Evaluation of CMAQ estimated gas and aerosol carbon using STN, IMPROVE, and CALNEX field measurements

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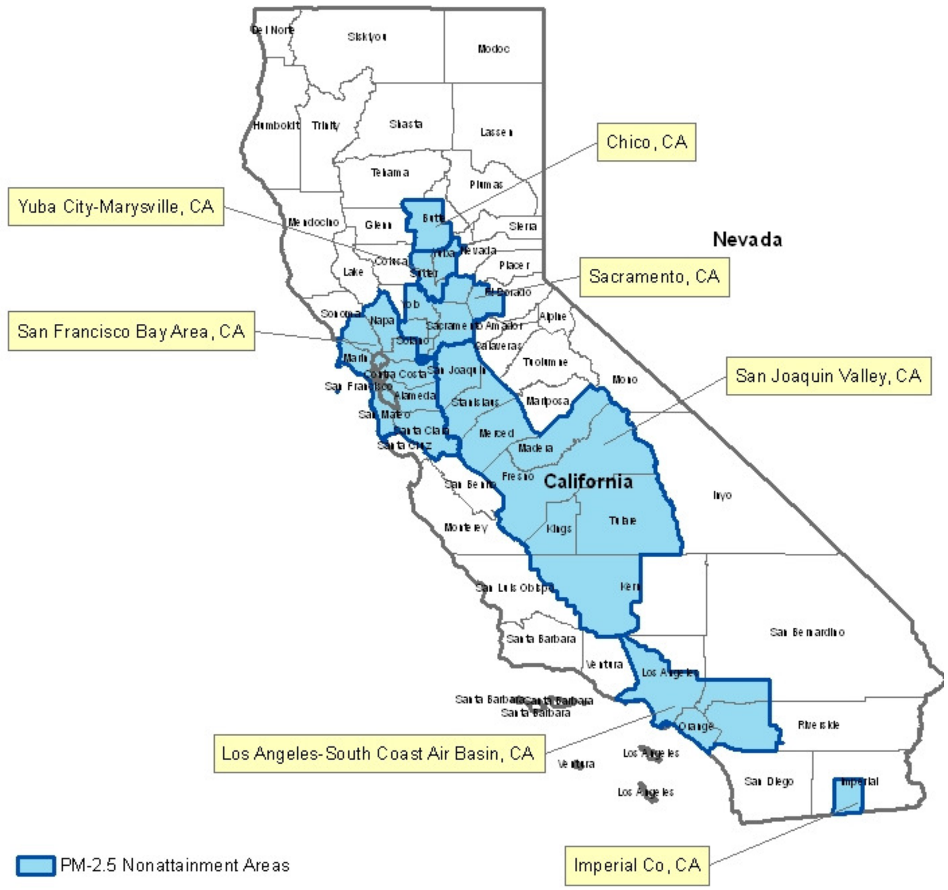
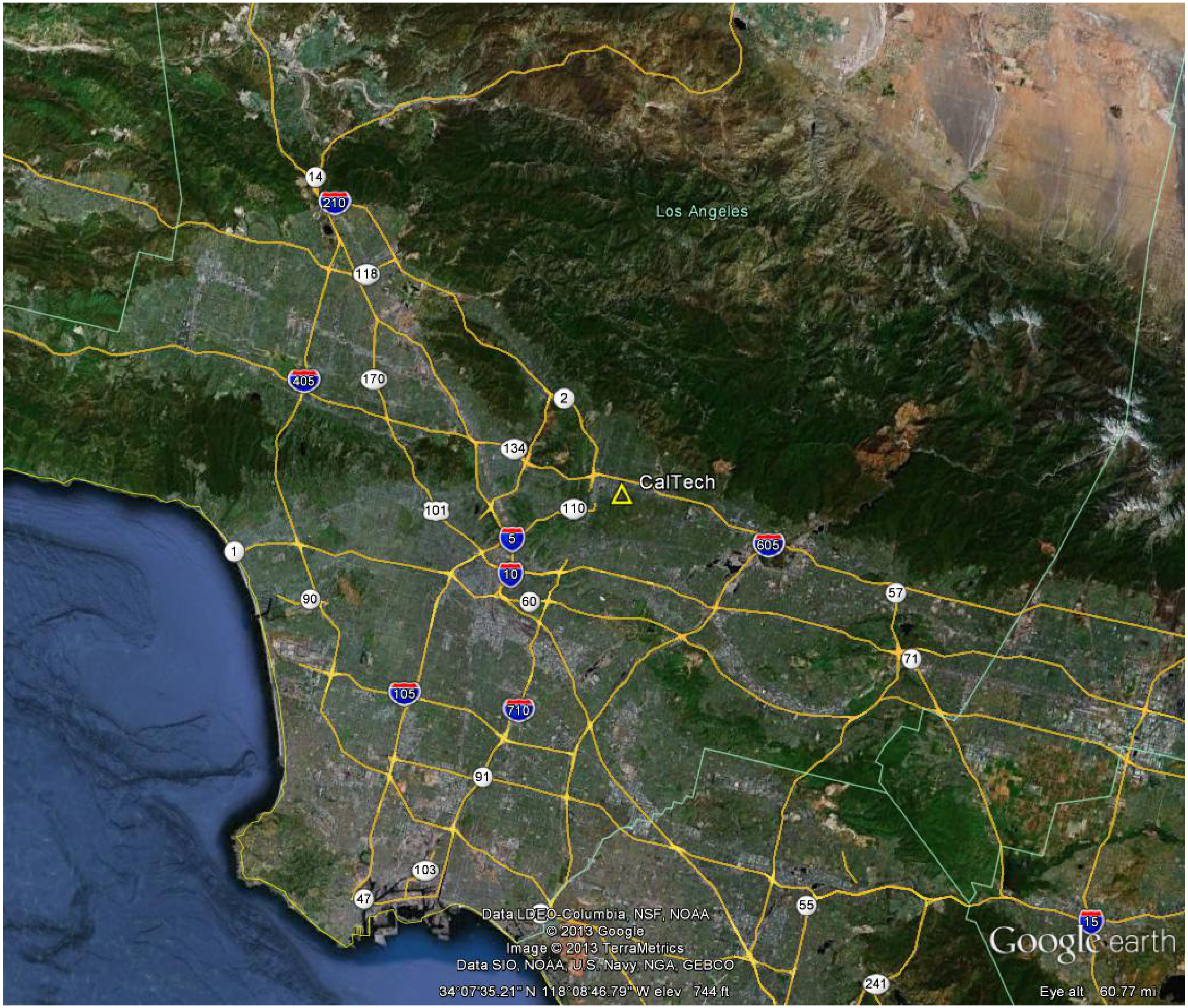
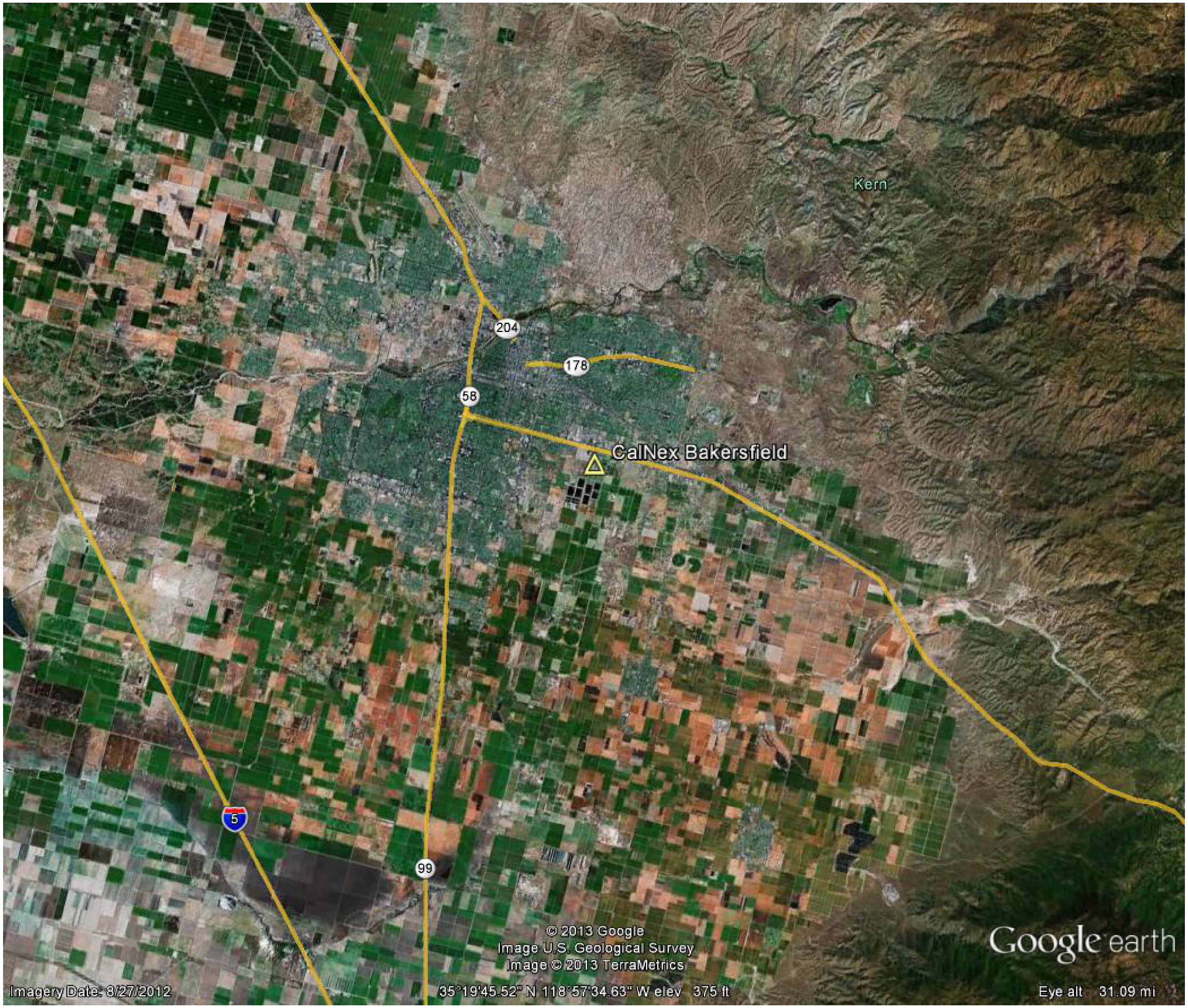
Motivation

