# Emission, pollutants transport and boundary conditions during ARCTAS/CARB -- A regional-scale modeling study

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# Outline

- Objectives and scientific questions
- Flights information and model introduction
- Results and preliminary analysis
- Summary and future work

# Objectives and scientific questions

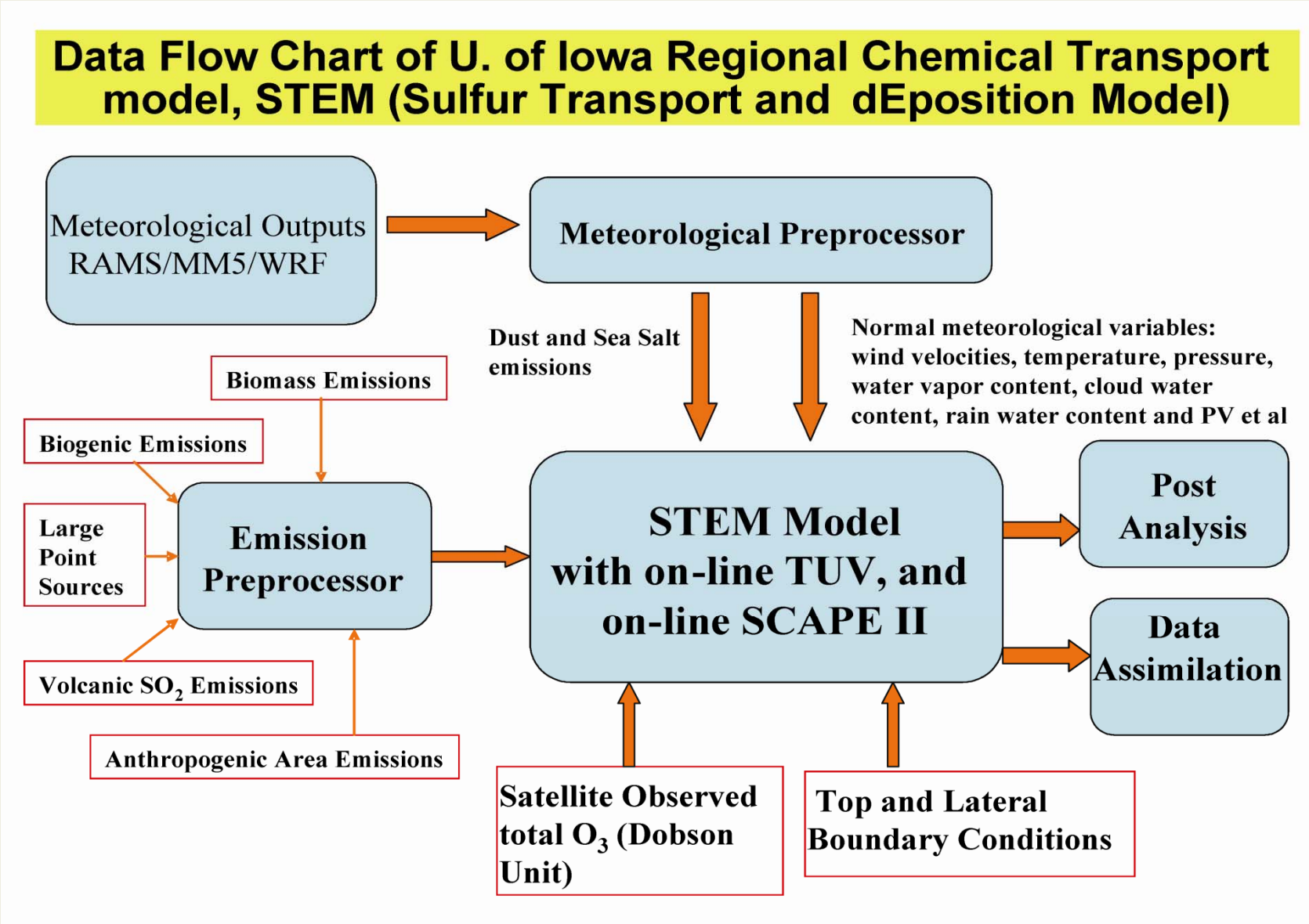
By using a regional chemical transport model STEM

- Assess California emission inventories
- CO and O3 transport
- Evaluate impact of oceanic boundary conditions on inland air quality

# Flights information

- 4 full flight days (6.18, 6.20, 6.22, 6.24)
- 1 transitional flight (6.26)
- DC-8 and P-3B aircrafts

# Model introduction



# Model setup

- Domain **North America**
- Grids **124x124; 60 km**
- Layers **18 ~10.5km**
- Time period and interval **June 10- June 30; 6 hours**
- Meteorology input **WRF**
- Column ozone data

  **Ozone Mapping Spectrometer (OMI)**
- Anthropogenic emission **NEI2001 for US**
- Biomass burning Regional Air Quality Modeling System

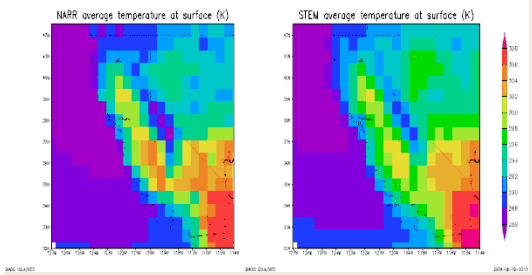
  **(RAQMS)**
- Boundary condition **RAQMS**
- Chemical mechanism **SAPRC99**

# Results and preliminary analysis

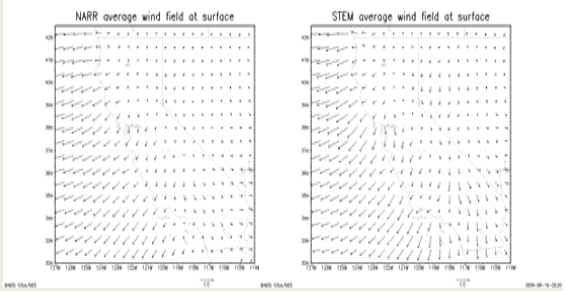
Examine WRF performance as meteorology input

**FOUNDATION**

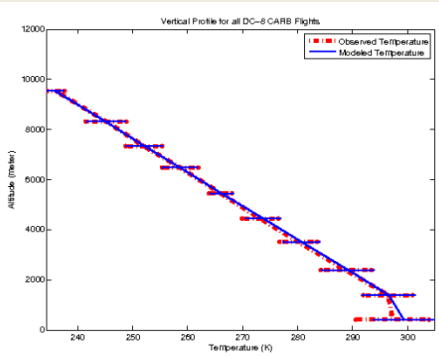
- Assess California emission inventories
- CO and O3 transport
- Evaluate impact of oceanic boundary conditions on inland air quality

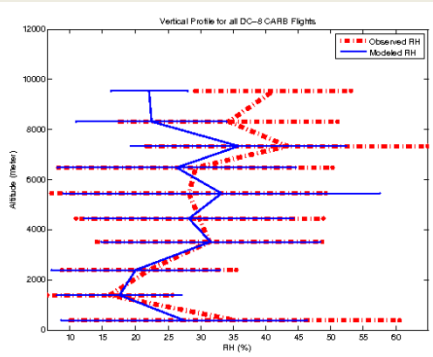


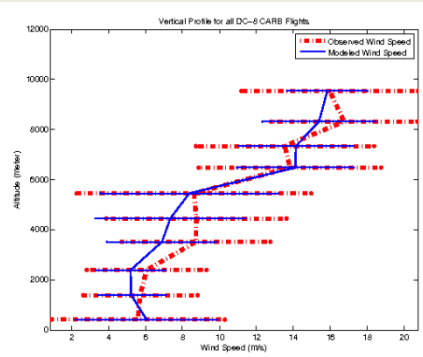

# WRF evaluation

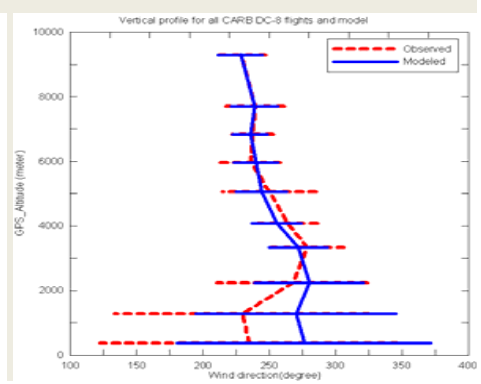



- Comparison
  - o North American Regional Reanalysis (NARR)
  - o Flight observations
  - o Walnut Grove Tower (WGT)
- A few biases: surface wspd (-), RH (-)
- Discrepancies can be used to explain STEM results



# Results and preliminary analysis

Examine WRF performance as meteorology input

FOUNDATION

- Assess California emission inventories
- CO and O3 transport
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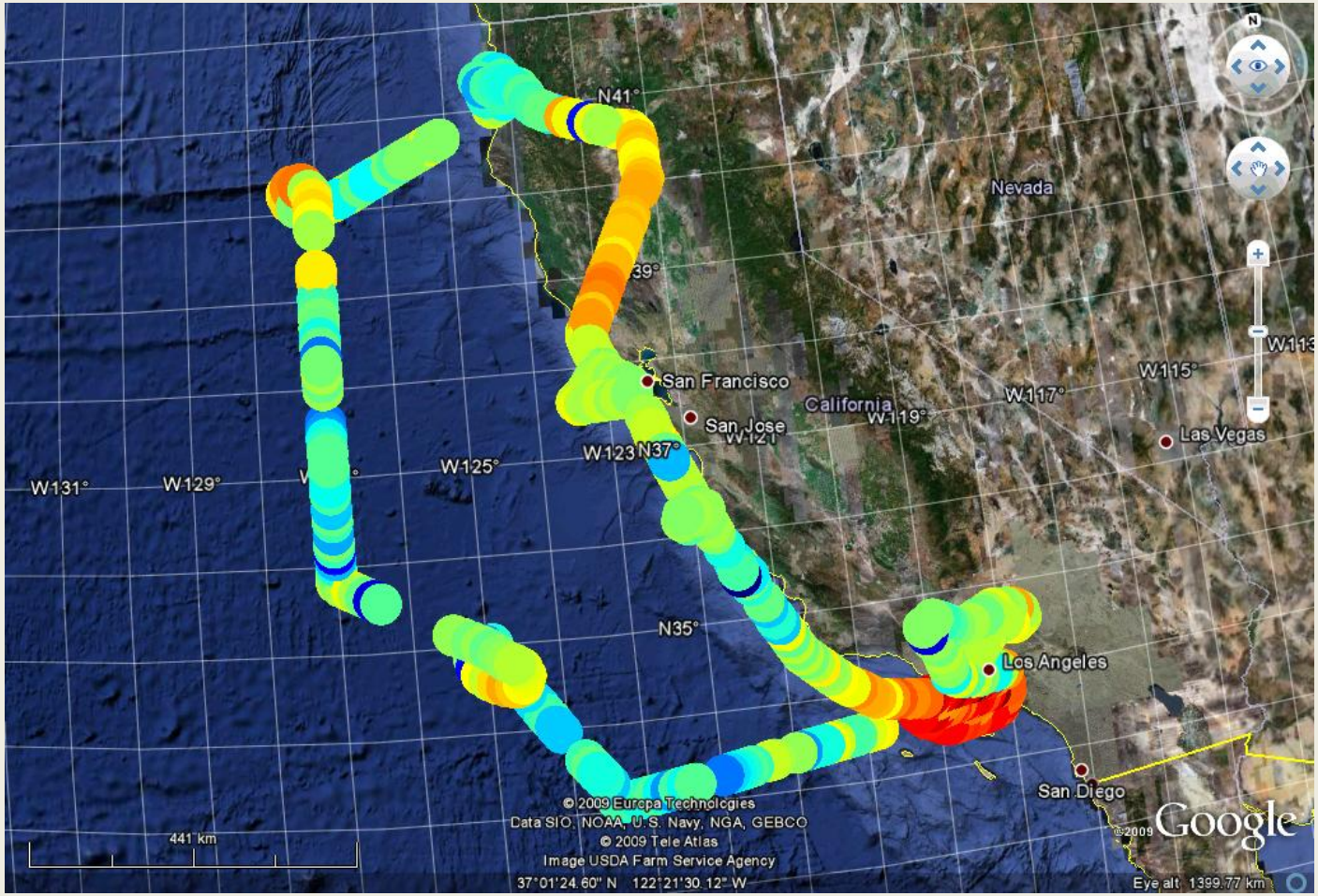
# Emission inventories (EI)
# Do recent changes improve model predictions?

| | VOC | NOx | SO2 | CO | NOx/VOC |
|---|---|---|---|---|---|
| NEI 2008/2001, anthrop * | 1.03 | 0.75 | 0.8 | 0.8 | 0.73 |
| CARB2008/2000 anthrop, summer** | 0.71 | 0.81 | 0.94 | 0.66 | 1.14 |

- Emission inventories changes vary between NEI and CARB reports.
- David Streets also developed EI for ARCTAS
- A series of sensitivity studies have been conducted

*NEI 2008 values were interpolated from NEI 2005 and 2009 prediction
**CARB data: http://www.arb.ca.gov/app/emsinv/cepam_emssumcat_query.php

# SO2 sensitivity studies




Jun 22 flight path colored with log (SO2)-red high, blue low

http://code.google.com/p/googleearthtoolbox/, customized by Charles Stanier, same below

- From figure, flight observed high SO2 around ports.
- LA and long beach ports in SoCal rank 1st &2nd busiest in the US in terms of volume cargo processed.*
- world-wide avg. S% in ship fuel 2.7% Vs  CA on road diesel 0.0015%*
- Ship emissions outside of ports excluded from NEI
- SO2 sensitivity studies

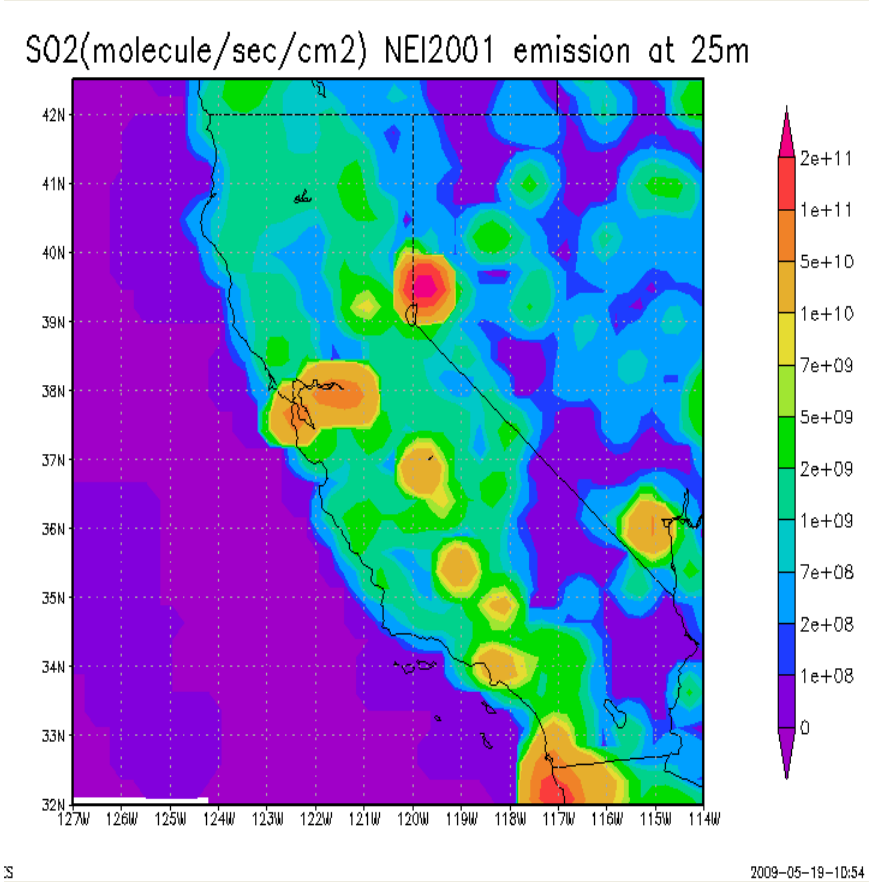
  Run 1 NEI 2001

  Run 2 NEI 2001 SO2 × 2

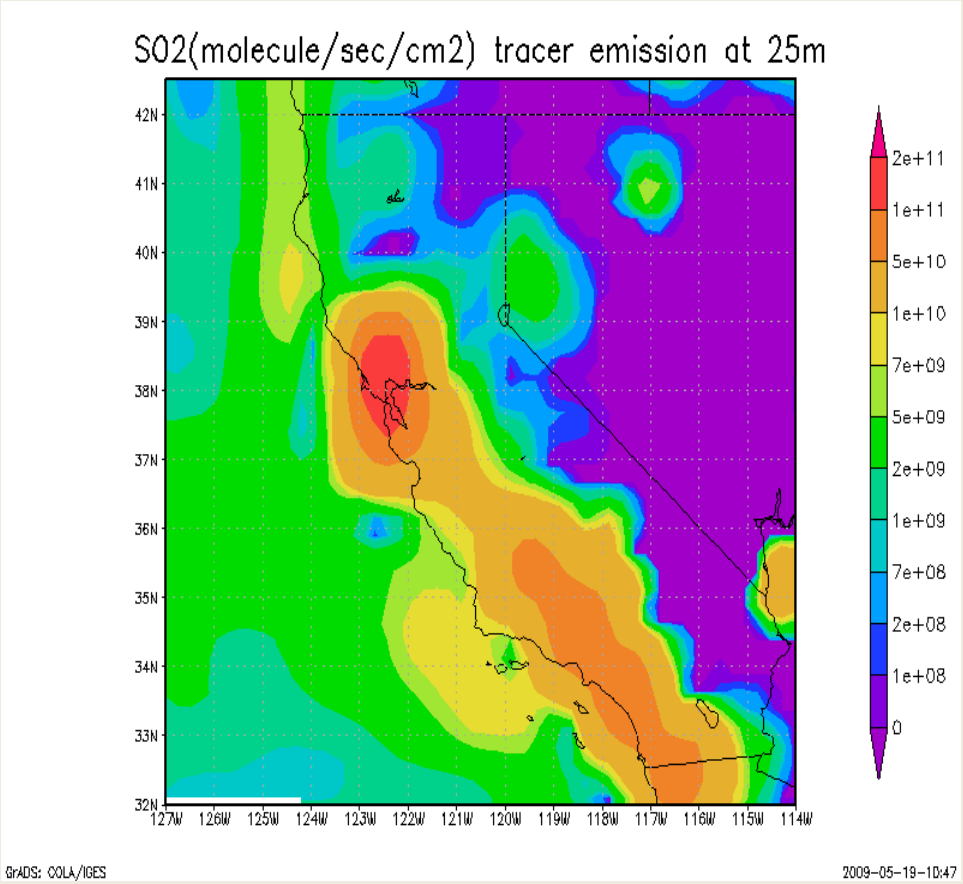
  Run 5 NEI 2001 SO2 replaced by David Streets' March-2008 version 1.0 for ARCTAS**

