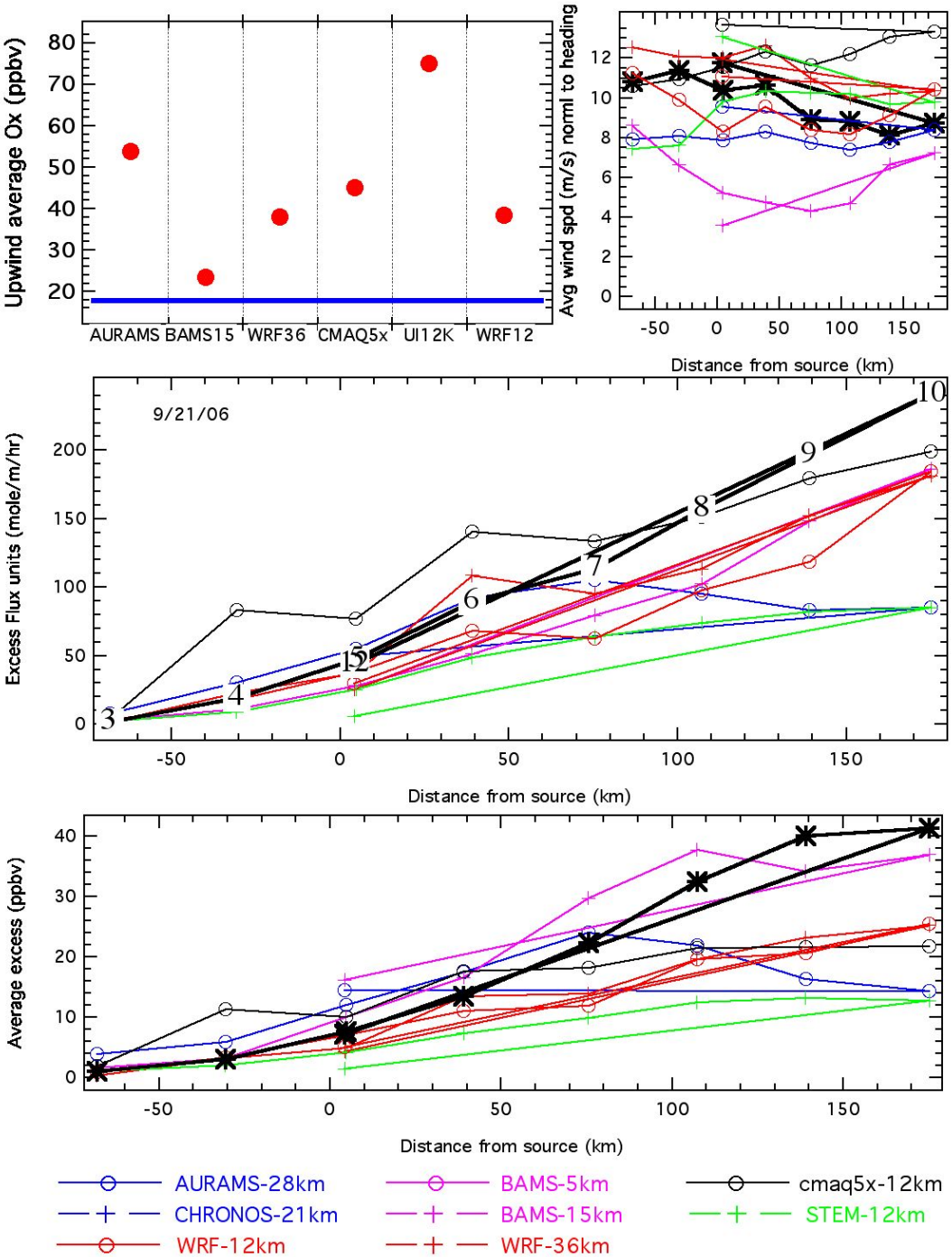
[if $X_i > X_{upwind}$, otherwise 0]