- California currently has many counties violating the 8-hr ozone and/or PM2.5 NAAQS
- Many counties still projected to be nonattainment in the future
- Model performance challenges in California: complex terrain, land-ocean interactions, large emissions sources
- Objective is to combine routine observation data with non-routine measurements from field campaigns like CalNex to evaluate meteorological and photochemical model performance in California



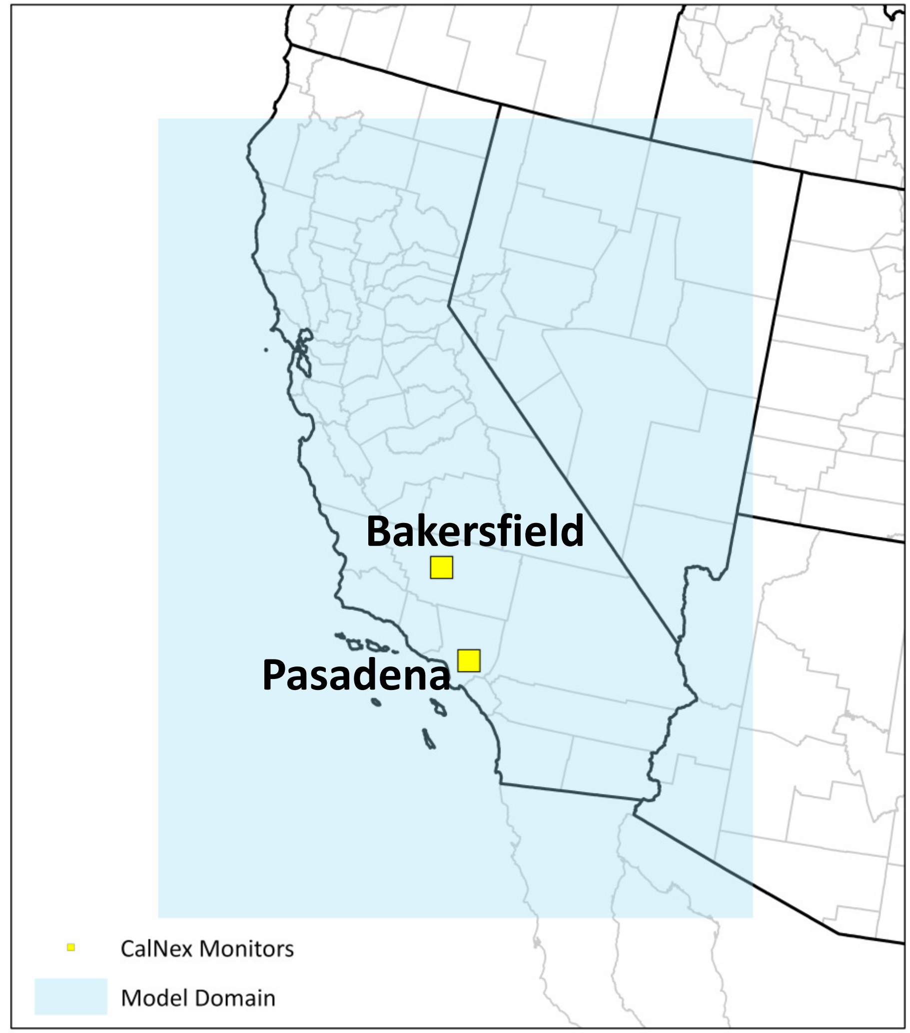

Los Angeles
CalTech
14
210
118
405
170
2
134
101
110
5
1
10
605
90
60
57
71
105
710
91
103
47
55
15
241
Data LDEO-Columbia, NSF, NOAA
© 2013 Google
Image © 2013 TerraMetrics
Data SIO, NOAA, U.S. Navy, NGA, GEBCO
34°07'35.21" N 118°08'46.79" W elev 744 ft
Google earth
Eye alt 60.77 mi


204
178
58
CalNex Bakersfield
Kern
5
99
© 2013 Google
Image U.S. Geological Survey
Image © 2013 TerraMetrics
Google earth
Imagery Date: 8/27/2012
35°19'45.52" N 118°57'34.63" W elev 375 ft
Eye alt 31.09 mi

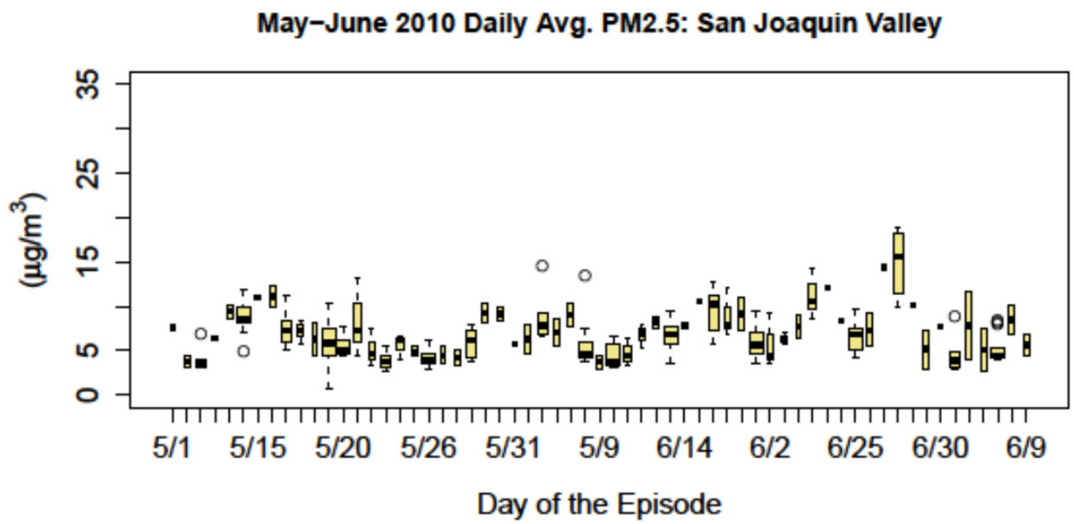
MODEL SETUP & APPLICATION

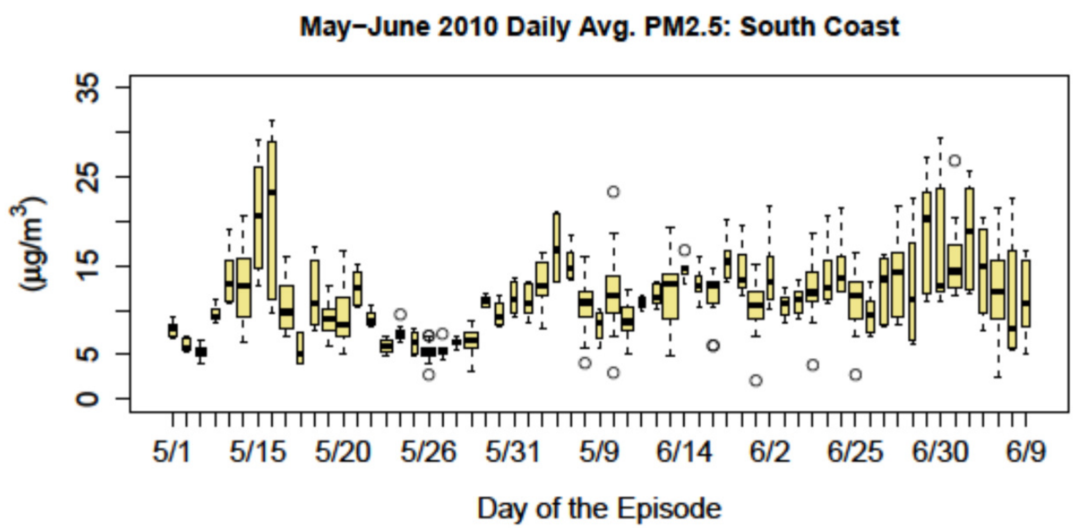
•4 km horizontal grid spacing
•NX=236, NY=317, NZ=34
•34 vertical layers (1 to 1 mapping with WRF)
•**CMAQ v5.0.2 – SAPRC07 – AERO6**
•Boundary inflow from coarser CMAQ simulation (boundary inflow to that from GEOS-CHEM)
•Ignoring the first 10 days to minimize initial condition influence