**S. Vutukuru, 2008*
**http://mic.greenresource.cn/data/arctas_premission

NEI

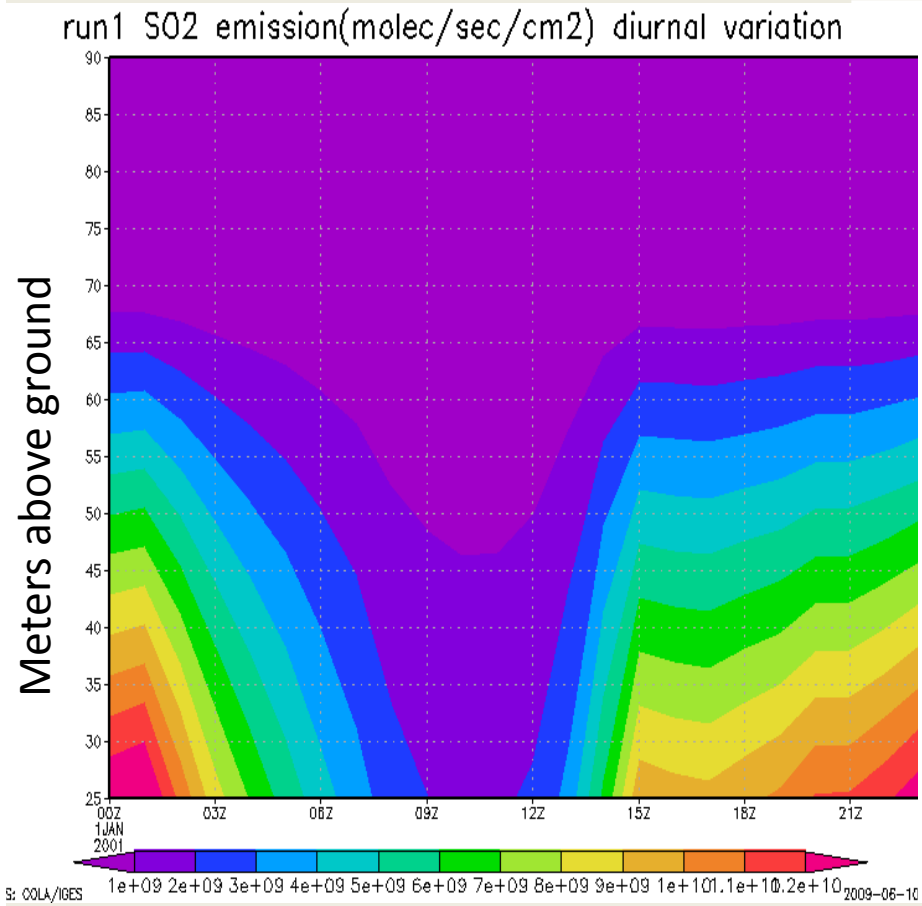

SO2(molecule/sec/cm2) NEI2001 emission at 25m
42N
41N
40N
39N
38N
37N
36N
35N
34N
33N
32N
127W 126W 125W 124W 123W 122W 121W 120W 119W 118W 117W 116W 115W 114W
2e+11
1e+11
5e+10
1e+10
7e+09
5e+09
2e+09
1e+09
7e+08
2e+08
1e+08
0
2009-05-19-10:54

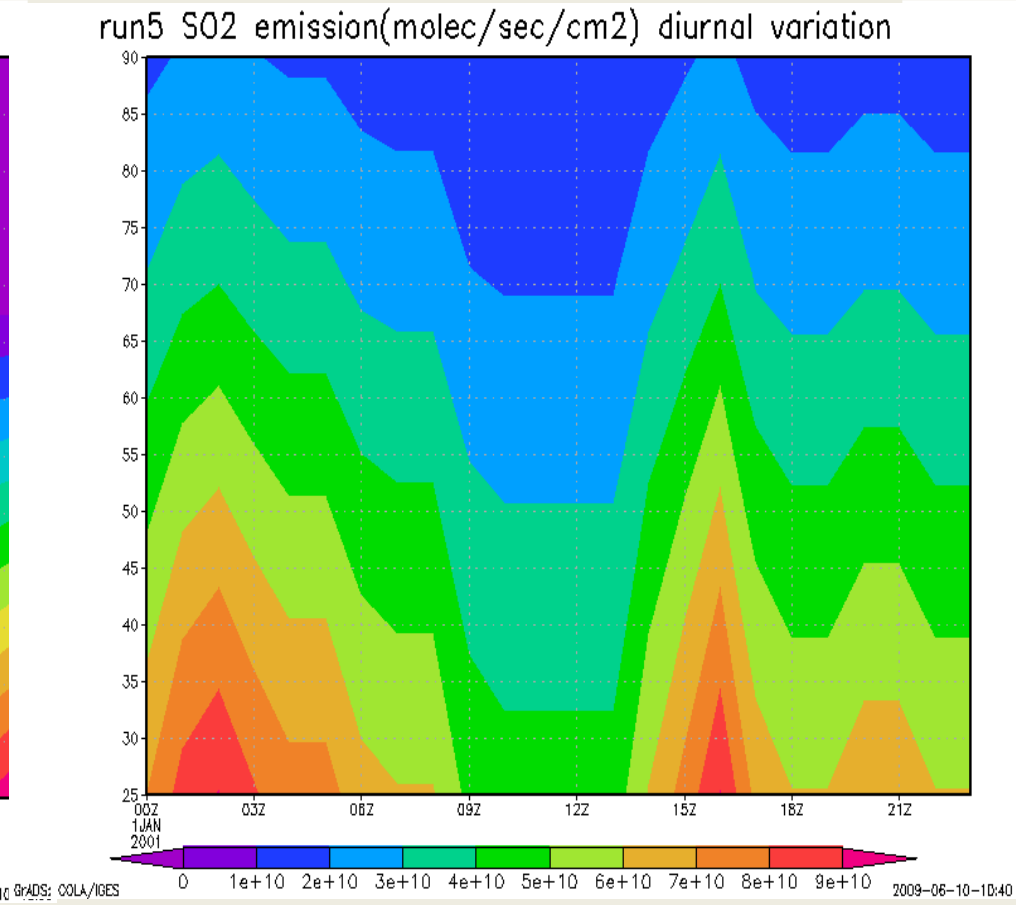
Streets'


SO2(molecule/sec/cm2) tracer emission at 25m
42N
41N
40N
39N
38N
37N
36N
35N
34N
33N
32N
127W 126W 125W 124W 123W 122W 121W 120W 119W 118W 117W 116W 115W 114W
2e+11
1e+11
5e+10
1e+10
7e+09
5e+09
2e+09
1e+09
7e+08
2e+08
1e+08
0
GrADS: COLA/IGES
2009-05-19-10:47

NEI

Streets'

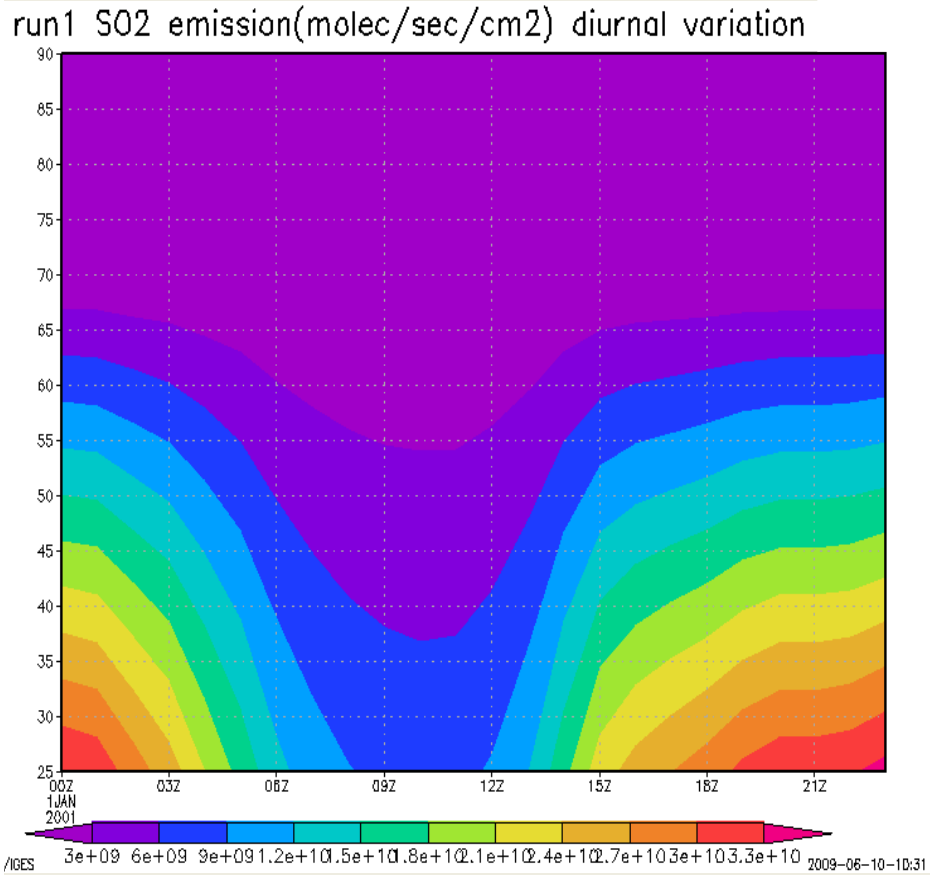


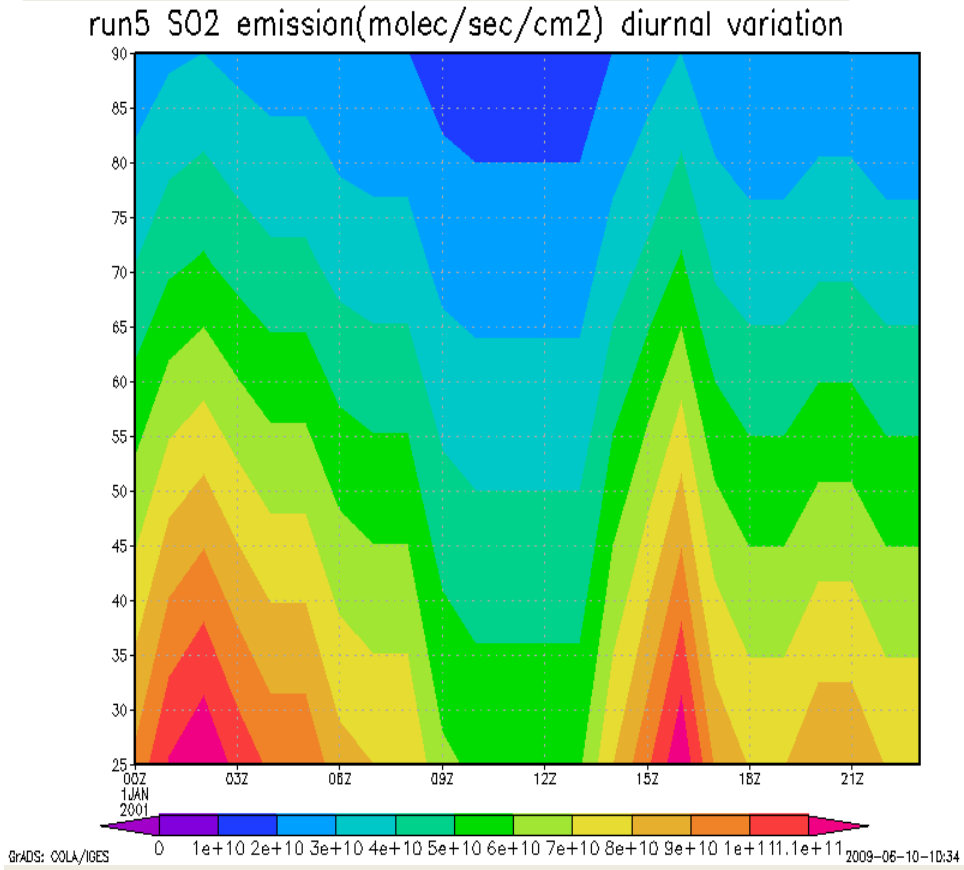




**Los Angeles**

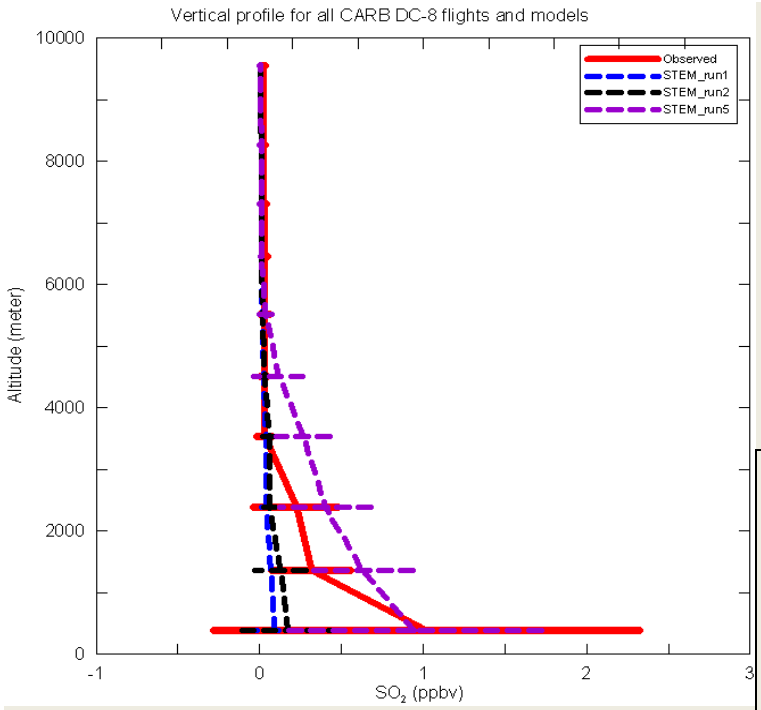
NEI

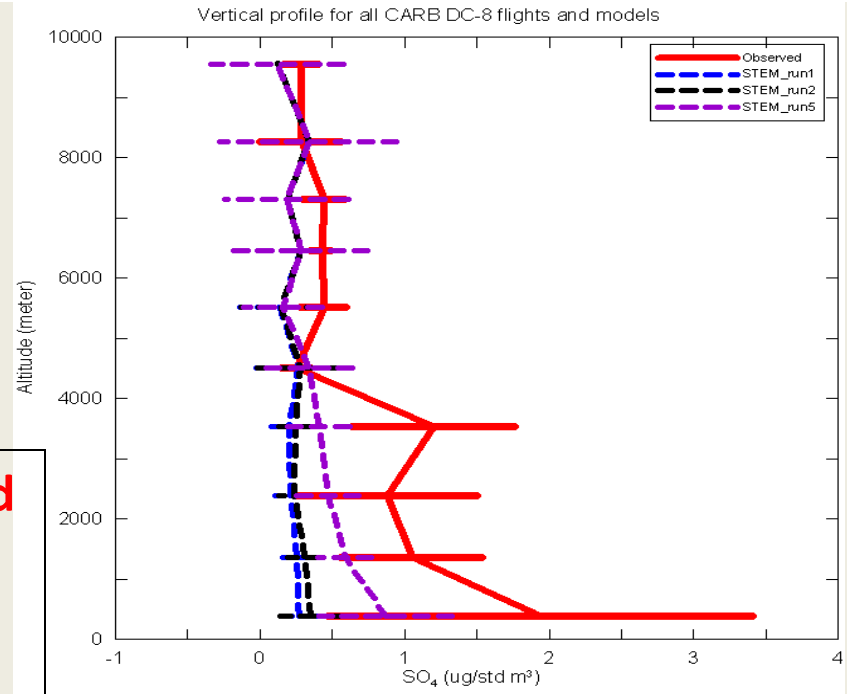
Streets’



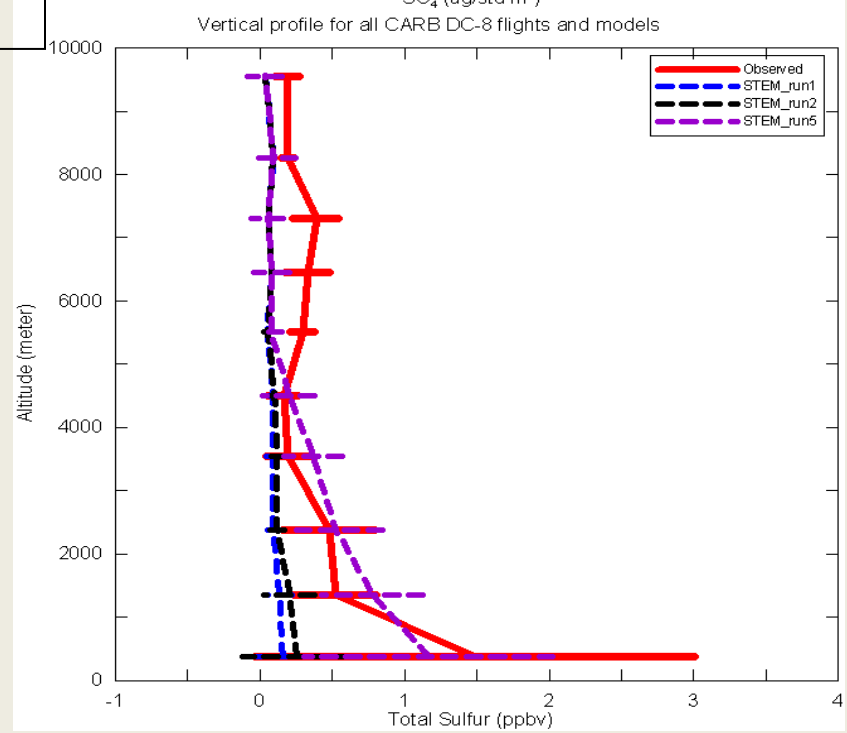




**San Francisco**




**Observed**
**RUN1**
**RUN1×2**
**Streets'**

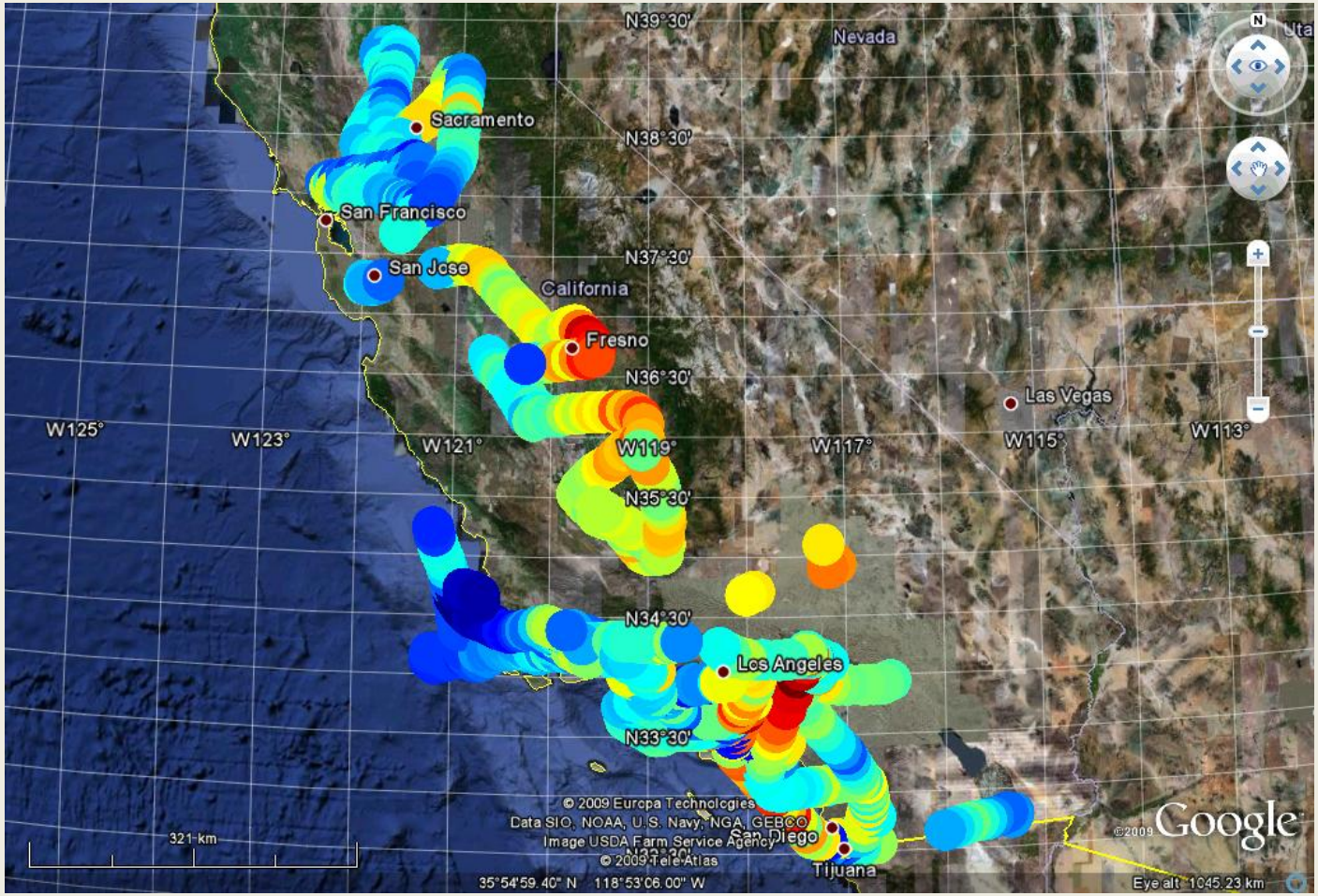



1) NEI 2001 EI resulted in low sulfur species prediction, doubled SO2 emission did not improve significantly