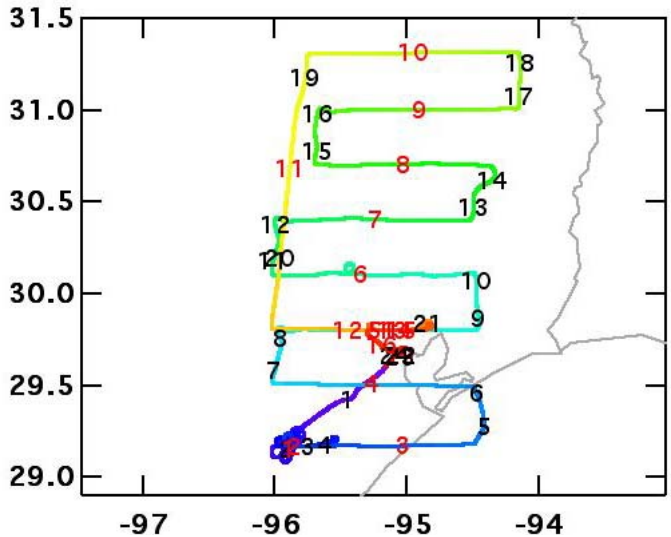
4) Average mixing ratio above background

Applied identically to observations and models

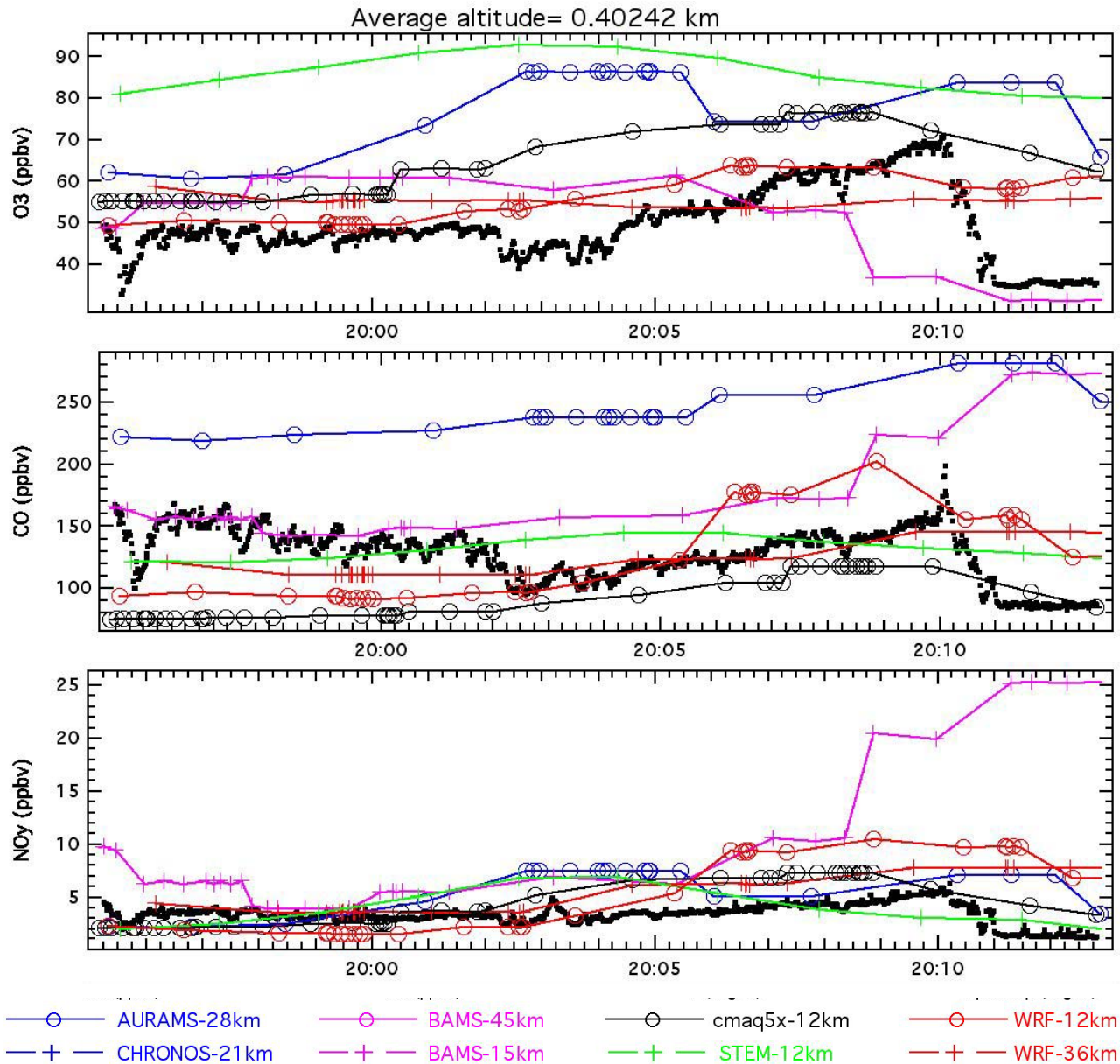
Flux units - moles/hr per meter(vertical)