•Modeled May and June 2010 to match CALNEX field campaign
•BEIS v3.14 biogenic emissions
•**2010/2011 based emissions: 2011 NEI v1**
Many published studies have noted the importance of using the emissions inventory closest to the year being modeled (here 2010)

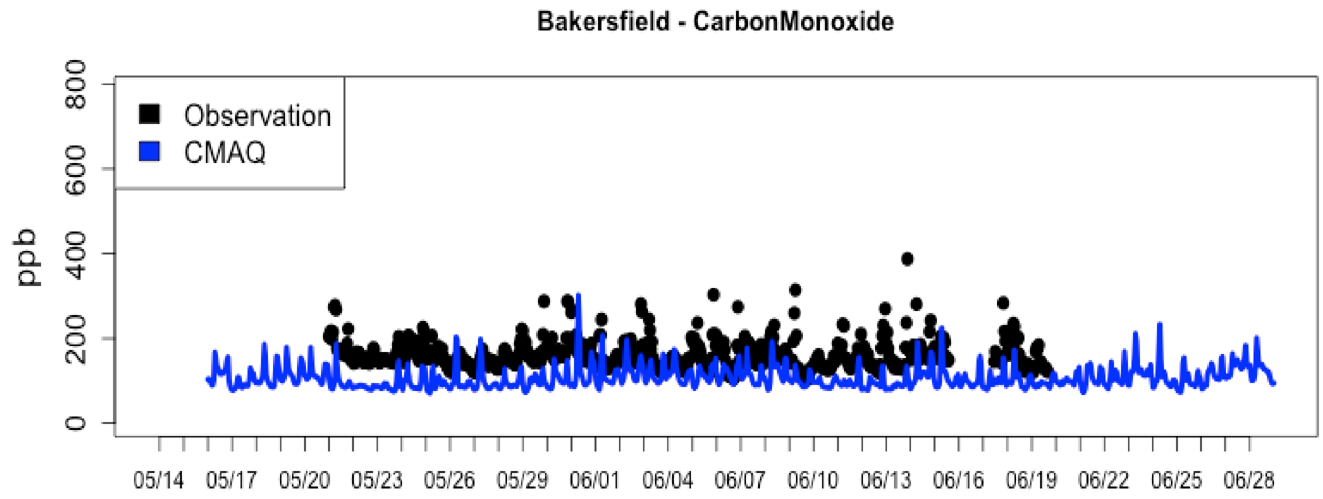


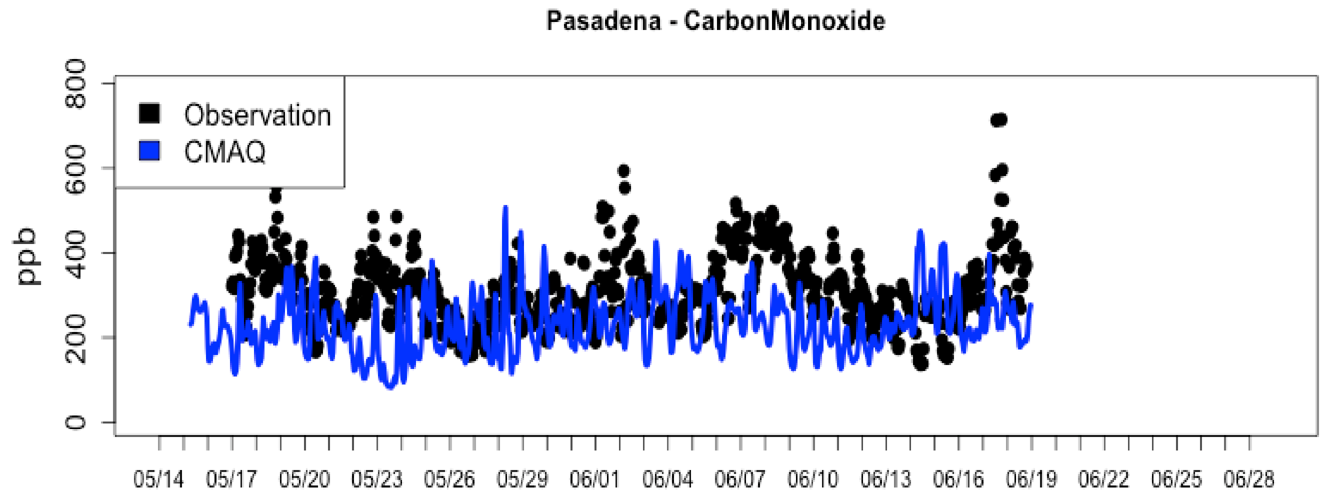
Episode PM2.5





Carbon Monoxide





Gas and Particle Carbon Species

Examine gas and particle phase carbon at Pasadena and Bakersfield sites

- Compare CMAQ estimated PM2.5 organic and elemental carbon to daily measurements
- Compare CMAQ estimated VOC against speciated 3-hr morning measurements and daily averages of hourly VOC
- Compare CMAQ estimated SOC against daily SOC tracer measurements
- Modern (non-fossil) and fossil components of PM2.5 carbon
- Primary and secondary PM2.5 at Pasadena