2) David Streets improved SO2 EI, for both continent and ocean areas around ports

3) Over prediction in SO2 and under prediction in SO4 with good potential sulfate (SO2+sulfate)may be due to conversion rates, which is sensitive to temperature and RH biases

# Sensitivity studies on O3-related species

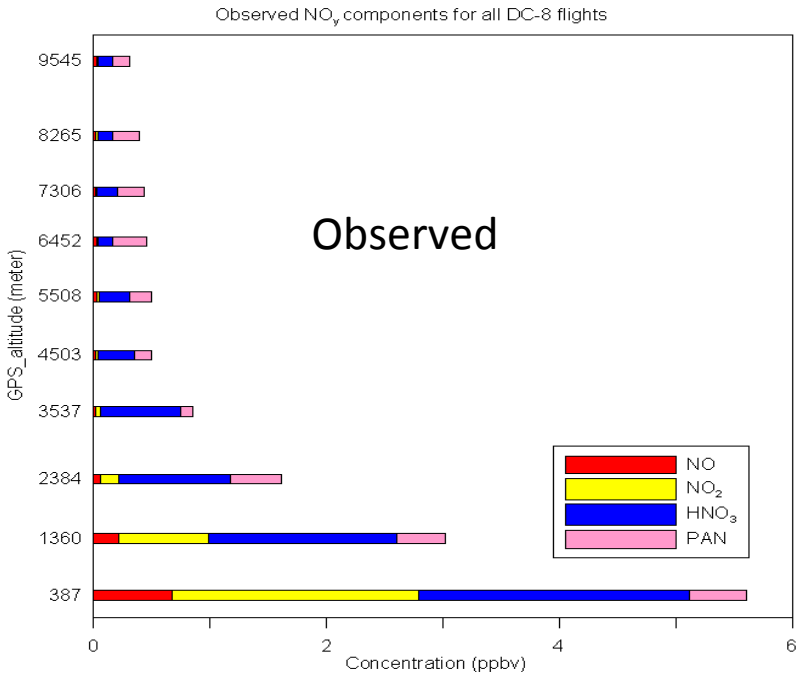



O3 was observed high from flight in central valley & SoCal below 1000m

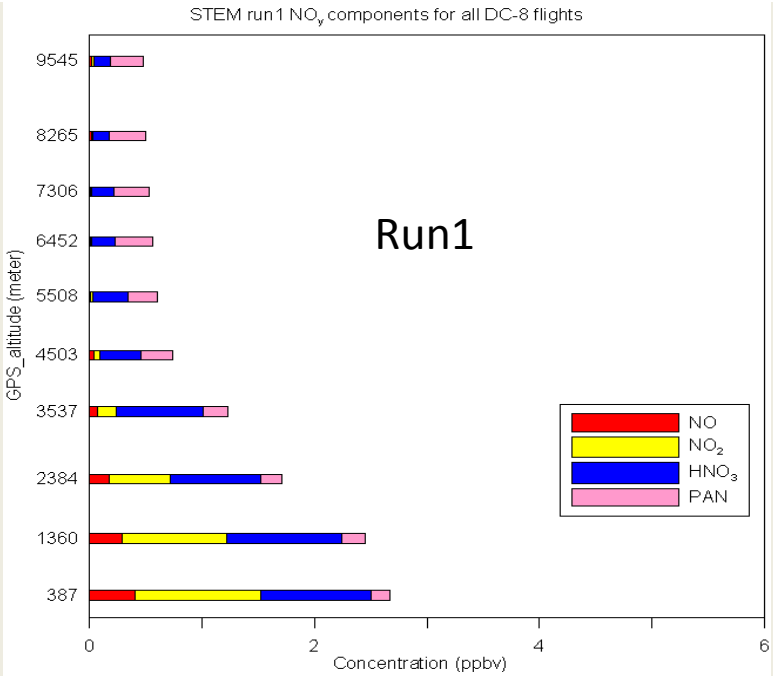
Sensitivity studies

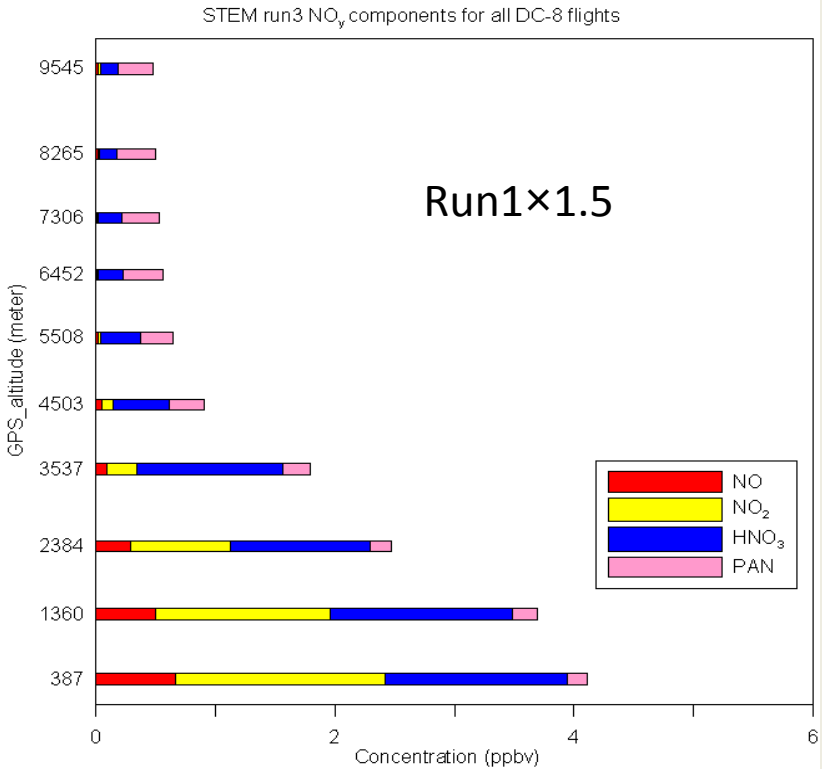
Run 3 NEI 2001 NO×1.5; NO2×1.5; CO×0.8 (NEI 2008/2001 for CO)

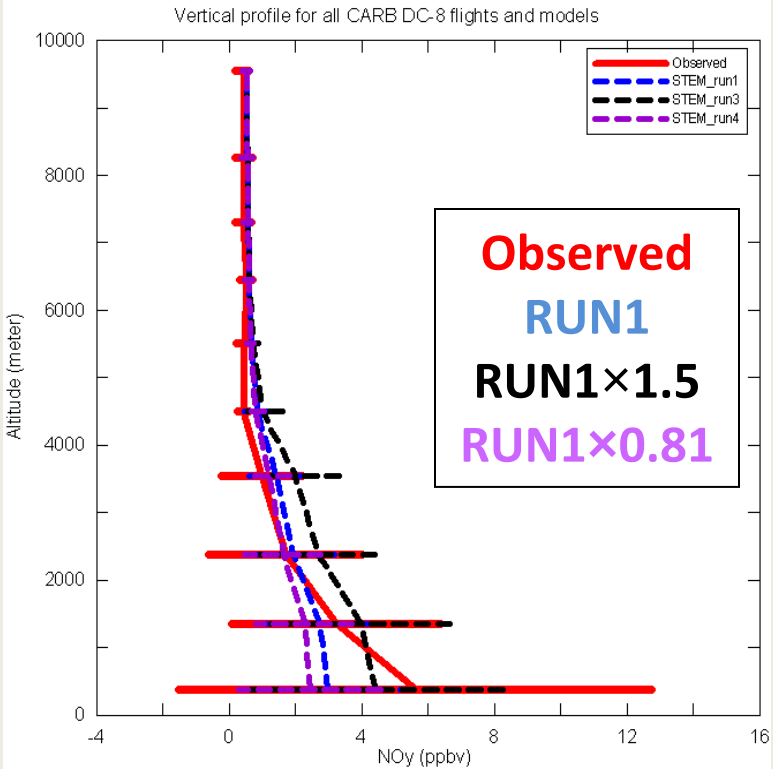
Run 4 NEI 2001 CO×0.66; NO×0.81; NO2×0.81; VOC all species×0.71 (CARB 2008/2000)




NOy (HNO3_SAGA MC shown)



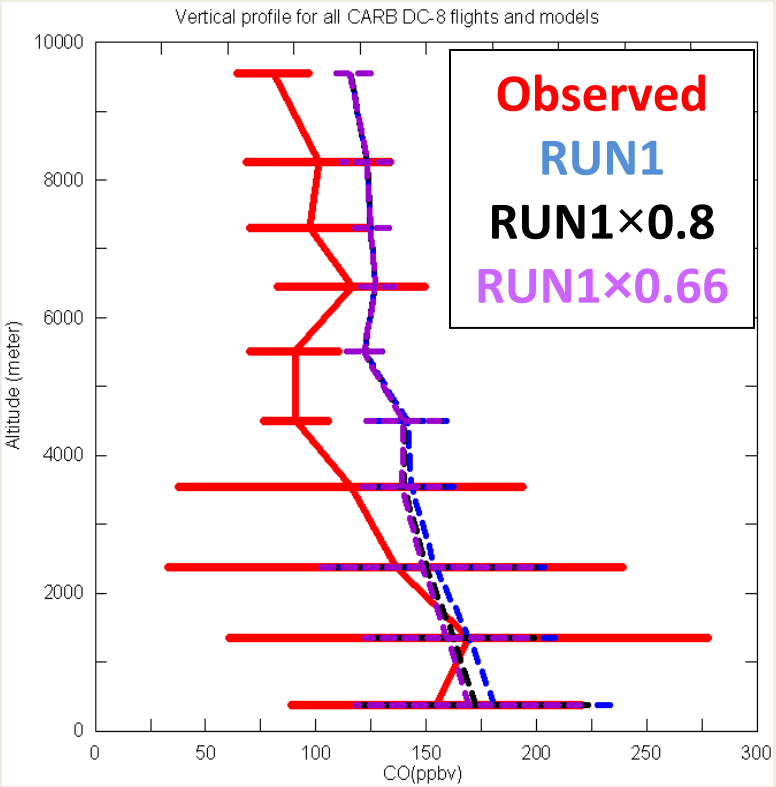



1) Run 3 improves NOy prediction

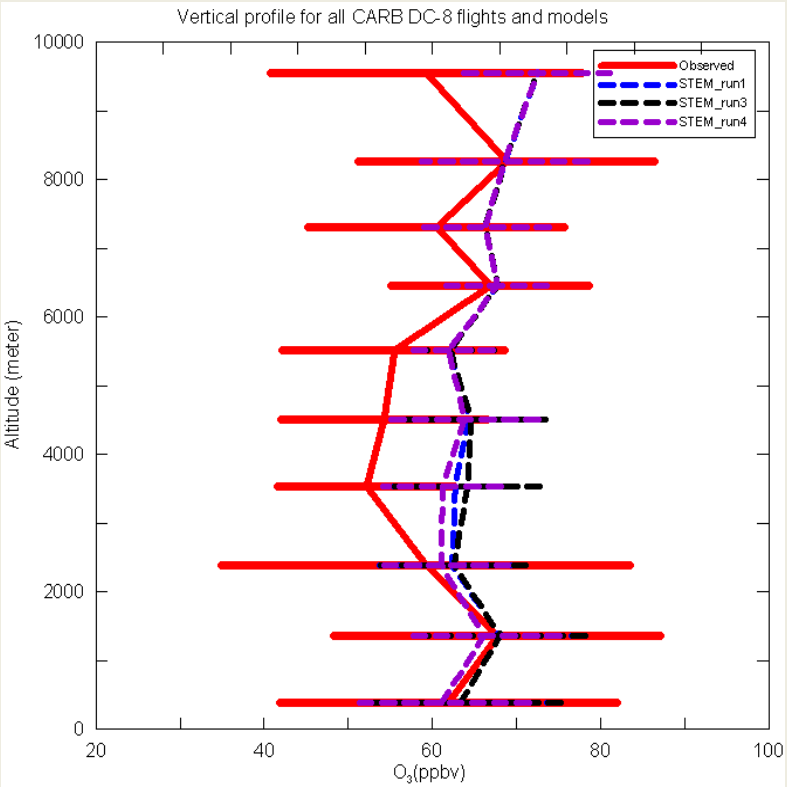
- NOx increased
- HNO3 increased, but not enough
- PAN stayed low in run 3

2) All NOy species were reduced in Run 4(figure not shown)

CO




O3




1) Below 2000m, CO and O3 were well predicted
2) CO and O3 were slightly sensitive to emissions

# Sub-summary for EI sensitivity studies

- David Streets' SO2 EI significantly improves model performance on sulfur species
- Multiplying NOx EI by 1.5, NOy prediction was improved - expecting more in future
- Lower altitudes CO and O3 captures observation well, and were not sensitive to emissions.
- Sensitivity studies evaluate existing EI and give clues for pollutant control strategies

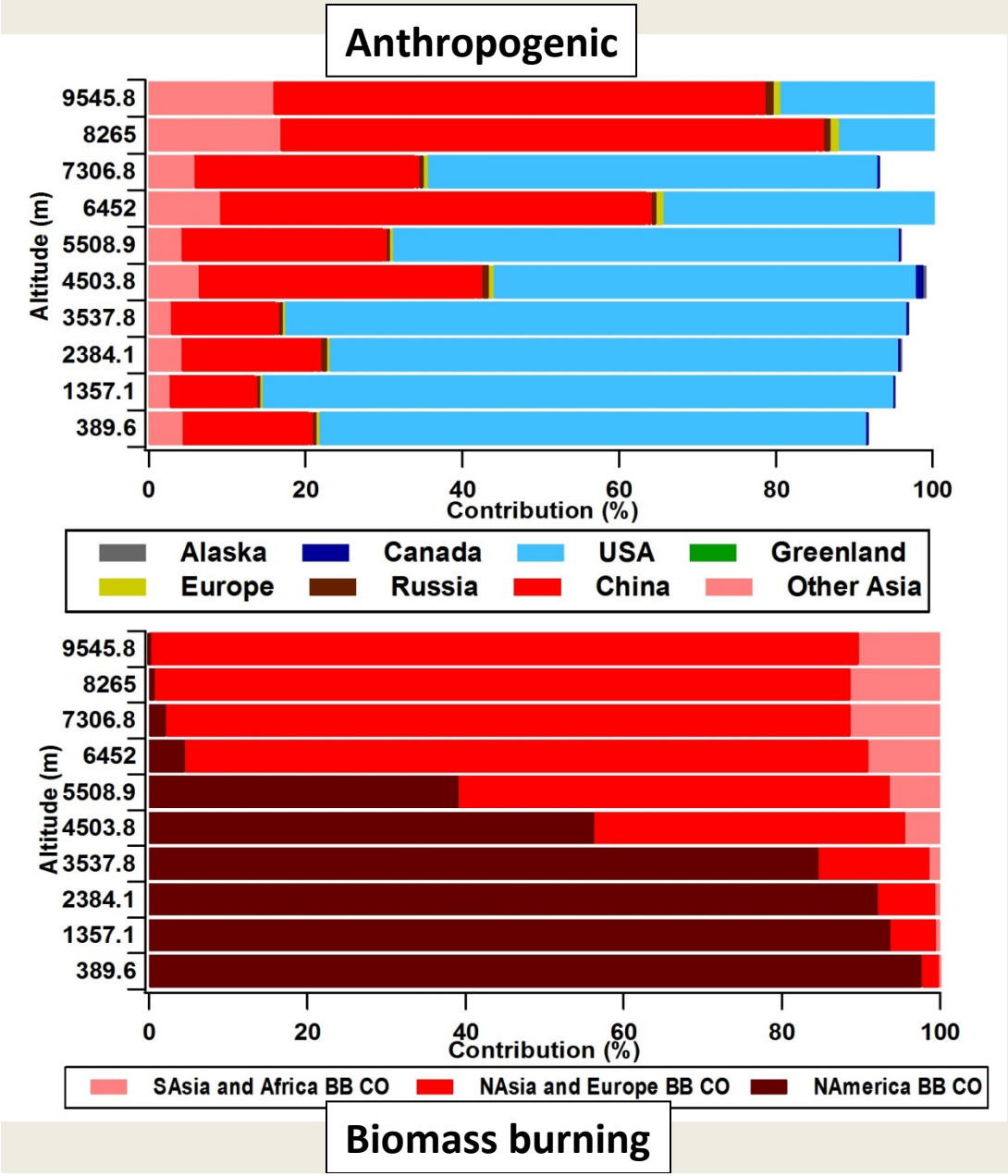
# Results and preliminary analysis

Examine WRF performance as meteorology input

FOUNDATION

- Assess California emission inventories
- CO and O3 transport
- Evaluate impact of oceanic boundary conditions on inland air quality

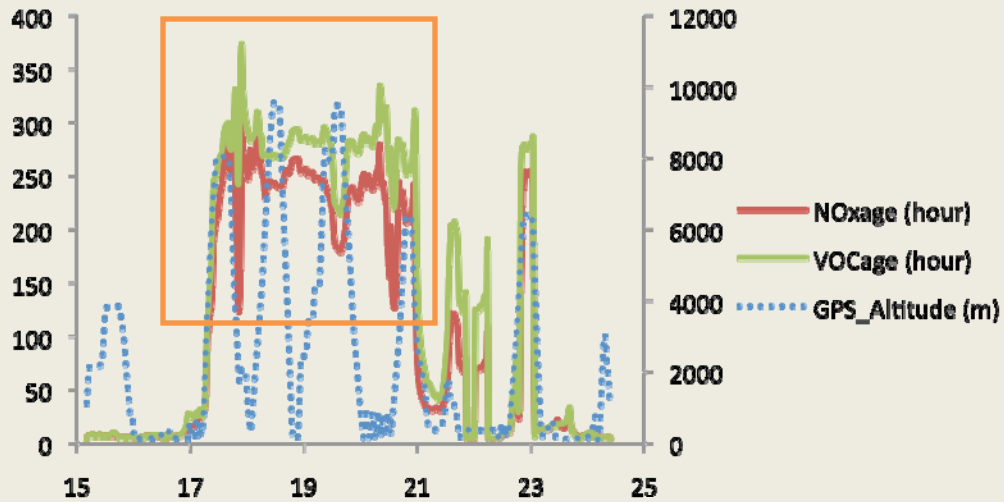
# CO transport

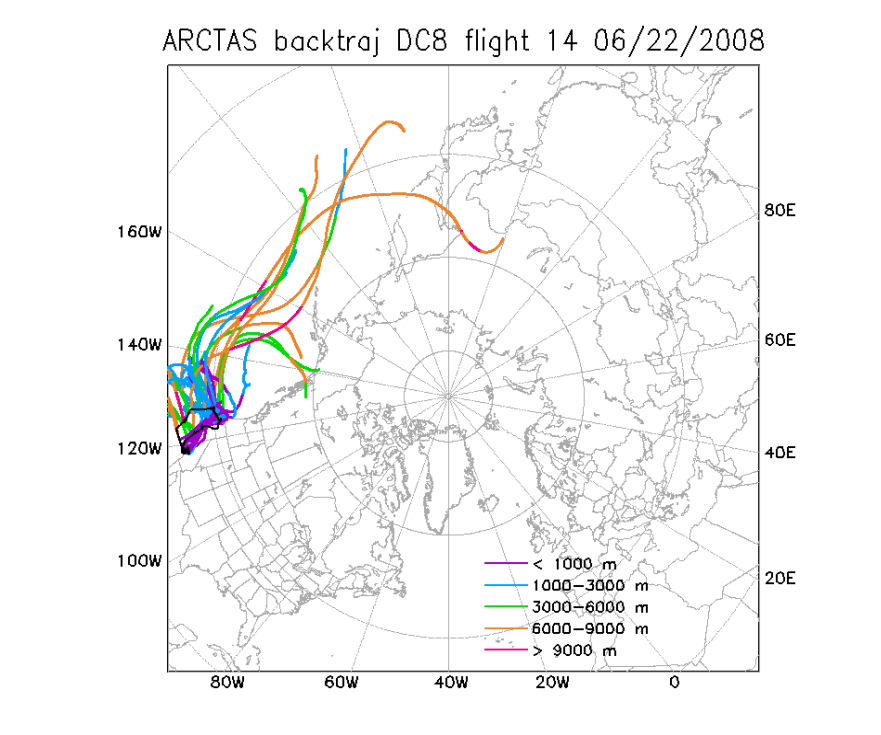



For all flight days-

Lower altitudes CO mainly comes from local sources;

Higher altitudes strongly influenced by Asian sources




1) Boxed was the period when DC8 flew along boundary, high NOx and VOC ages (qualitative indicator of air mass age) indicate inflows from sources in long distances.

