



College of Environmental Sciences and Engineering

Peking University

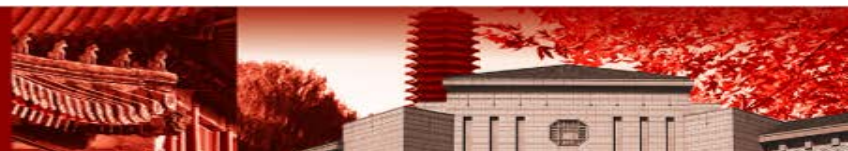
Seasonal variations of model bias in simulations of major PM_{2.5} chemical components in China

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2018-05-21

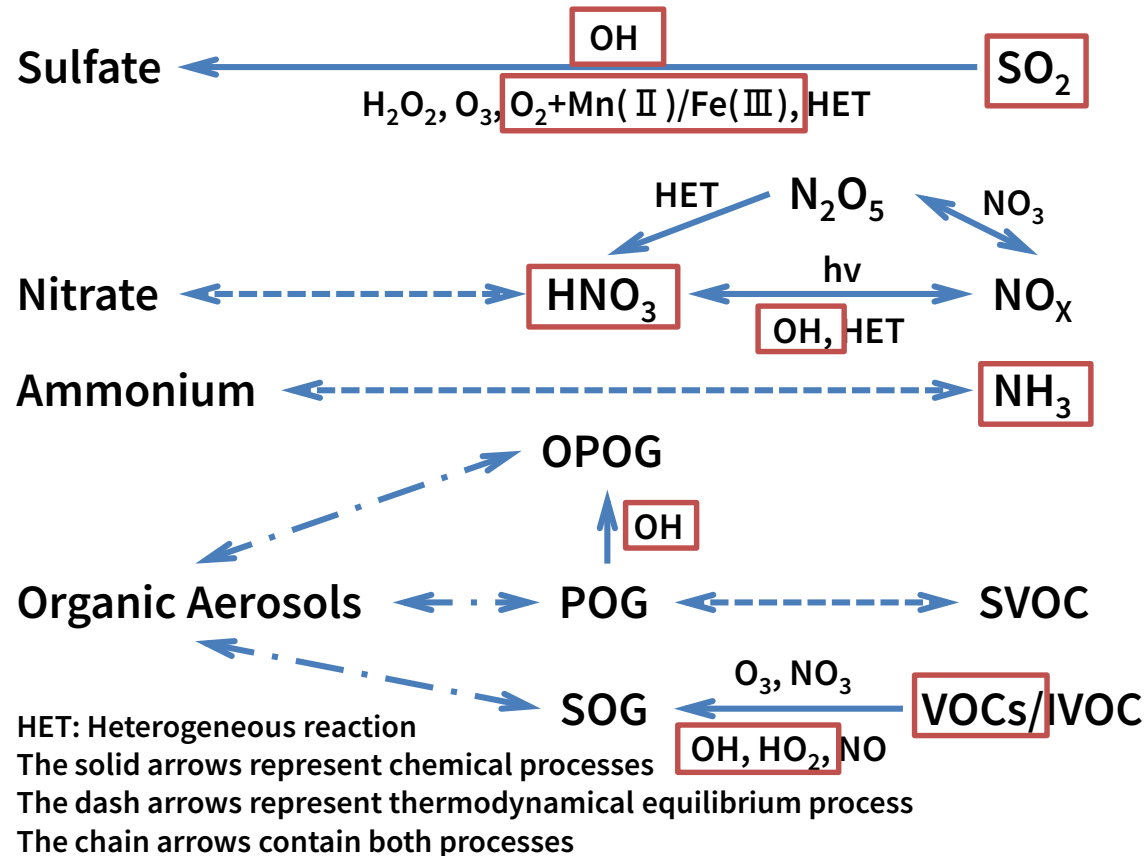


北京大学



Simulations by GEOS-Chem

Meteorological Parameters: e.g., PBL height, T, RH, wind etc.



