WRF/Chem Simulation of Ozone and Precursors in the LA Basin During the 2010 CalNex Campaign

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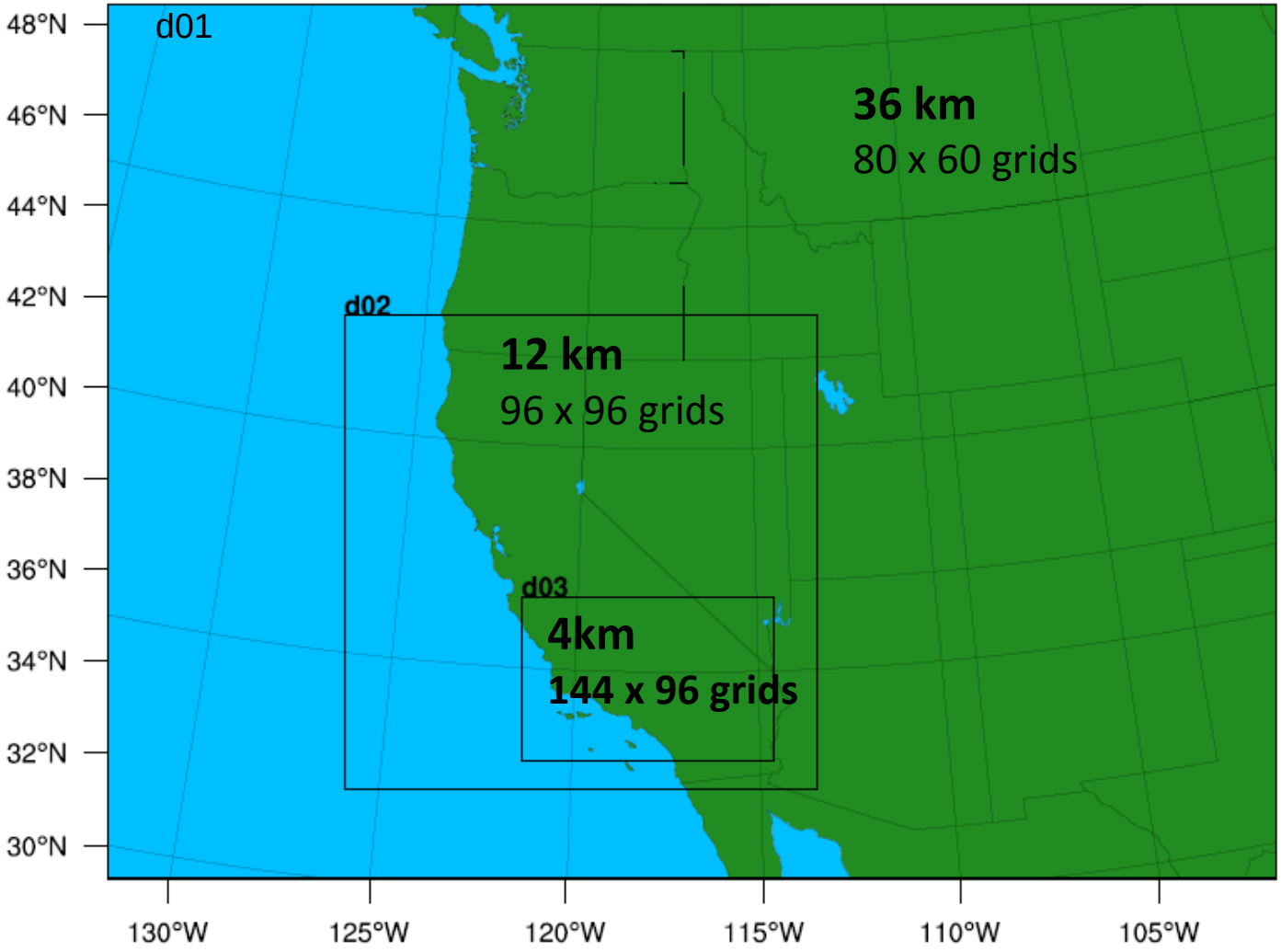
WRF/Chem (one-way) Nested Domains for This Study

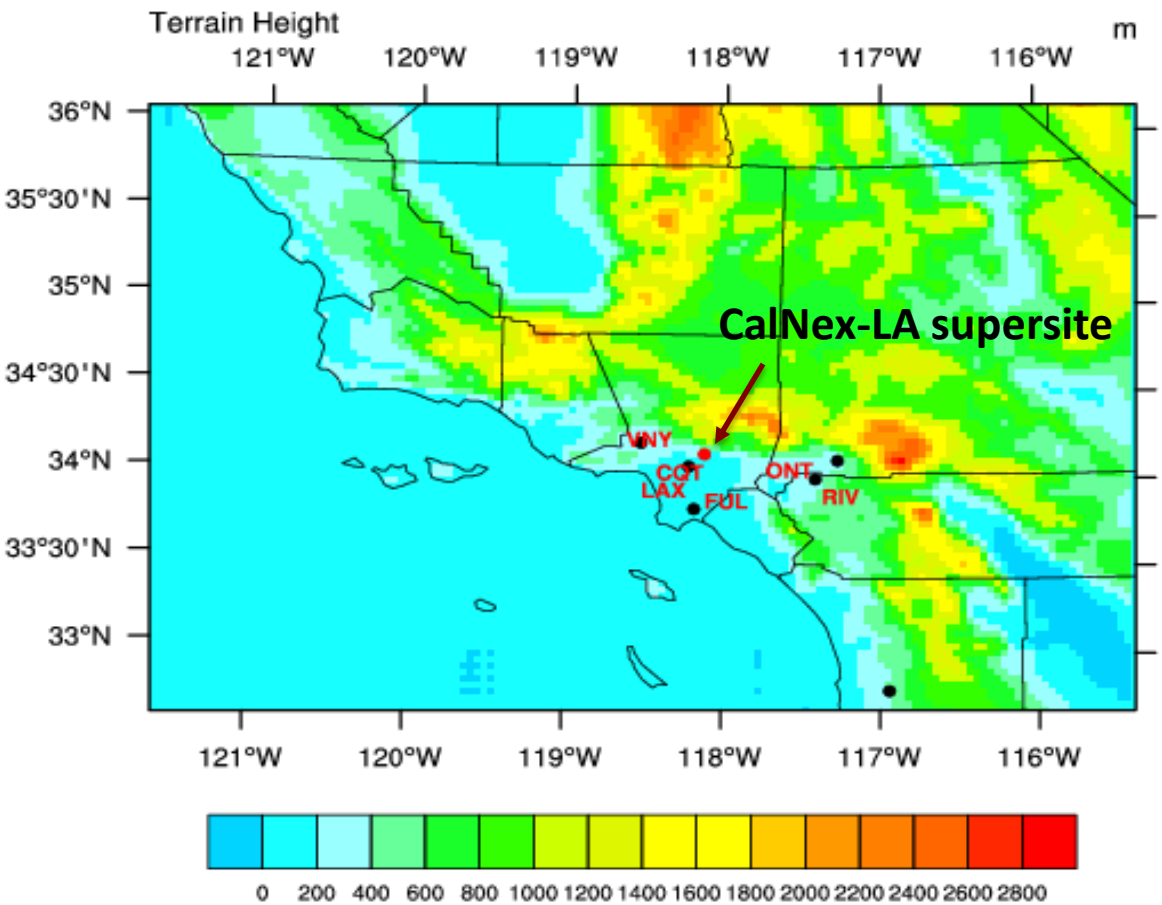
Simulation May 27–June 15



WRF/Chem (v3.1.1) Configuration for this study

Aerosol scheme	MOSAIC (4 bin) [*Zavier et al,* 2007]
Photolysis scheme	Fast-J [*Wild et al,* 2000]
Gas phase chemistry	CBM-Z [*Zavier et al,* 1999]
Long-wave radiation	*Mlawer et al.* [1997]
Land-surface model	NOAH [*Chen and Dudhia,* 2001]
Boundary layer scheme	YSU [*Hong et al.,* 2006]
Chemistry initialization	5-day spin-up
Meteorological initial and boundary conditions	NARR (32-km), initialized every 2 days
Chemical boundary condition	Climatology [*McKeen et al.,* 2002]
Vertical layers	30 (lowest grid box height 56 m)
Anthropogenic emissions	NEI'05 with adjustments
Biogenic emission	*Guenther et al.* [1993,1994]

ASOS (T, Winds) and ARB (O_3, NO_x) Surface Observations

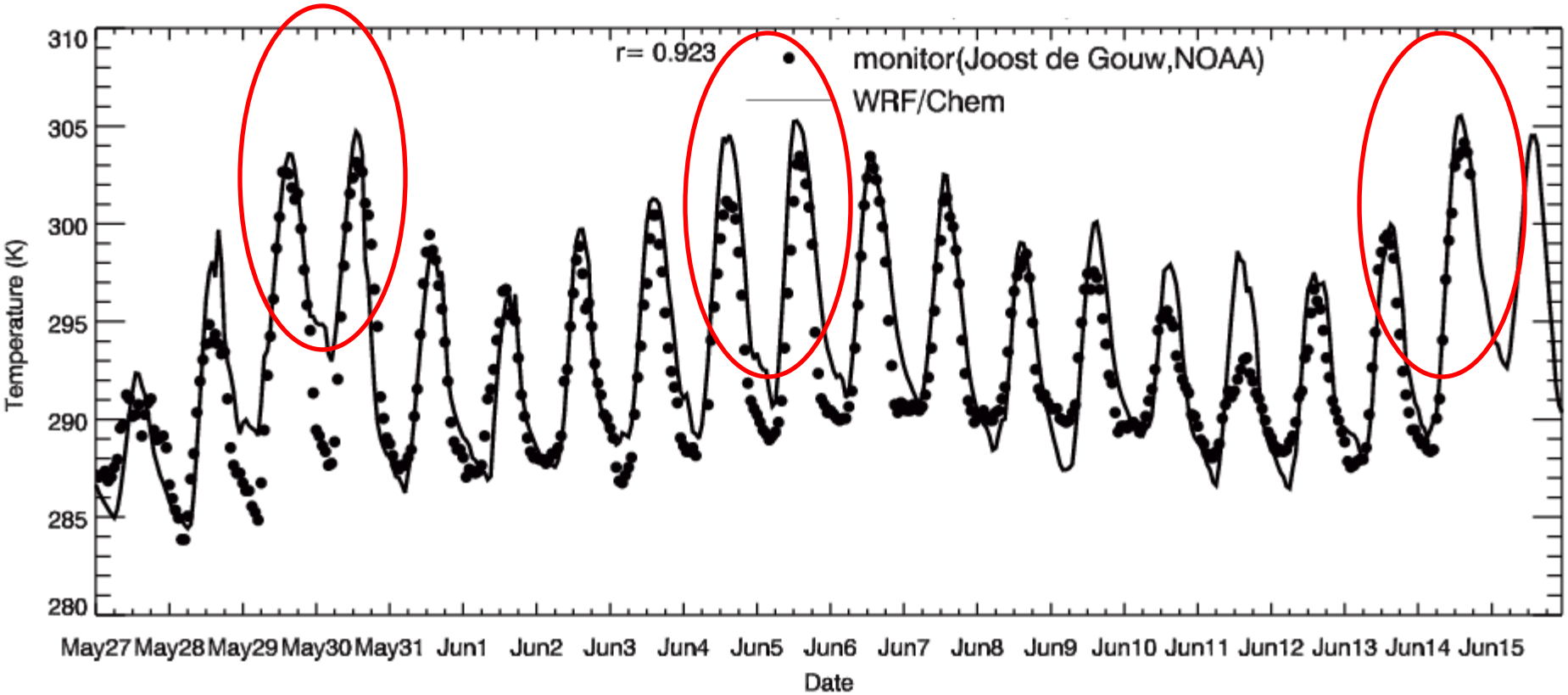


Site	Name	Alt.
CQT	Downtown LA	56
FUL	Fullerton	29
LAX	LA Intl Airport	38
ONT	Ontario	287
RIV	Riverside	353
VNY	Van Nuys	244
Los Angeles	N. Main Street	27
Los Angeles	N. Long Beach	2
Los Angeles	Reseda	69
Riverside	Rubidoux	76
San Bernardino	4th Street	0
San Diego	El Cajon	44