2) Back trajectories along ocean boundary shows mid and high-altitude Asian inflow

# O3 transport

- Despite low population, northern CA includes O3 non-attainment area*
- Background O3 - O3 transported to the site from marine environment contributes observed O3 together with locally-formed O3*
- Previous model work concluded that background O3 in NA is generally 15-35ppb and decreases at polluted days*

**Parrish et al, 2009 (in draft)*

- Parrish et al argues that observed O3 is directly proportional to transported background
- *OUR WORK: Potential source contribution function (PSCF) – 3 day back trajectories from coastal Trinidad Head(THD) and 3 inland sites; source contribution analysis*
- Parrish et al conclude that it takes 20-30 hours for O3 to transport from coast to inland*
- *OUR WORK: correlate modeled O3 at THD (multiple heights) and 3 inland sites to determine best time offset*

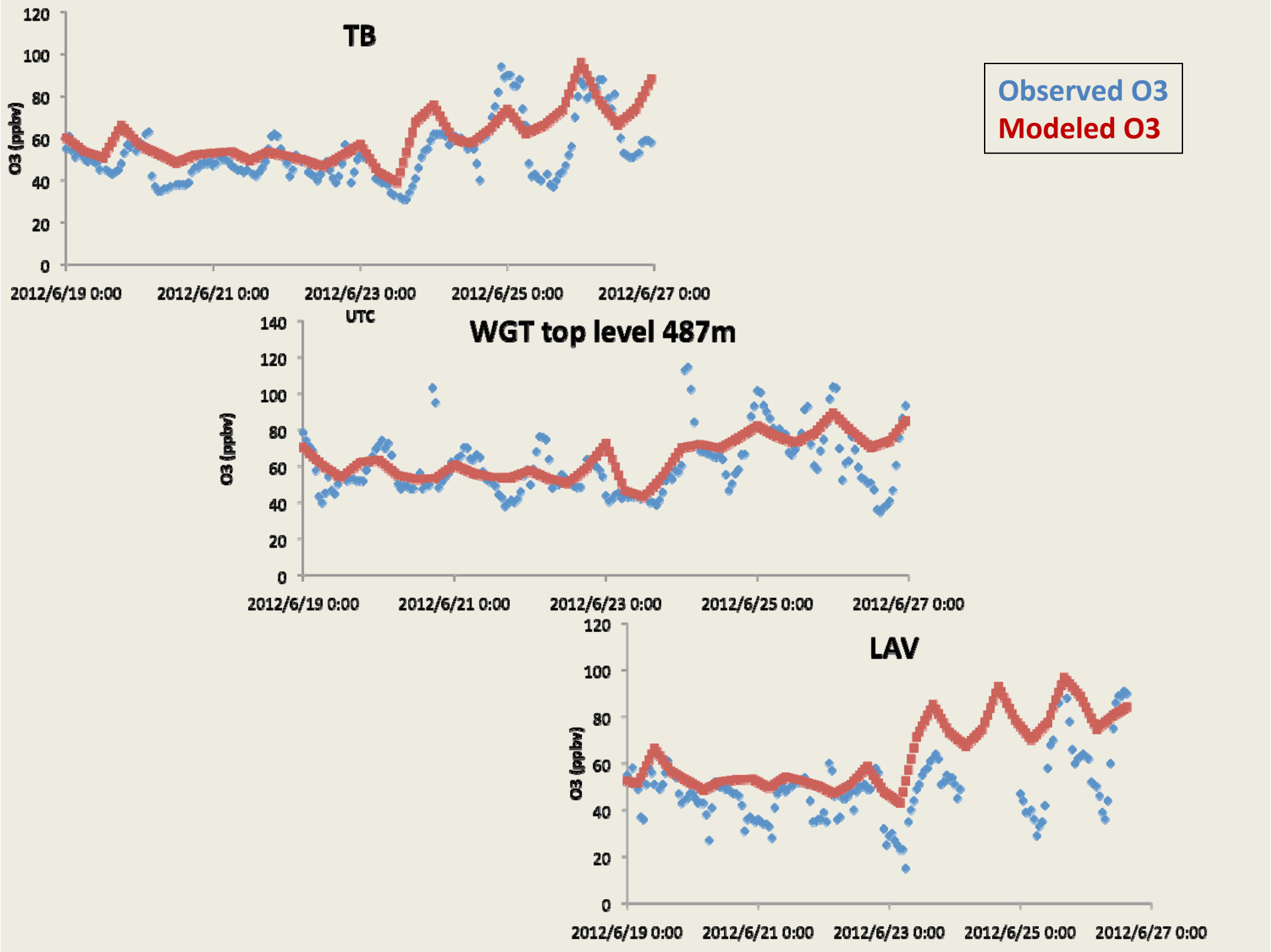
**Parrish et al, 2009 (in draft)*

# Sites information

- THD (sounding at 400, 1000, 1500, 3000m)*
- WGT (suburban, top level 487m)
- LAV NP(CASTNET site, remote,1756m)
- Tuscan Butte (isolated rural site, ranks the highest O3 in Northern Sacramento valley,** 570m)

*ftp://ftp.cmdl.noaa.gov/ozwv/ozone/ARCIONS/CARB/

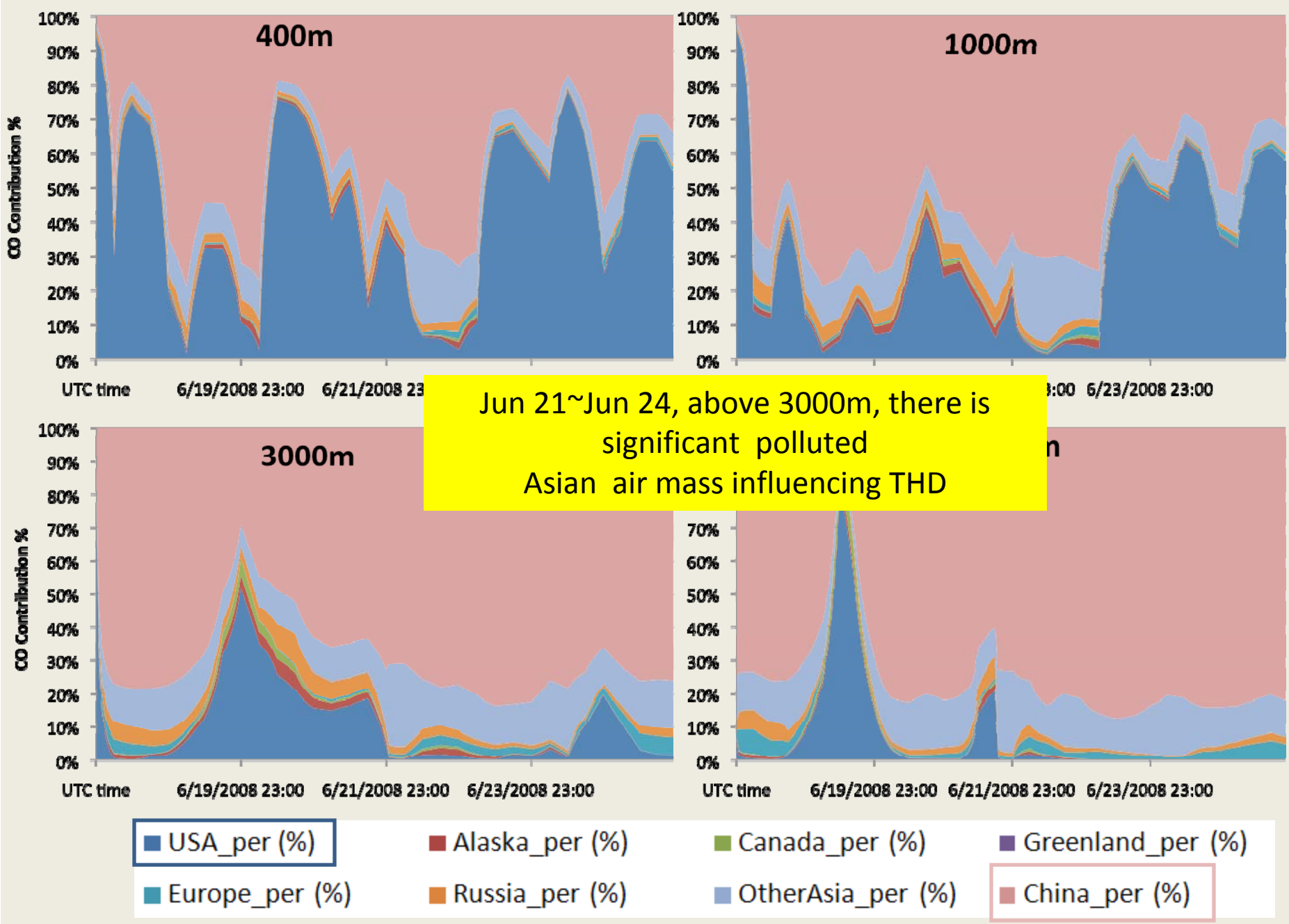
***Parrish et al, 2009 (in draft)*


TB
Observed O3
Modeled O3
O3 (ppbv)
120
100
80
60
40
20
0
2012/6/19 0:00
2012/6/21 0:00
2012/6/23 0:00
2012/6/25 0:00
2012/6/27 0:00
UTC
WGT top level 487m
140
LAV

# Back trajectories

- CA suggests 1 hour average O3 not to exceed 90ppb. *
- Three inland sites -Trajectories ending date were determined by days exceeded 90ppb (high) and days with 1 hour O3 staying below 60ppb (low)
- THD- source contribution analysis to determine at what level (and what time) it was highly influenced by sources out of NA

*http://www.arb.ca.gov/research/aaqs/caaqs/ozone/o-hist/o-hist.htm#2005

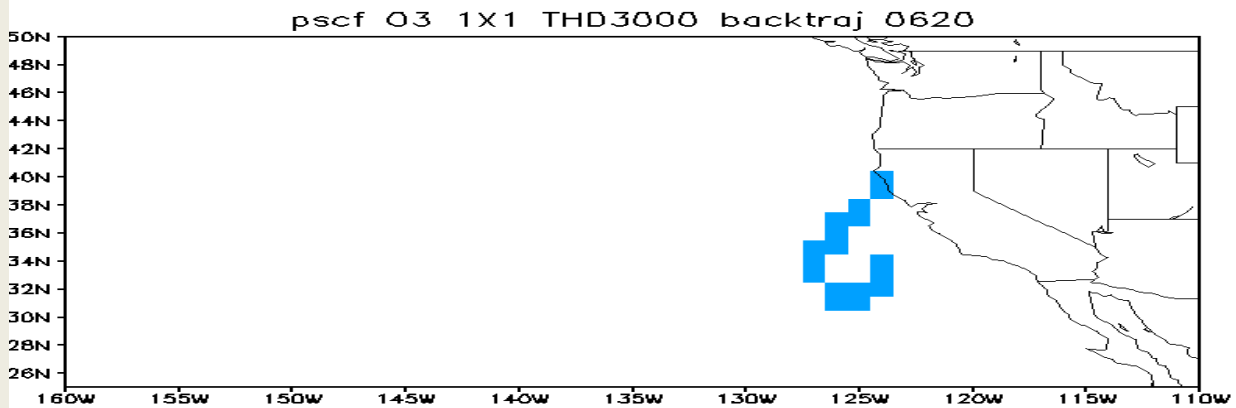



Jun 21~Jun 24, above 3000m, there is significant polluted Asian air mass influencing THD

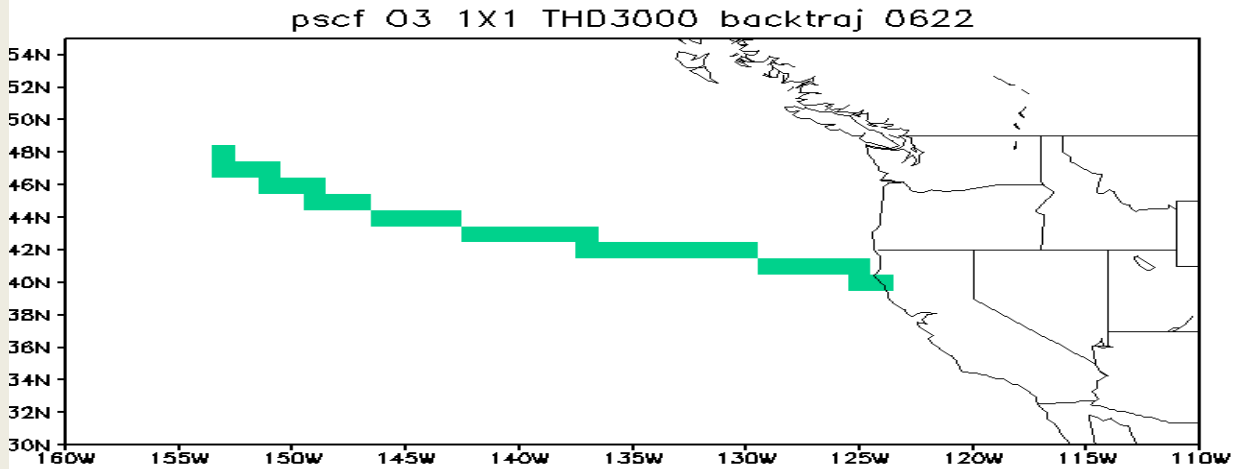
At THD, as altitude increases, local contribution decreases while Asian contribution increases