Nested GEOS-Chem
v11-01/v11-02d

Period: 2011.7-2013.5

Site: IAP (Beijing)

Emission Inventories:
MEIC(2012)+MIX(2010)

Meteorology Input:
MERRA2 0.5°x0.625°
(GEOS-FP 0.25°x0.3125°)

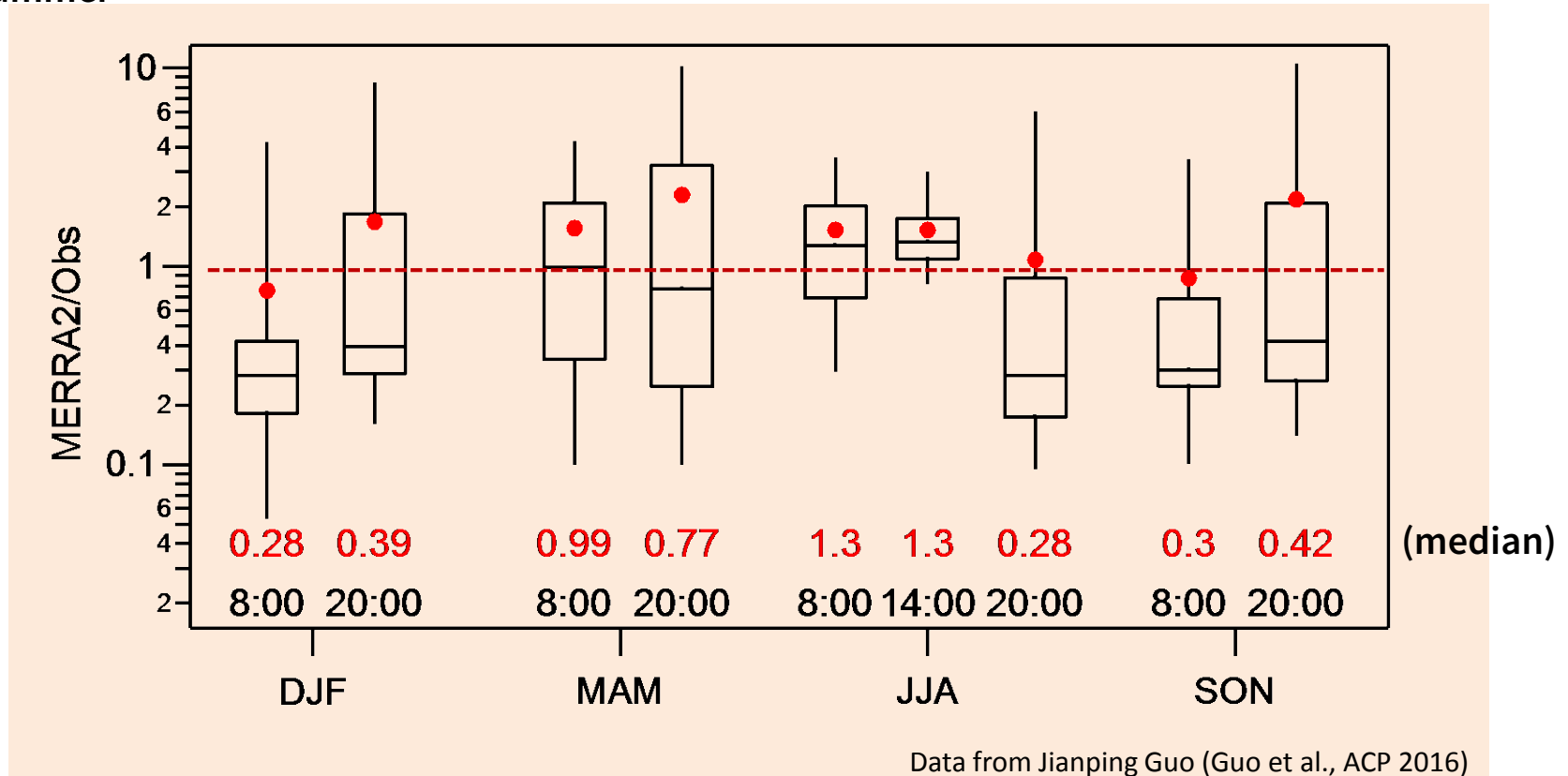
Output: Hourly mean

Real-time measurements from ACSM:

- NR-PM₁
- a PM₁ to PM_{2.5} ratio of ~0.7 is considered while comparing the observations to the model (unpublished results from PKU)

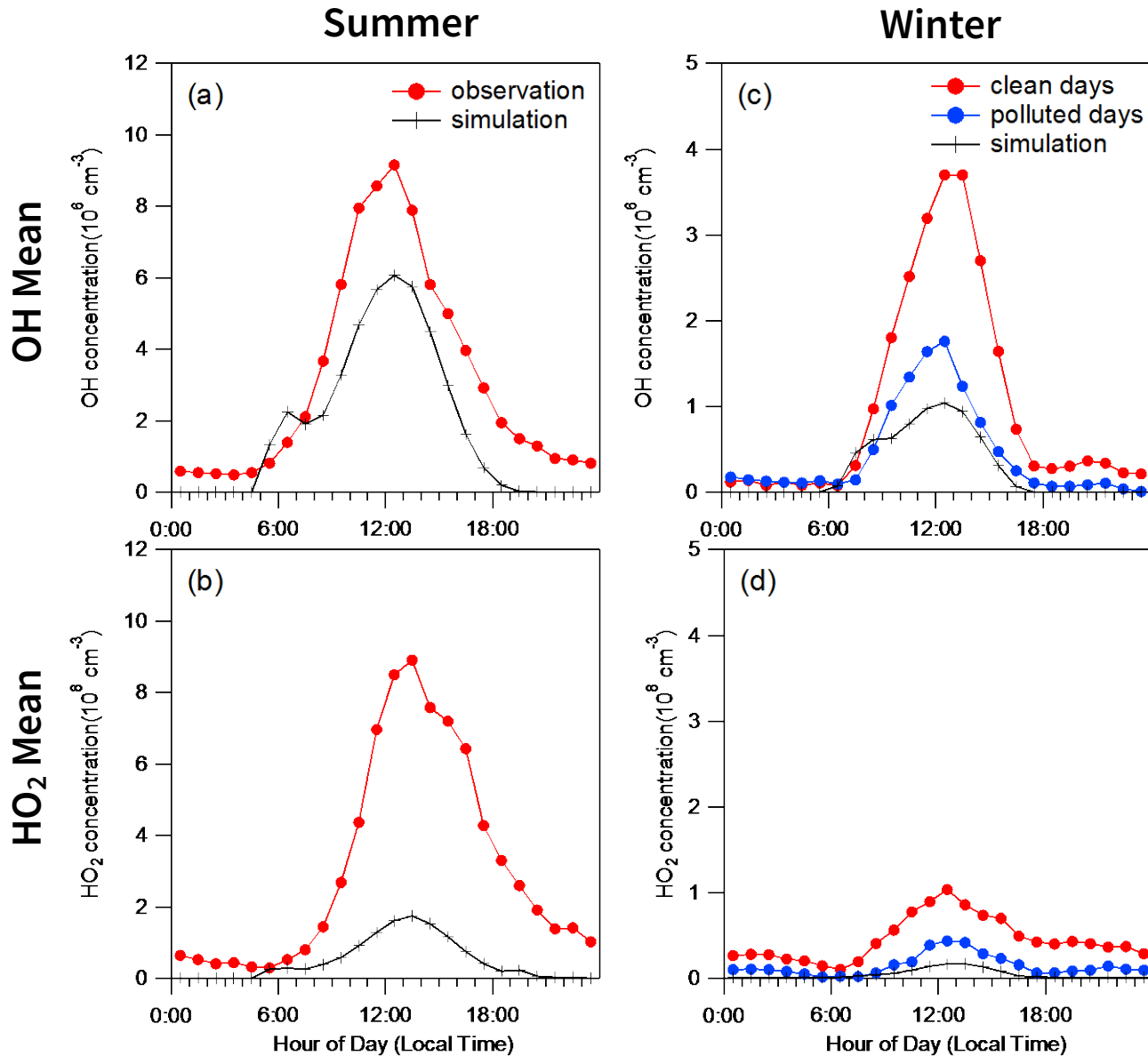
PBL height: underestimated in fall and winter

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.