Automated Surface Observing System (ASOS)

Surface Temperature (2-m) at Caltech Supersite

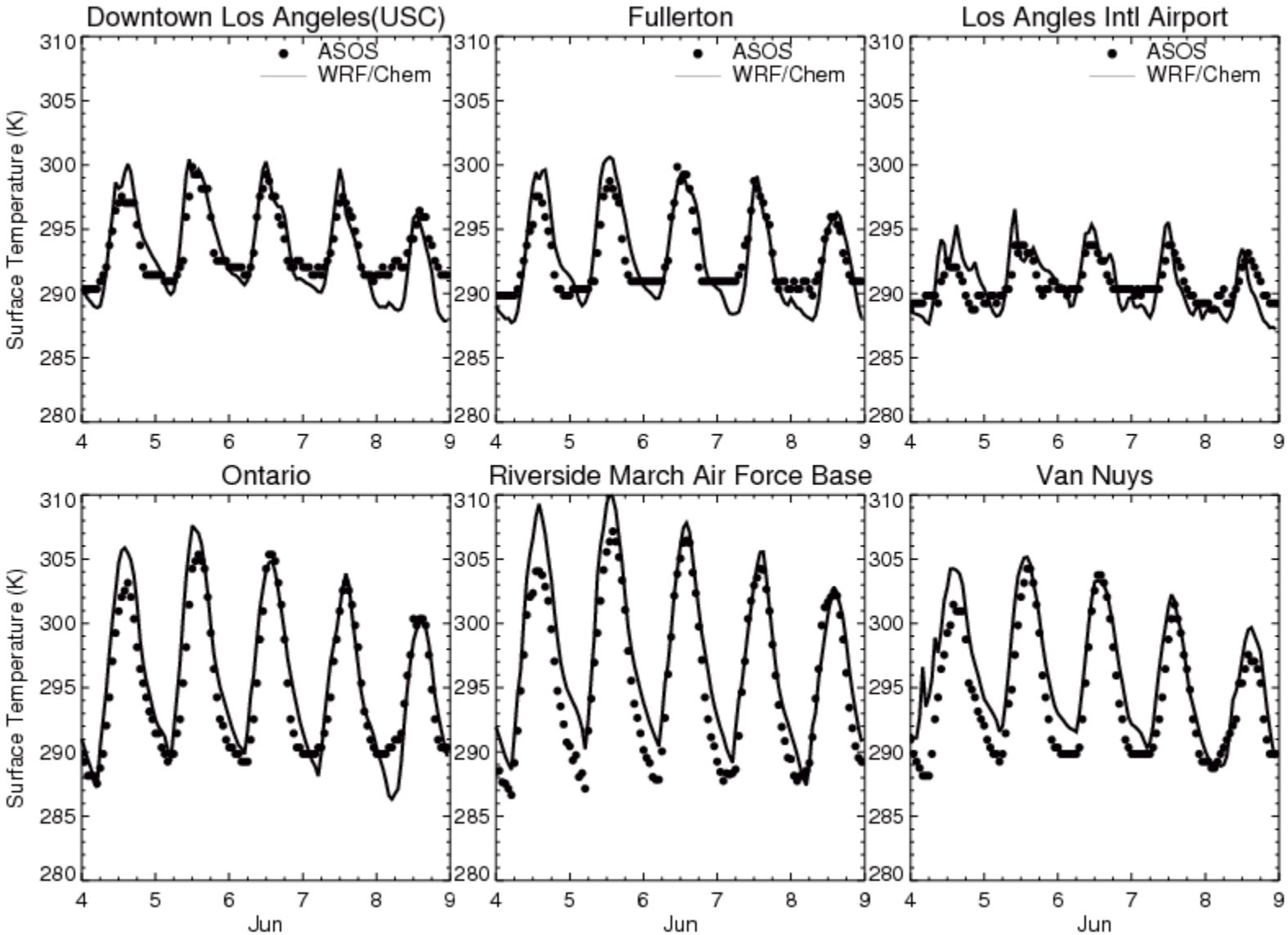
May 27–June 15



Temperature generally well captured, including the high temperatures during the weekends (e.g., r^2=0.94, n=120, p=0.01 for June 4 – 8) with positive nighttime biases.

Surface Temperature at Other ASOS Sites

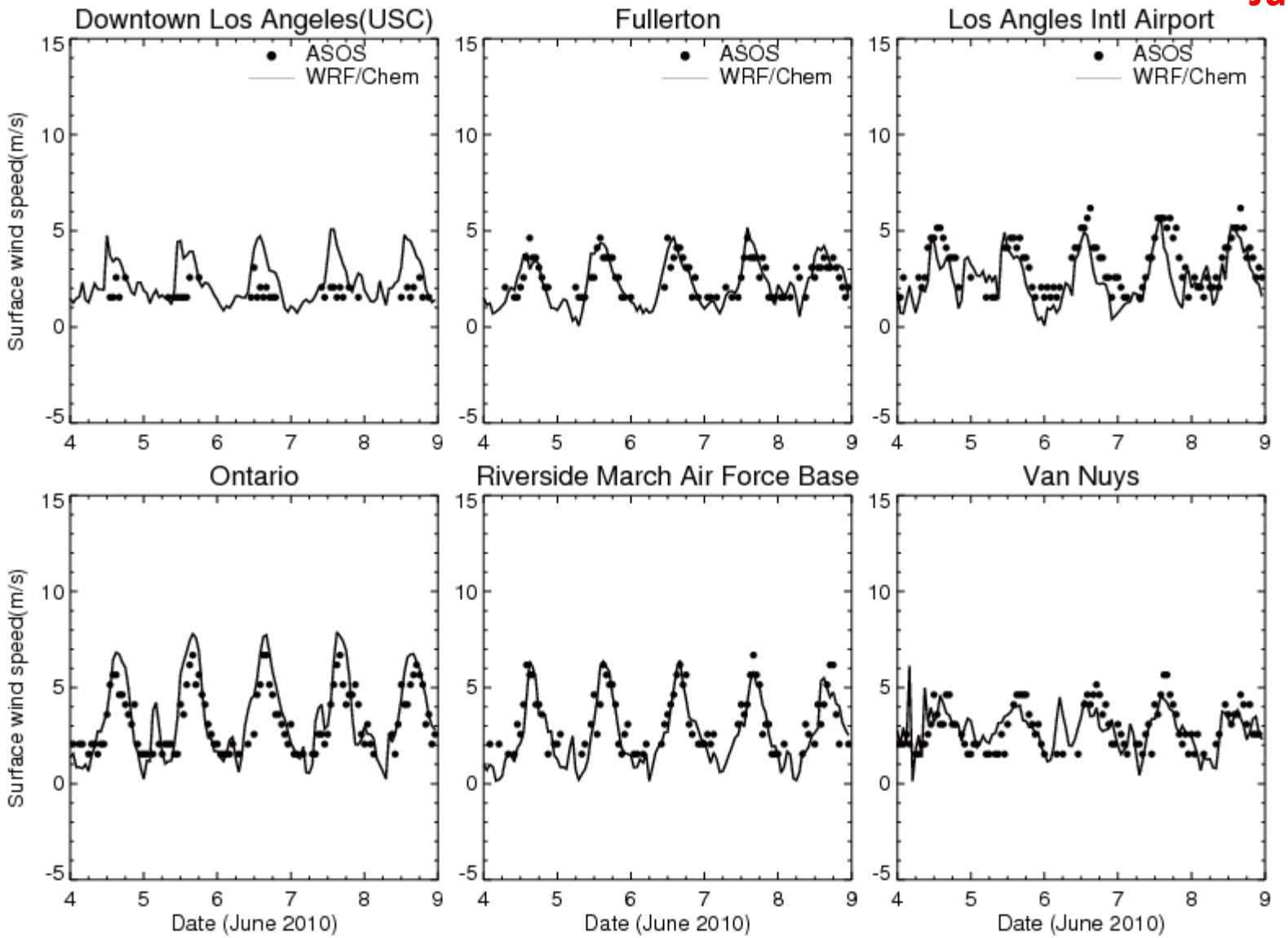
June 4–8



Day-to-day and diurnal variations reproduced by the model. A ~2 K positive nighttime bias at foothill sites.

Surface Wind Speed at Other ASOS sites

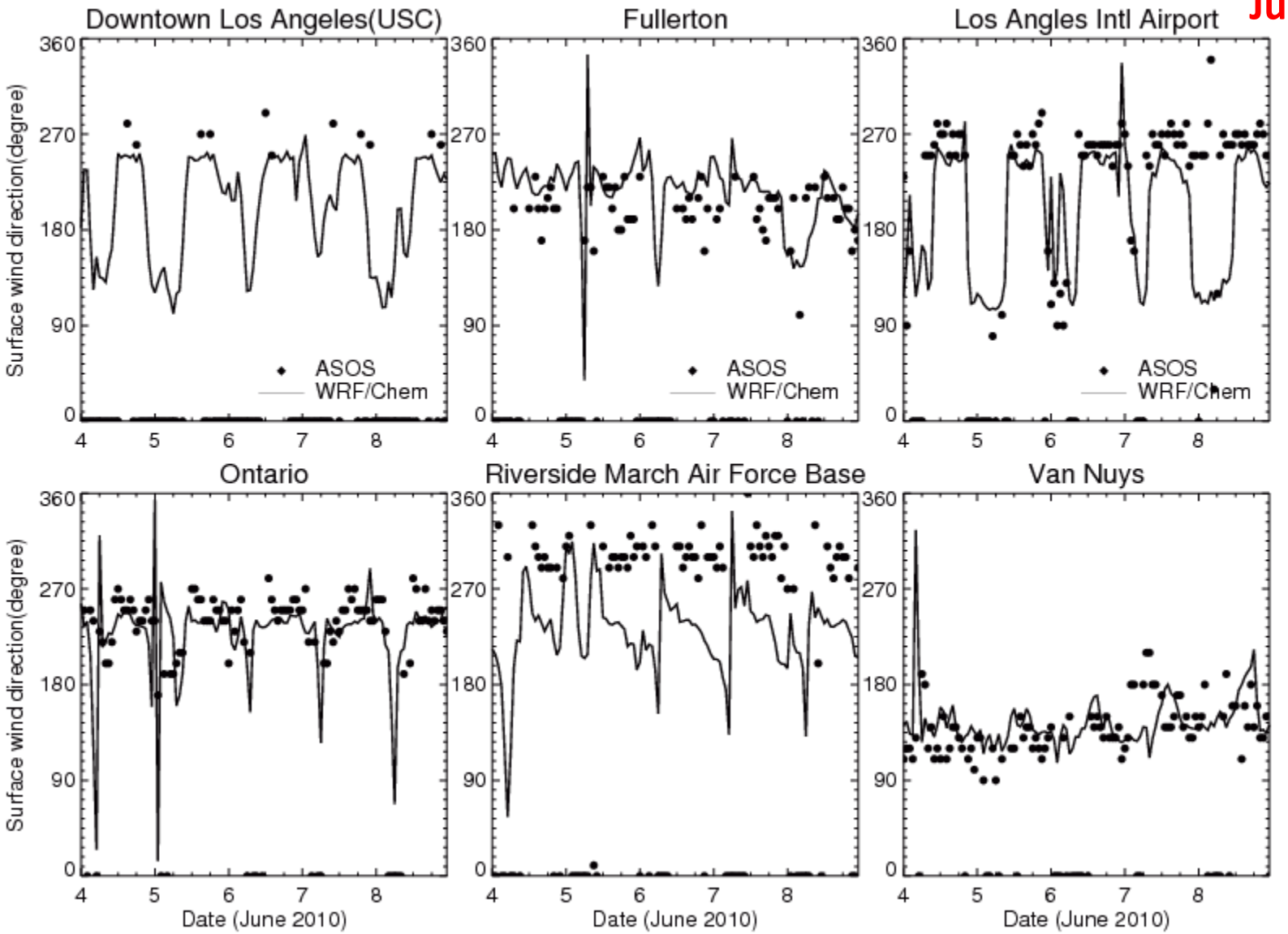
June 4–8



Model has difficulty at predicting near-zero wind speed.

