College of Environmental Sciences and Engineering
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Simulations of Organic Aerosol in China

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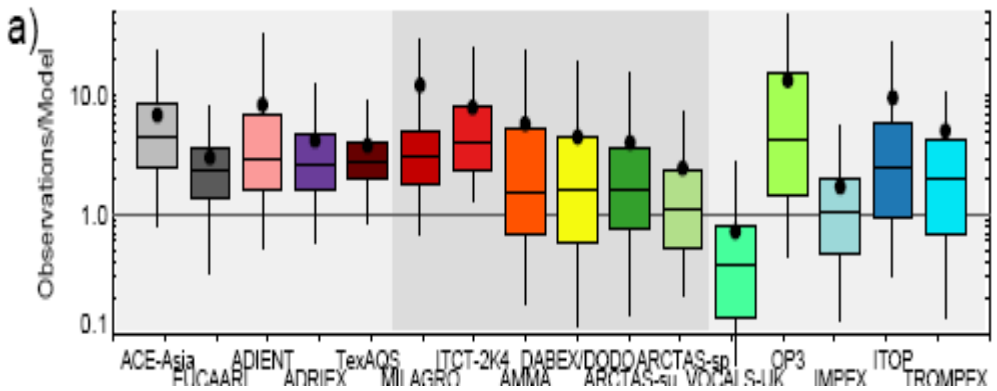
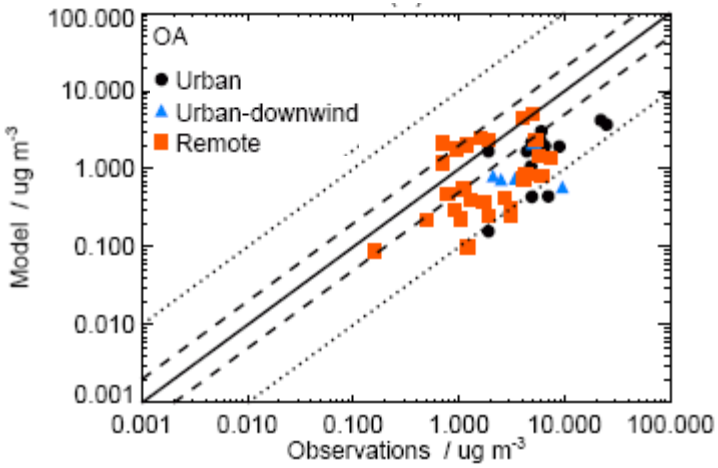
Funded by MOST of CHINA

Insufficient Understanding of OA



(Heald et al., ACP, 2011)



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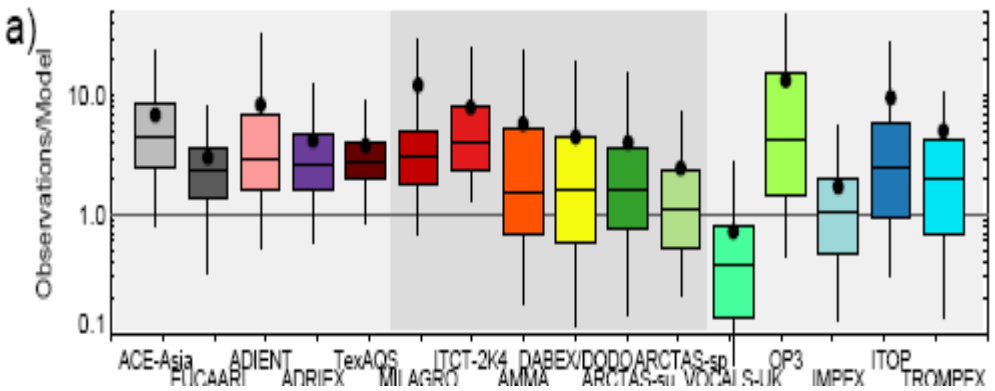

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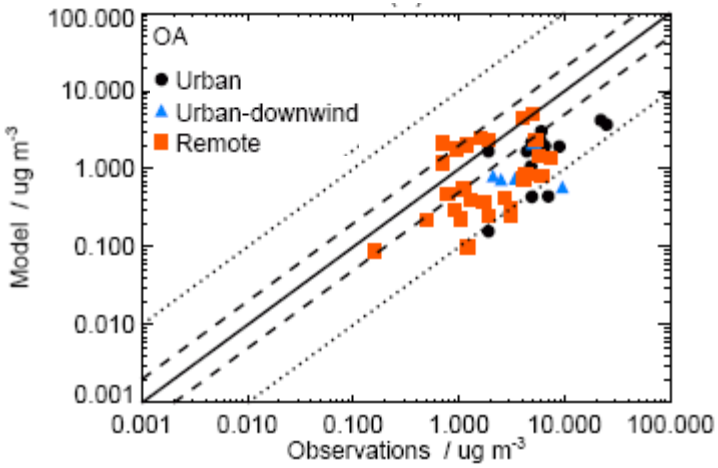

