Application of a volatility basis set model to secondary organic aerosol simulations across the U.S.

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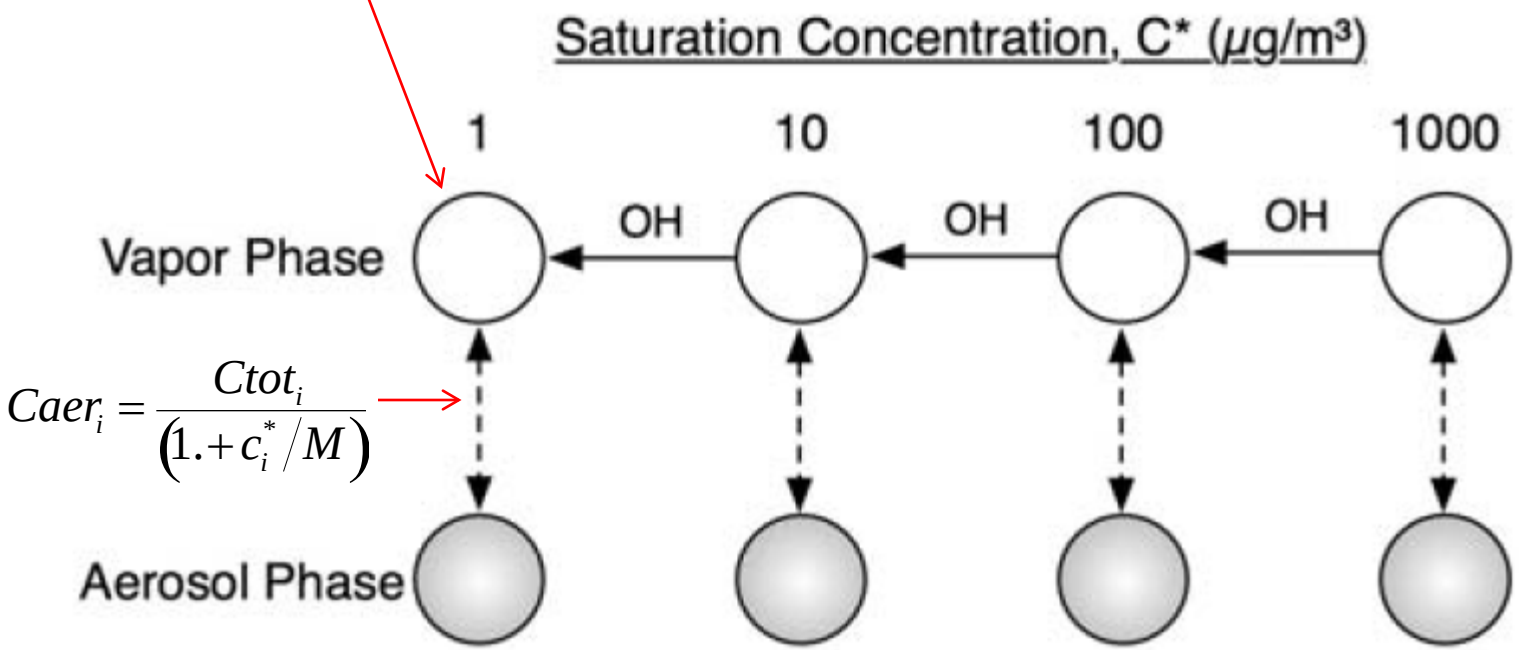
Outline

- VBS mechanism
- WRF-CHEM evaluation for the eastern U.S., August-September, 2006
- DWH oil spill
- CalNex-2010 simulations – preliminary results

Volatility Basis Set (VBS)

Organic condensable vapors (OCVs)

Farina et al., 2010



Faster aging takes place in the gas phase, deposition of these vapors can be significant removal mechanism

SOA yields – RACM mechanism

VOC	High NO_x conditions				Low NO_x conditions			
	1	*10*	*100*	*1000*	*1*	*10*	*100*	*1000*
HC5	0.0000	0.0375	0.0000	0.0000	0.0000	0.0750	0.0000	0.0000
HC8	0.0000	0.1500	0.0000	0.0000	0.0000	0.3000	0.0000	0.0000
OLT	0.0008	0.0450	0.0375	0.1500	0.0045	0.0090	0.0600	0.2250
OLI	0.0030	0.0255	0.0825	0.2700	0.0225	0.0435	0.1290	0.3750
TOL	0.0030	0.1650	0.3000	0.4350	0.0750	0.2250	0.3750	0.5250
XYL, CSL	0.0015	0.1950	0.3000	0.4350	0.0750	0.3000	0.3750	0.5250
ISO	0.0003	0.0225	0.0150	0.0000	0.0090	0.0300	0.0150	0.0000
SESQ	0.0750	0.1500	0.7500	0.9000	0.0750	0.1500	0.7500	0.9000
API, LIM	0.0120	0.1215	0.2010	0.5070	0.1073	0.0918	0.3587	0.6075

Updates to Murphy and Pandis (2010)