Surface Wind Direction at Other ASOS sites

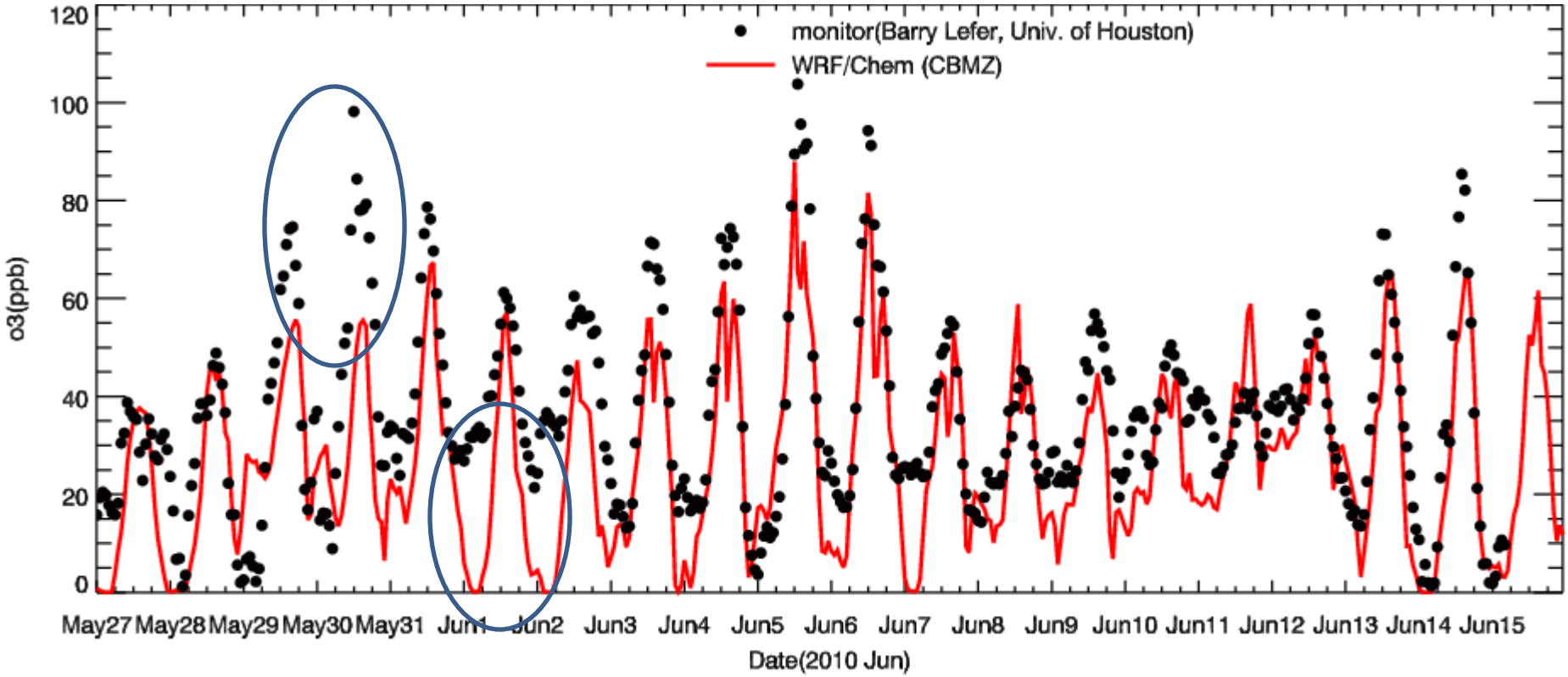
June 4–8



The prevailing direction and day/night direction change is captured by the model, but the frequent direction changes are difficult for model to predict.

Surface O_3 at Caltech Supersite

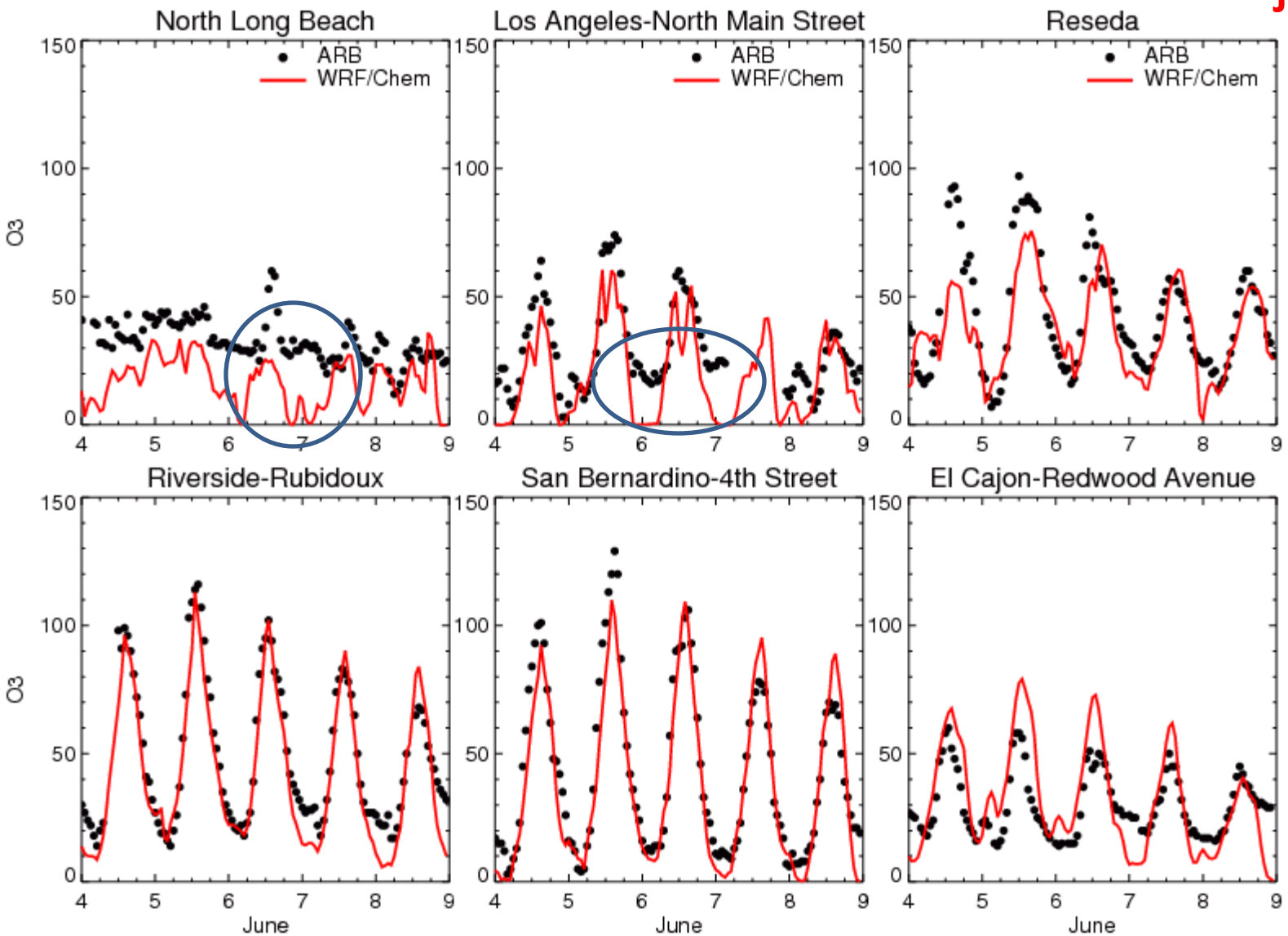
May 27–June 15



- **Model captures the diurnal, day-to-day, and synoptic variations of surface O_3.**
- **The nighttime depletion of O_3 (e.g., June 1, 2, 7) due to excessive emissions of NO_x.**
- **Model underestimates O_3 during May 29-30 (by 20–40 ppb) because of unusually deep boundary layer in the model.**

Surface O_3 at Other ARB sites

June 4–8

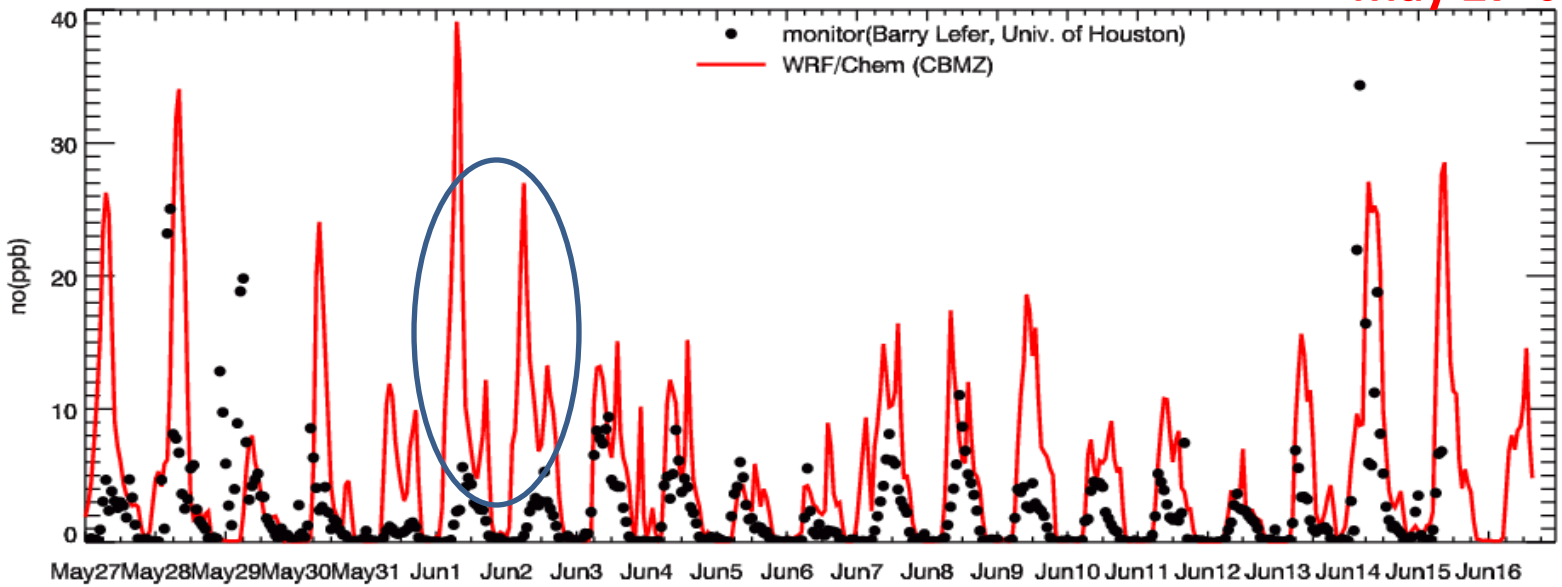


- **Downwind surface O_3 generally well captured.**
- **The nighttime depletion of O_3 due to excessive emissions of NO_x in source region.**