9/21/06

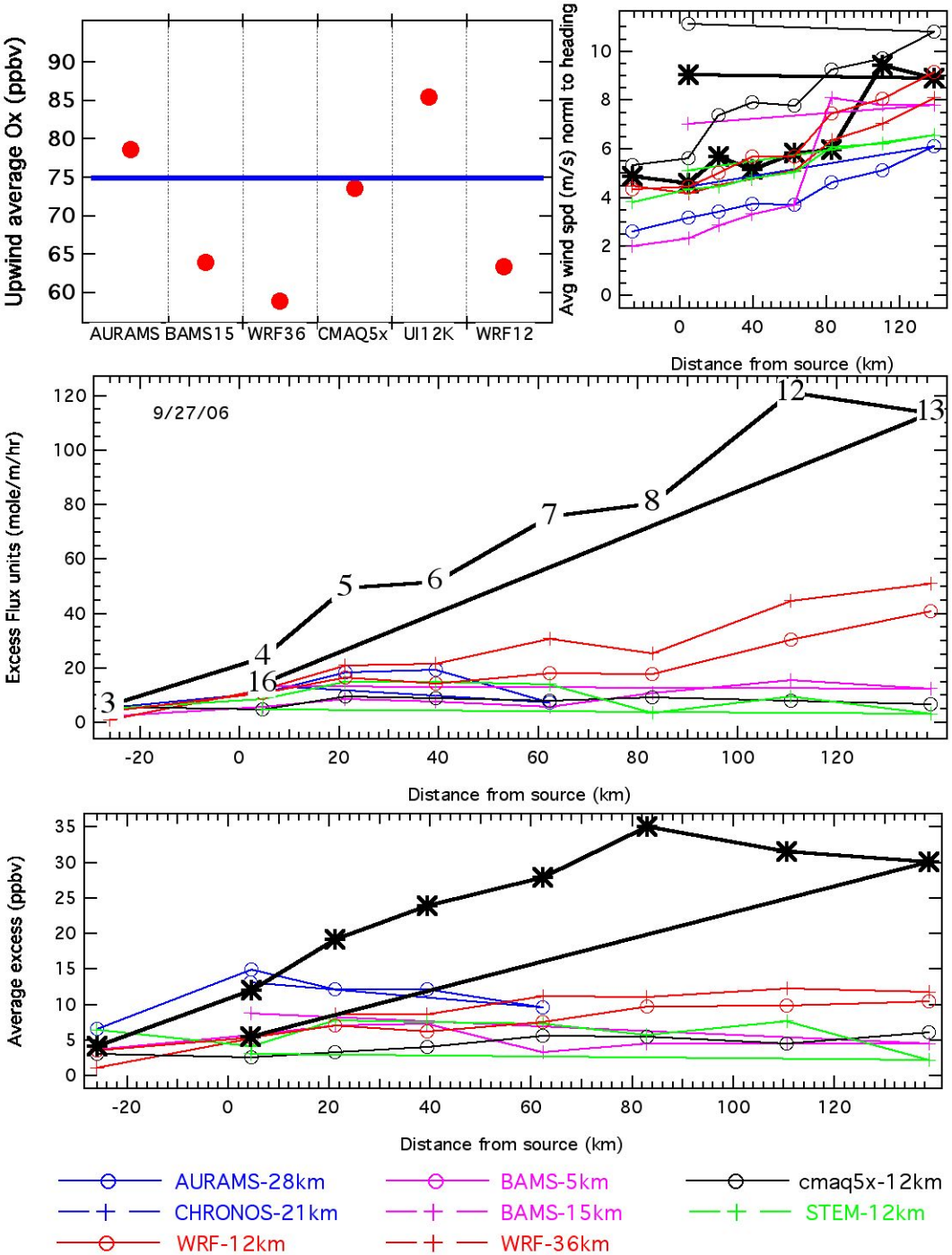

Upwind average Ox (ppbv)
AURAMS BAMS15 WRF36 CMAQ5x UI12K WRF12
Avg wind spd (m/s) norml to heading
Distance from source (km)
9/21/06
Excess Flux units (mole/m/hr)
Distance from source (km)
Average excess (ppbv)
Distance from source (km)
AURAMS-28km
CHRONOS-21km
WRF-12km
BAMS-5km
BAMS-15km
WRF-36km
cmaq5x-12km
STEM-12km