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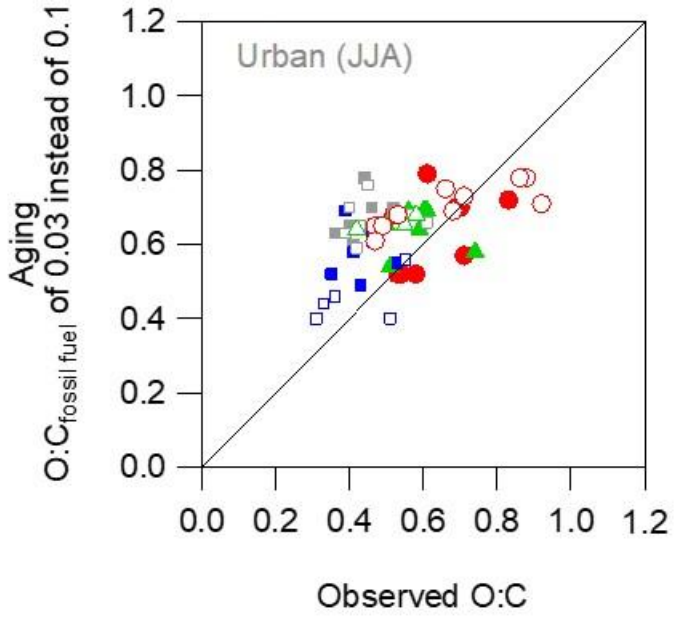
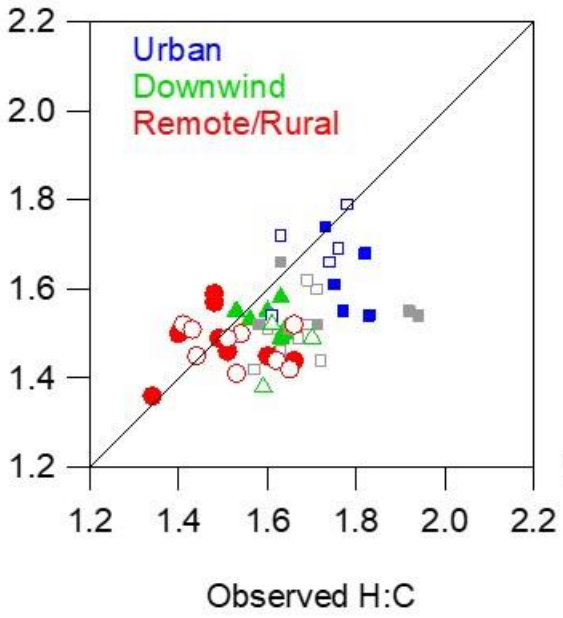
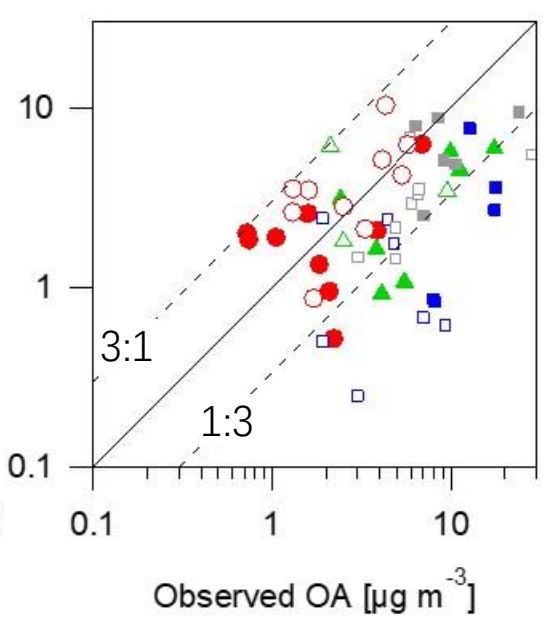






SOA Schemes in GEOS-Chem

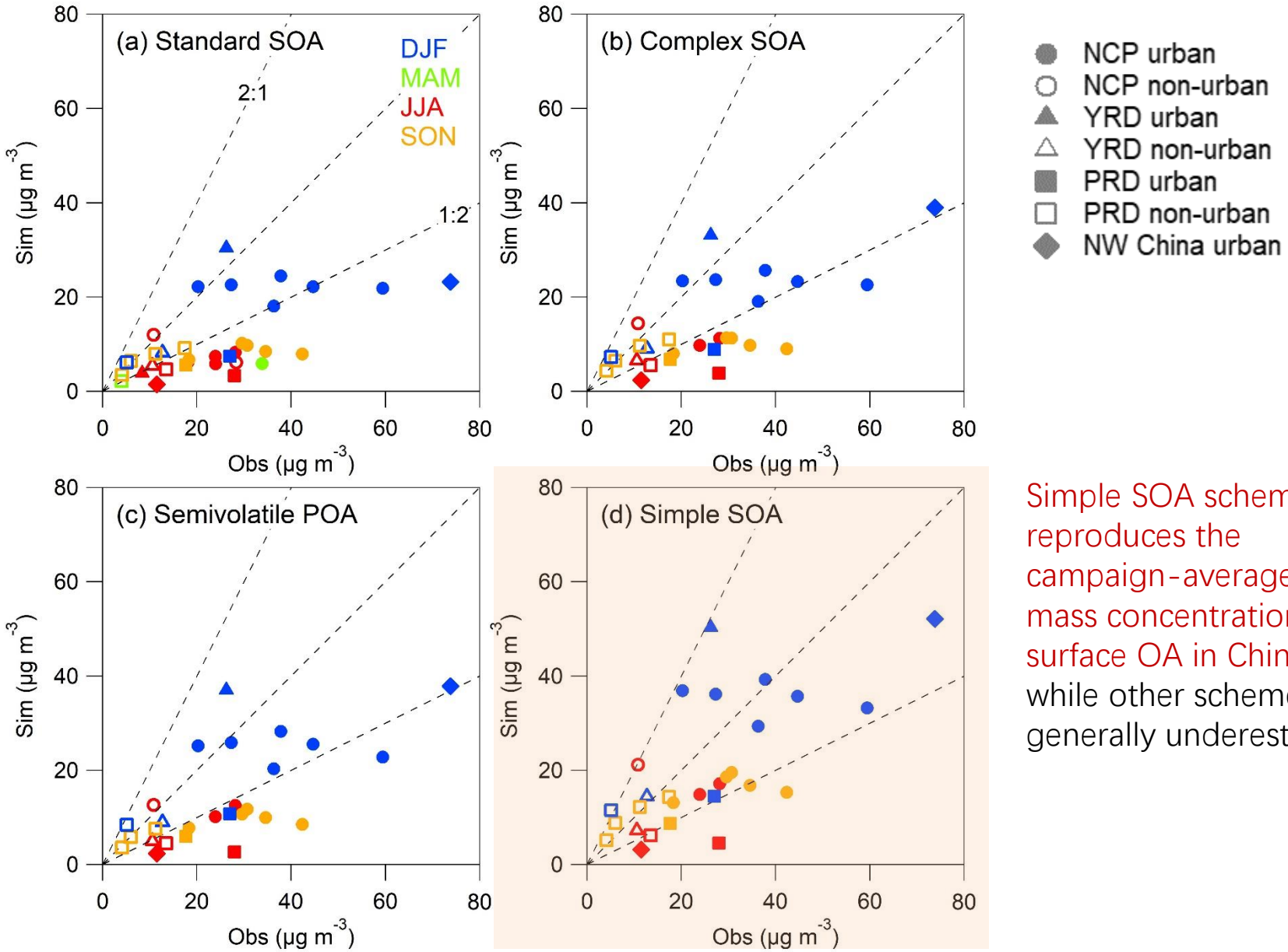
v11-02d: Nested grid; Base year: 2011-2013