WRF-CHEM sensitivity runs

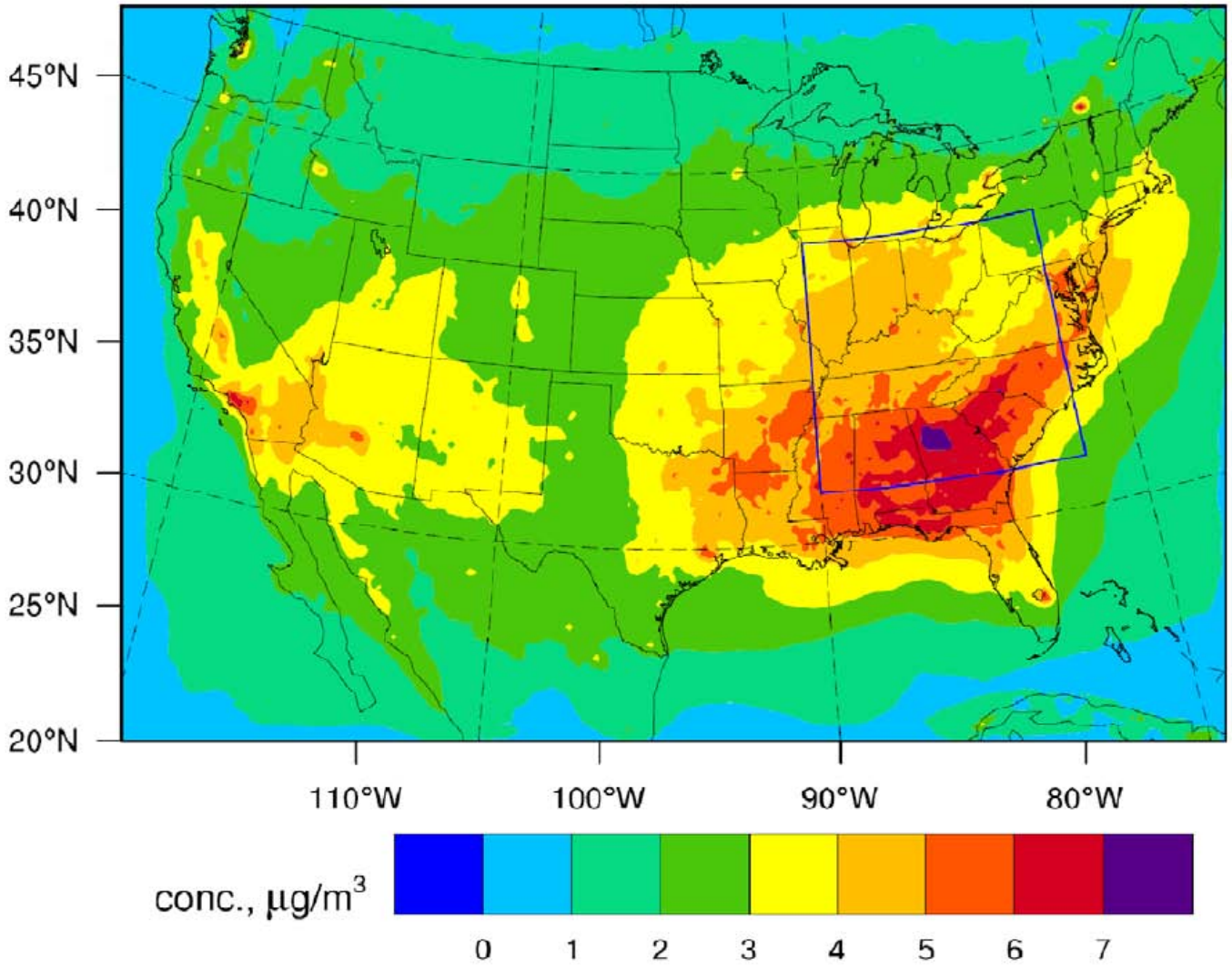
- Anthropogenic OCV reaction rate with OH
- Biogenic OCV reaction rate with OH
- Deposition Velocity of OCVs
- Model Horizontal Resolution
- Planetary Boundary Layer Scheme

Optimum Values – Based on Evaluation Statistics

- Both Anthropogenic and Biogenic OCV age
- OCV - OH rx rate = 1. 10^{-11} 1/cm^3-s
- Deposition velocity of OCV = 0.25*(HNO3 deposition velocity)
- No additional SVOC or IVOC

Ahmadov et al., submitted

Near surface organic aerosol concentrations, daily averaged during 08/04– 09/28, 2006