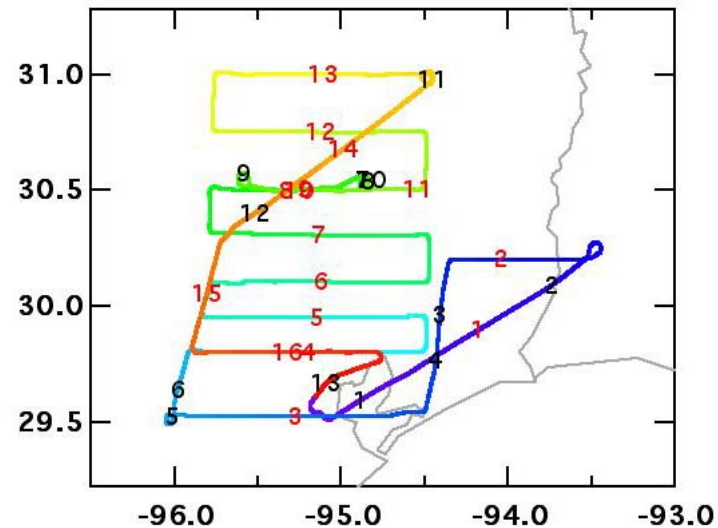

31.5
31.0
30.5
30.0
29.5
29.0
-97
-96
-95
-94

9/21/06 - 110 km north of Houston

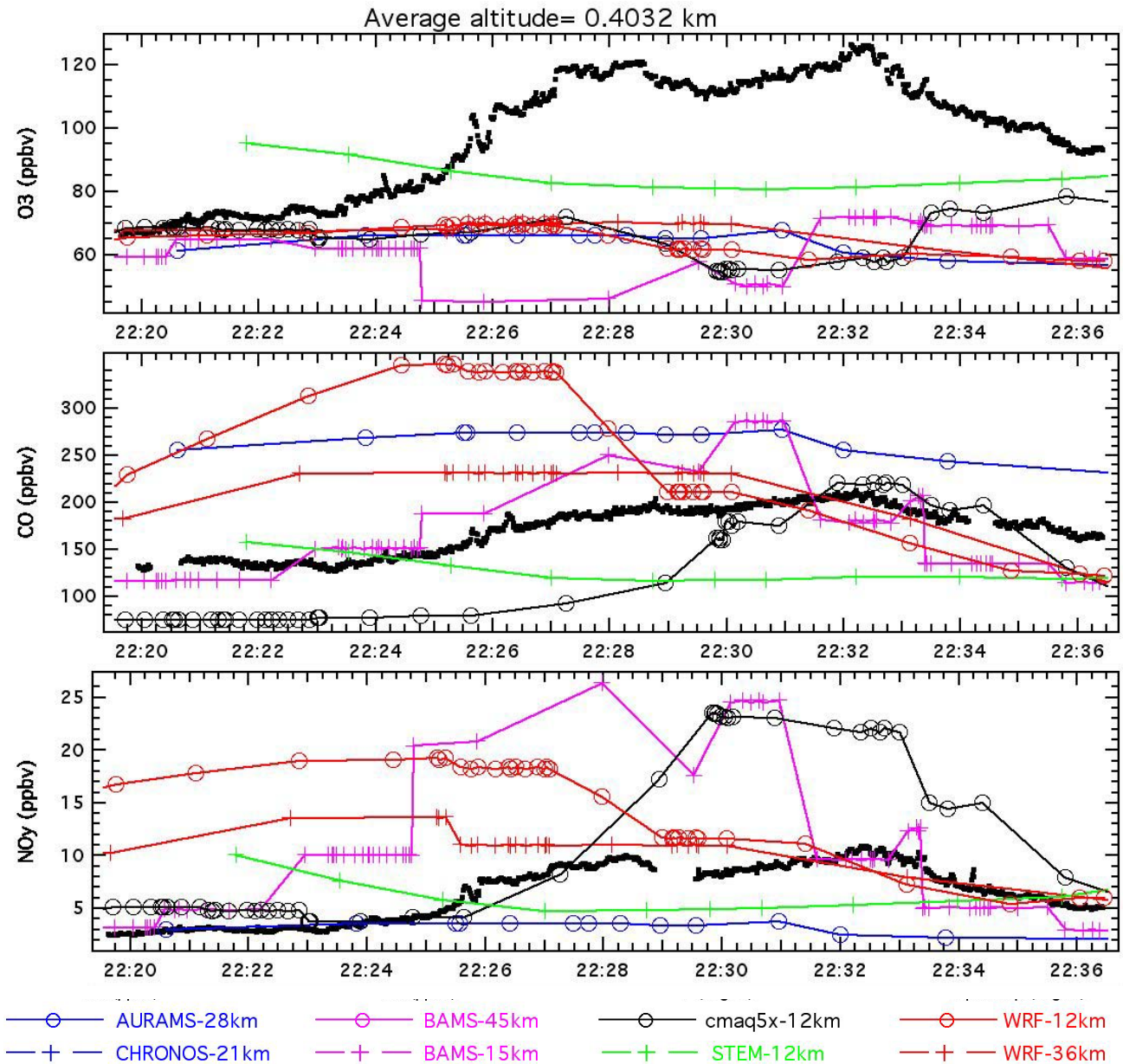


9/27/06