MERRA2 0.5° x 0.625°(also has tested on GEOS-FP 0.25° x 0.3125°)

OA Scheme Names	Description
Standard SOA	POA is treated as nonvolatile; SOA is simulated by the volatility basis set (VBS) method both high and low NO_x regimes
Complex SOA	SOA formation from aqueous isoprene uptake is included on the basis of standard SOA scheme.
Semivolatile POA (SVOC and IVOC)	POA is treated as semivolatile; SOA from SVOC and IVOC are included; Aqueous isoprene uptake is included.
Simple SOA	POA is treated as nonvolatile; No detailed SOA chemistry; The emission of SOA precursor is tied directly to emissions of monoterpenes, isoprene, biomass burning CO, biofuel CO, and fossil fuel CO in HEMCO.

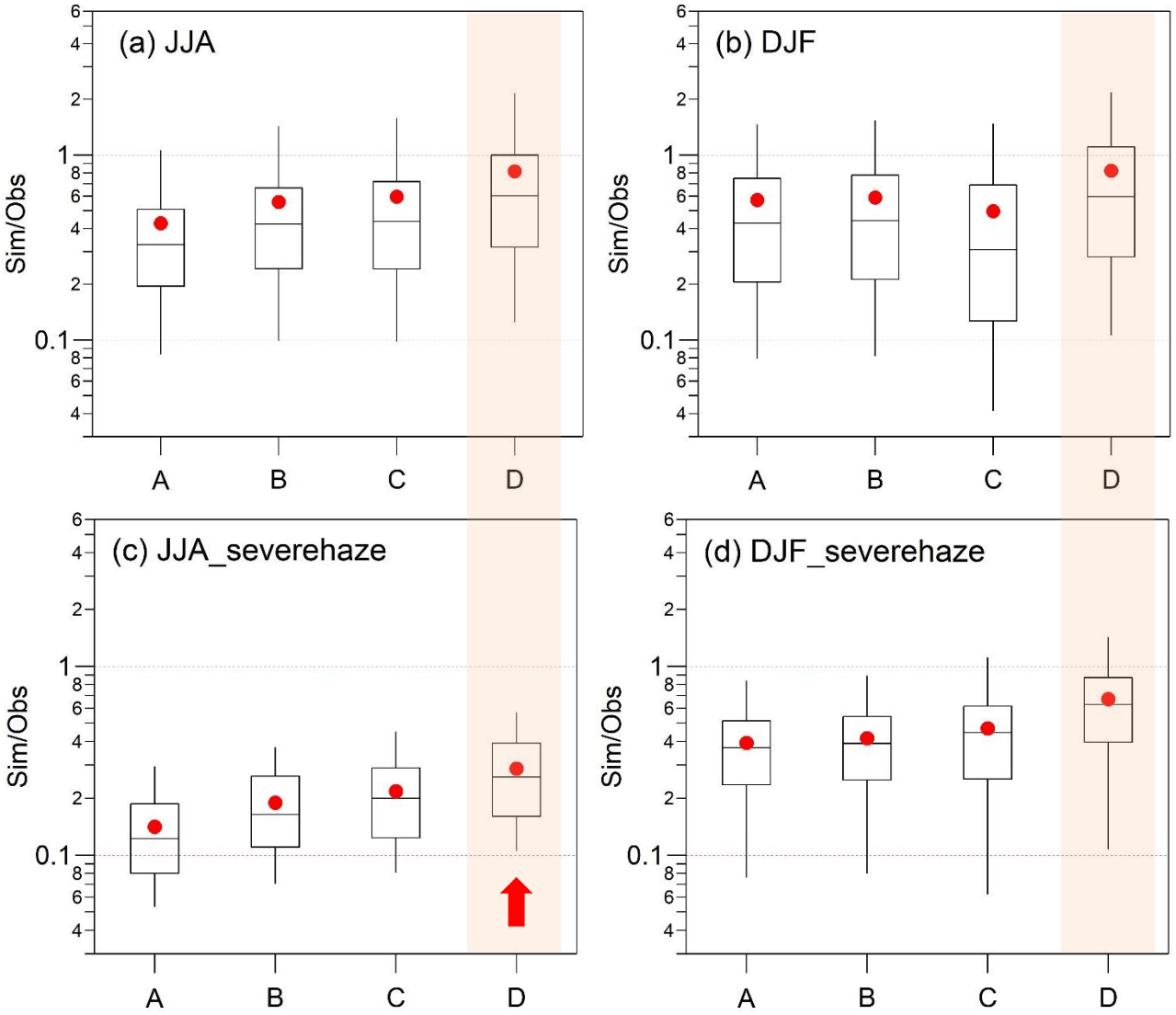
Anthropogenic emissions of CO, NO_x, SO_2, NH_3, BC, OC, and aromatic VOCs are from MEIC (2012) for China and MIX (2010) for the rest of Asia.