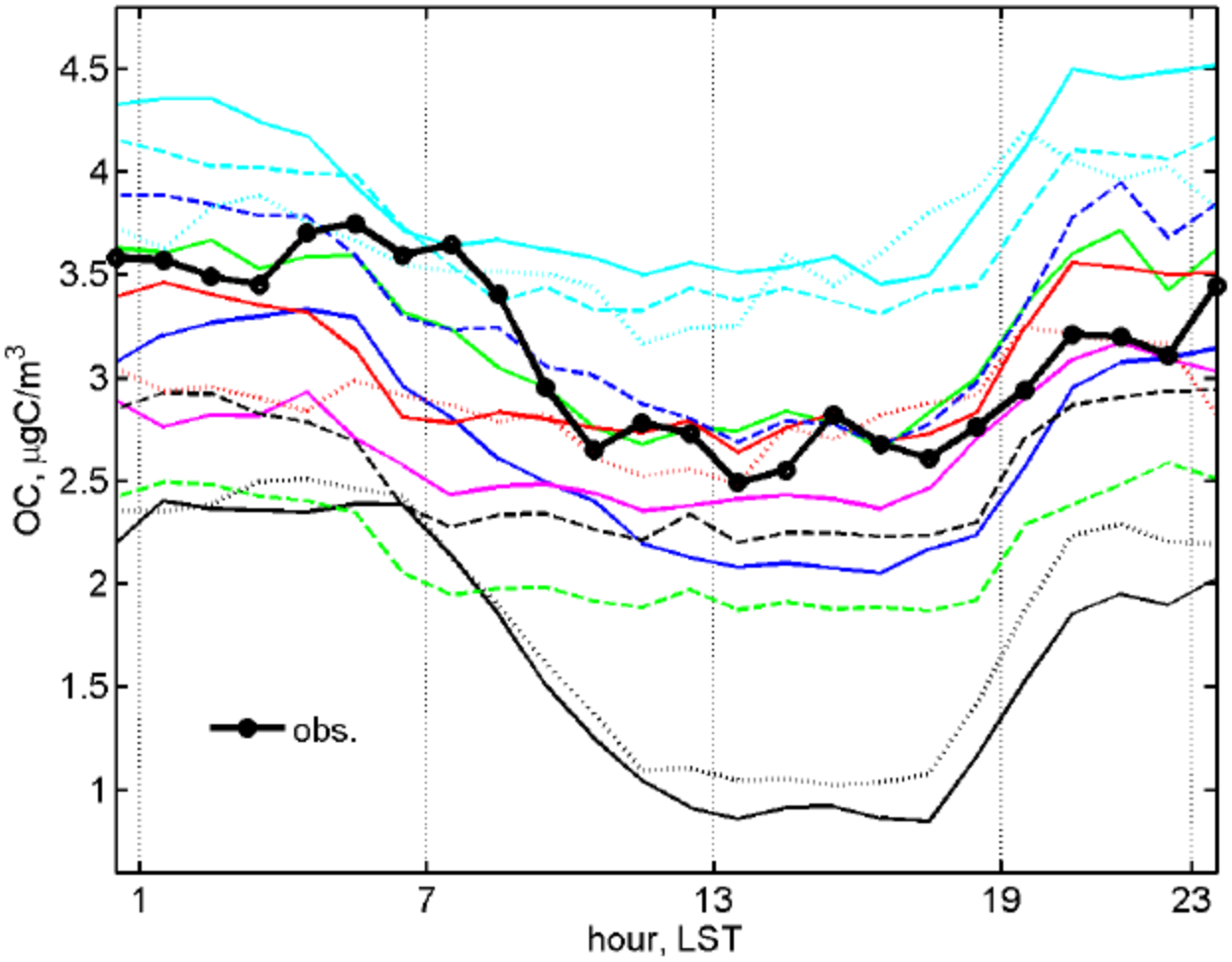


Ahmadov et al., submitted

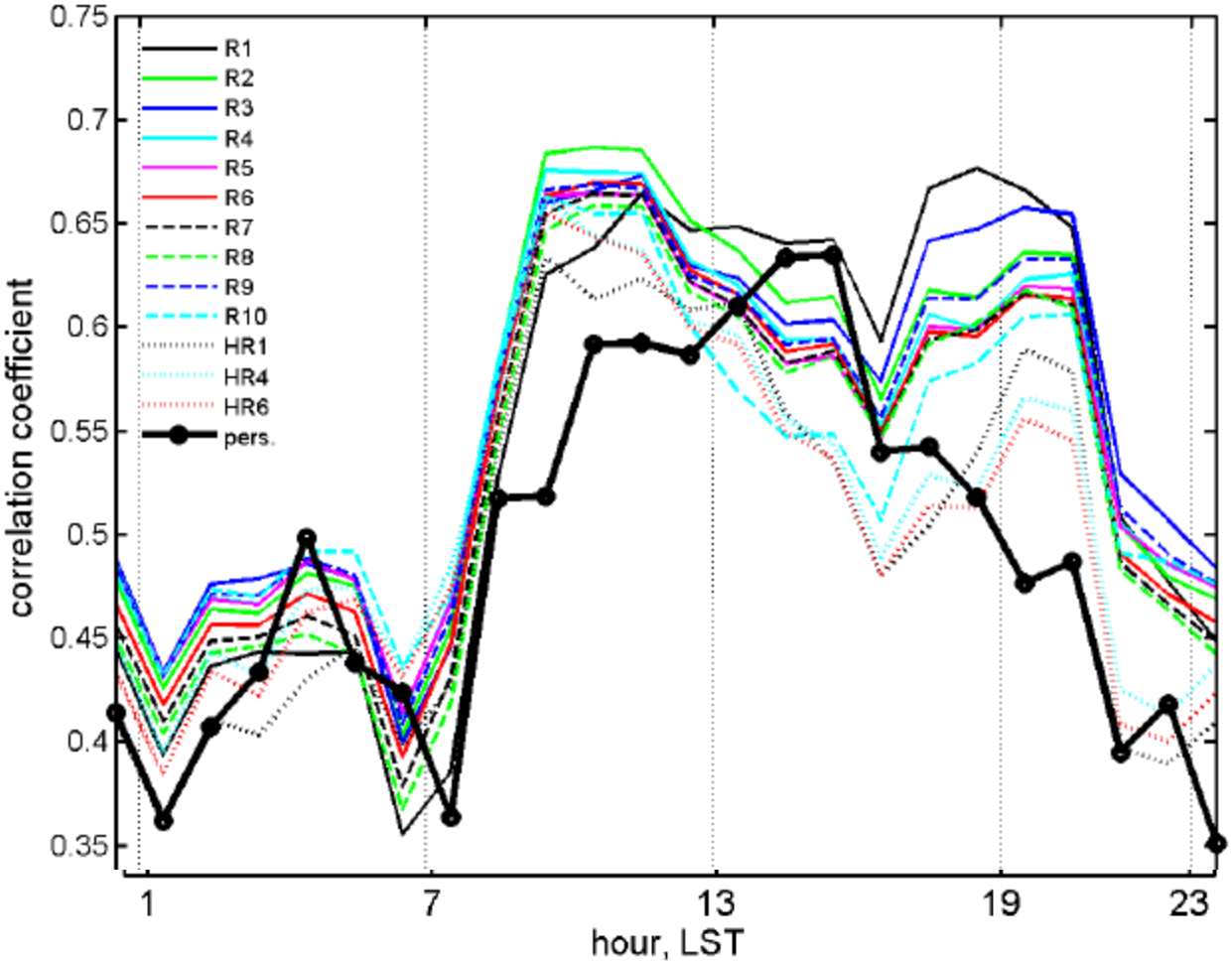
Observation data

Network	OC, μgC/m^3	EC, μg/m^3	Number of sites meeting criteria		Number of valid points	
			OC	EC	OC	EC
IMPROVE	1.09	0.29	37	37	621	619
STN	2.48	0.53	134	132	1508	1493
SEARCH	3.39	0.34	7	7	338	340