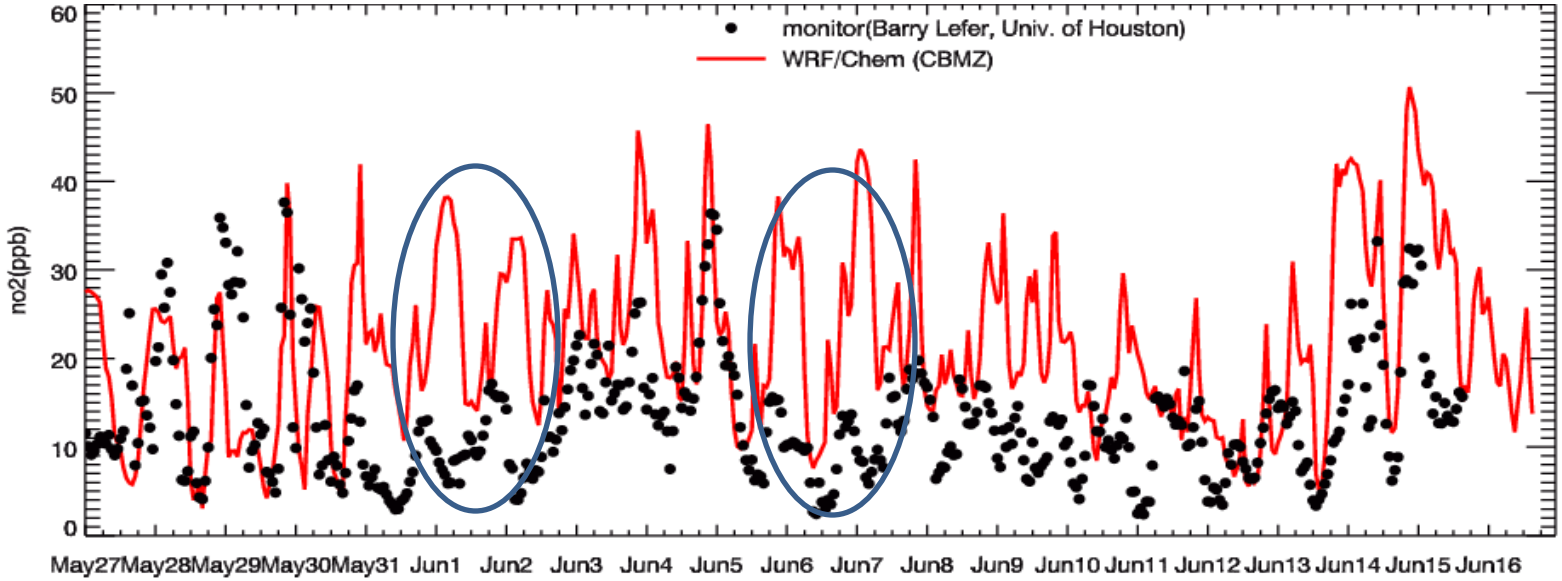
Surface NO and NO_2 at Caltech Supersite

May 27–June 15

NO

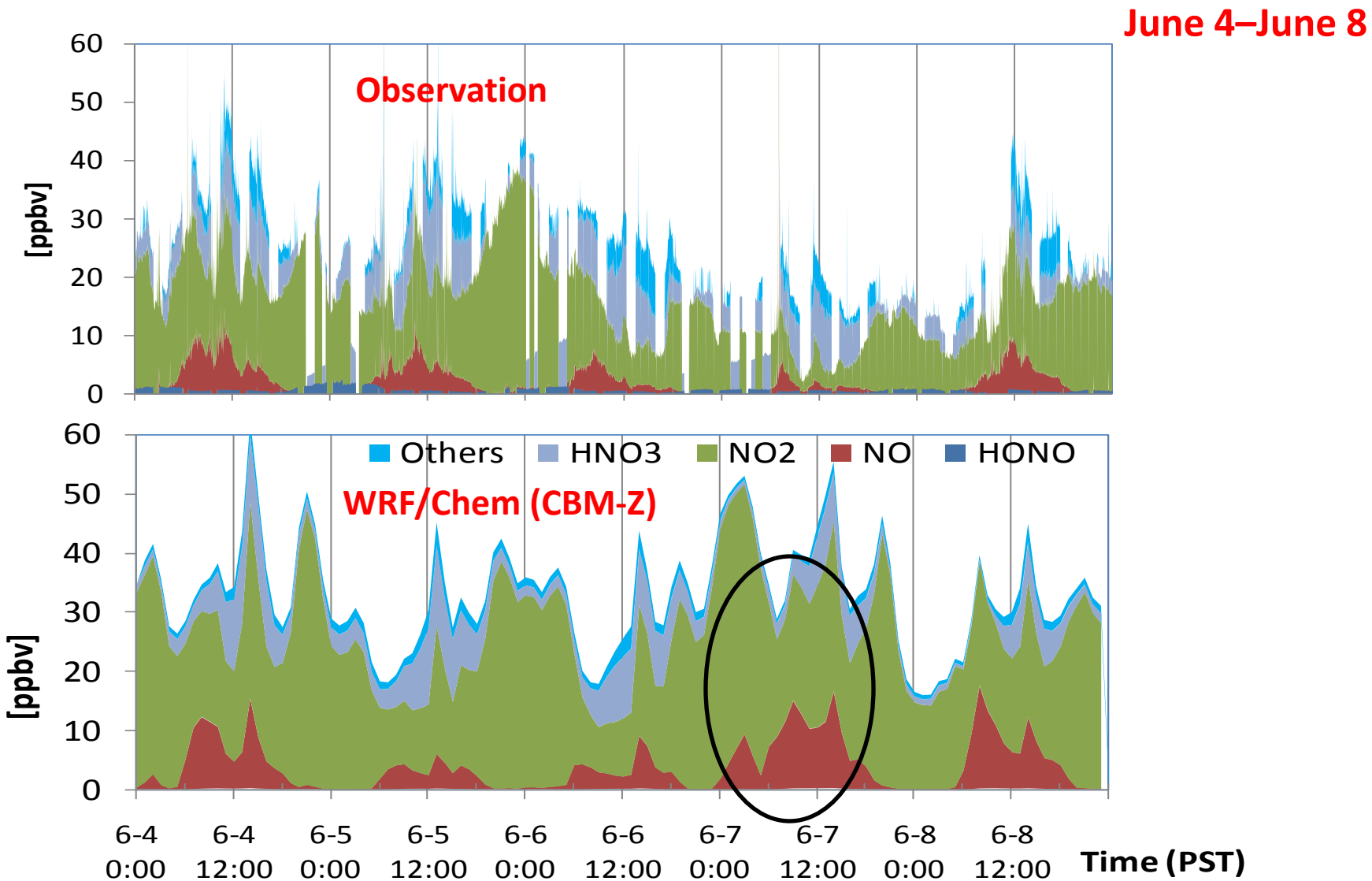


NO_2



- **The nighttime NO_x are consistently overestimated.**

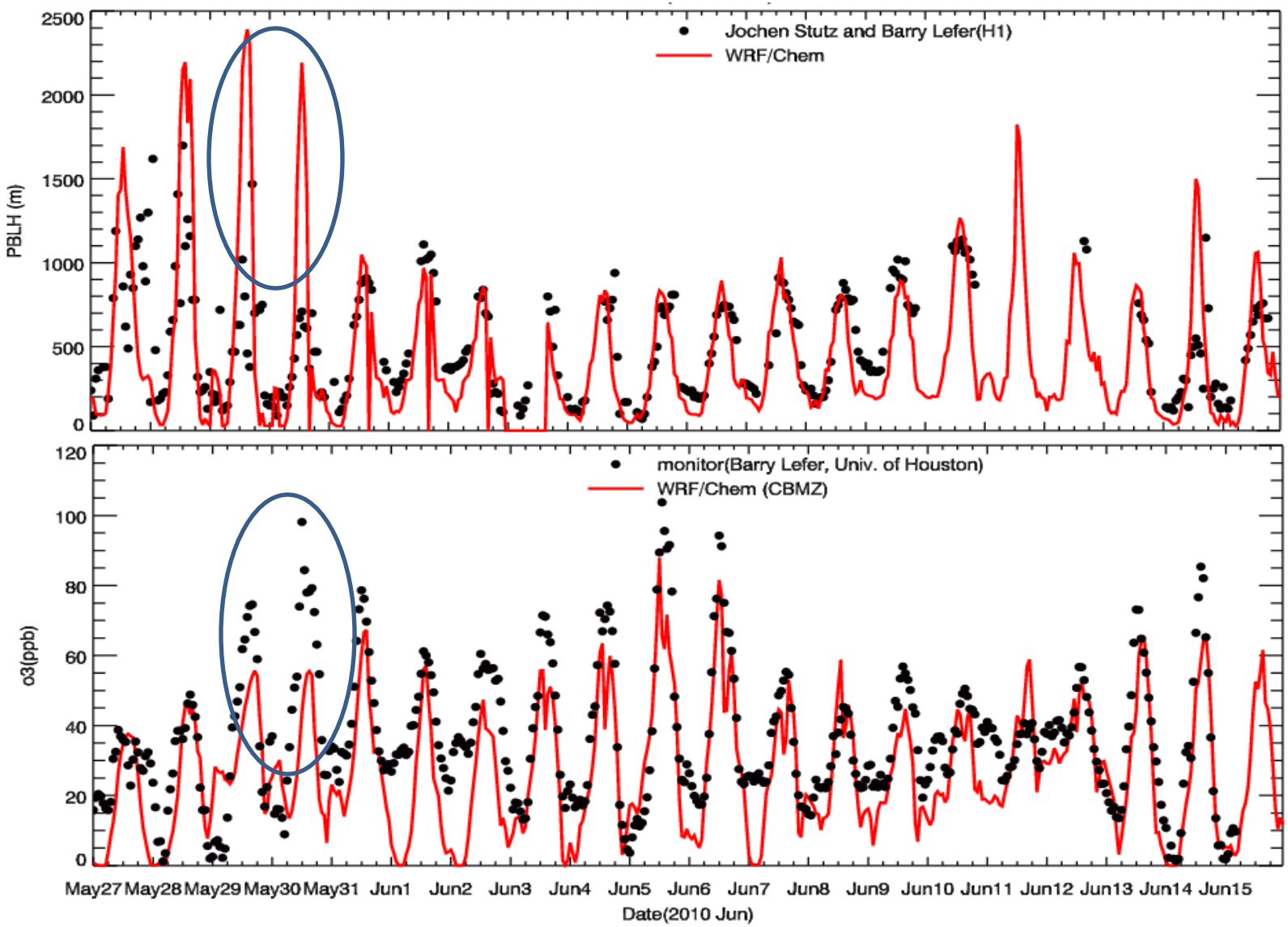
Surface NO_y Partitioning at Caltech Supersite