Observed O3 at THD

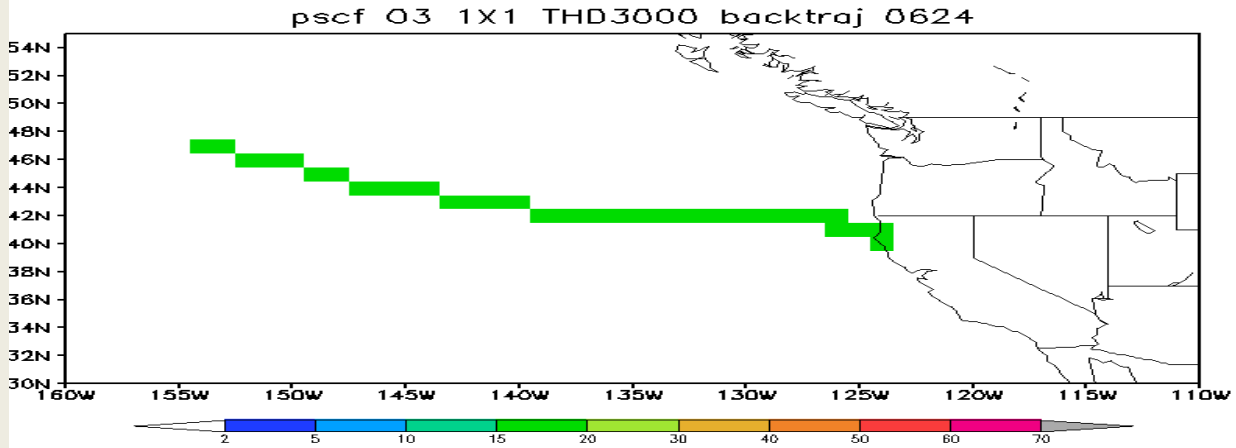
41.9ppb

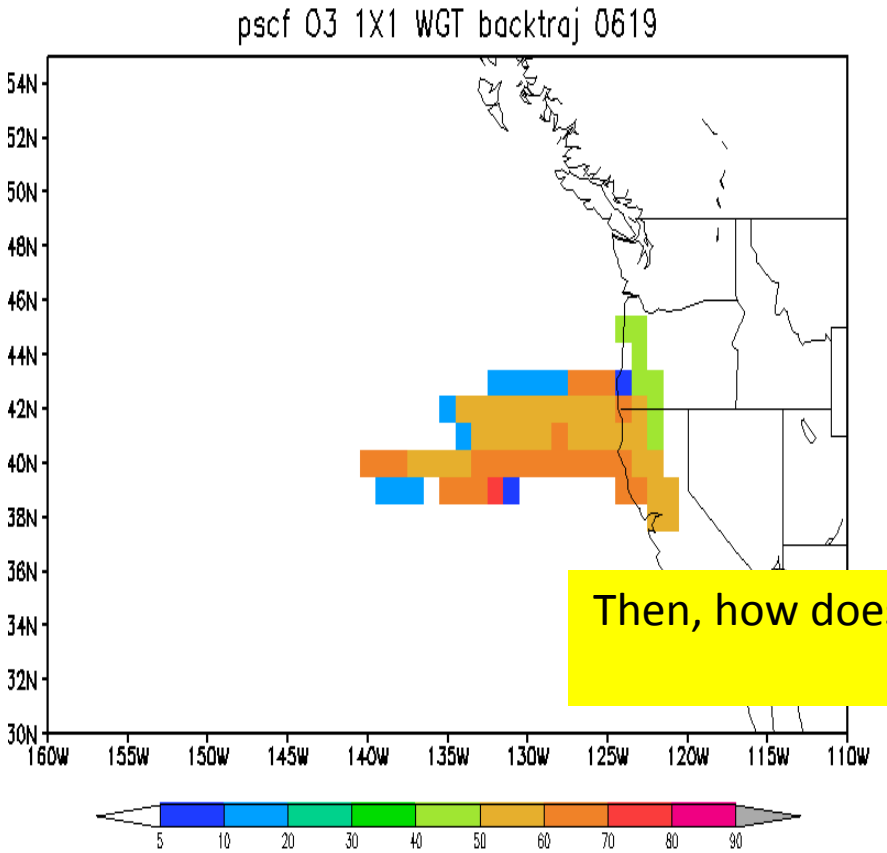


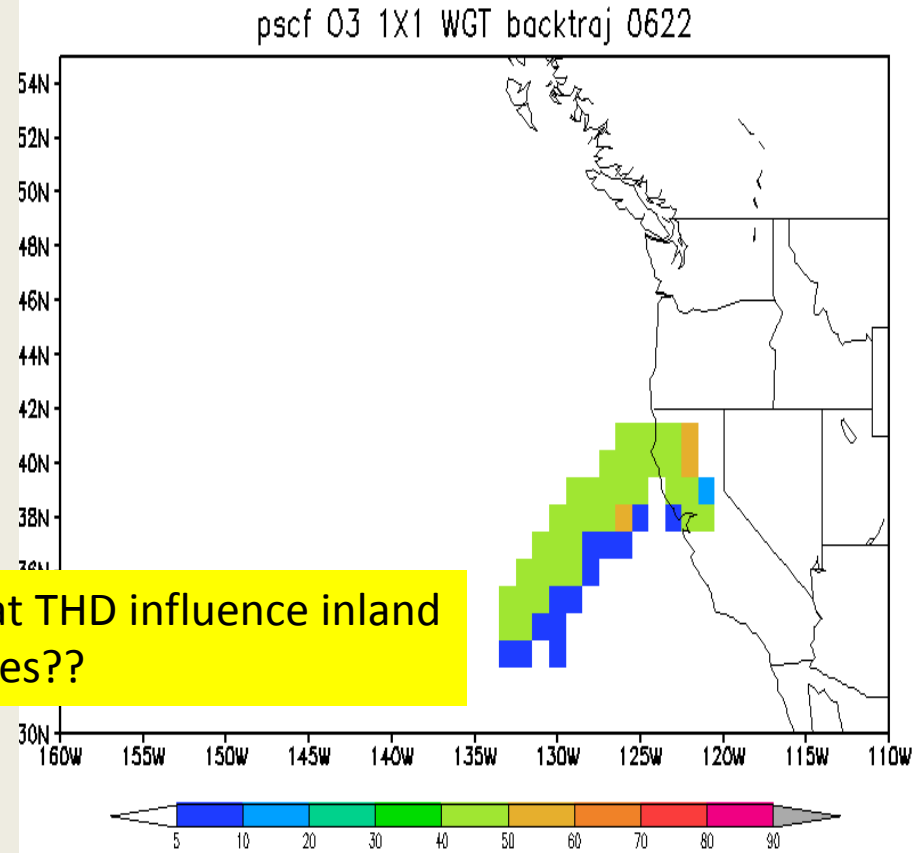

62.2ppb




77.3ppb





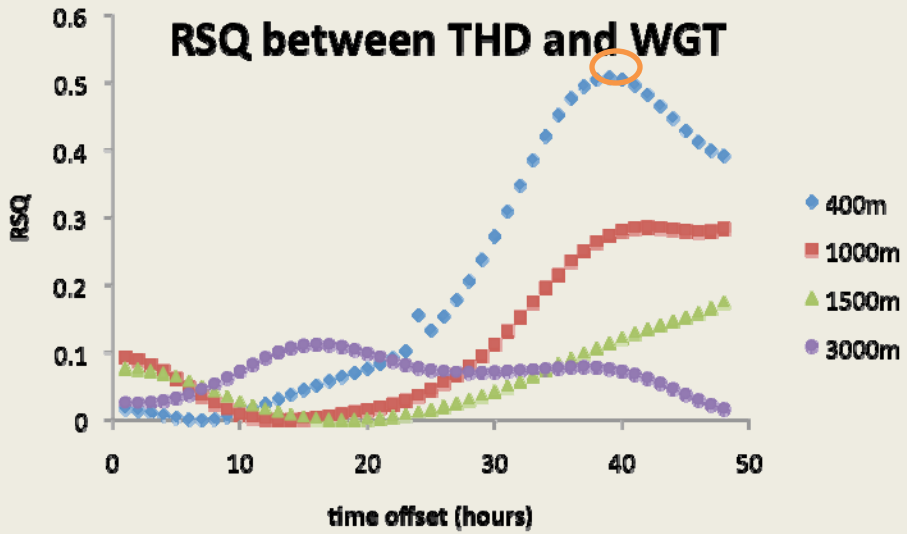

Then, how does O3 at THD influence inland sites??

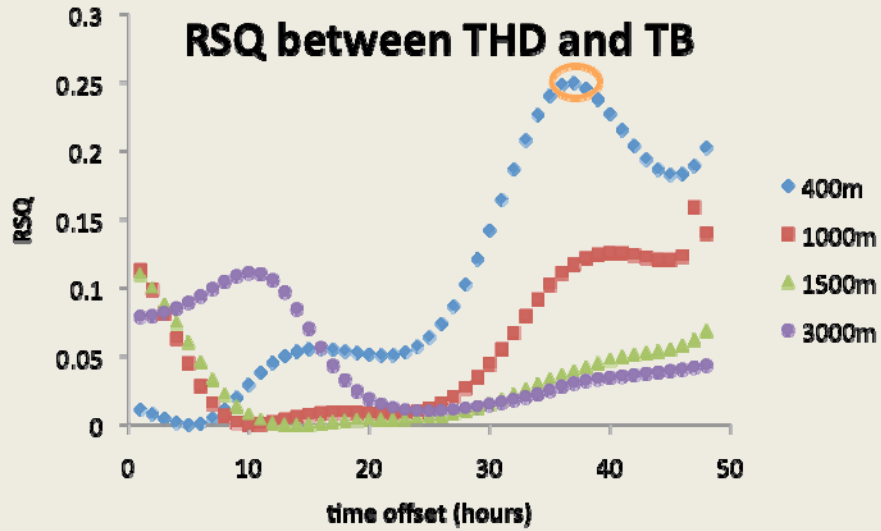
Observed high O3 day

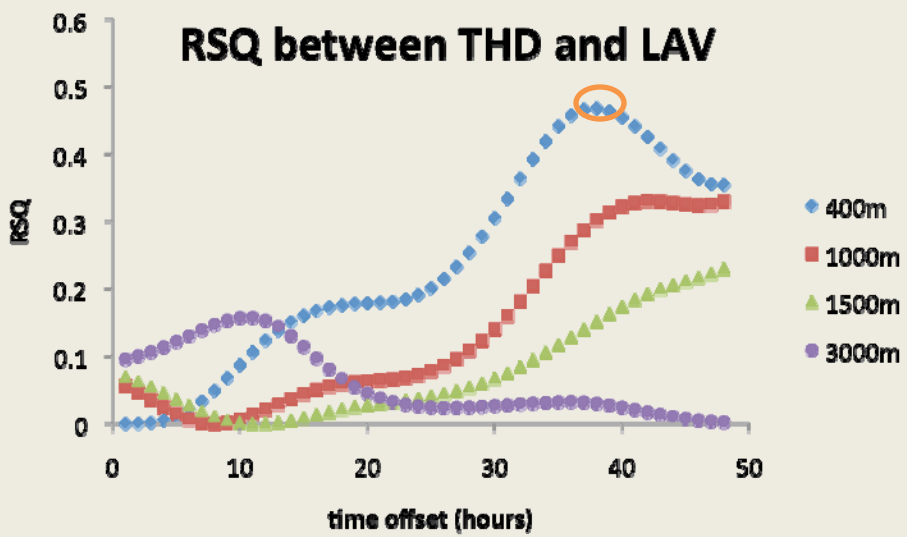
Observed low O3 day

Although cases with background O3 were limited within the short period, we qualitatively conclude - observed O3 is proportional to background O3

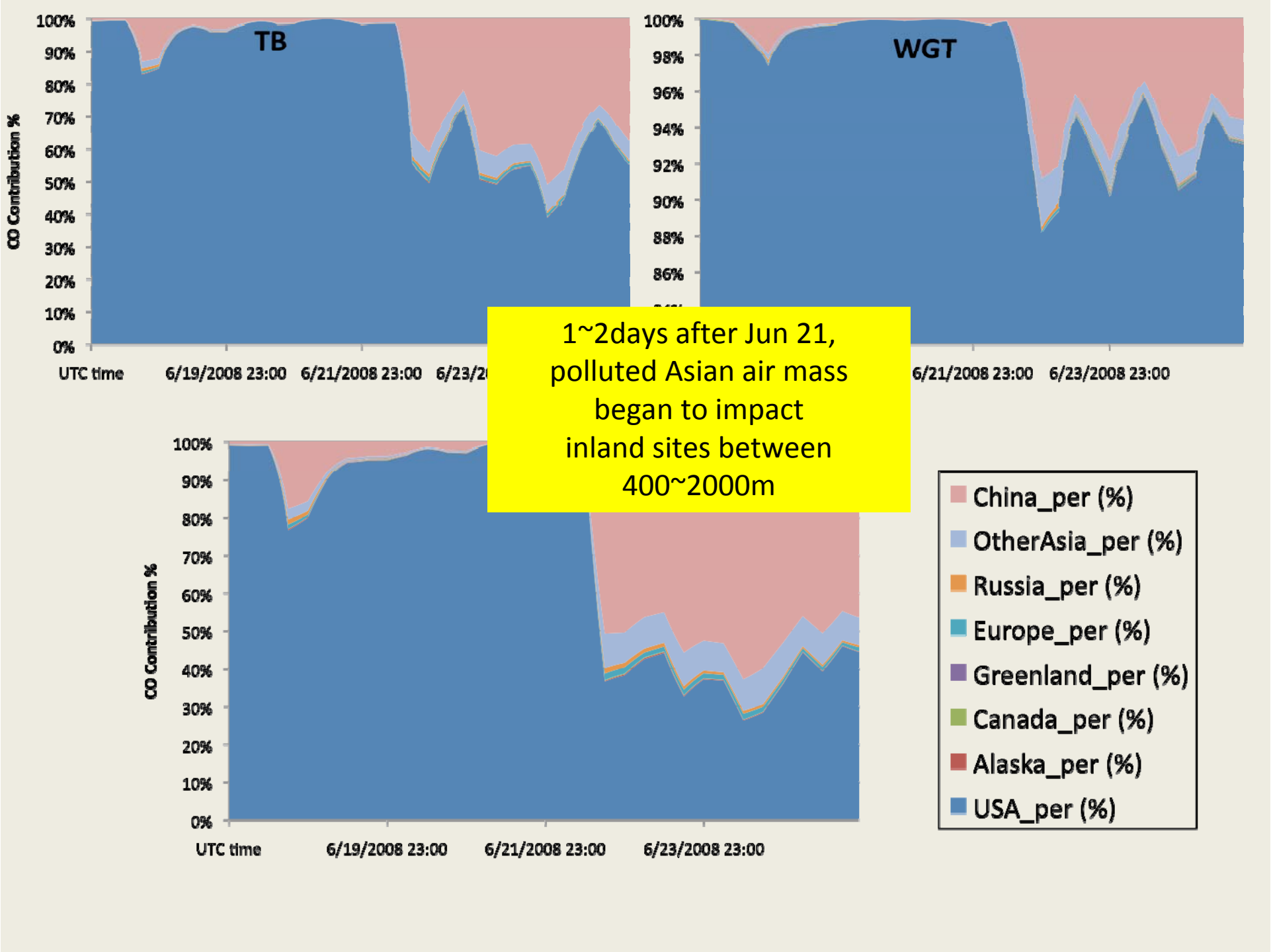
# Correlation study



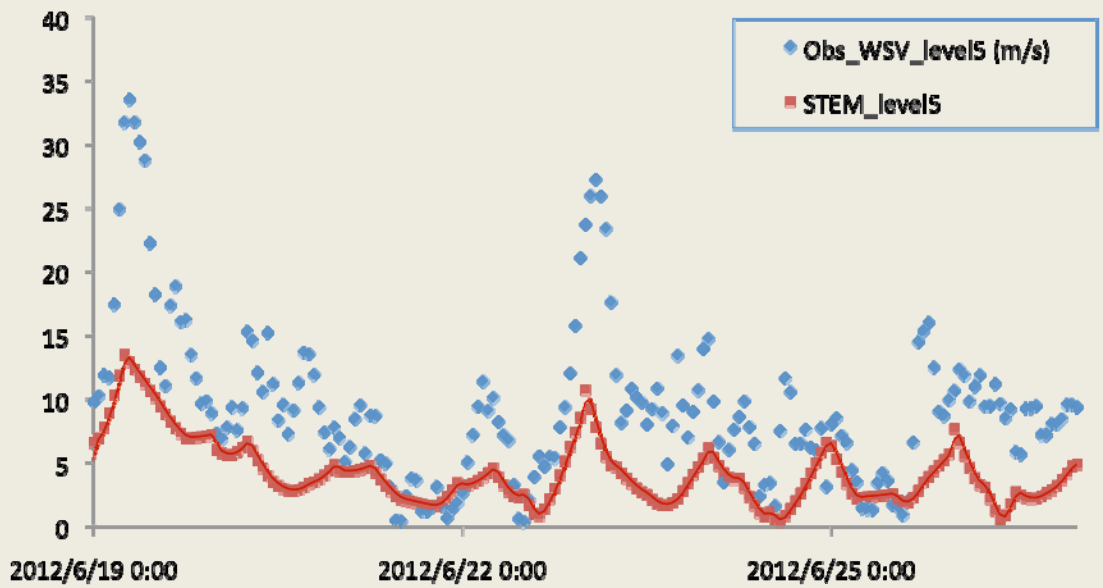




- Model outputs show highest correlation between THD 400m-1000m and inland sites
- Correlations between THD – WGT and LAV are stronger than THD – TB during that period
- Model indicates O3 from THD impacts inland sites after 36~39hours transport


TB
WGT
CO Contribution %
100%
90%
80%
70%
60%
50%
40%
30%
20%
10%
0%
98%
96%
94%
92%
88%
86%
UTC time
6/19/2008 23:00
6/21/2008 23:00
6/23/2008 23:00
1~2days after Jun 21, polluted Asian air mass began to impact inland sites between 400~2000m
China_per (%)
OtherAsia_per (%)
Russia_per (%)
Europe_per (%)
Greenland_per (%)
Canada_per (%)
Alaska_per (%)
USA_per (%)

- lower wind speed predicted by WRF may result in longer transport time




| | Observed | STEM 60km, 6hr | WRF 12km, 1hr | WRF 60km |
|---|---|---|---|---|
| WS rsq | | 0.6 | 0.48 | 0.1 |
| WS avg (m/s) | 9.38 | 4.26 | 4.1 | 2.86 |
| WS bias | | -5.12 | -5.28 | -6.52 |
| WS error% | | -54.62 | -56.33 | -69.54 |

# Sub-summary for transport study

- CA is a receptor of CO and O3 from sources out of NA
- Asian CO inflows impact high altitudes
- Observed O3 is proportional to background O3 at northern CA
- O3 transported from coast at top ocean boundary mainly over ~400~1000m and impact inland the next 1~2days
- The conclusions may only represent this particular period, various research methods can be applied for different cases

# Results and preliminary analysis

Examine WRF performance as meteorology input

FOUNDATION

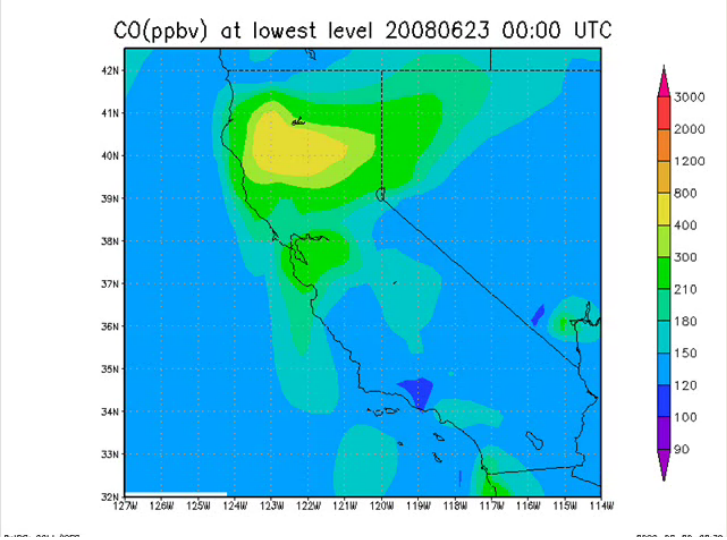
- Assess California emission inventories
- CO and O3 transport
- Evaluate impact of oceanic boundary conditions on inland air quality

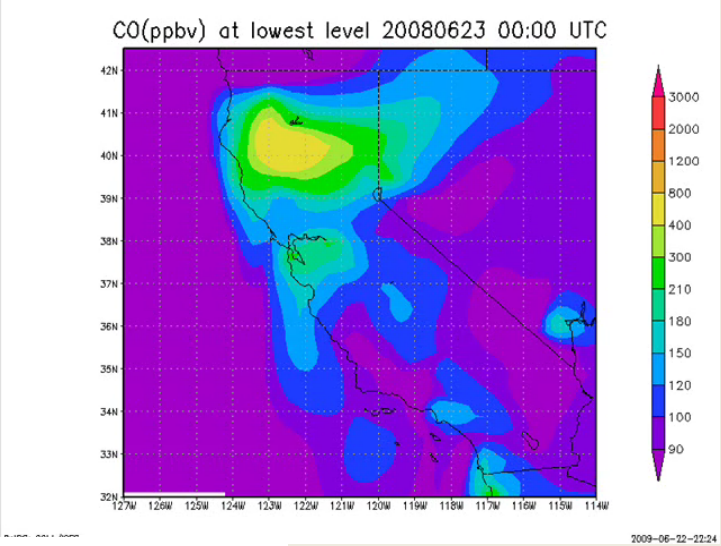
# Oceanic boundary conditions (BC)