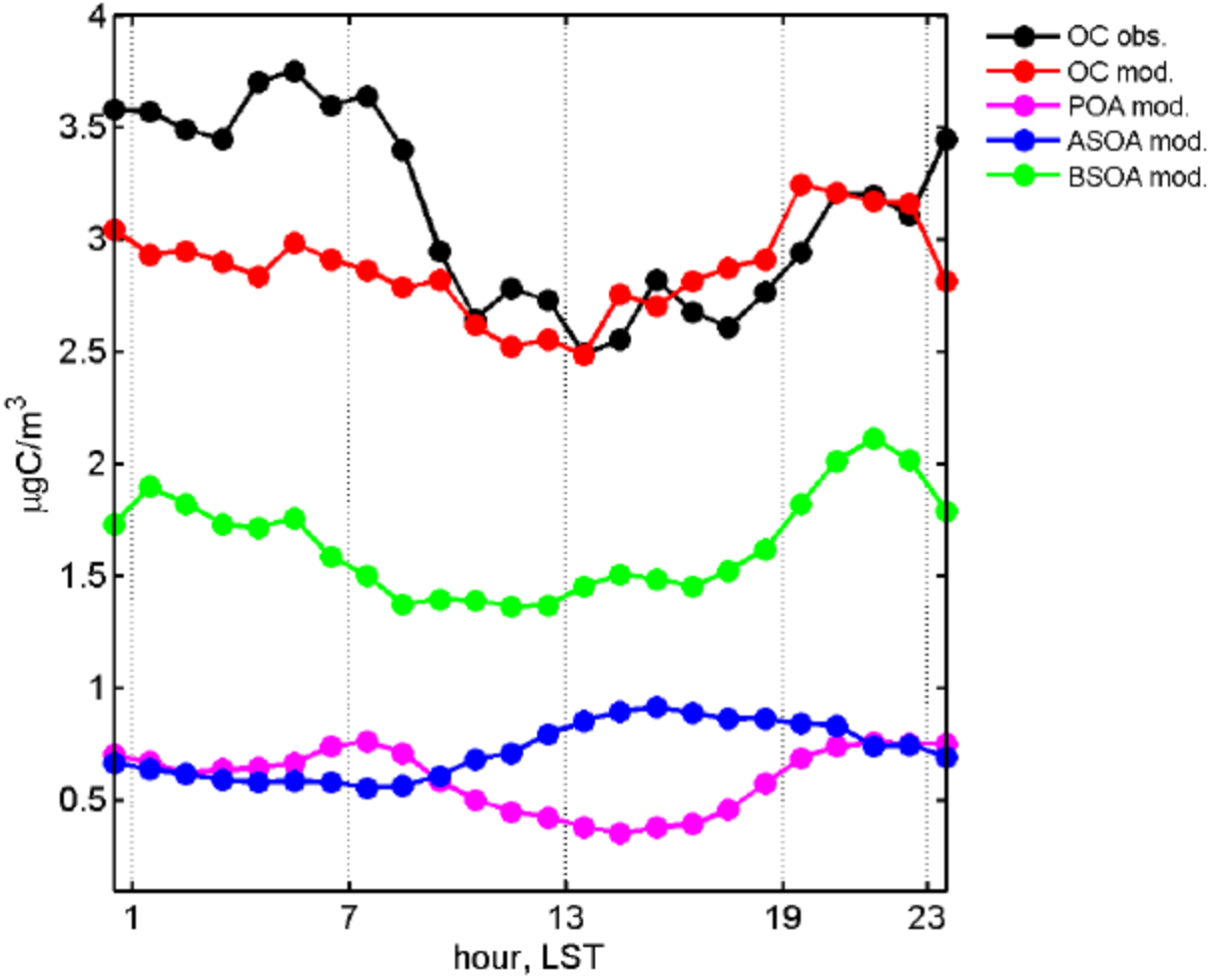
Comparison with the SEARCH data



Comparison with the SEARCH data

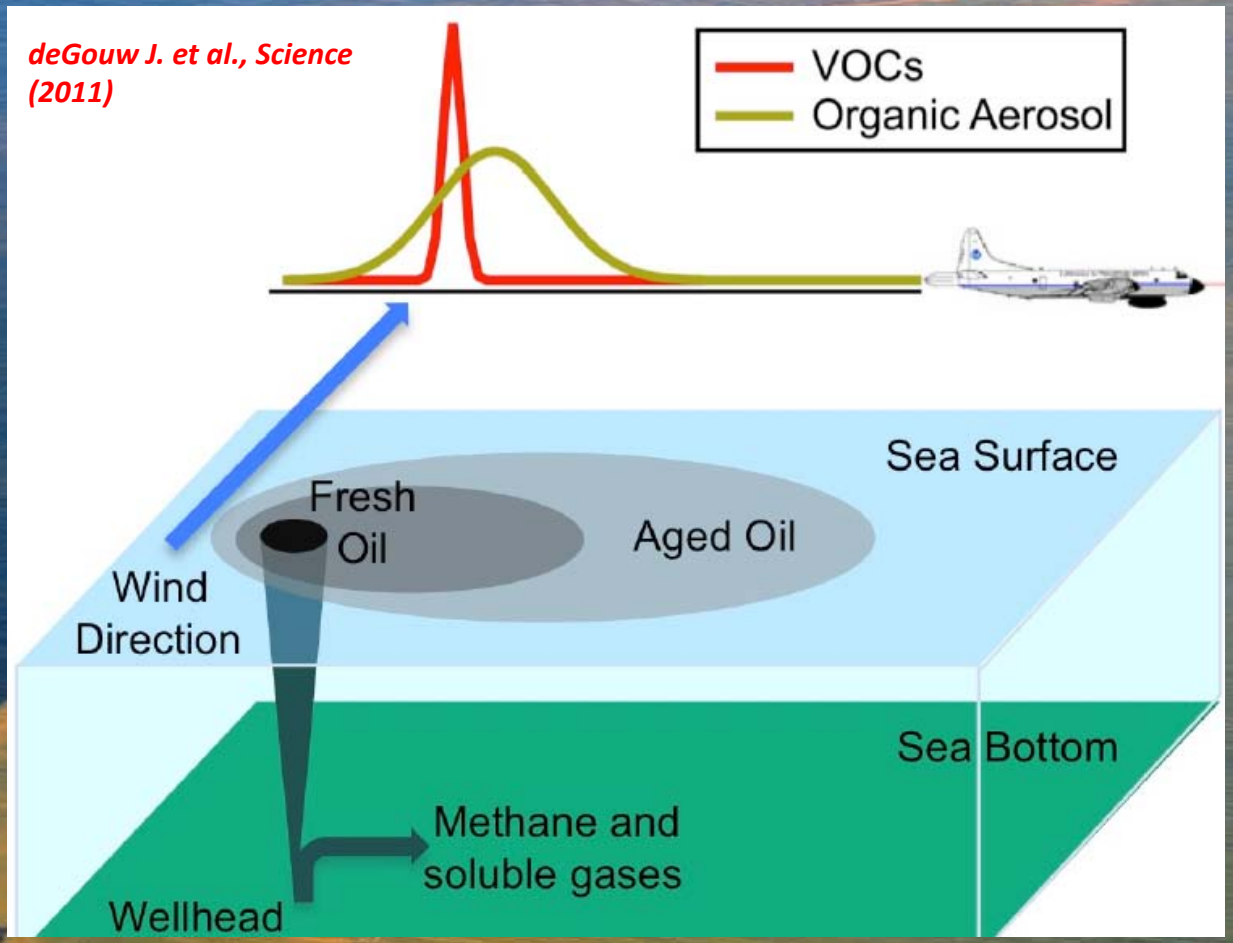


Comparison with the SEARCH data

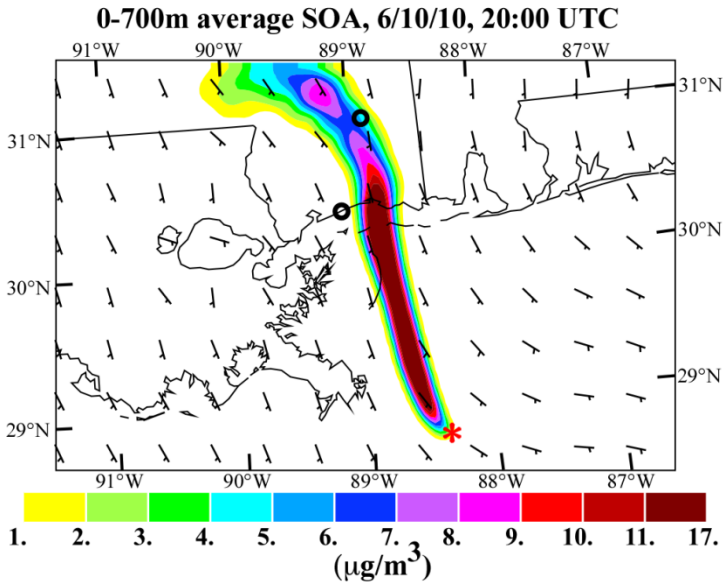


Mexican Gulf oil spill from DWH

- NOAA P3 aircraft's 2 flights on 8th and 10th of June