Surface OA: Model vs. AMS/ACSM Obs. in China



Simple SOA scheme reproduces the campaign-average mass concentrations of surface OA in China while other schemes generally underestimate.

Surface OA: Model vs. AMS/ACSM Obs. in Beijing



A: Standard SOA
B: Complex SOA
C: Semivolatile POA
D: Simple SOA

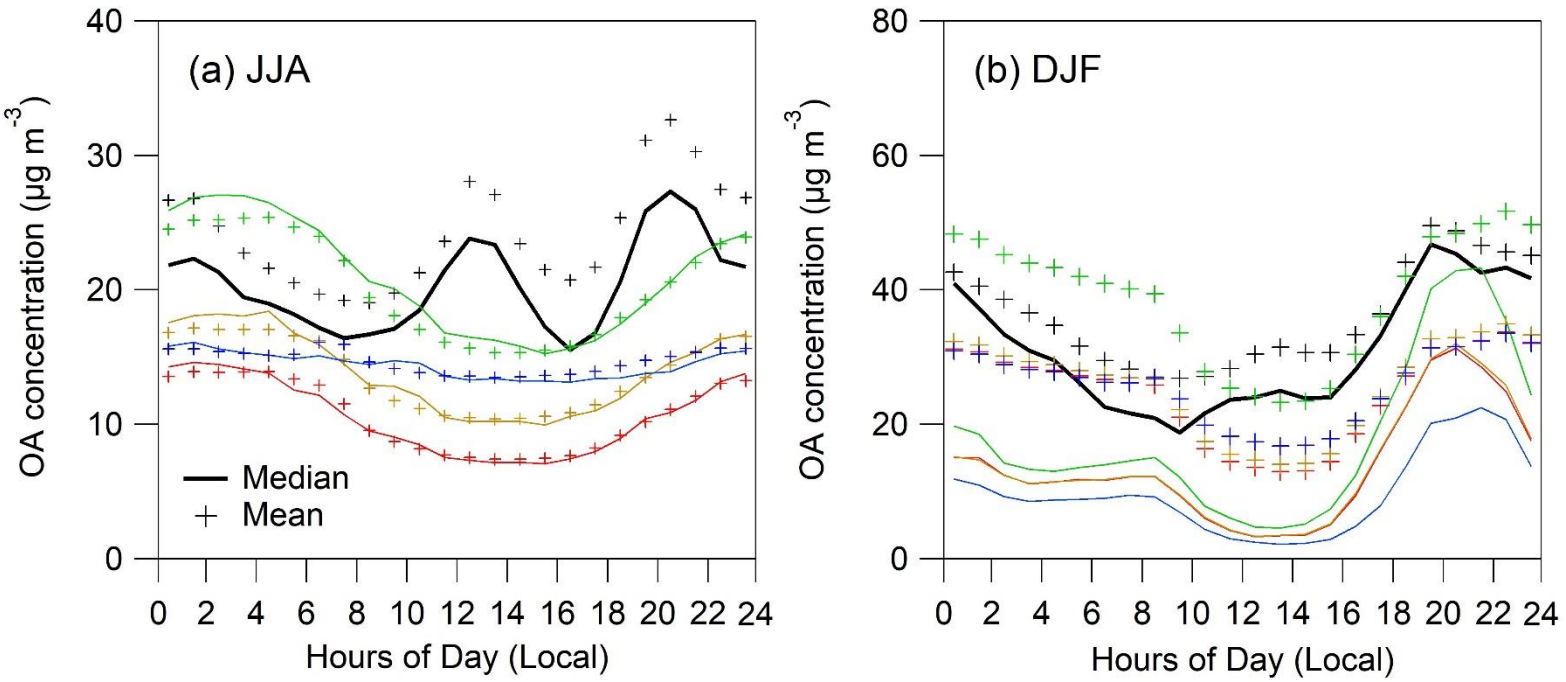
The variance in model bias for simple SOA is similar to those for other schemes, although it captures the mean OA mass better.

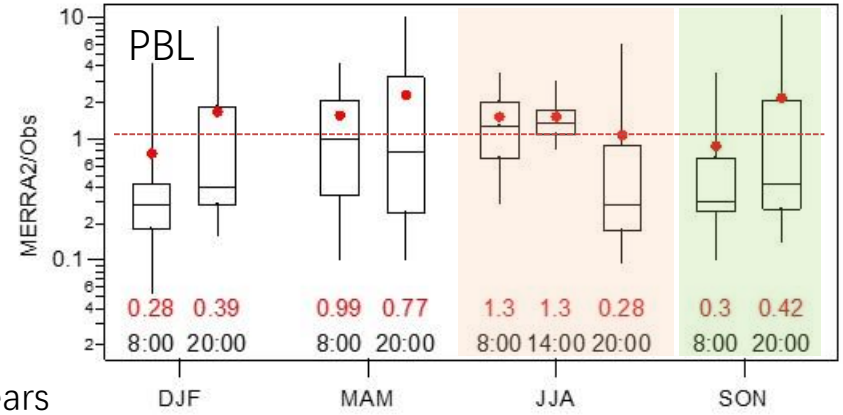
Even with simple SOA scheme, summer OA mass in Beijing during severe haze events is still largely underestimated.