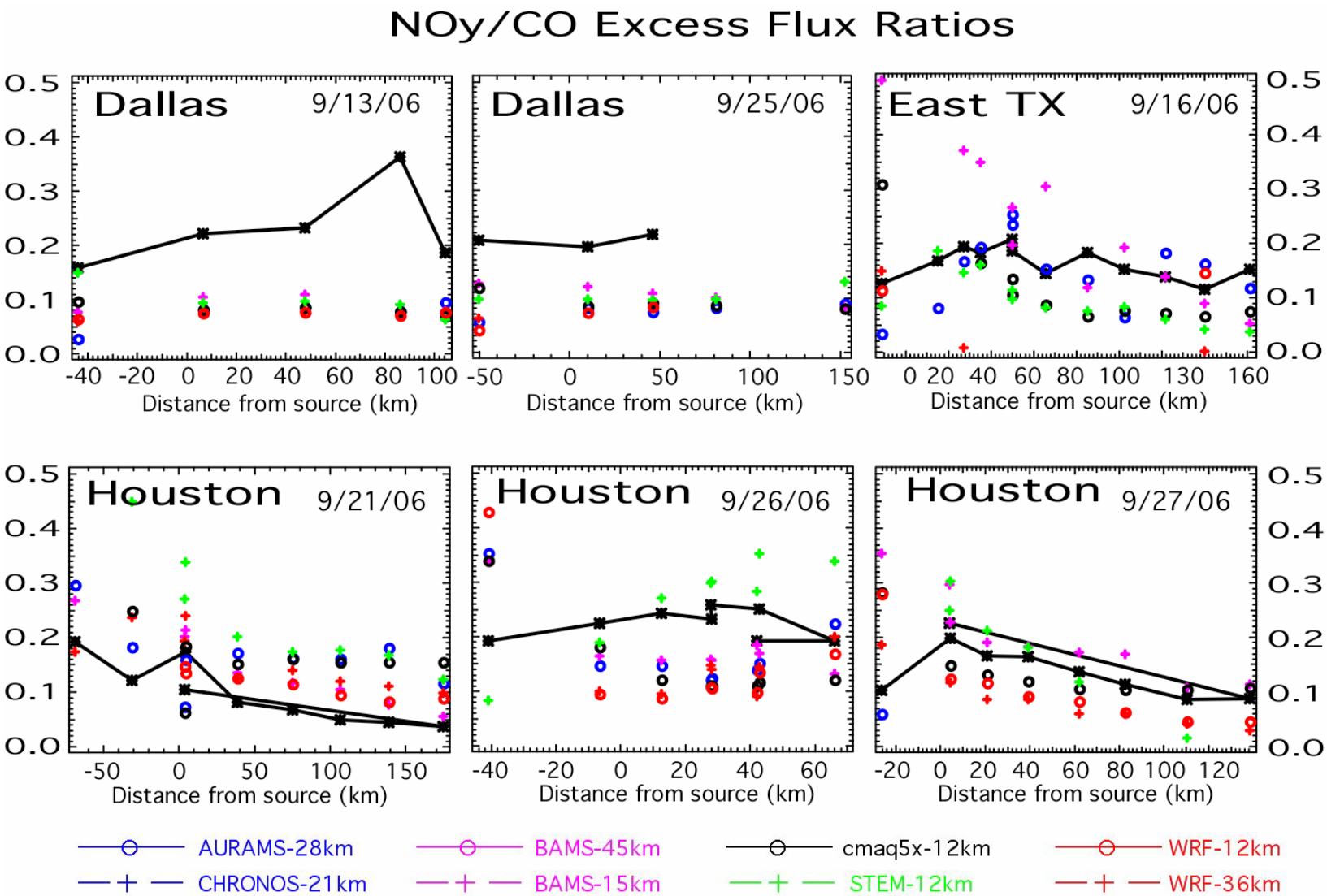

Upwind average Ox (ppbv)
AURAMS BAMS15 WRF36 CMAQ5x UI12K WRF12
Avg wind spd (m/s) norml to heading
Distance from source (km)
9/27/06
Excess Flux units (mole/m/hr)
Distance from source (km)
Average excess (ppbv)
Distance from source (km)
AURAMS-28km
CHRONOS-21km
WRF-12km
BAMS-5km
BAMS-15km
WRF-36km
cmaq5x-12km
STEM-12km