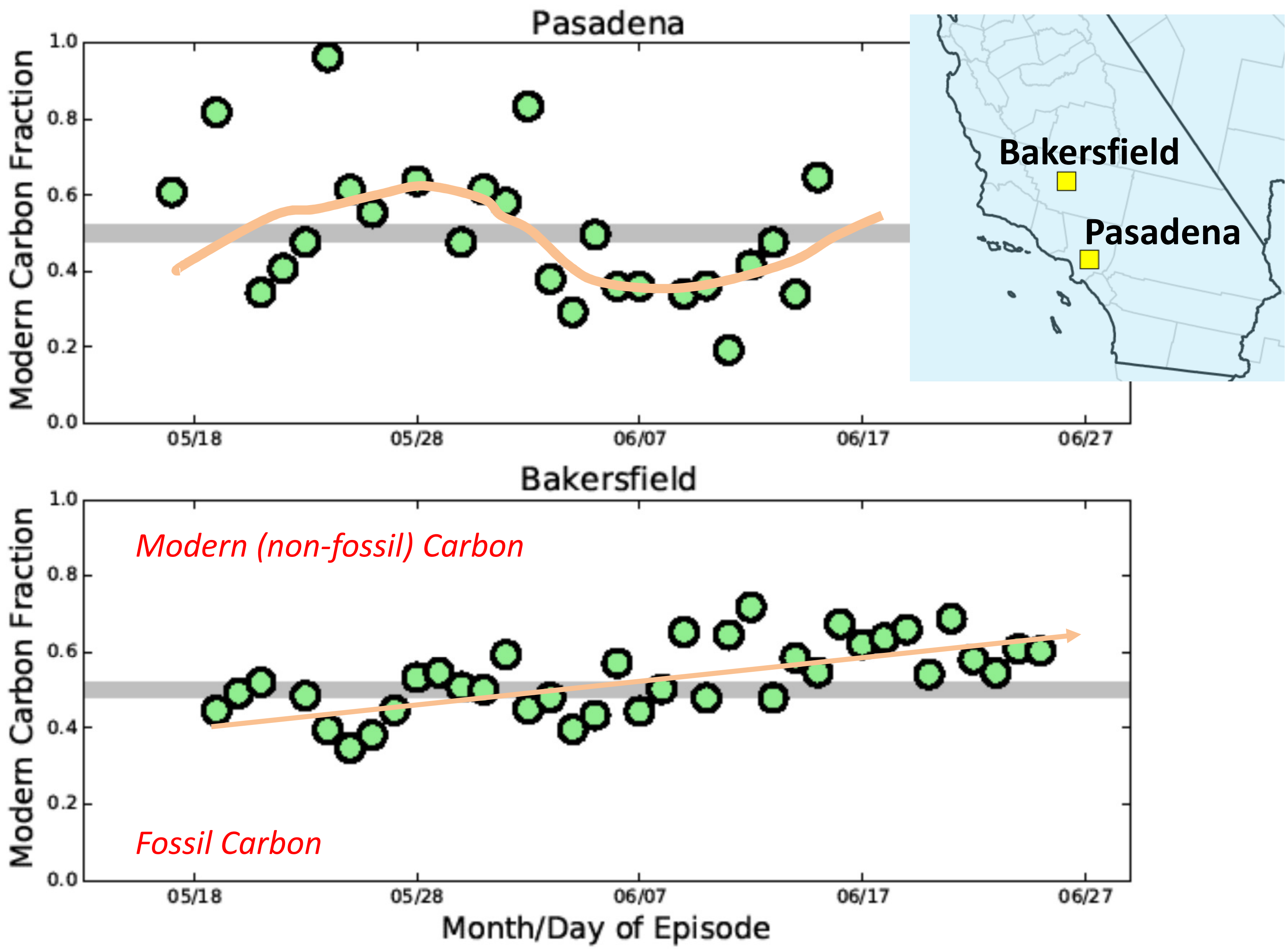
NEI2011 v1 Sources of POA and BTX

	Primarily emitted PM2.5 organic carbon				Benzene + Toluene + Xylenes			
Sector	SSJV (tons)	SSJV (%)	LA (tons)	LA (%)	SSJV (tons)	SSJV (%)	LA (tons)	LA (%)
Non-point area	139.9	33.8	410.1	40.8	326.7	37.2	1229.3	35.8
Onroad mobile	73.3	17.7	263.6	26.2	273.5	31.2	1190.9	34.6
Nonroad mobile	23.9	5.8	161.4	16.1	170.1	19.4	822.3	23.9
Point: non-electrical generating	61.3	14.8	56.3	5.6	68.3	7.8	177.7	5.2
Residential wood combustion	54.1	13.1	82.7	8.2	2.0	0.2	3.2	0.1
Oil & gas exploration and related	28.5	6.9	0.0	0.0	34.2	3.9	1.1	0.0
Fugutive dust	24.9	6.0	18.1	1.8	0.0	0.0	0.0	0.0
Commercial marine & rail	3.8	0.9	11.4	1.1	2.6	0.3	12.8	0.4
Point: electrical generating	4.3	1.0	1.7	0.2	0.1	0.0	1.0	0.0
Total Modern Carbon	218.9	52.9	510.9	50.8	2.0	0.2	3.2	0.1
Total Fossil Carbon	195.2	47.1	494.5	49.2	875.3	99.8	3435.1	99.9

- Modern Carbon
  - Meat cooking
  - Open burning of waste; residential wood combustion
  - Dust from livestock, agricultural tilling
- Fossil Carbon
  - Onroad and offroad engines burning gasoline and diesel

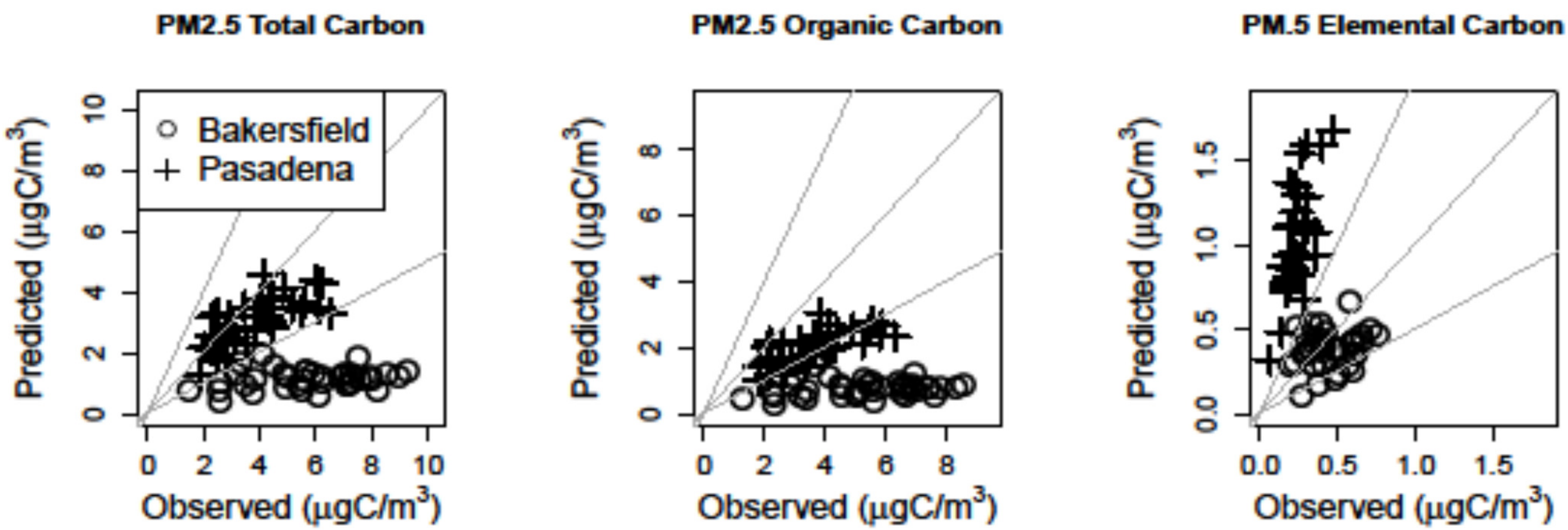
- Modern Carbon
  - Biogenic emissions (trees, crops, grasses)
- Fossil Carbon
  - Onroad and offroad engines burning gasoline and diesel