Jun 22 flight path-partially across ocean boundaries

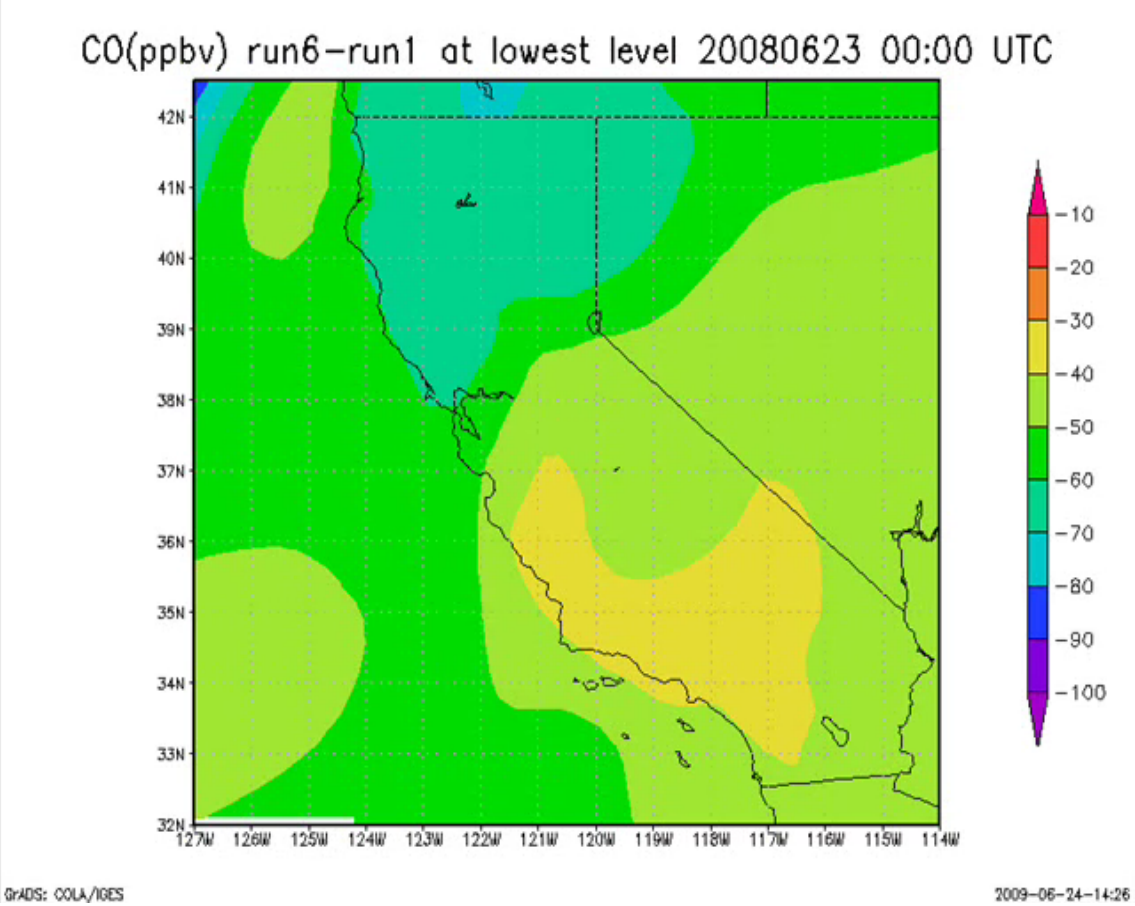
- Original BC: taken from RAQMS, time varied
- Contrasted Run 6: temporarily-fixed west boundary and time-varied RAQMS BC for rest three boundaries:
  - Flight-observed vertical profile (marked red in figure) for 8 species (CO, NO, NO2, O3, HNO3, PAN, H2O2, SO2) were interpolated into STEM grids and kept spatially constant over the west boundary
  - Other species were replaced with average RAQMS BC during that period
- Results analyzed by comparing O3 and CO over CA between both runs over 48 hrs after the June 22 flight

RUN



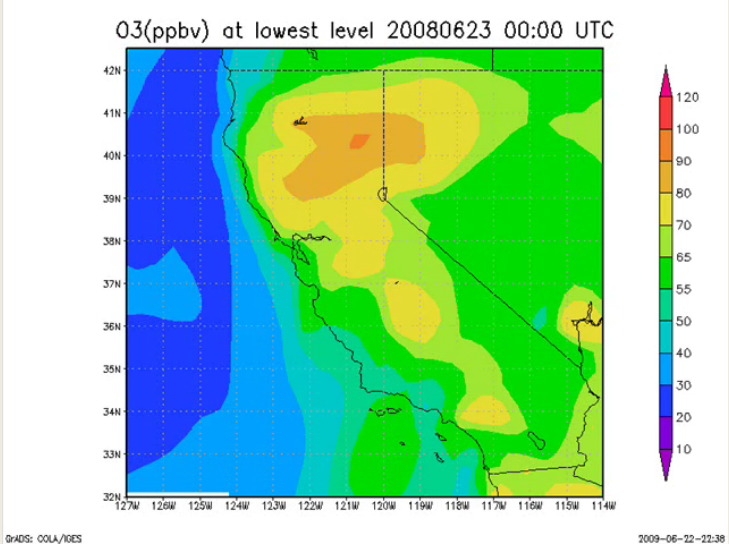



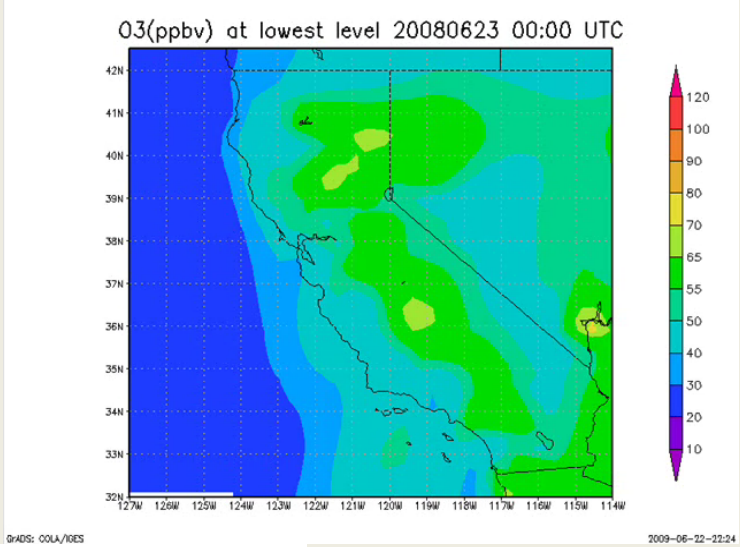

RUN6



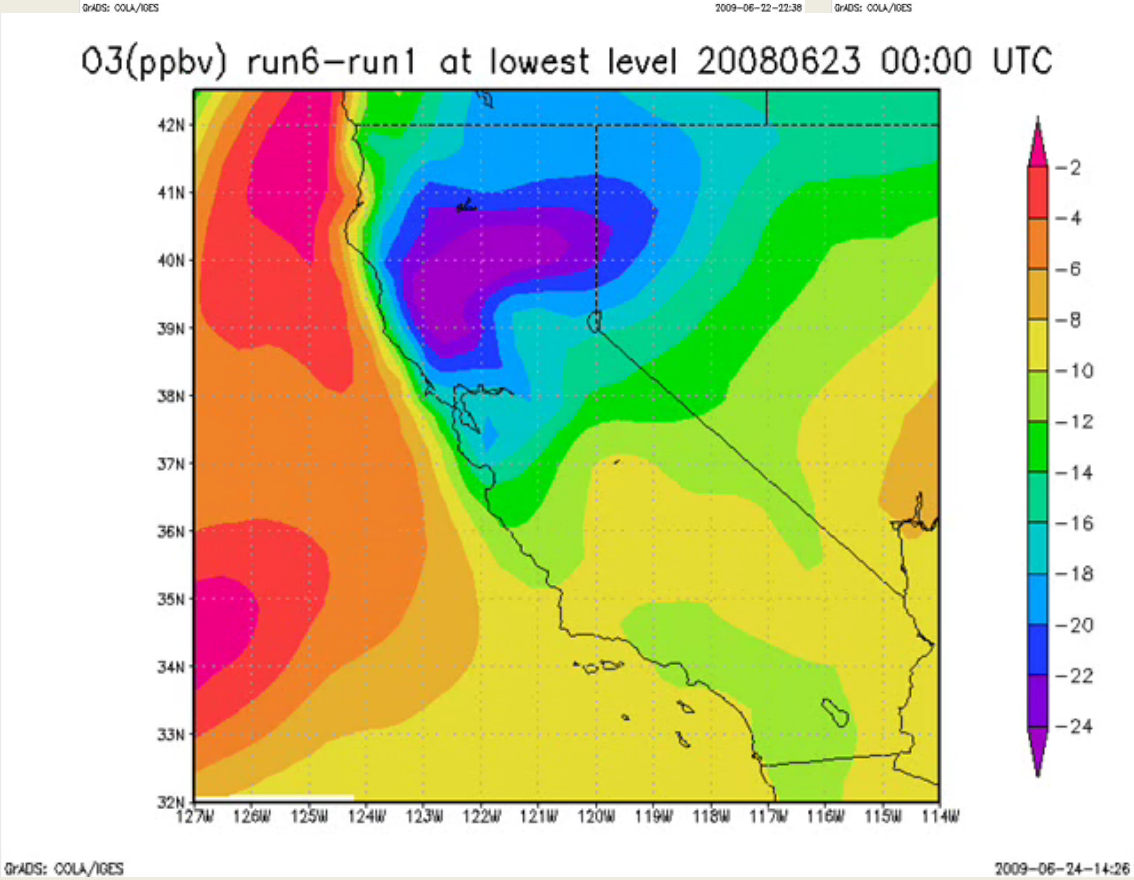

The influence to Northern CA is relatively constant, due to strong local Biomass burning

RUN1




RUN6




The most O3-reduced areas at surface moved– indicates the significance of using time and spatial varied BC

# Sub-summary for BC study

- CO and O3 concentrations were sharply reduced
- CO over Northern CA was strongly controlled by Bio burning
- BC sensitive study indicates the advantage of using time and spatial-varied BC, which will benefit future model forecasts and flight plans

# Summary

- WRF did fairly well in meteorology simulation,

  The bias affect STEM performance
- SO2 and NOy predictions were improved by emission sensitivity studies
- High altitude CO and northern CA O3 are affected by sources out of NA
- CO and O3 were not sensitive to emissions, but were highly reduced in fixed-boundary case
- Time and spatial-varied BC reduce predicted concentration biases substantially

# Future work

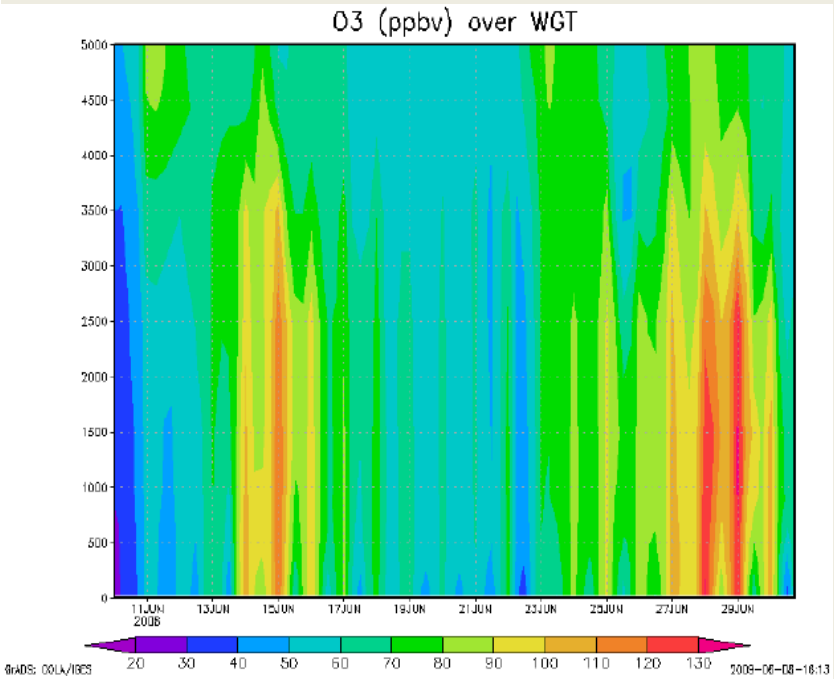
- Higher resolution
- Resolve emissions
- Improve forecast by BC sensitivity study
- Working on WRF-chem with different EI, resolutions, and domains, will add Bio burning and include chemistry-climate feedbacks

# Acknowledgement

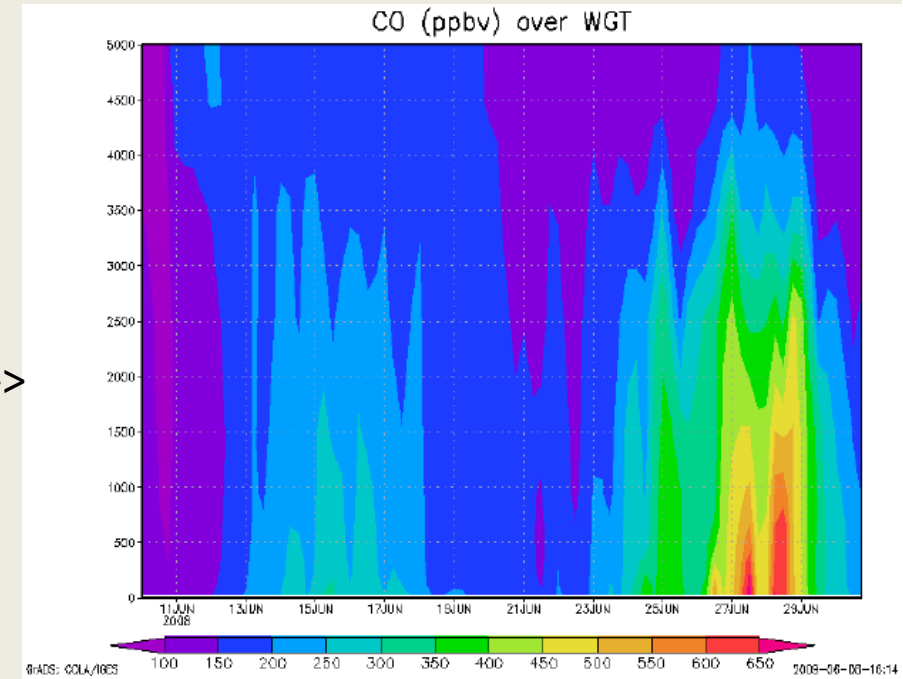

- CGRER, The University of Iowa
- ARCTAS Measurement Team
- NASA & CARB
- David Streets, Giuseppe Calori, Alessio D'Allura, Youhua Tang, Robert P. Pierce, Jassim A. Al-Saadi