31.0
30.5
30.0
29.5
-96.0
-95.0
-94.0
-93.0

9/27/06 - 110 km north of Houston



Surrogates for relative emission comparisons



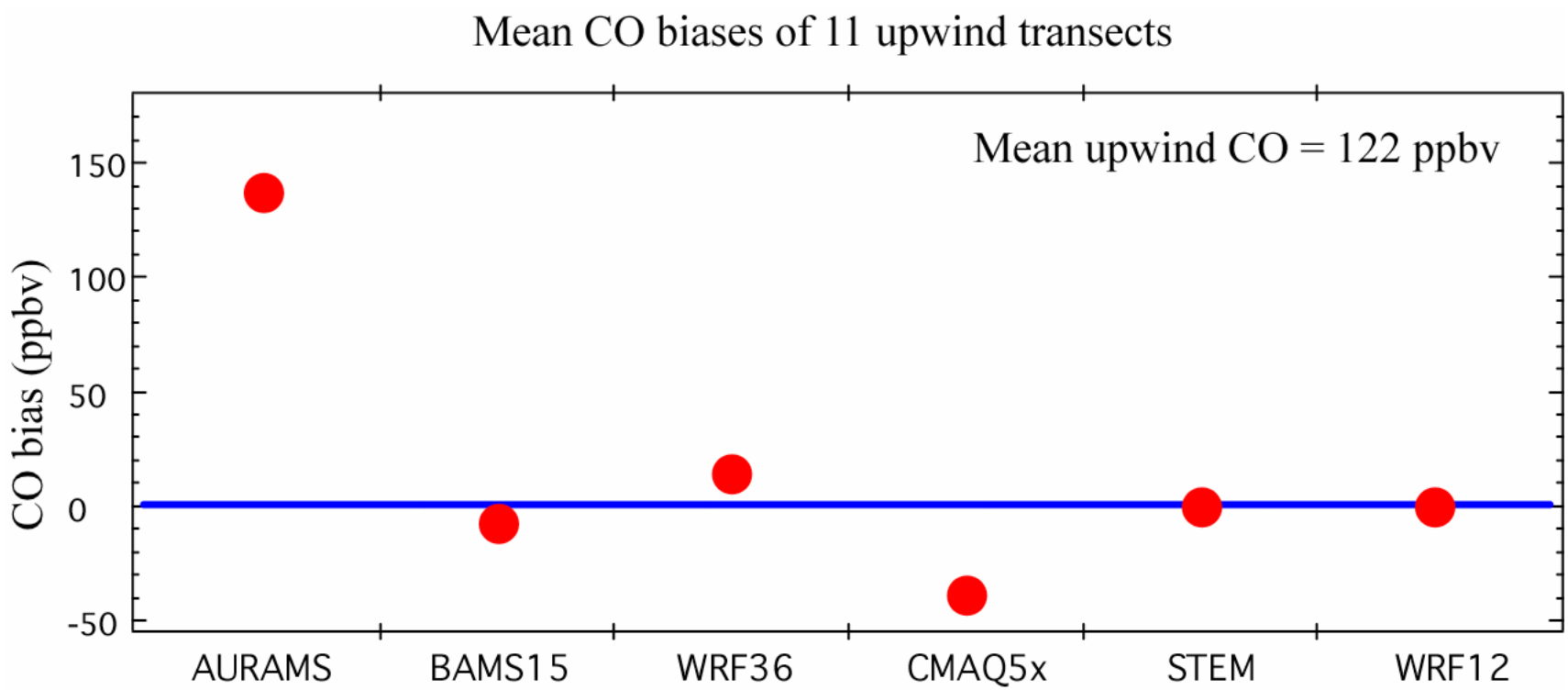
Species in Flux Comparisons on Web site

O_3	NOy	PM2.5	Ethylene
CO	NOx	PM2.5 sulfate	Toluene
H_2O	HNO_3	PM2.5 EC	Xylene
SO_2	PAN	PM2.5 OC	CH_3CHO
CH_2O	NH_3	Total sulfur	

Ratio Comparisons on Web site

O_3/CO	NOx/NOy	sulfate/PM2.5	O_3/(PAN+HNO_3)
NOy/CO	HNO_3/NOy	OC/PM2.5	
NOx/CO	PAN/NOy	EC/PM2.5	
SO_2/CO	PM2.5/NOy		
PM2.5/CO	O_3/NOy		
CH_2O/CO	CH_2O/NOy		
CH_3CHO/CO	CH_3CHO/NOy		
Ethylene/CO			
OC/CO			
EC/CO			

Example of Ongoing Statistical Evaluation



Summary:

Web site designed for AQ forecast evaluation
(Focus on fluxes upwind and downwind of source regions)

O_3 forecasts for Houston -

1) Highest O_3, narrow plumes missing in models
2) Downwind under-predictions on light wind days, better agreement on strong wind days

Emissions -

1) Evidence for high CO emissions in all models relative to NOy
2) Need for including inventories designed for compliance into air-quality forecast models