- **HNO_3 in good agreement, HONO underestimated, NO, NO_2 overestimated.**

PBL Height and O_3 at Caltech Supersite

May 27–June 15

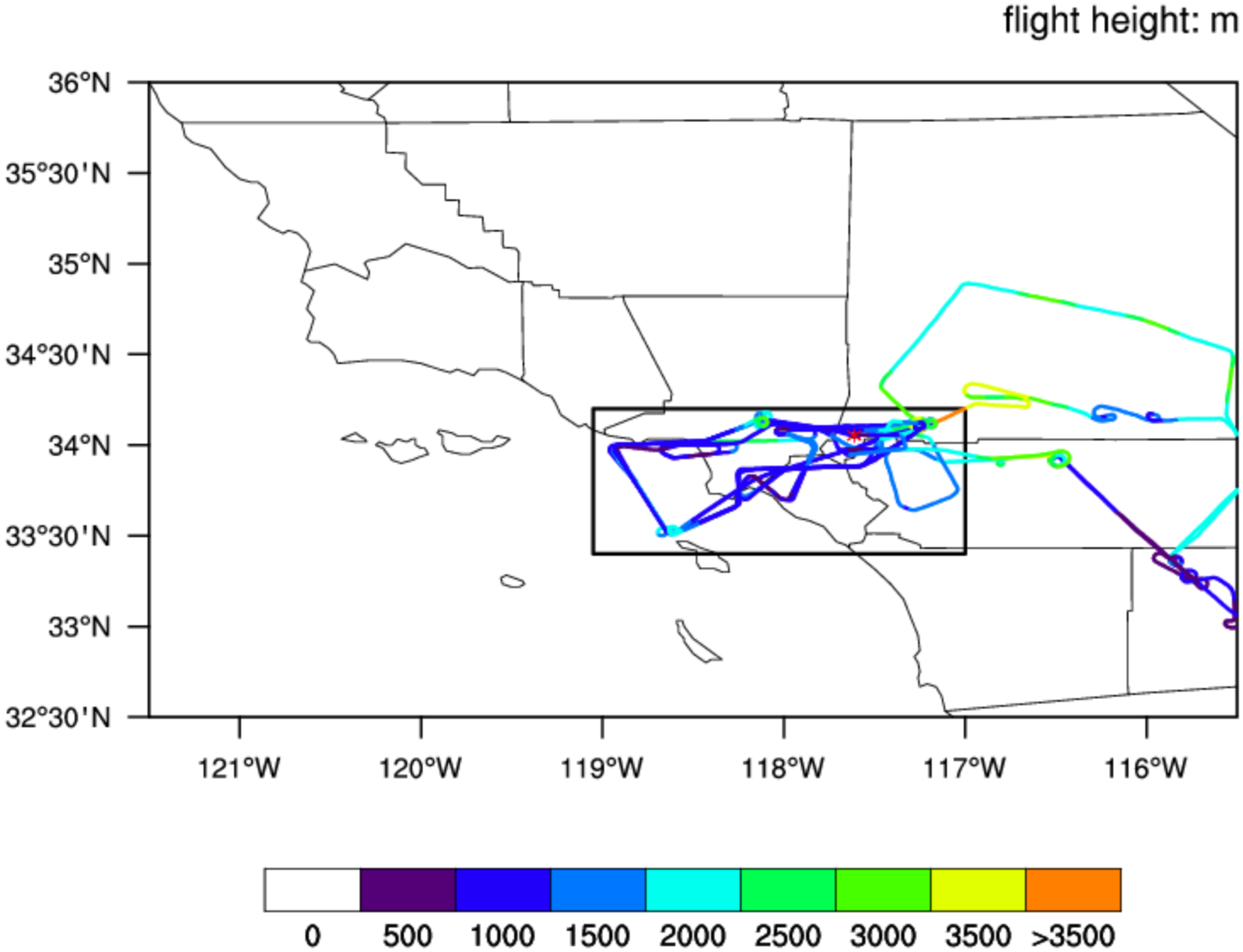


Model PBL heights were 2–3 times the lidar retrieved values for May 29-30 (leading to the corresponding low O_3 concentrations) but in excellent agreement for other days.