- IAP site; hourly mean over 2 years
- Haze period: the periods when the hourly mean concentrations of NR-PM_1 are greater than 75 μg m^{-3} for over 36 hours;
- Severe haze events: the periods when the hourly mean concentrations of NR-PM_1 are greater than 150 μg m^{-3} during a haze period.

Diurnal Patterns of Surface OA in Beijing

Obs. | Standard SOA | Complex SOA | Semivolatile POA | Simple SOA





- IAP site; hourly mean over 2 years

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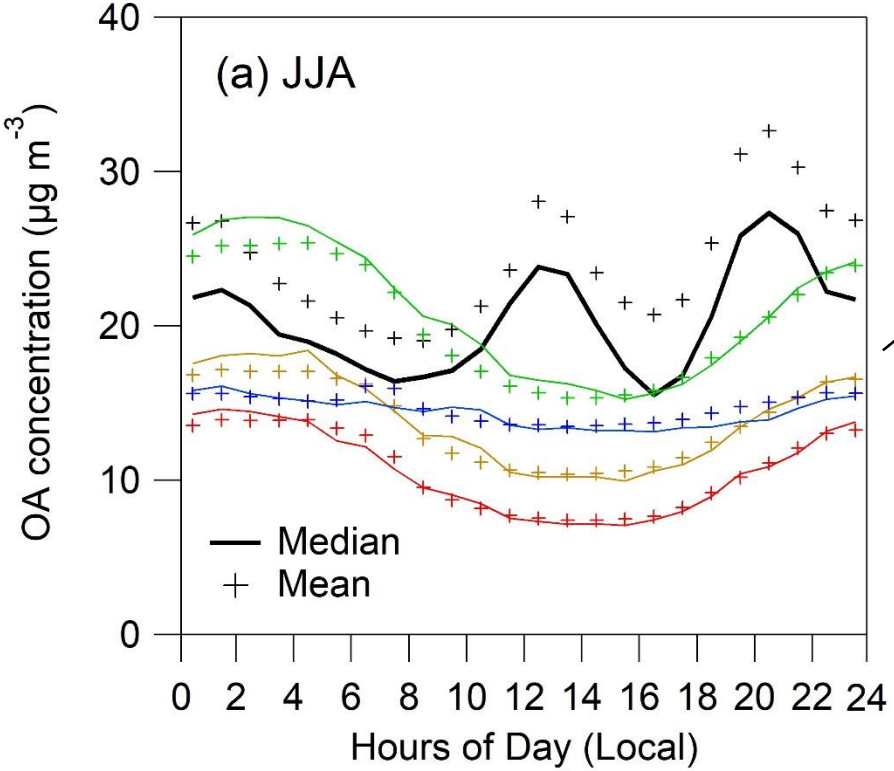
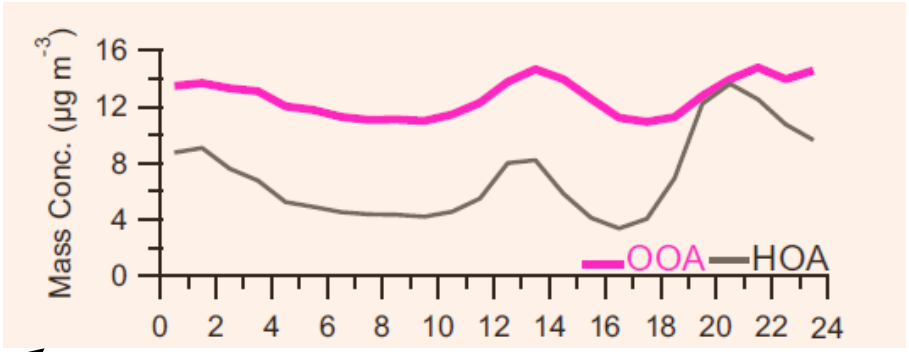
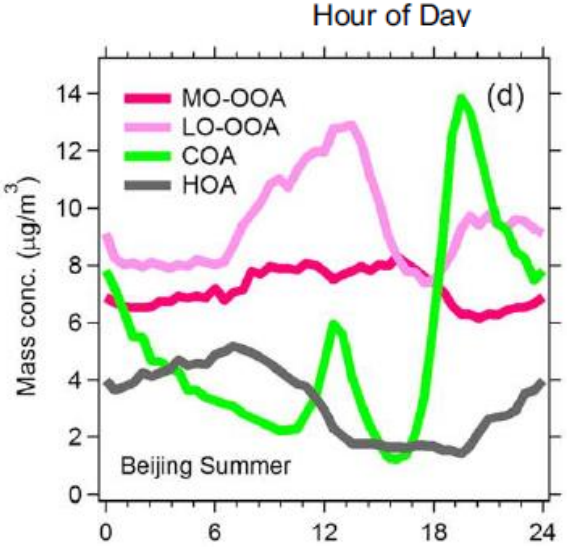




[Sun et al., 2012]