Observed daily average PM2.5 modern carbon fraction



PM2.5 Carbon Performance

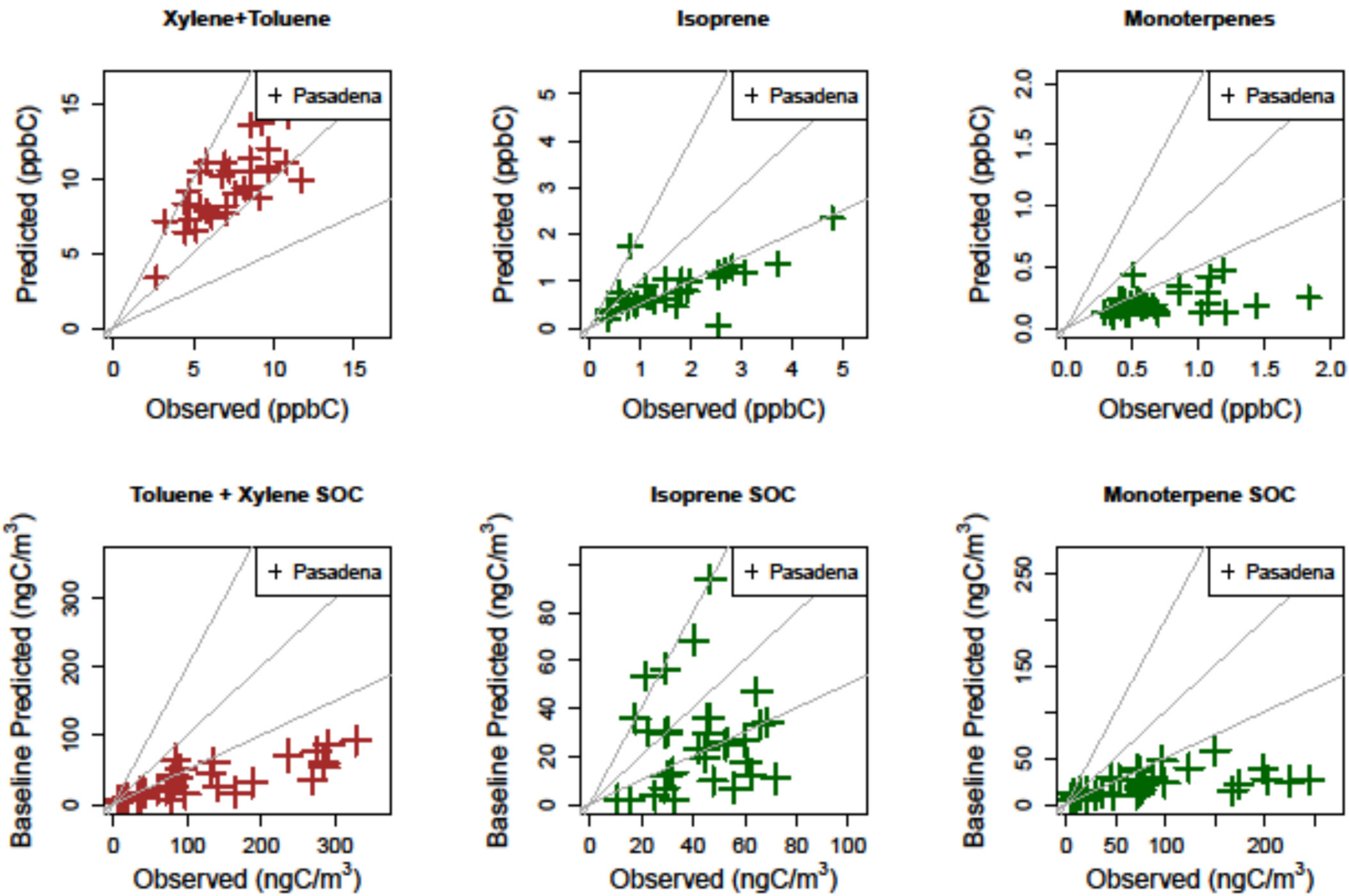
- Average observed modern PM2.5 carbon fraction 50% at Pasadena and 53% at Bakersfield; average modeled fraction is ~60% at both sites
- Modeled and observed daily average PM2.5 carbon shown below