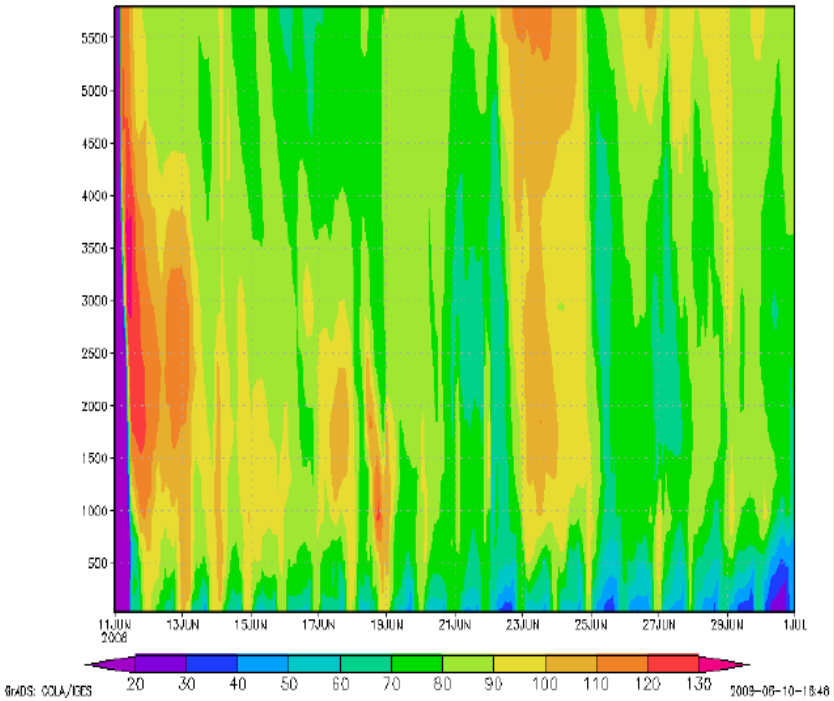

**THANK YOU!**

**QUESTIONS? COMMENTS?**

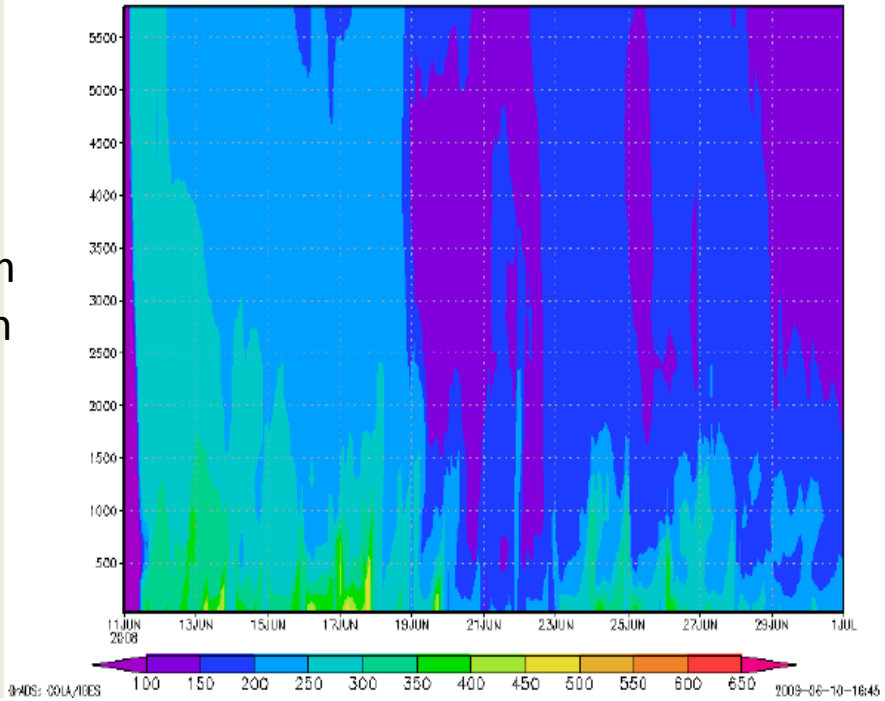


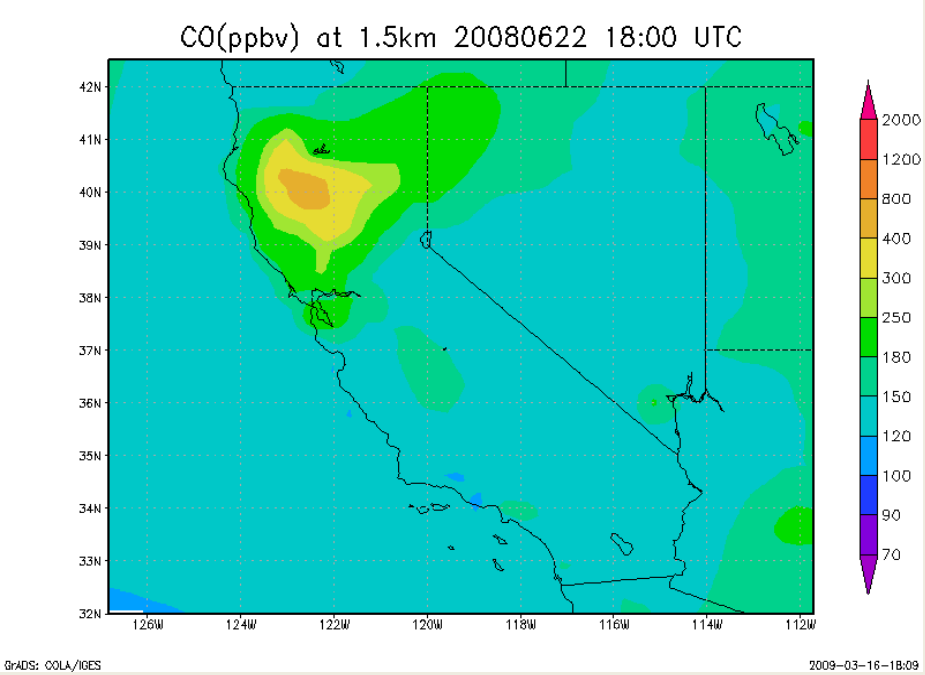

<- STEM ->



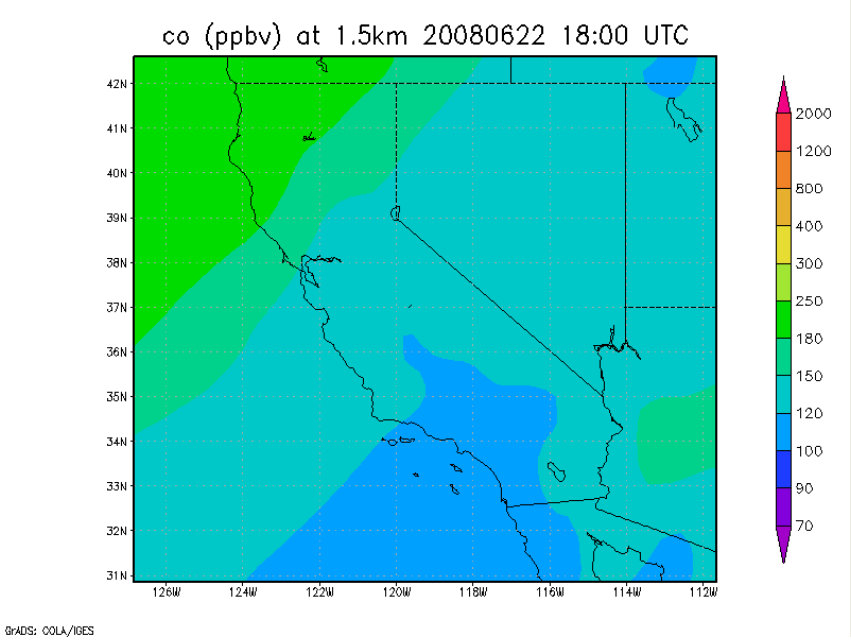




<- WRF-chem 12km with NEI 2005; no BB ->





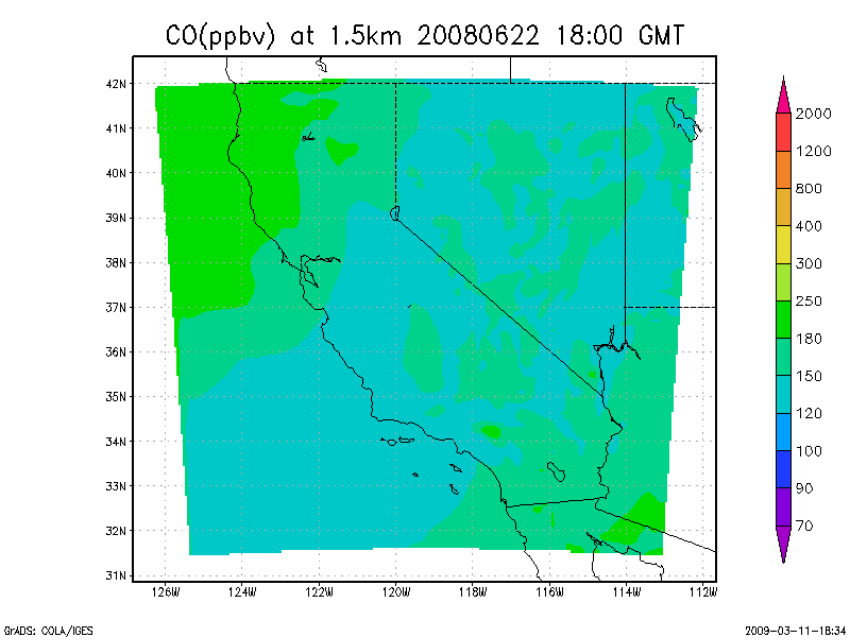

←STEM

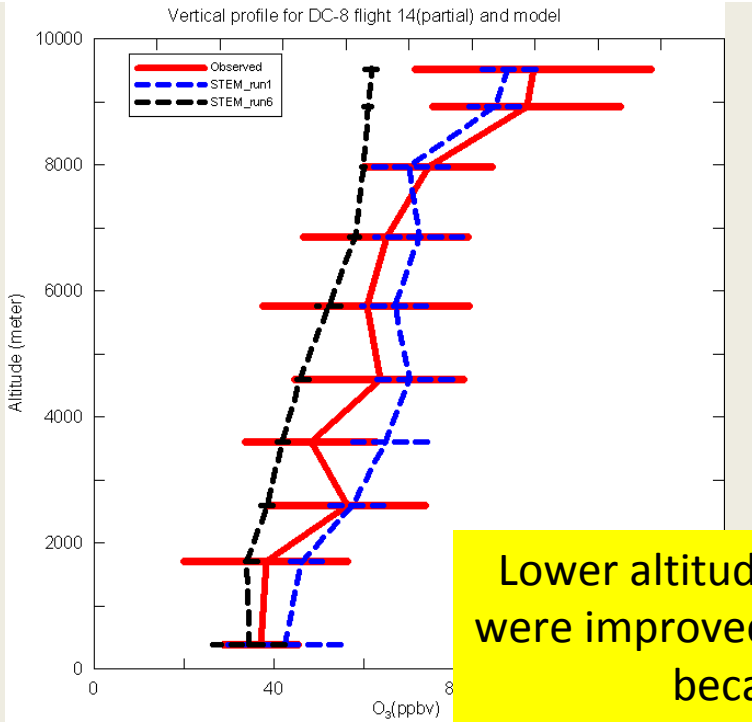



WRF-chem
w/o BB

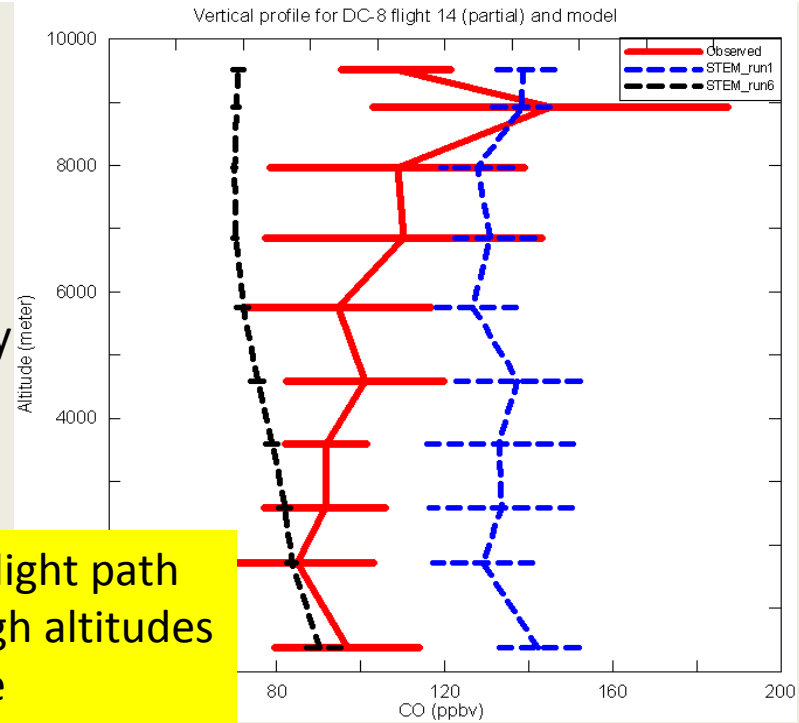
<-60km

12km->

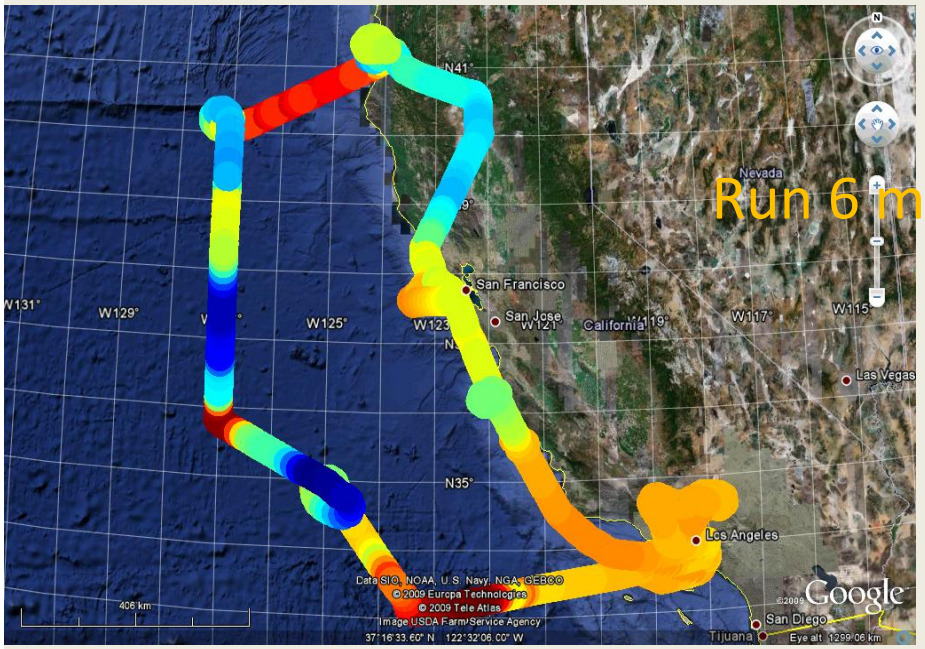


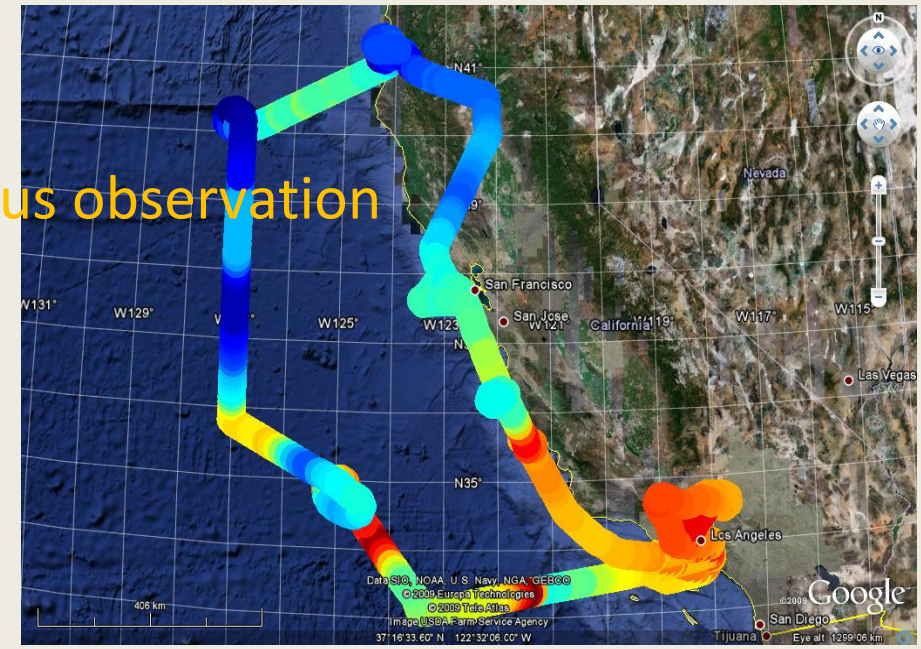



Partial vertical profiles across boundary layer




Lower altitudes along flight path were improved while high altitudes became worse



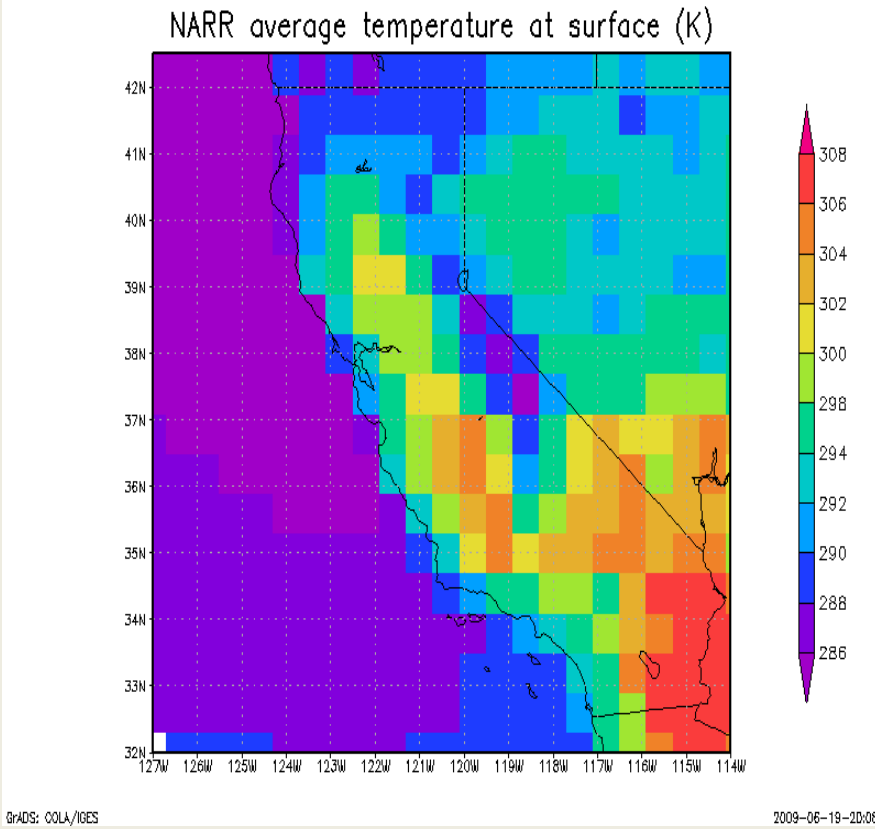



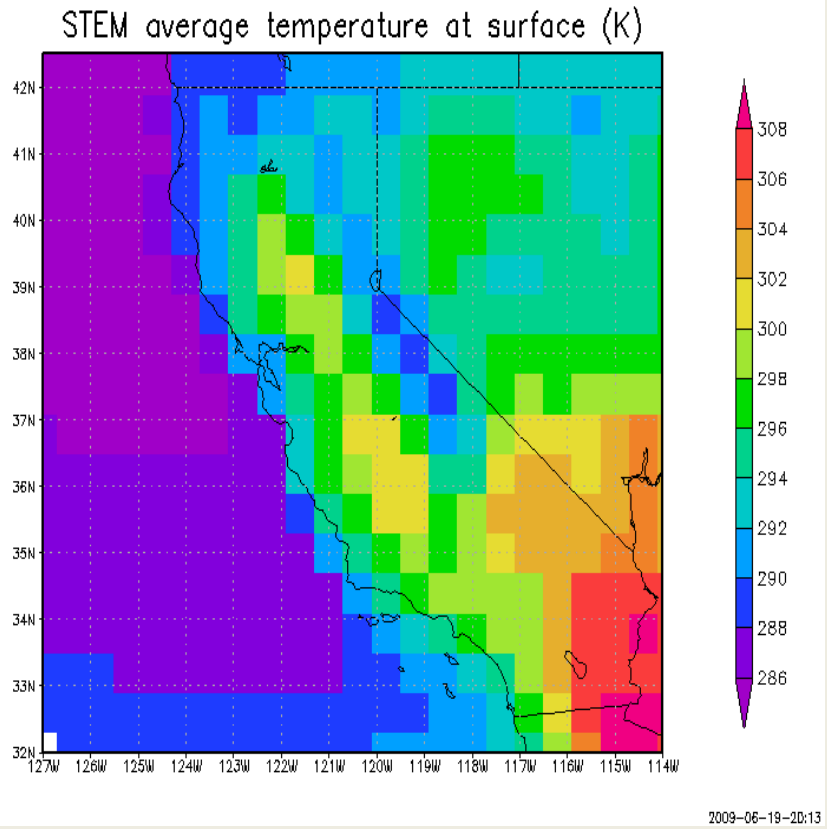
# Compared with NARR

- About NARR
  - Long-term, consistent, high-resolution (32km, 45 layers) climate dataset*
  - Near-surface temperatures and winds closer to observations, especially during summer*

- We compare 20 day (6.11-6.30) average meteorology variables for NARR and WRF results(after its interpolation into STEM grids)
- To keep NARR grids consistent with STEM, areas out of NARR domain were filled with NCAR FNL Final Analysis data

*http://www.emc.ncep.noaa.gov/mmb/rreanl/


NARR average temperature at surface (K)
42N
41N
40N
39N
38N
37N
36N
35N
34N
33N
32N
127W 126W 125W 124W 123W 122W 121W 120W 119W 118W 117W 116W 115W 114W
308
306
304
302
300
298
294
292
290
288
286
GrADS: COLA/IGES
2009-06-19-20:08 GrADS: COLA/IGES