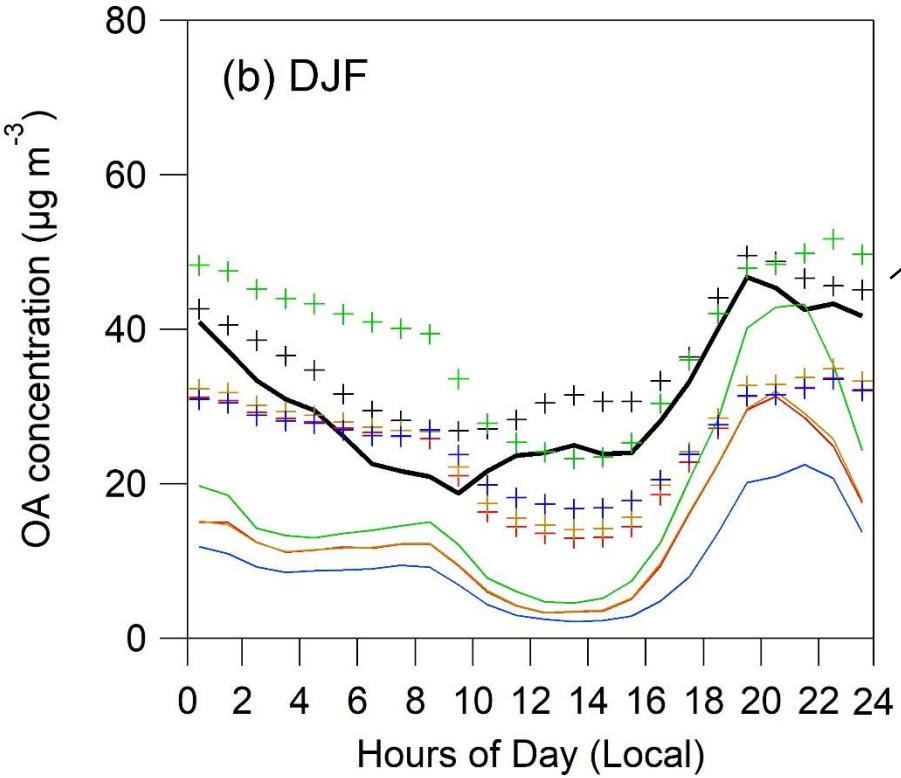


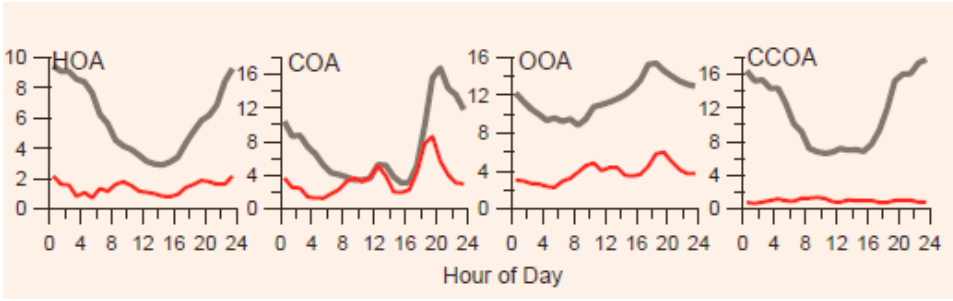
[Hu et al., 2016]

- In the summer, the model underestimates COA and OOA. OOA include OOA-1 (perhaps due to underestimated OH and VOCs) and OOA-2 (aged SOA that correlates with sulfate).

Diurnal Patterns of Surface OA in Beijing

Obs. | Standard SOA | Complex SOA | Semivolatile POA | Simple SOA





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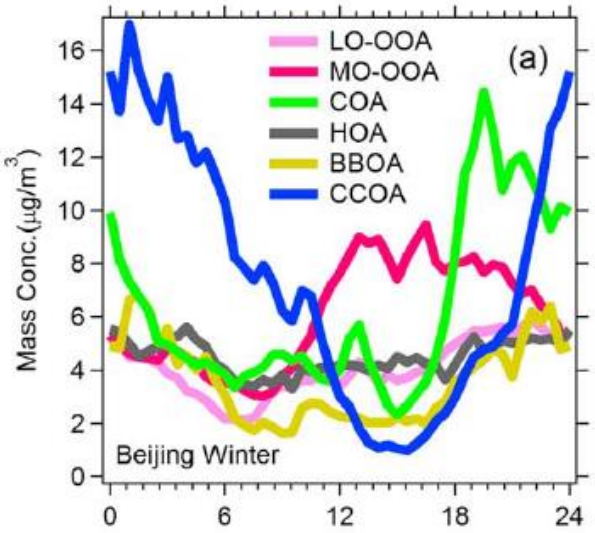


[Hu et al., 2016]

- In the winter, the model underestimates COA and OOA. OOA include OOA-1 (perhaps due to underestimated OH and VOCs) and OOA-2 (SOA that correlates with sulfate and RH – more studies suggest this as "aqueous SOA").

Summary

- Simple SOA scheme reproduces the mean OA mass in China, except during severe haze events in the summer.

- The variance in model bias for simple SOA scheme is similar to those for other schemes, suggesting some fundamental misunderstanding in the model.

- Comparisons of modeled diurnal patterns to the PMF results suggest that COA and aq-SOA are perhaps underrepresented in the model, causing the bias in the simulations of surface OA in urban area of China.

Thank you for your attention!

Nested GEOS-Chem Simulations

Anthropogenic emissions of CO, NO_x, SO_2, NH_3, BC, OC, and aromatic VOCs used MEIC (2012) for China and MIX (2010) for the rest of Asia