PM2.5 Organic Carbon Performance

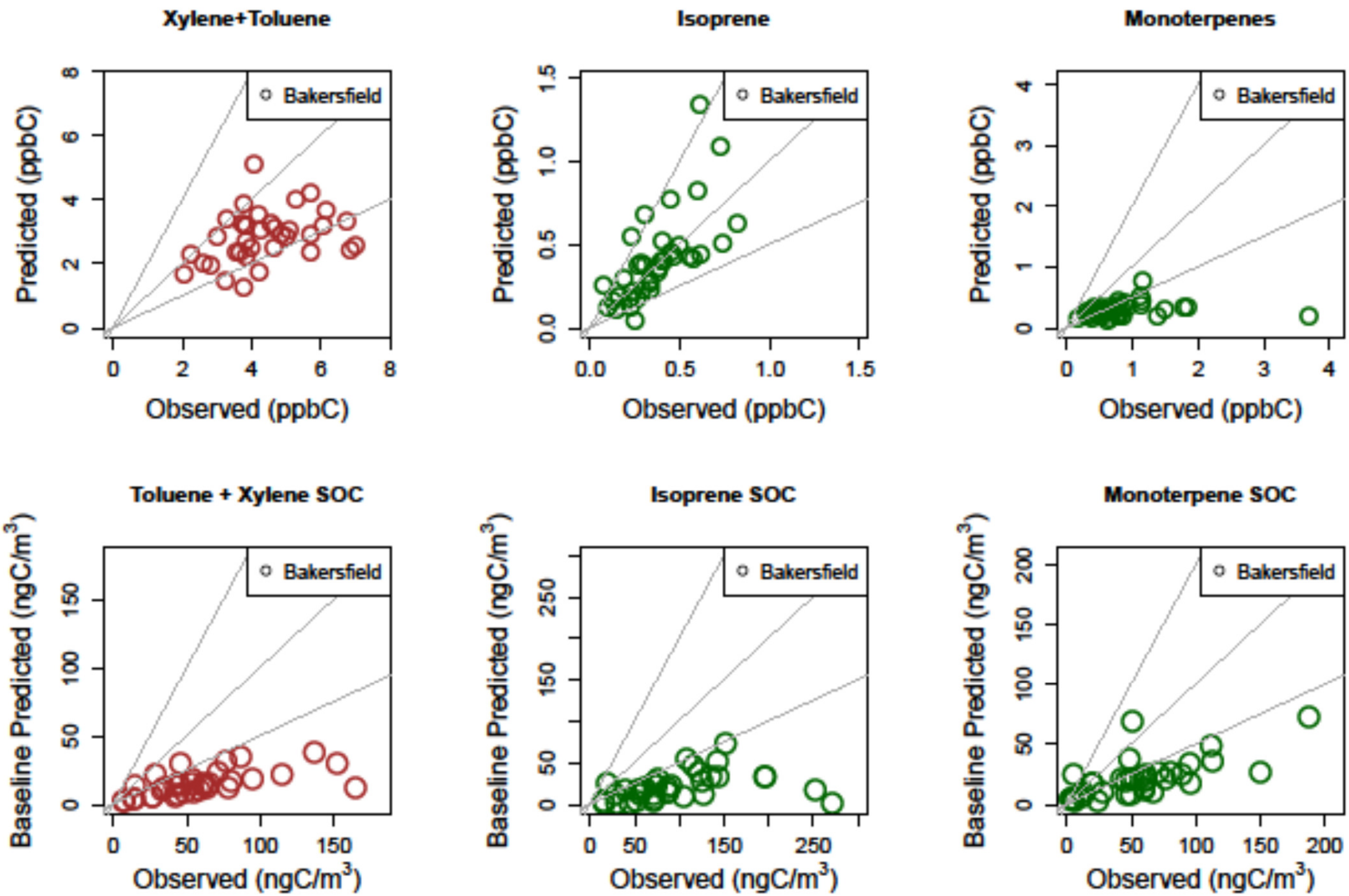
- Slight underestimate at Pasadena; are we getting the right answer for the right reasons?
- Large underestimate at Bakersfield; however large differences exist in co-located measurements
- AMS based measurements at Pasadena suggest organic aerosol there is ~2/3 secondary
- Similar observation based approaches at Bakersfield suggest of that organic aerosol is secondary
- Baseline CMAQ AE6 simulation has 10% of organic aerosol from secondary production

PASADENA

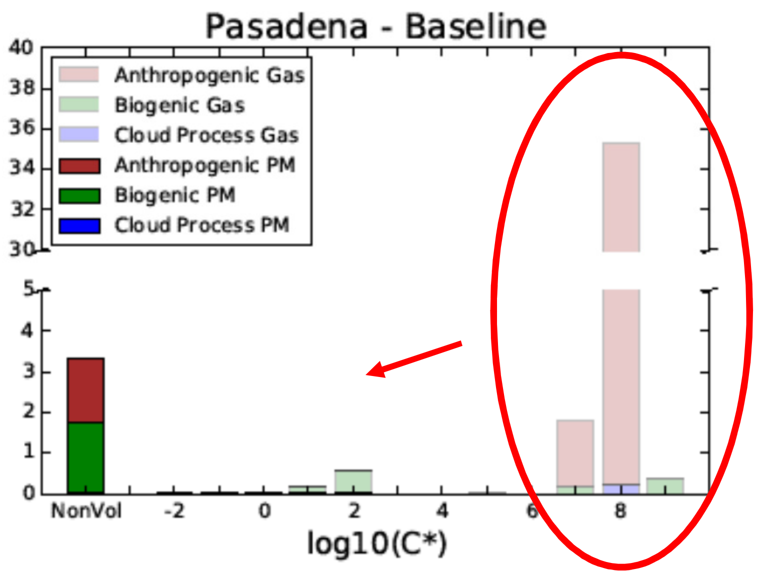


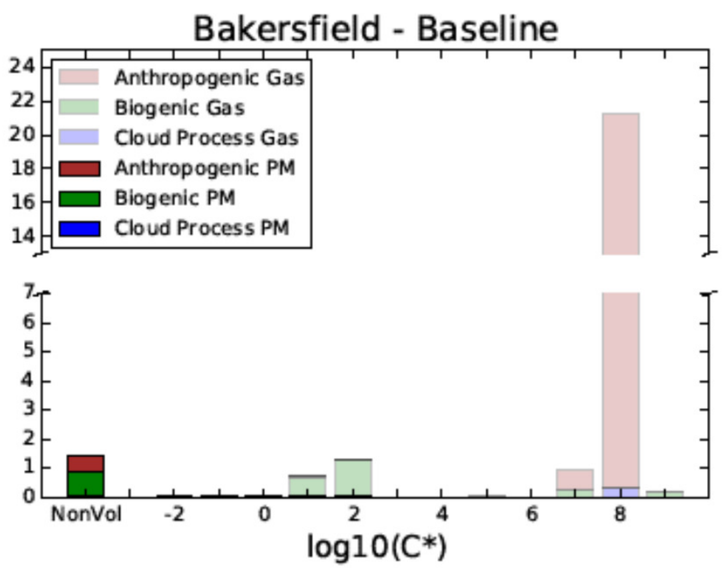
Xylene+Toluene
Isoprene
Monoterpenes
Predicted (ppbC)
Observed (ppbC)
+ Pasadena
Toluene + Xylene SOC
Isoprene SOC
Monoterpene SOC
Baseline Predicted (ngC/m3)
Observed (ngC/m3)
+ Pasadena