STEM average temperature at surface (K)
42N
41N
40N
39N
38N
37N
36N
35N
34N
33N
32N
127W 126W 125W 124W 123W 122W 121W 120W 119W 118W 117W 116W 115W 114W
308
306
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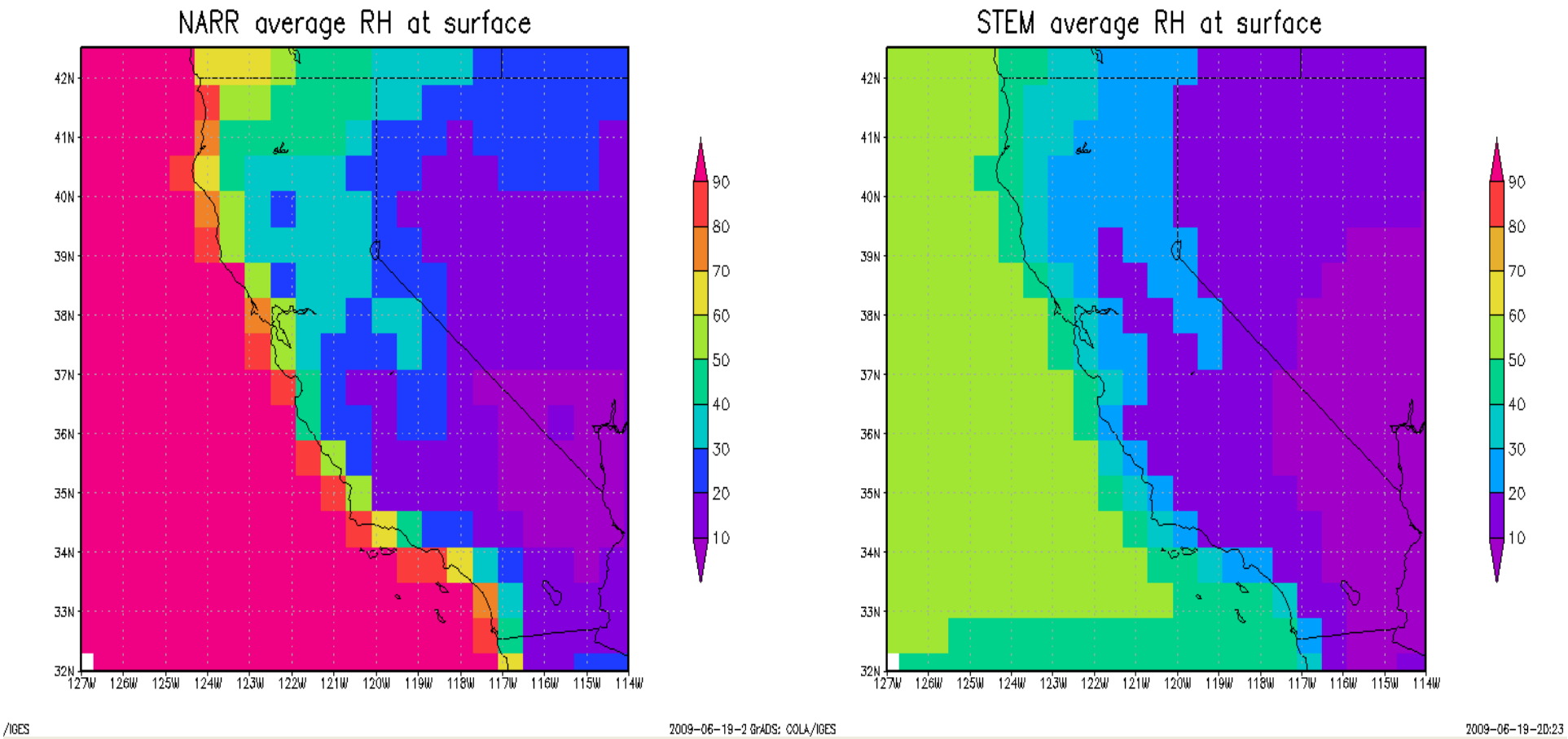
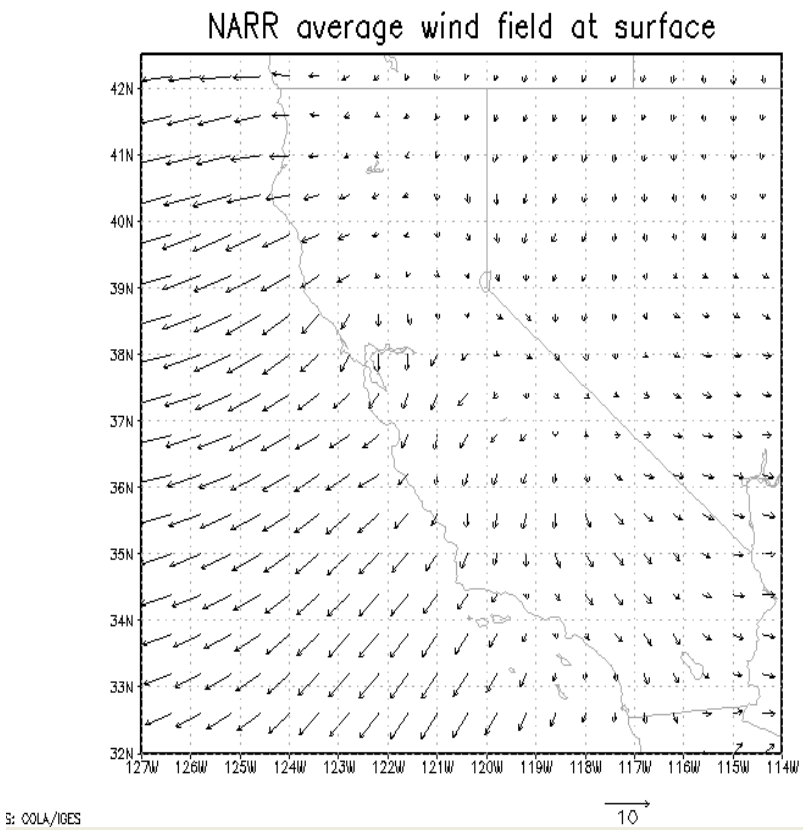
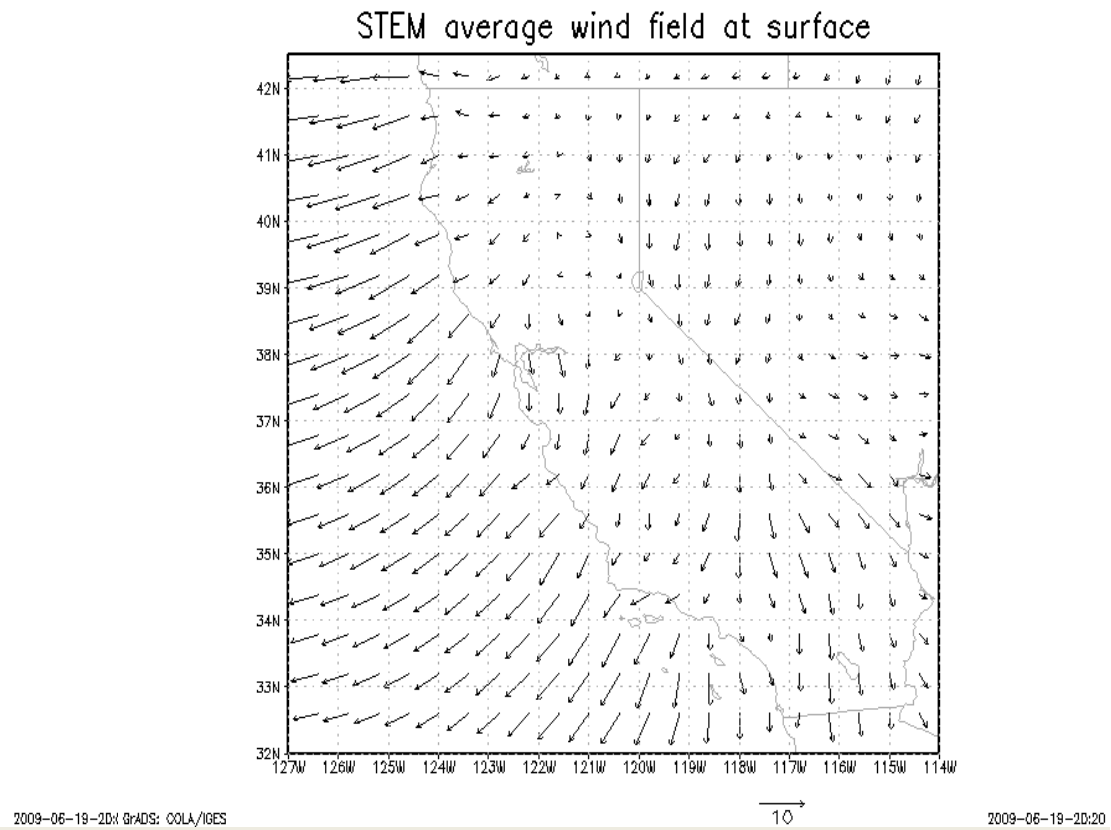
300
298
296
294
292
290
288
286
2009-06-19-20:13




Discrepancies of RH over ocean may be due to their different 1st layer heights above the ground

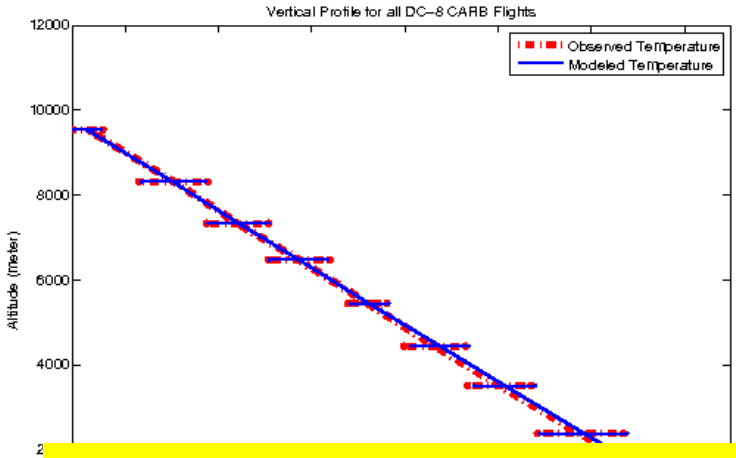


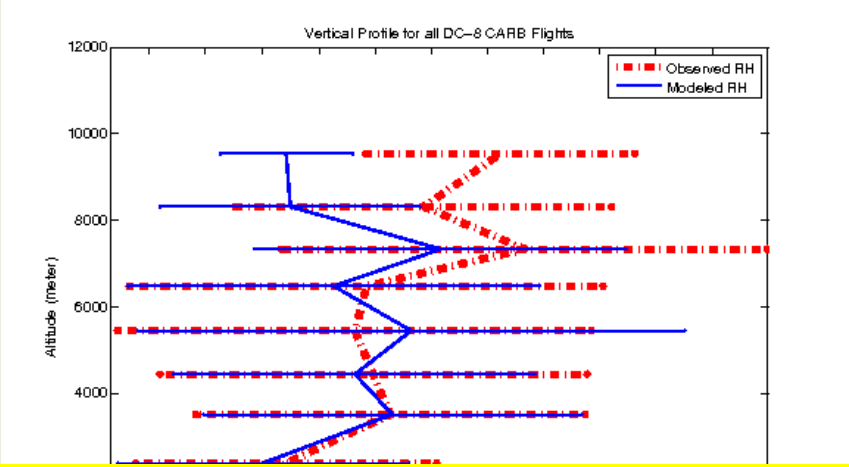




2009-06-19-20:X GrADS: COLA/IGES

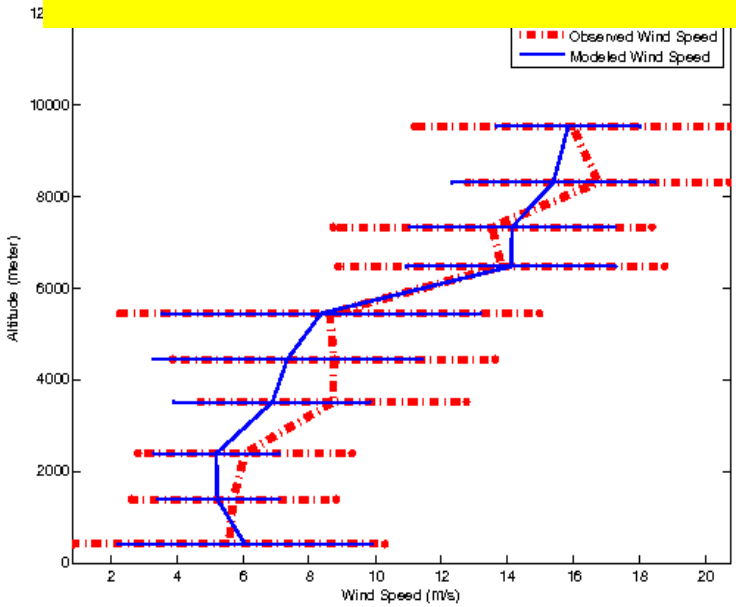
- WRF generally provided good meteorology prediction at surface compared with NARR
- NARR shows advantages of higher resolution

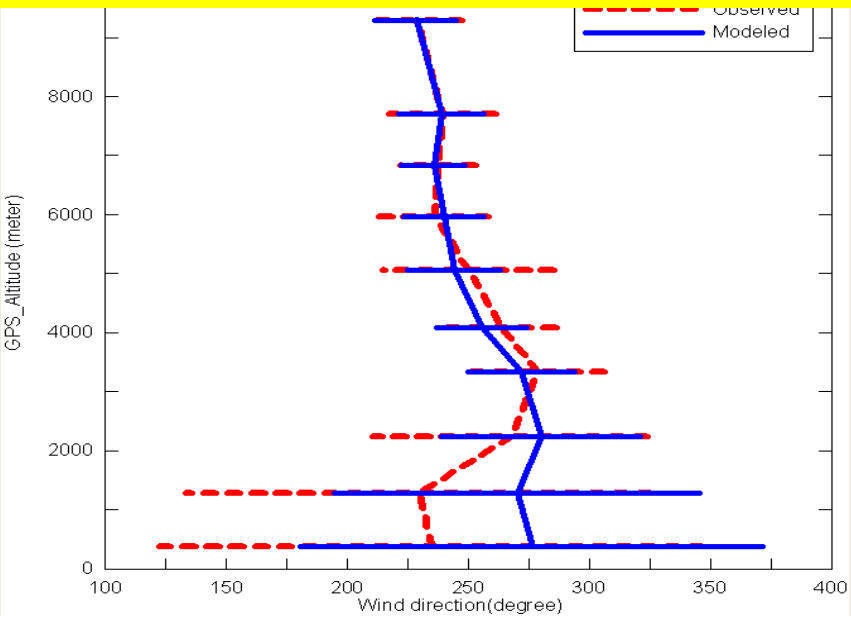
# Compared with Flight observations




WRF did fairly well but still needs improvement at lower levels

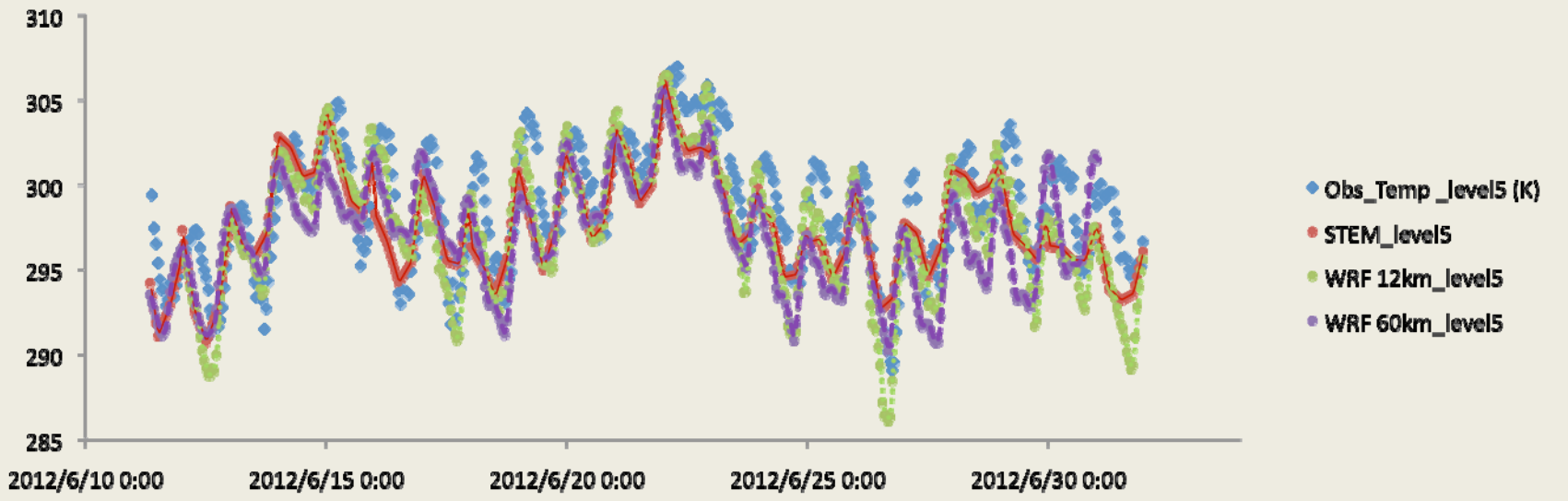


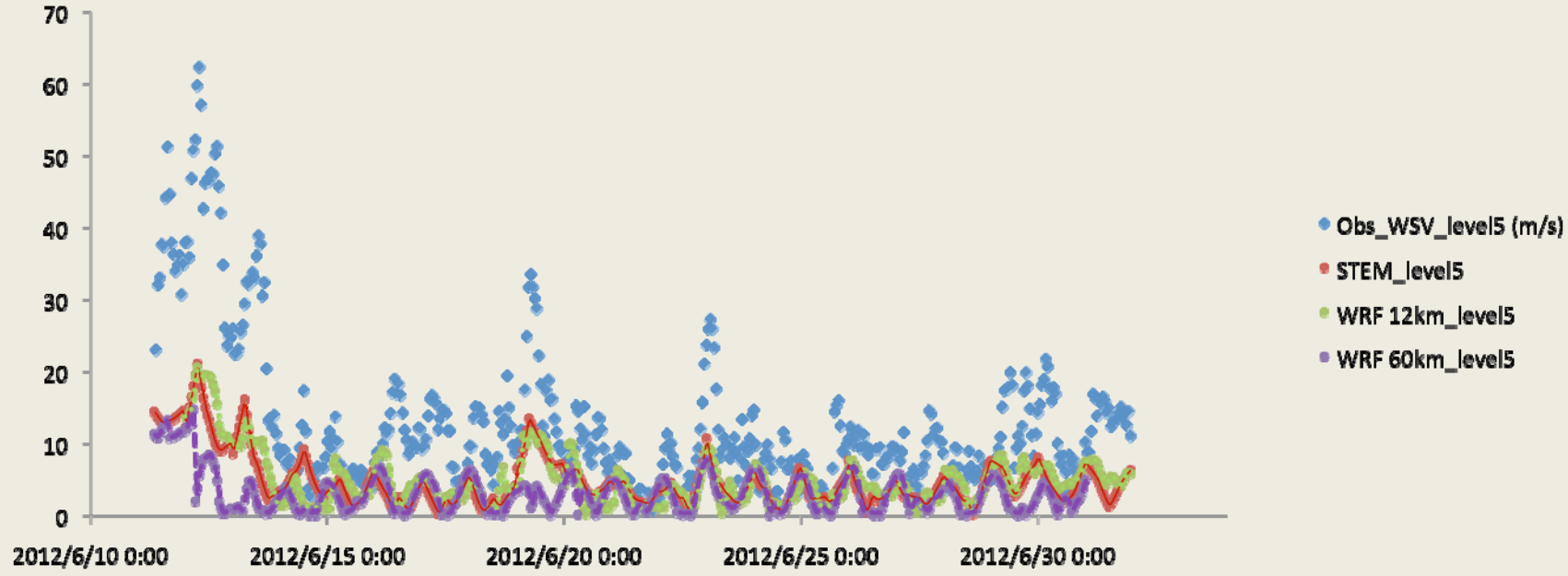



# Compared with WGT observations

- 20 miles south of Sacramento
- Tower measures O3, CO, temperature and wind field at 5 levels: 30, 400, 800, 1200,1600 feet.*
- Also have compared results from WRF-chem using two resolutions during the same period
- In this presentation, only show results of top level to connect with transport study

*Data source :http://tbsys.serveftp.net/wg/wgup/tower.htm


310
305
300
295
290
285
2012/6/10 0:00
2012/6/15 0:00
2012/6/20 0:00
2012/6/25 0:00
2012/6/30 0:00
Obs_Temp _level5 (K)
STEM_level5
WRF 12km_level5
WRF 60km_level5


70
60
50
40
30
20
10
0
2012/6/10 0:00
2012/6/15 0:00
2012/6/20 0:00
2012/6/25 0:00
2012/6/30 0:00
Obs_WSV_level5 (m/s)
STEM_level5
WRF 12km_level5
WRF 60km_level5

| | Observed | STEM | WRF 12km | WRF 60km |
|---|---|---|---|---|
| temp rsq | | 0.56 | 0.64 | 0.45 |
| temp avg (K) | 298.72 | 297.61 | 297.50 | 297.21 |
| temper bias | | -1.10 | -1.21 | -1.51 |
| temp error % | | -0.37 | -0.41 | -0.50 |
| | | | | |
| WS rsq | | 0.61 | 0.67 | 0.23 |
| WS avg (m/s) | 12.97 | 4.86 | 4.90 | 3.08 |
| WS bias | | -8.11 | -8.07 | -9.89 |
| WS error% | | -62.50 | -62.21 | -76.23 |

1) Good capture of temperature for all three
2) Wind speeds are bias low for all three
3) From RSQ between model and observed data: STEM 60km is close to WRF 12km;
4) From average values: STEM did best for temperature,
performance of WS was close to WRF 12km