- High concentrations (10-20 ppb) of aromatics C9-11 were detected
- 10-20 µg/m3 organic particles were observed too!



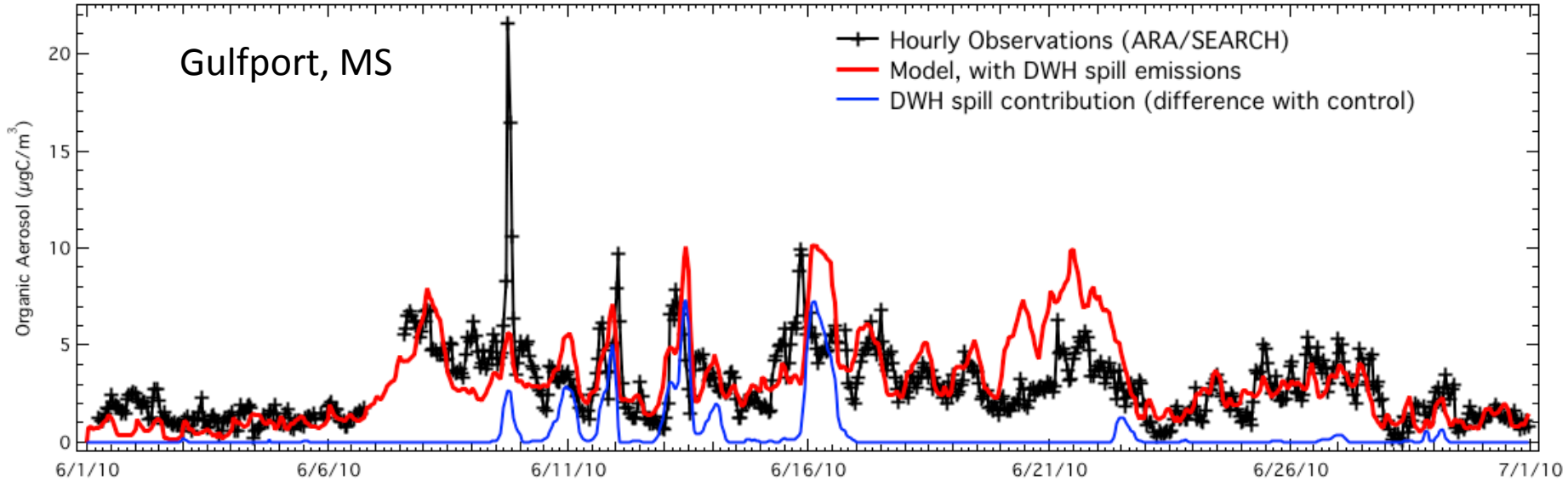
Comparison against the surface data: search network



Model shows good overall correlation with observations during June, 2010.