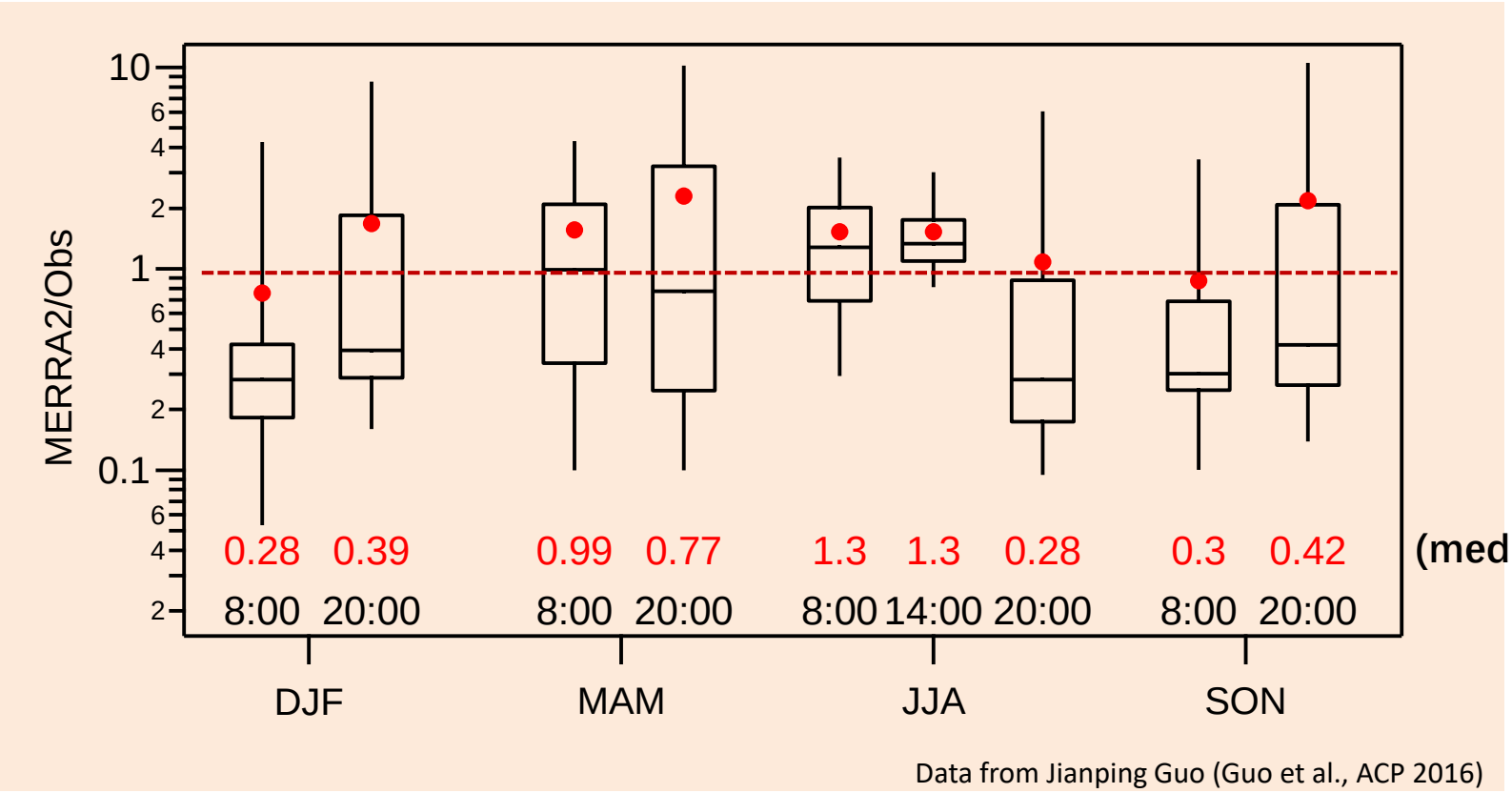
Unit: ppbv

Period of Sampling	Species	Obs	Sim	Obs/Sim
3 Aug 2011 – 13 Sep 2011	Benzene	1.29	0.75	1.72
	Toluene	2.23	1.57	1.42
	Xylene	1.75	0.76	2.30
	isoprene*	0.41	0.33	1.24
29 Dec 2011 – 18 Jan 2012	benzene	2.34	1.35	1.74
	toluene	2.67	2.44	1.09
1 Aug 2012 – 31 Aug 2012	benzene	0.98	0.74	1.33
	toluene	1.99	1.50	1.33
	xylene	1.50	0.75	1.99

*Daytime (7:00-19:00) averages; Site: Beijing

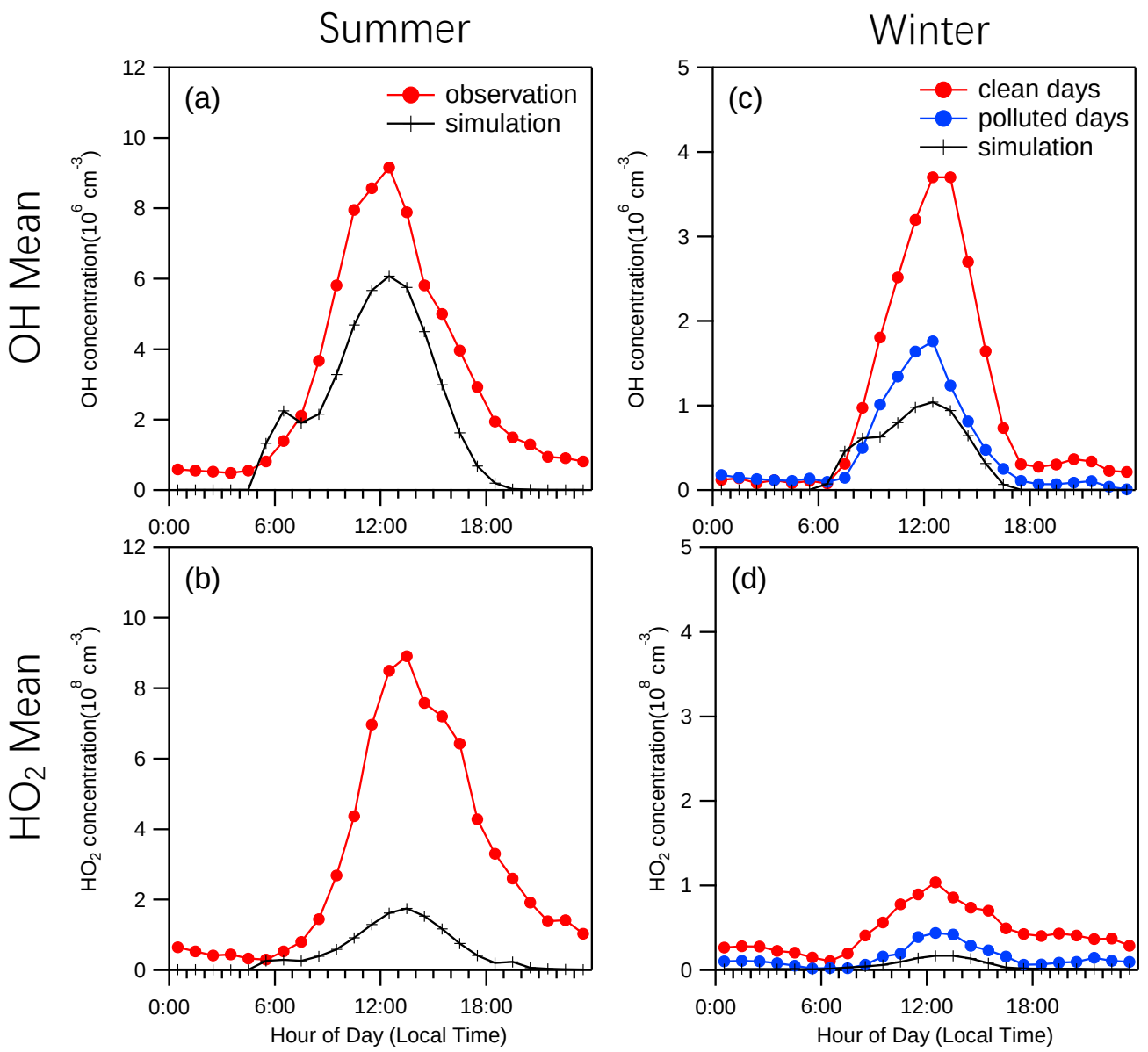
PBL height: underestimated in fall and winter