WP-3 Flight Tracks over the LA Basin

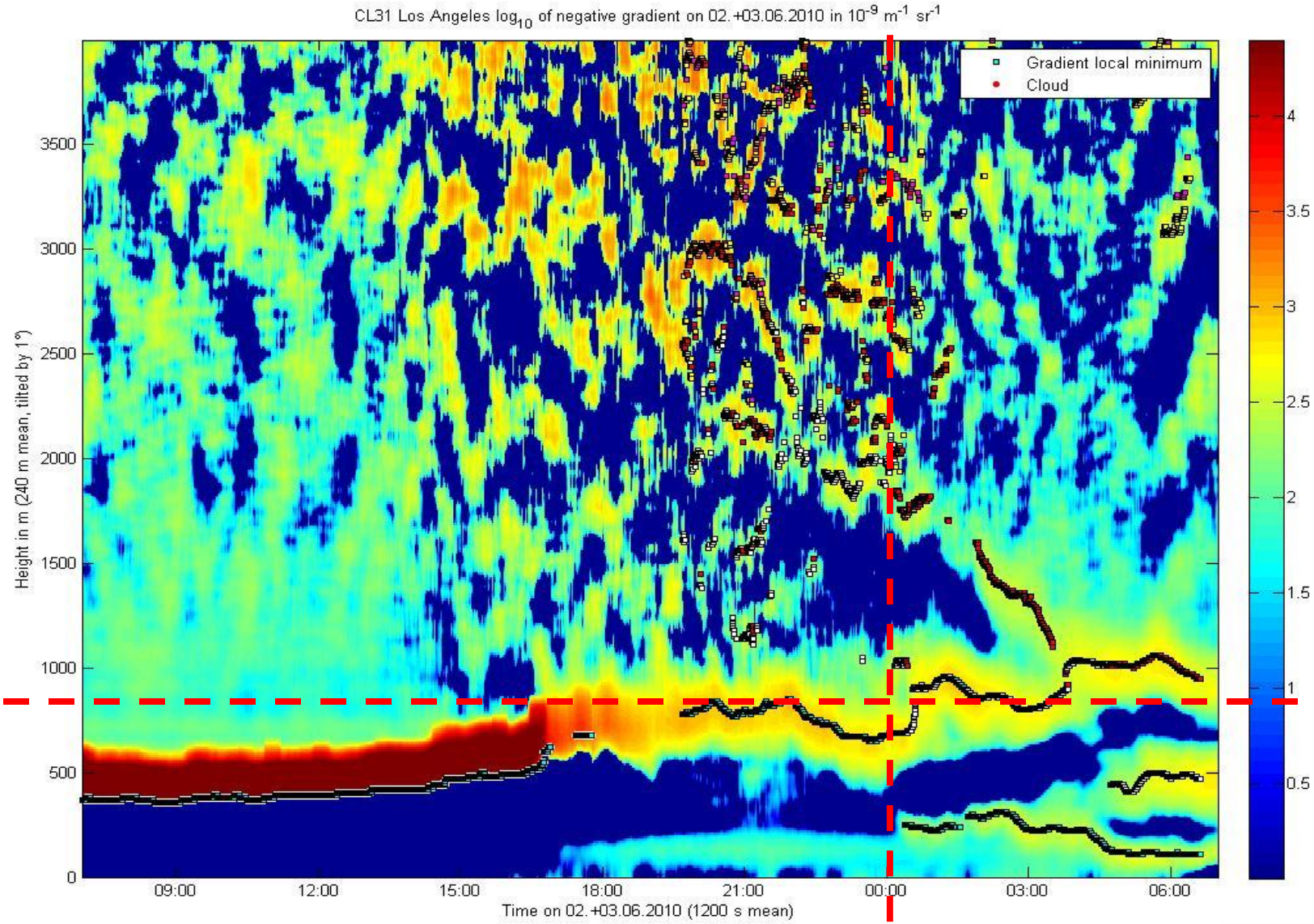
June 2–3

Targeting nighttime chemistry



The Residual Layer

June 2

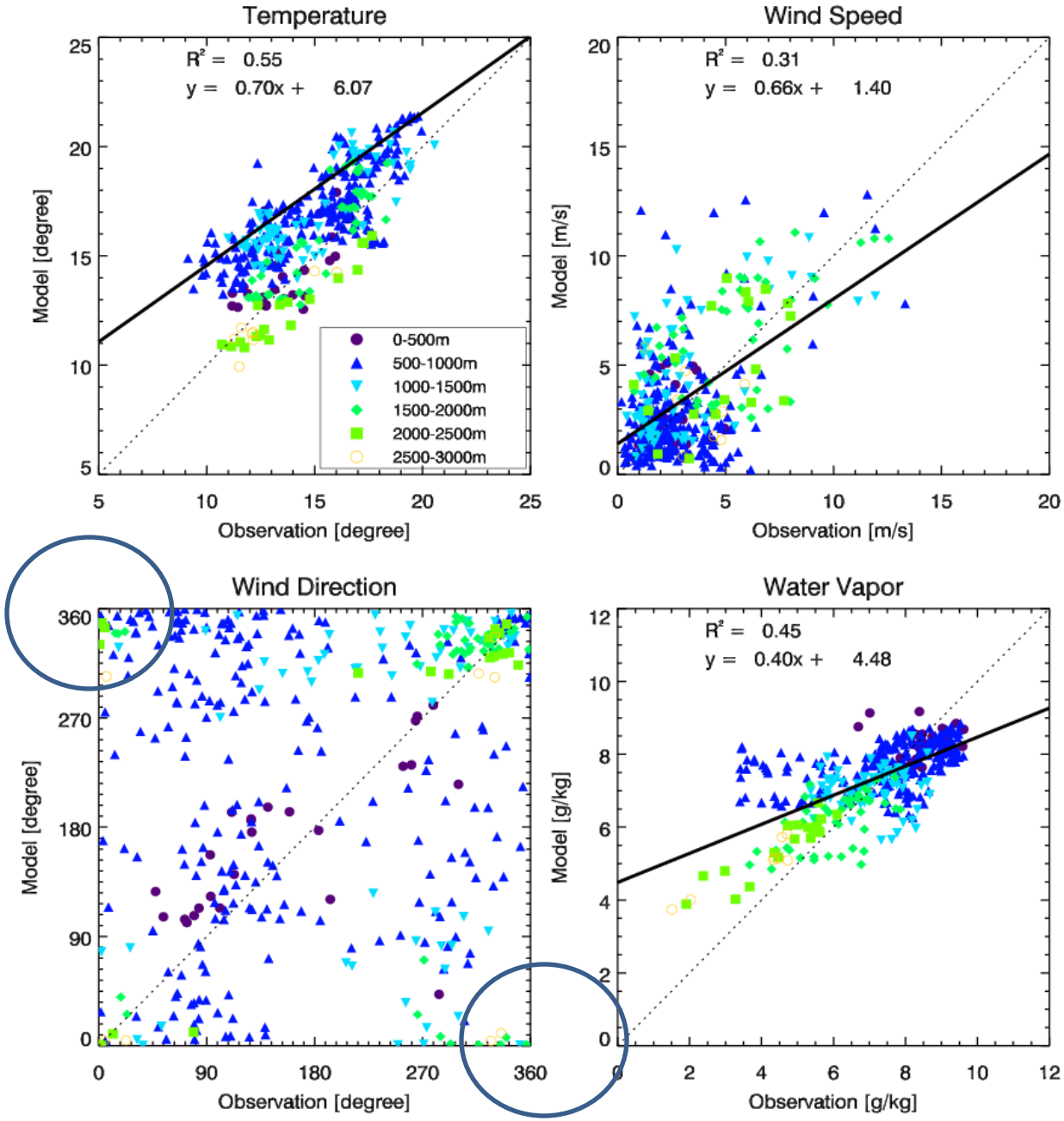


0 2 5 8 11 14 17 20 23

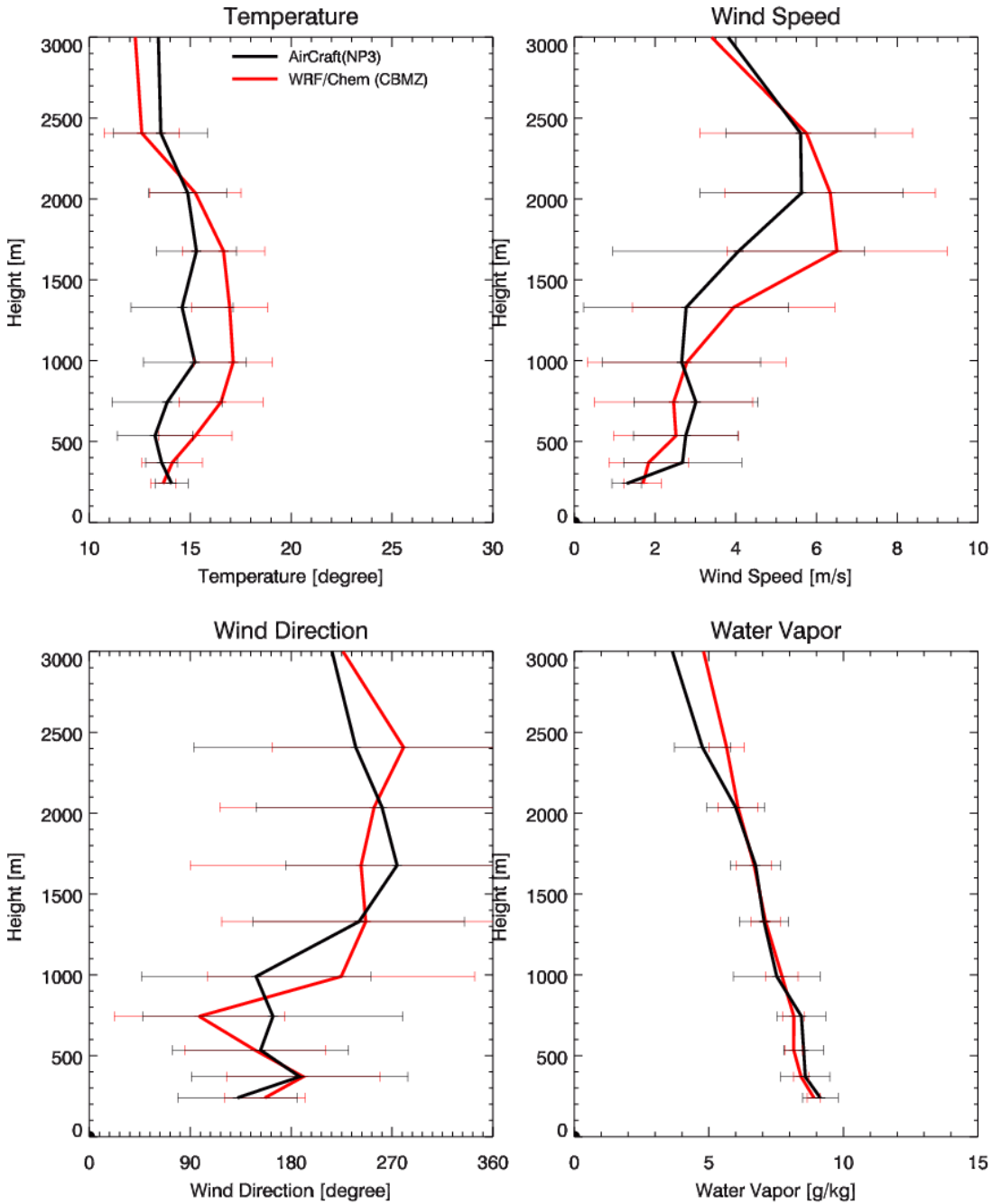
Local Time

Spatial Variations of T, Winds and Water Vapor in LA Basin

June 2–3
Night



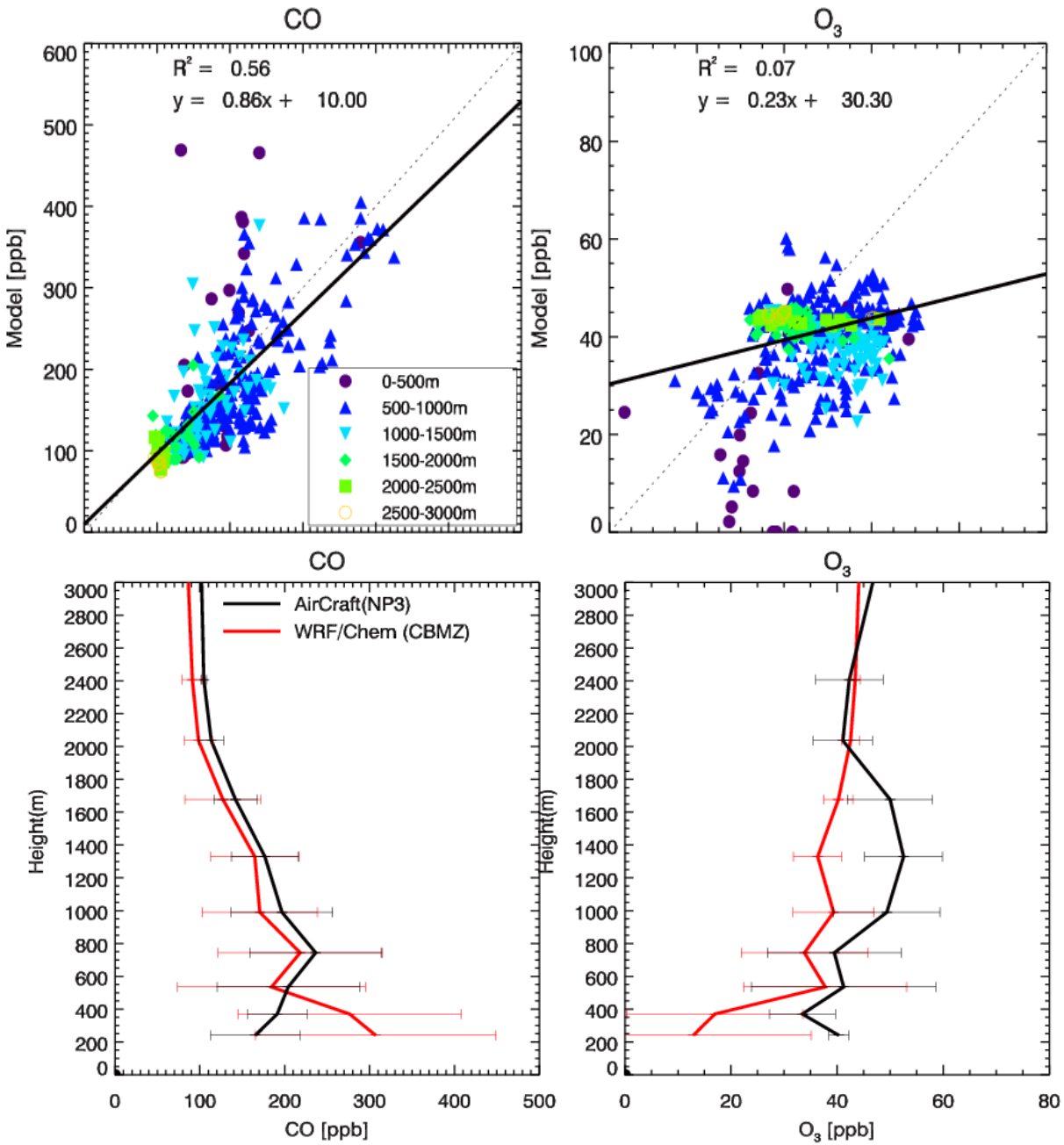
Vertical Profiles of T, Winds and Water Vapor in LA Basin



June 2–3 Night

- **Model captures the overall vertical distributions.**
- ***T* inversion layer below 1 km. Model *T* positive bias of ~2–3 K at 0.5–2 km.**
- **Model winds too strong at 1–2 km and too weak below 1 km.**

Vertical Distributions of CO and O_3 in the LA Basin



June 2–3 Night

- **Good agreement for CO at 0.5–3 km.**
- **Surface CO overestimated in the model (weaker winds and excessive emissions?).**
- **O_3 underestimated below 2 km with largest discrepancies at 1–2 km (excessive dilution due to strong winds? Or less daytime O_3 production due to NO_x?) and near the surface (titration).**

Conclusions

- **Diurnal, day-to-day and synoptic variations of Surface temperature, wind speed and direction, PBLH and surface O_3 were generally reproduced (temperature: r^2=0.94, n=120; wind speed: r^2 =0.75, n=104; PBLH: r^2=0.70, n=94, O_3: r^2=0.92, n=114) except for May 29-30.**
- **The high O_3 levels during May 29-30 were under-predicted by 20-40 ppbv by the model, in large part due to the deeper than observed PBL heights in the model.**
- **3-Dimensional temperature, winds and water vapor were well predicted in the LA basin during June 2-3 night.**
- **Modeled CO below 3 km showed good agreement with the aircraft observations while were overestimated below 500 m. Modeled O_3 showed significantly underestimation at 800-1600 m and it was associated with overestimated NO_2, HNO_3 and NO_y in RL. The vertical profiles of CO, O_3 and NO_x indicate that the emissions of CO and NO_x in the model are too high.**

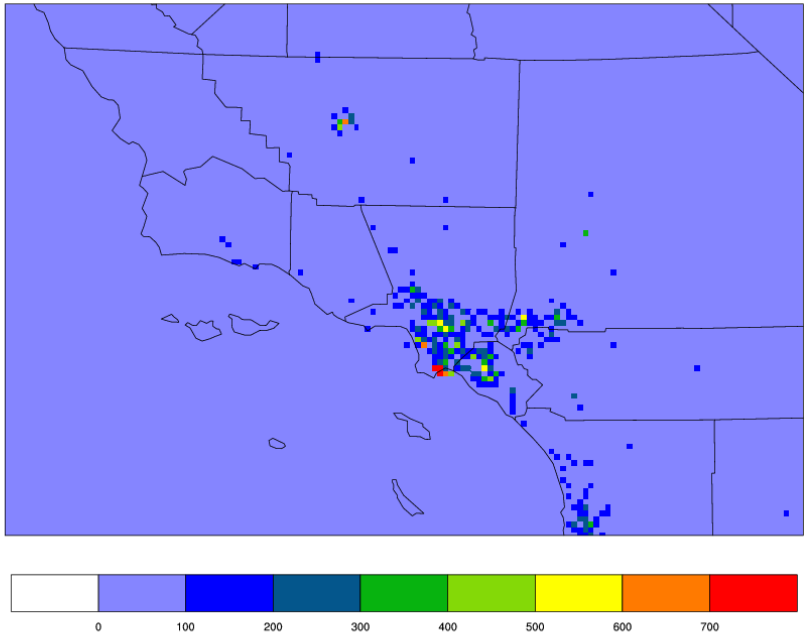
Spatial and Temporal Distribution of Emissions