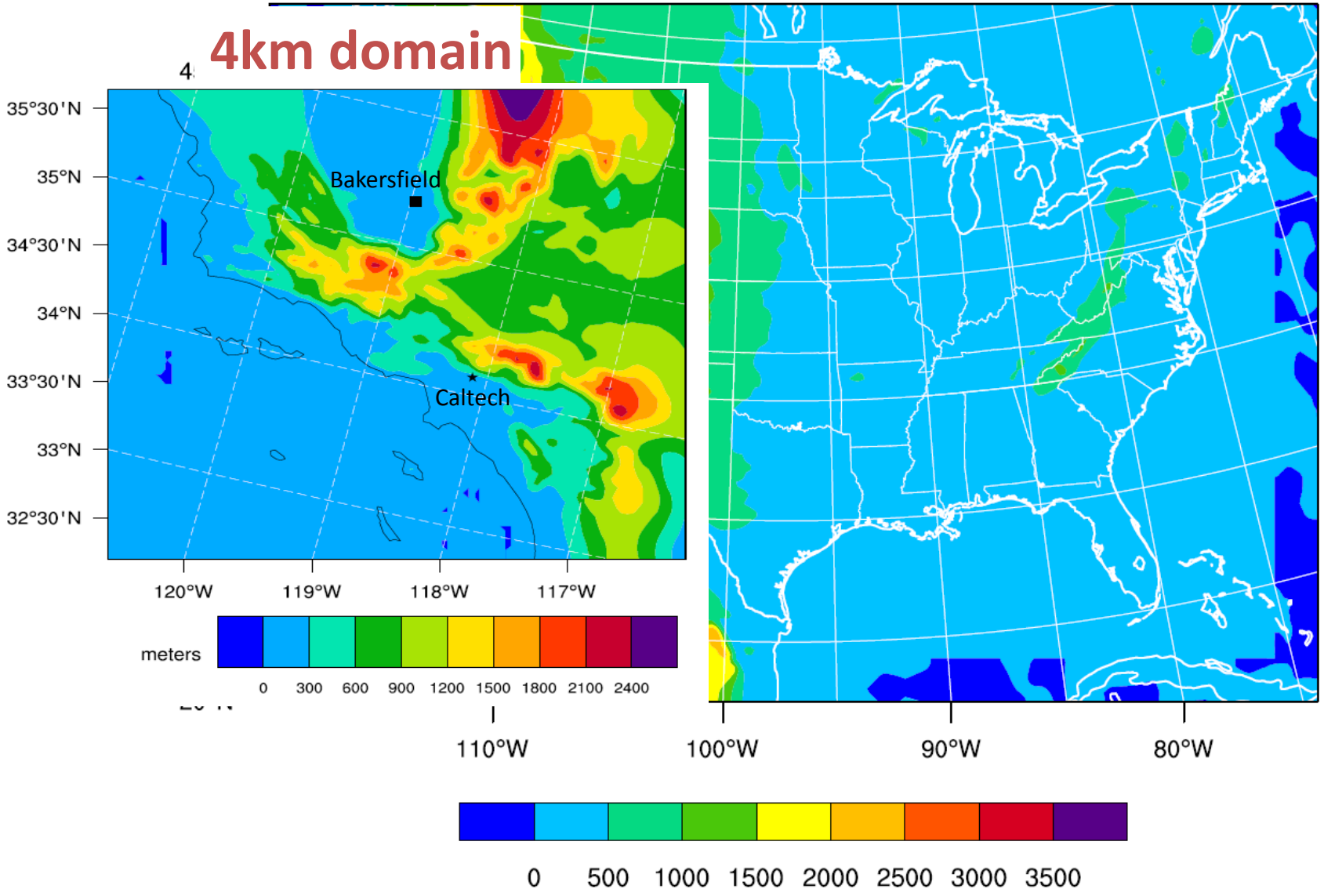
When model shows an impact from the DWH spill, there is a corresponding peak in the observations.

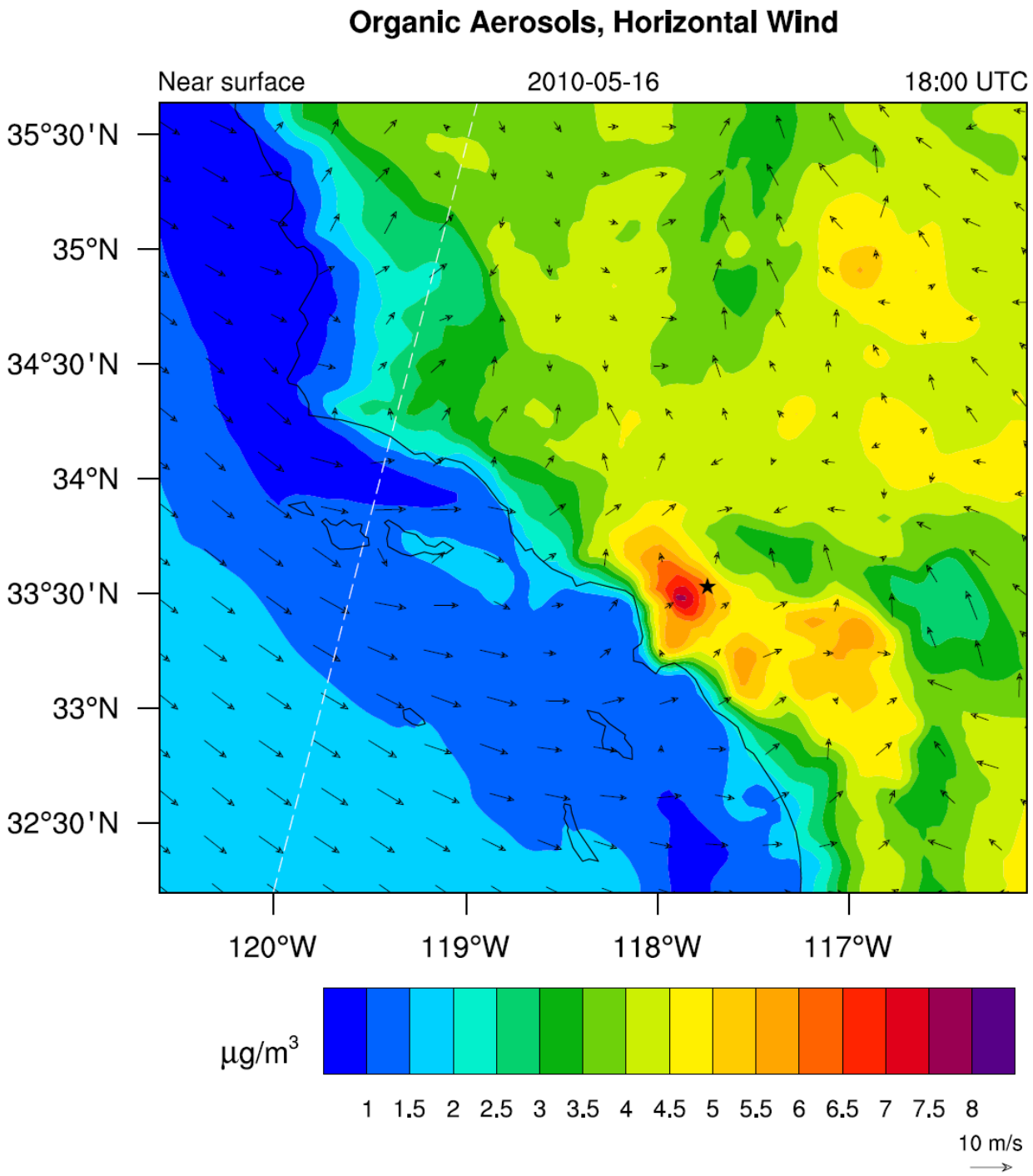
The magnitude and timing of the peaks are not always coincident.