BAKERSFIELD

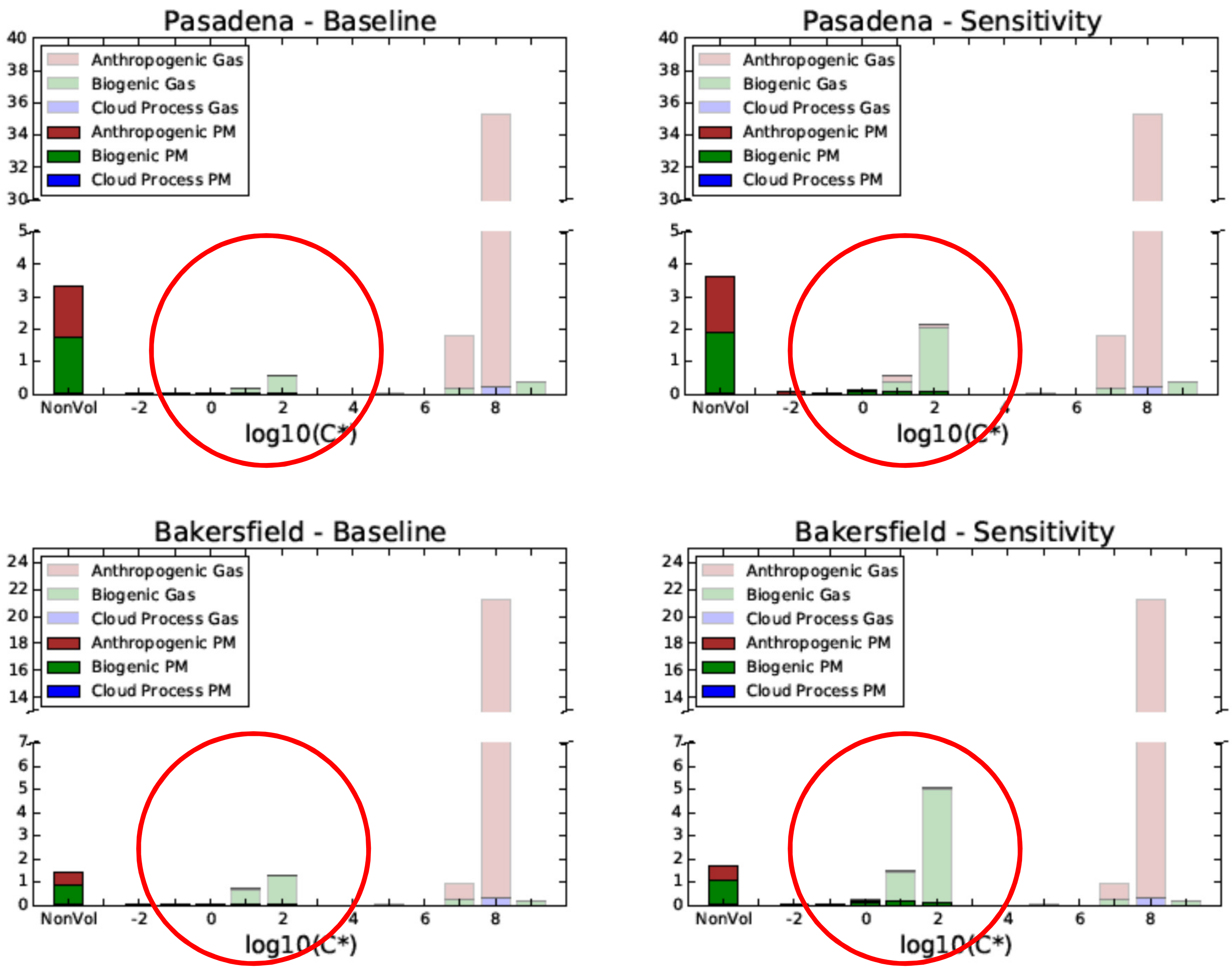


CMAQ Sensitivity Simulation





- VOC (especially BTX) fairly well characterized
- How to get more VOC to participate in SOA parameterization?
- Increased semi-volatile yields by a factor of 4 for anthropogenic and biogenic VOC
- This sensitivity intended to provide a sense about how much more SOA may be formed if yields were higher—not suggesting this is a needed change to CMAQ


Pasadena - Baseline
Pasadena - Sensitivity
Bakersfield - Baseline
Bakersfield - Sensitivity
Anthropogenic Gas
Biogenic Gas
Cloud Process Gas
Anthropogenic PM
Biogenic PM
Cloud Process PM
NonVol
-2
0
2
4
6
8
log10(C*)

Remarks

- PM2.5 organic carbon estimated by CMAQ AE6 for 2010 CALNEX period and sites is too "modern" and too "primary"
- Likely missing both modern and fossil sources (e.g. IVOC)
- Underestimating SOC from known modern and fossil sources as well (e.g. missing production pathways such as isoprene IEPOX/MAE, alkanes, PAHs)
- Both CMAQ and measured tracer SOC explain little of total modeled or measured PM2.5 organic carbon at these sites for this time period
- Increasing semivolatile VOC yields results in some improvements
- Mobile sector seems well characterized in NEI2011 for this area
- Better representation and possibly microscale transport of biogenic precursors emissions
- May need to treat POA as semi-volatile for this area/period

Related Future Work

- Apply VBS for this platform
  - Evaluation of CMAQ VBS Organic Aerosol Model Predictions during the CalNex-2010 Field Study (Woody, M. et al; CMAS 2014)
- Improved IVOC emissions characterization
- Updated version of BEIS and NEI (version 2)

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- Drew Genter, Jessica Gilman, Jose Jimenez, Patrick Hayes, Allan Goldstein
- CALNEX field study participants

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