Anthropogenic Emission raw Data: National Emission inventory 2005 (Stu McKeen)
Spatial Allocation: according to geography (land use) , population and economy info.
Temporal Allocation: hourly factors are included

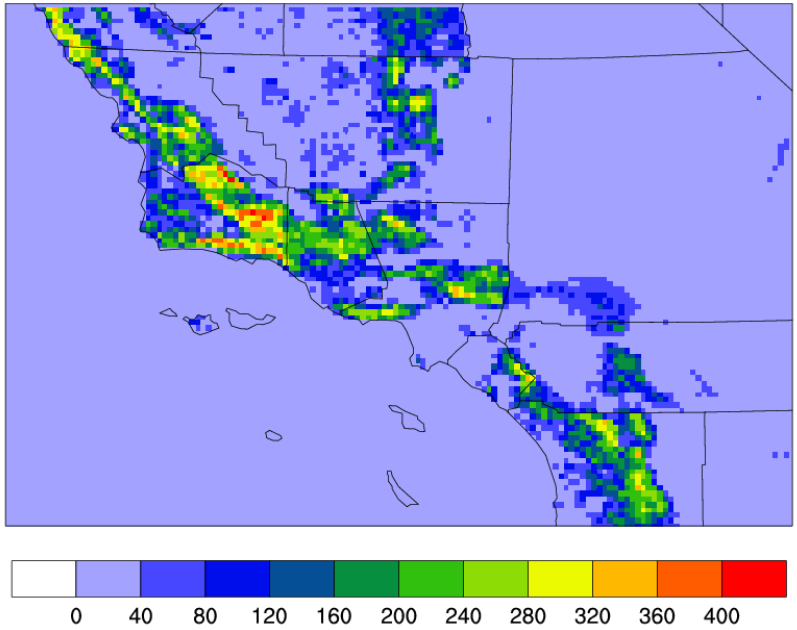
4 x 4 km Gridded data aggregated into 36, 12, 4km

Biogenic Emissions: Guenther Online, Based on the distribution of vegetation, and calculated to temperature and radiation.