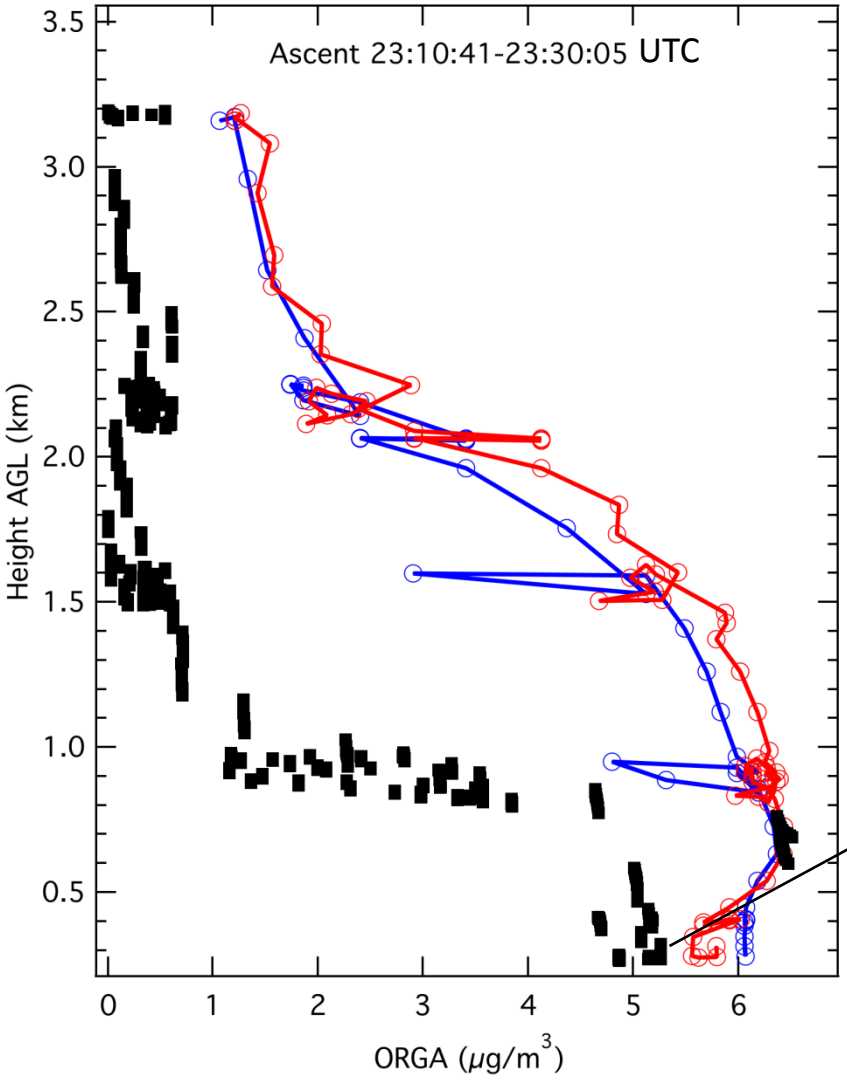
Middlebrook et al., in press

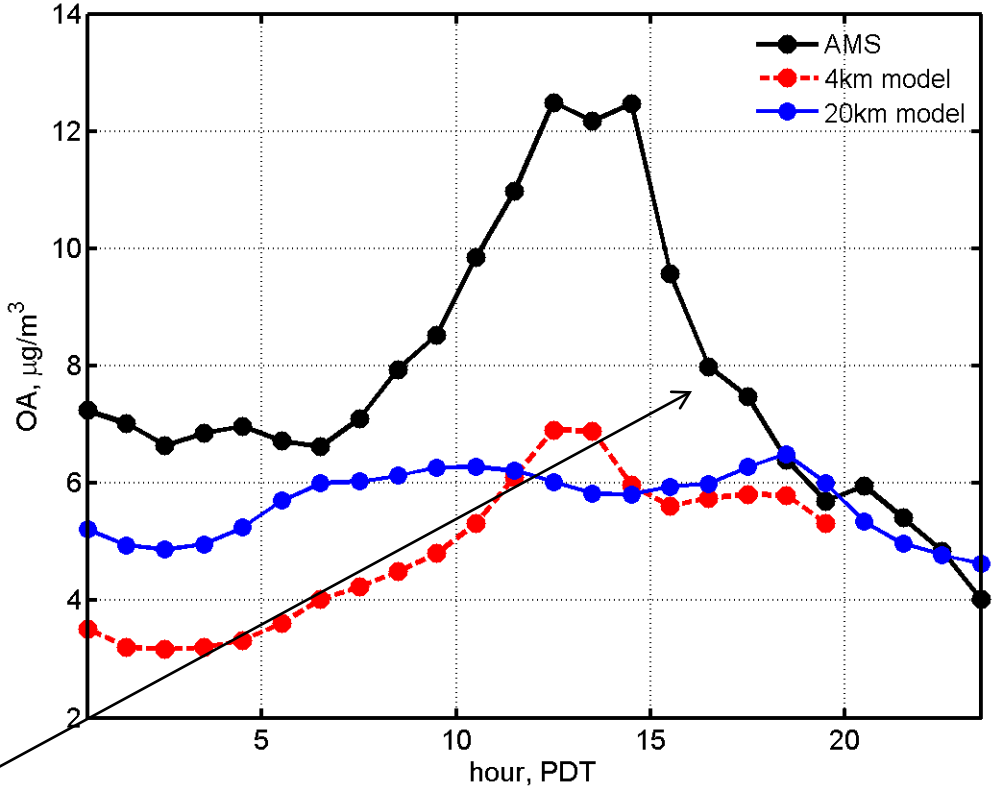
CalNex-2010 domain,
20km resolution domain, topography