PBL is calculated using bulk Richardson algorithms, depending on profiles measured by GTS1 digital electronic radiosonde at 8:00 BJT and 20:00 BJT as well as 14:00 BJT in summer



- PBL height is underestimated by 60-70% (median) in fall and winter with uncertainties in both MERRA2 and the measurements.

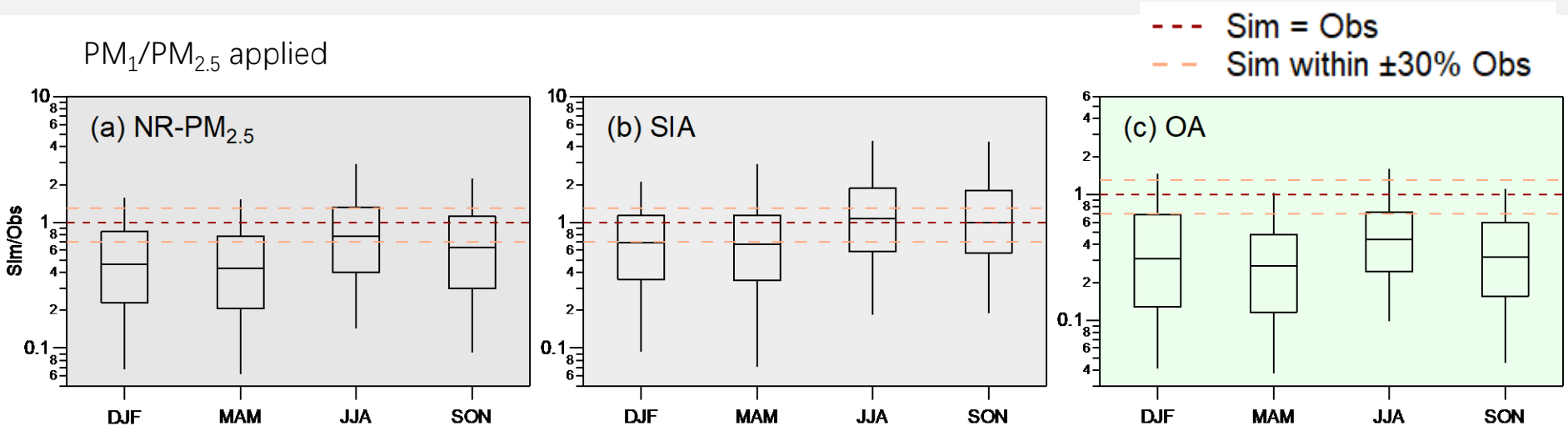
Oxidants: Underestimated in the models



Surface OH and HO_2 concentrations are underestimated in Beijing by a factor of 1.5 to 4 (more in the winter).

Major chemical components of $PM_{2.5}$

$PM_1/PM_{2.5}$ applied



Sim/Obs	NR-$PM_{2.5}$				SIA				OA			
Percentile	DJF	MAM	JJA	SON	DJF	MAM	JJA	SON	DJF	MAM	JJA	SON
25	0.23	0.21	0.39	0.30	0.35	0.35	0.58	0.57	0.13	0.12	0.24	0.16
50	**0.46**	**0.43**	**0.82**	**0.63**	**0.69**	**0.67**	**1.07**	**1.00**	**0.31**	**0.27**	**0.44**	**0.32**
75	0.85	0.78	1.40	1.12	1.14	1.14	1.85	1.81	0.69	0.48	0.72	0.59
0.7 Obs < Percent of data <1.3 Obs	**26%**	**25%**	**26%**	**25%**	**27%**	**29%**	**23%**	**25%**	**20%**	**21%**	**29%**	**24%**

- $PM_{2.5}$: underestimated, particularly in winter and spring, driven by OA underestimation
- SIA: fine as a total
- OA: consistently underestimated, along with underestimated OH, VOC but mixed PBL effects

Correlation with HRions – 2017 PKU Winter AMS – HR – r2