Anthropogenic NO_x

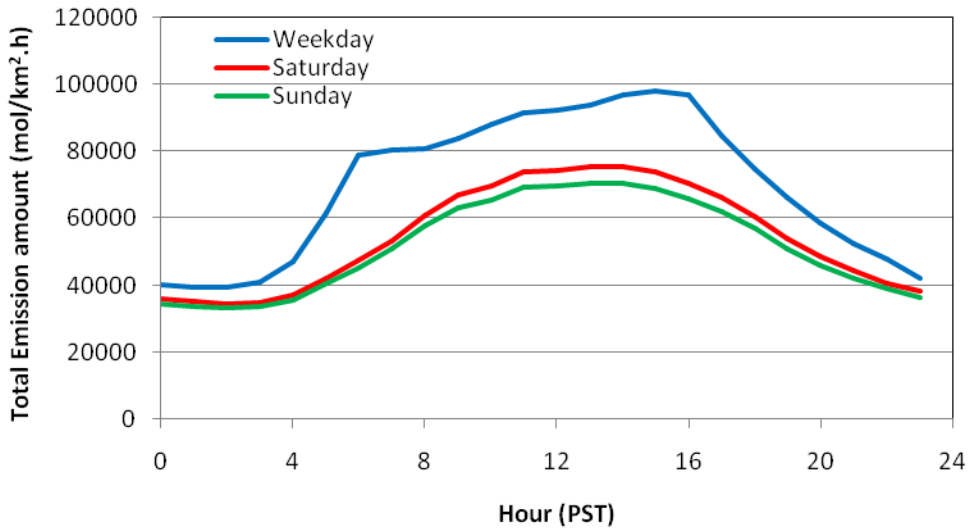


Biogenic Isoprene

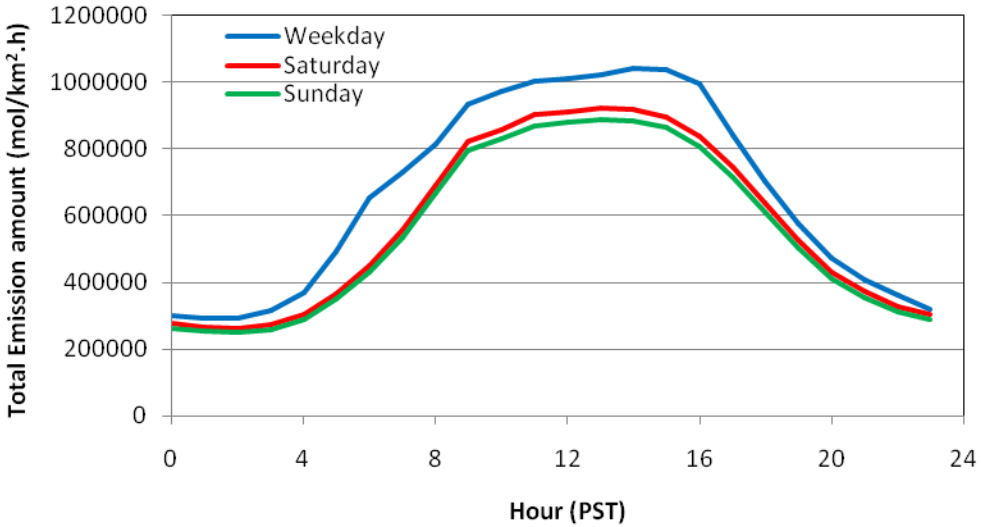


Reduction of 28% of CO and 24% of NO_x from 2005 to 2010 according to CARB

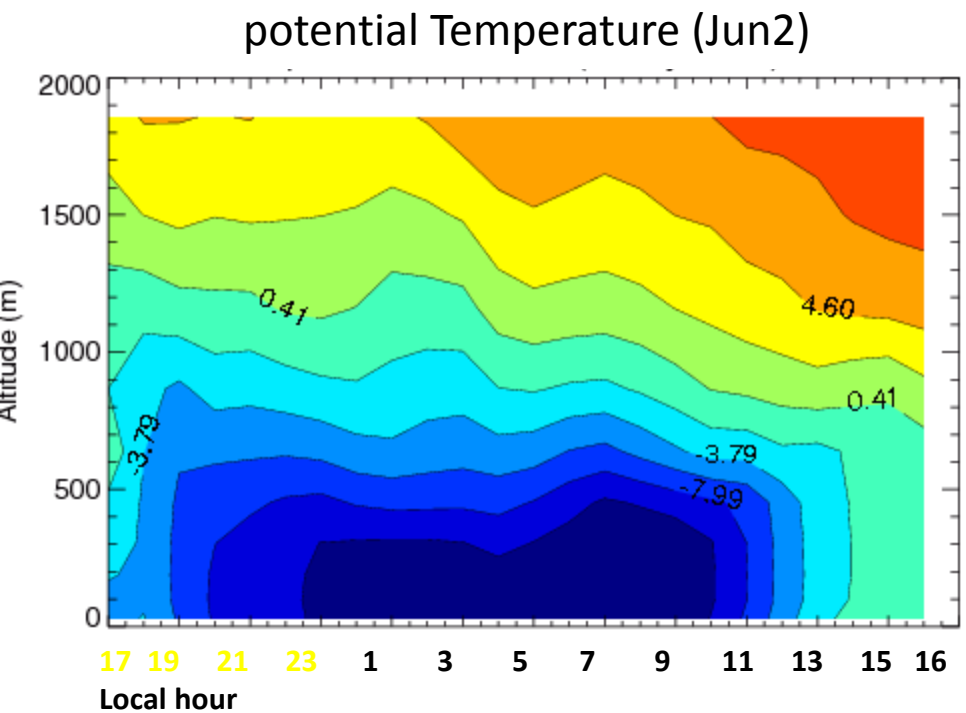
Hourly NO_x variation for 4km domain

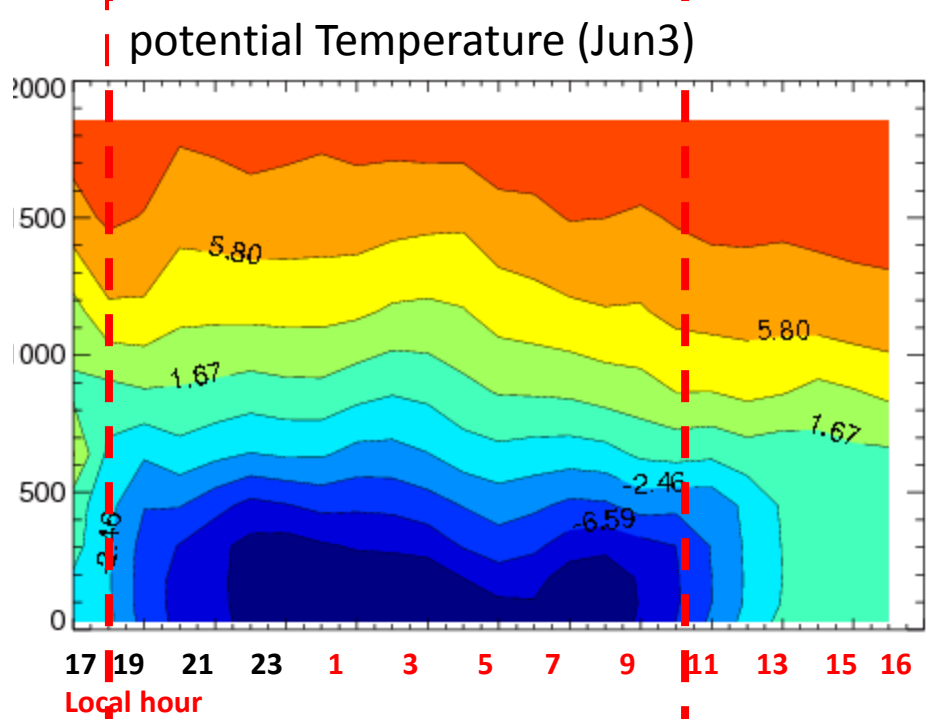


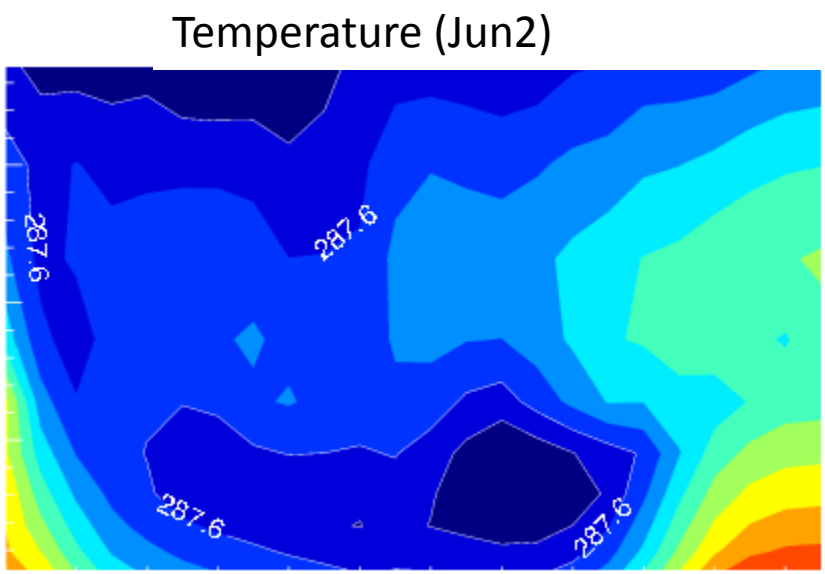
Hourly CO variation for 4km domain

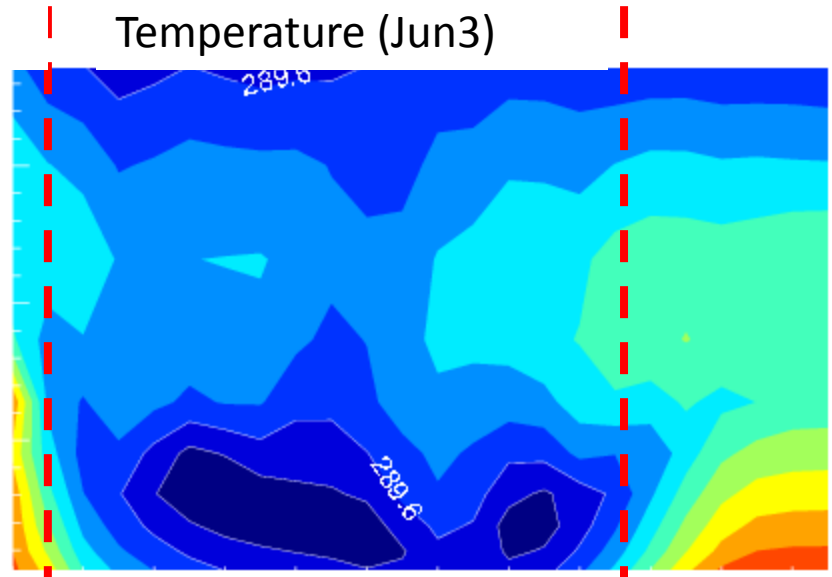


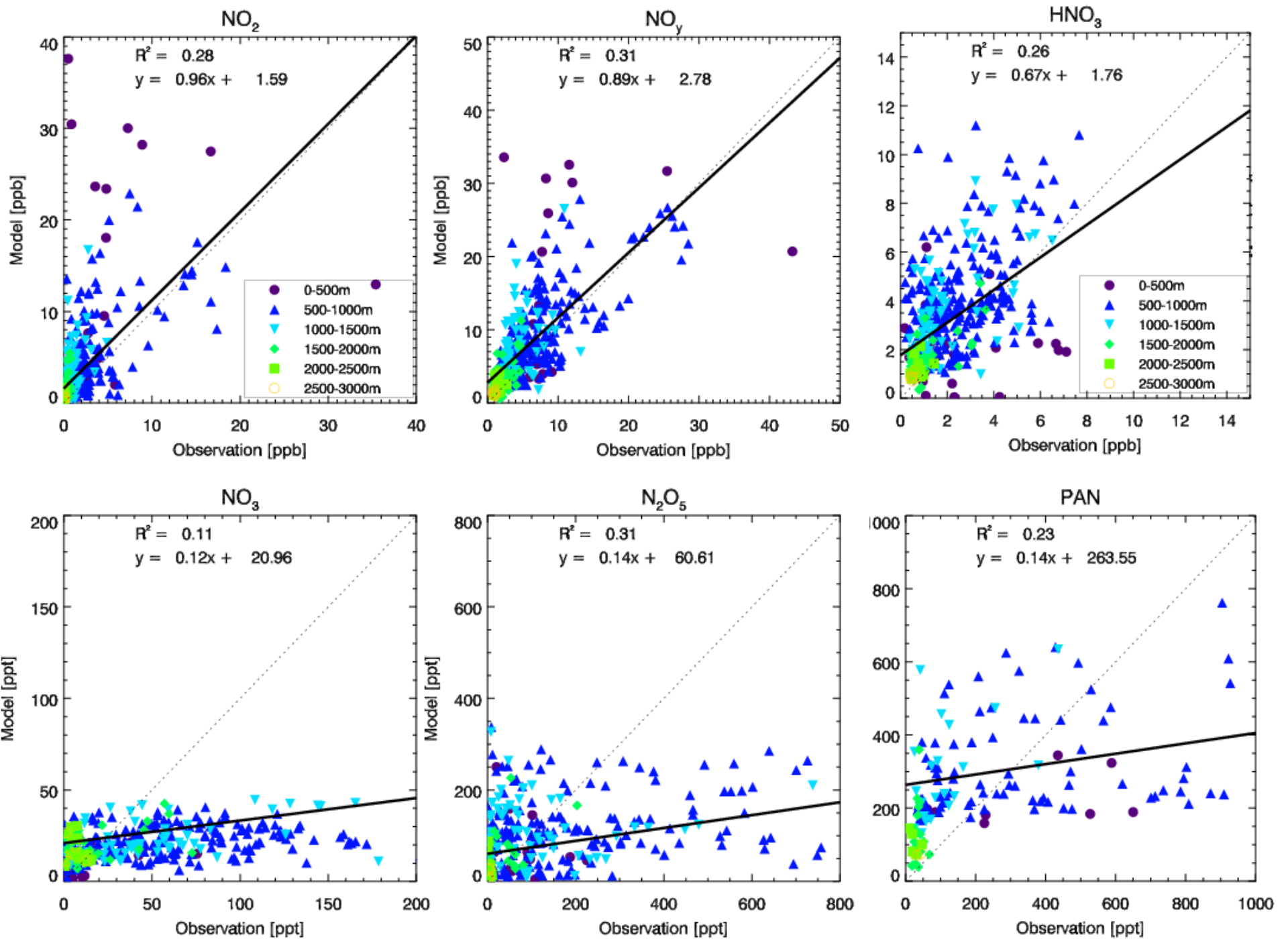
kg/km^2.hr	Weekday	Saturday /Weekday	Sunday Weekday
E_SO_2	162428	0.98	0.97
E_NO	1365922	0.82	0.78
E_CO	11749318	0.90	0.86
E_ISO	230	1.13	1.13
E_ETH	267446	1.00	1.00
E_HC3	322526	1.06	1.03
E_HC5	167418	1.09	1.06
E_HC8	117918	0.91	0.89
E_XYL	42358	1.10	1.08
E_OL2	55850	1.07	1.04
E_OLT	39632	1.07	1.03
E_OLI	51954	1.12	1.07
E_TOL	55160	1.06	1.03
E_CSL	404	1.00	1.00
E_HCHO	34684	0.93	0.90
E_ALD	11334	0.95	0.92
E_KET	26372	1.00	0.98
E_ORA2	432	1.00	1.00
E_NH3	483030	1.01	0.98
E_VOC (total)	1193718	1.04	1.01

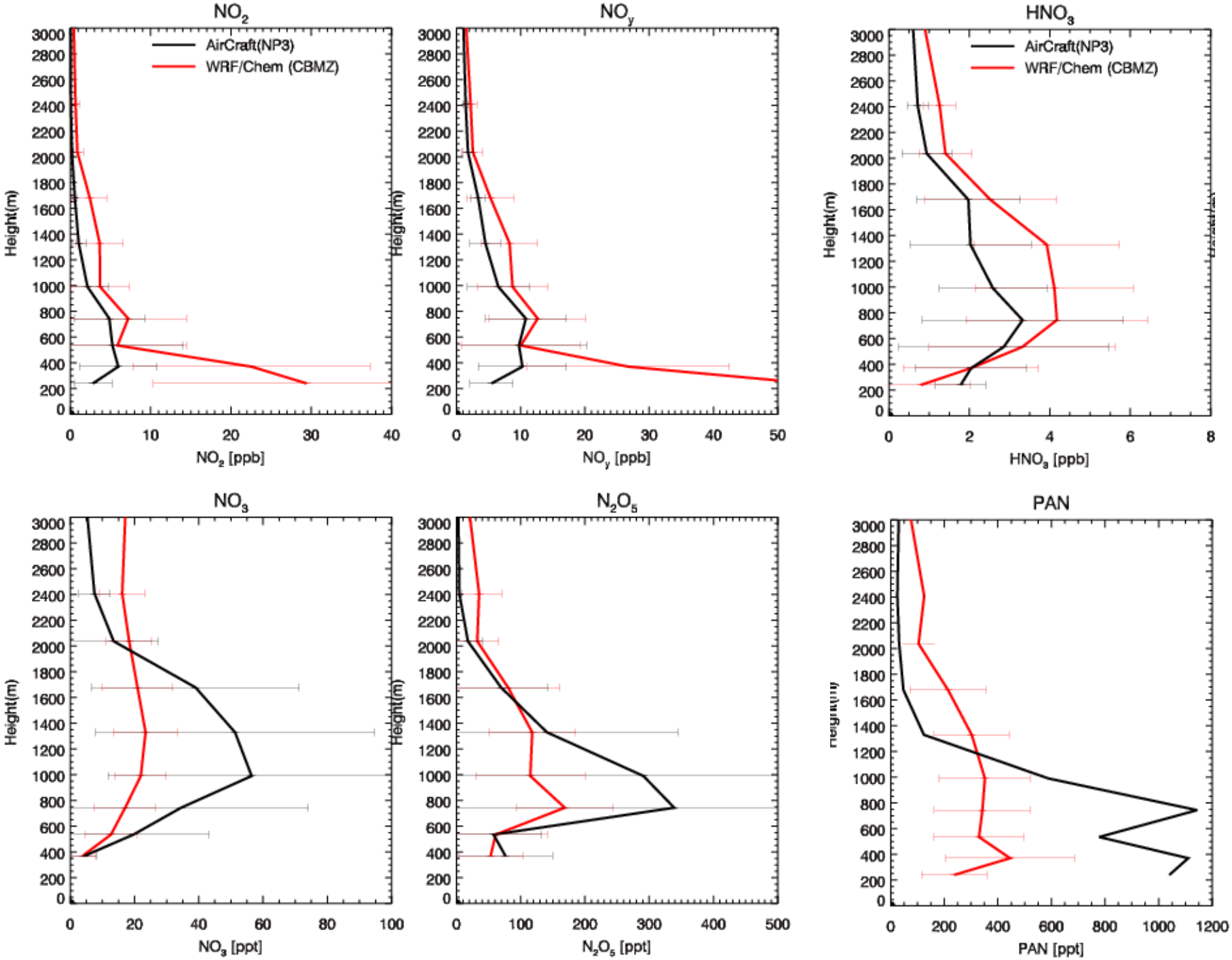

potential Temperature (Jun2)
Altitude (m)
2000
1500
1000
500
0
0.41
4.60
0.41
-3.79
-3.79
-7.99
17 19 21 23 1 3 5 7 9 11 13 15 16
Local hour


potential Temperature (Jun3)
5.80
5.80
1.67
1.67
-2.46
-6.59
17 19 21 23 1 3 5 7 9 11 13 15 16
Local hour


Temperature (Jun2)
287.6
287.6
287.6
287.6


Temperature (Jun3)
289.6
289.6


NO2
R² = 0.28
y = 0.96x + 1.59
Model [ppb]
Observation [ppb]
0-500m
500-1000m
1000-1500m
1500-2000m
2000-2500m
2500-3000m
NOy
R² = 0.31
y = 0.89x + 2.78
Model [ppb]
Observation [ppb]
HNO3
R² = 0.26
y = 0.67x + 1.76
Observation [ppb]
NO3
R² = 0.11
y = 0.12x + 20.96
Model [ppt]
Observation [ppt]
N2O5
R² = 0.31
y = 0.14x + 60.61
Model [ppt]
Observation [ppt]
PAN
R² = 0.23
y = 0.14x + 263.55
Observation [ppt]


NO2
NOy
HNO3
NO3
N2O5
PAN
AirCraft(NP3)
WRF/Chem (CBMZ)
Height(m)
NO2 [ppb]
NOy [ppb]
HNO3 [ppb]
NO3 [ppt]
N2O5 [ppt]
PAN [ppt]