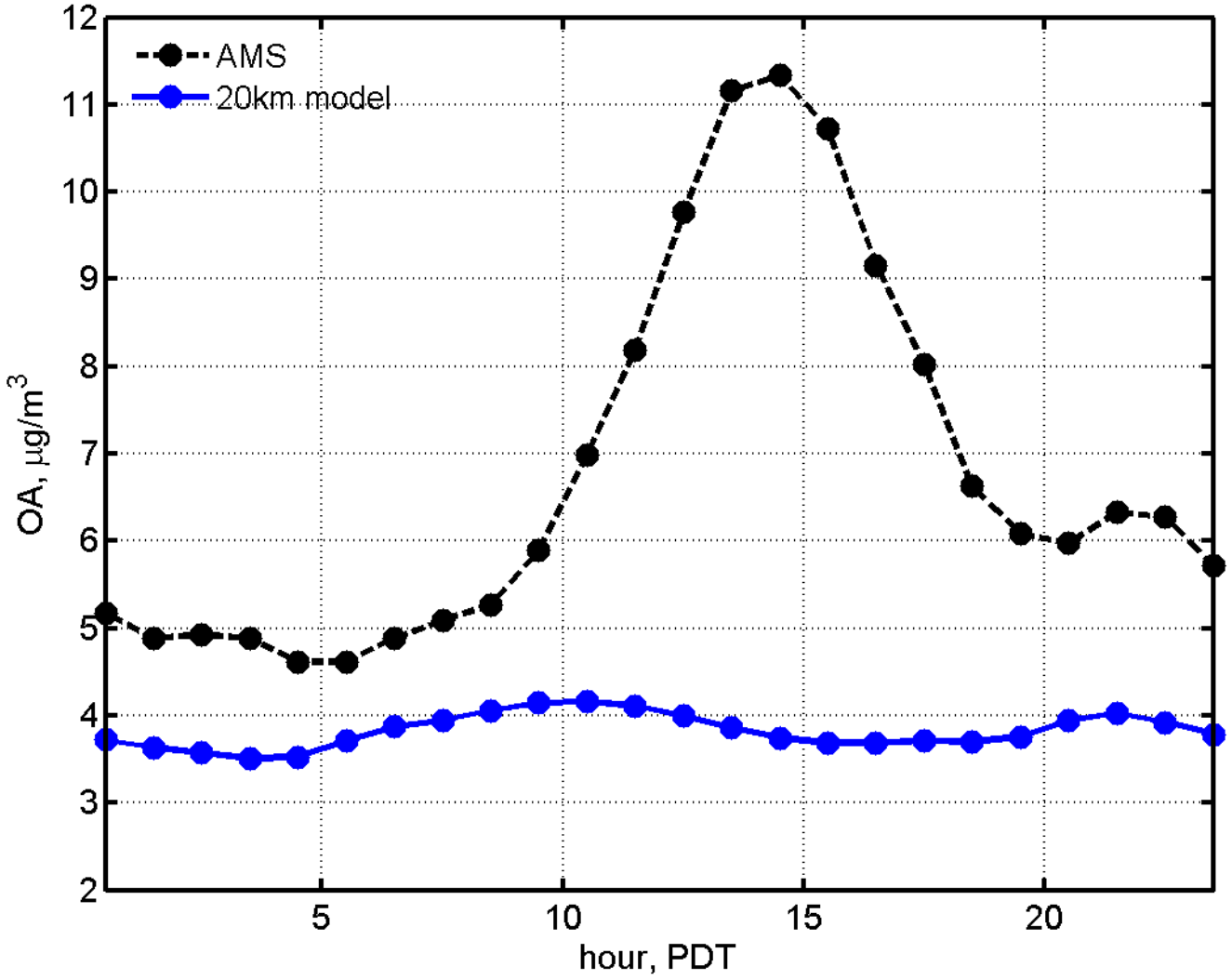

Organic Aerosols, Horizontal Wind
Near surface
2010-05-16
18:00 UTC
35°30'N
35°N
34°30'N
34°N
33°30'N
33°N
32°30'N
120°W
119°W
118°W
117°W
µg/m3
1
1.5
2
2.5
3
3.5
4
4.5
5
5.5
6
6.5
7
7.5
8
10 m/s

Vertical profile of OA over Caltech, May-16th (weekend)





Evaluation of the organic aerosol simulation, Caltech site, 14/05-15/06, 2010



Concluding remarks

- The new SOA scheme based on the VBS approach, the updated SOA yields and the aging mechanism substantially improves OA simulations by WRF-CHEM
- The new SOA scheme within the MADE module of WRF-CHEM is a computationally efficient and suitable tool for a wide range of air quality modeling applications
- More OA measurements across the U.S. with high spatiotemporal resolution is needed to better constrain the SOA models (e.g. drawback of daily concentrations)
- Additional measurements/variables for better evaluation are necessary: e.g. O:C ratios, PMF analysis, C14…