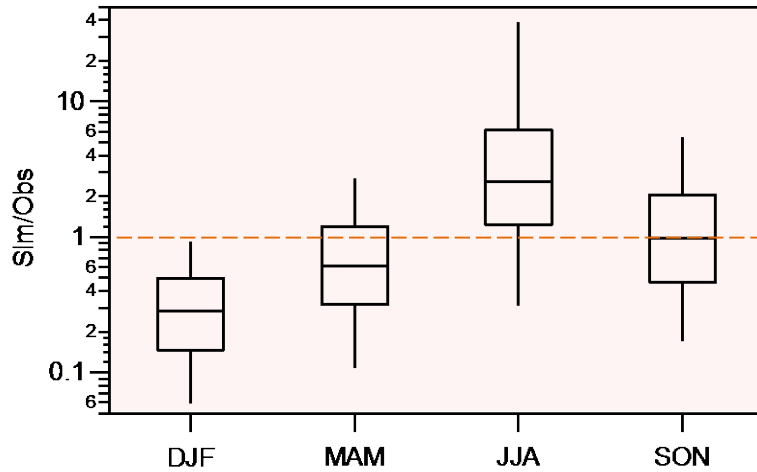
Oxidants: underestimated in both summer and winter



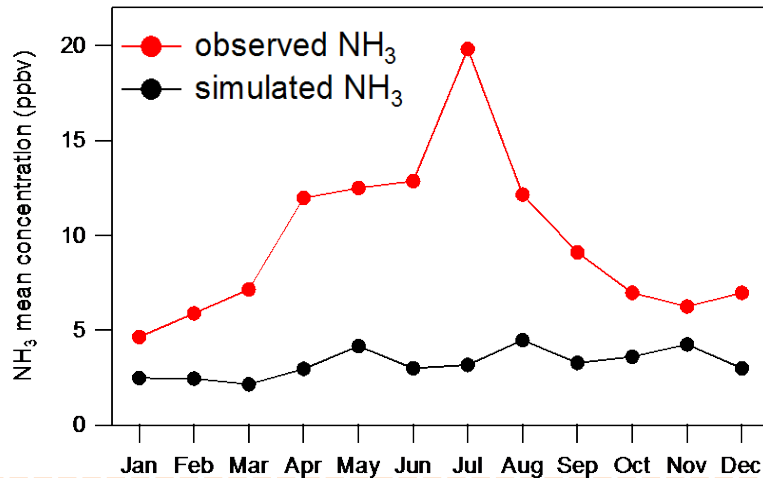
Surface OH and HO₂ concentrations are underestimated in Beijing by a factor of 1.5 to 4 (more in the winter).

Major Precursors: complex behavior

SO₂



NH₃



Aromatics

*daytime (7:00-19:00) averages

Unit: ppbv		Obs	Sim	Sim/Obs
3 Aug – 13 Sep 2011	Benzene	1.29	0.75	0.6
	Toluene	2.23	1.57	0.7
	Xylene	1.75	0.76	0.4
	Isoprene*	0.41	0.33	0.8
29 Dec 2011 – 2011 – 18 Jan 2012	Benzene	2.34	1.35	0.6
	Toluene	2.67	2.44	0.9
1–31 Aug 2012	Benzene	0.98	0.74	0.8
	Toluene	1.99	1.50	0.8
	Xylene	1.50	0.75	0.5

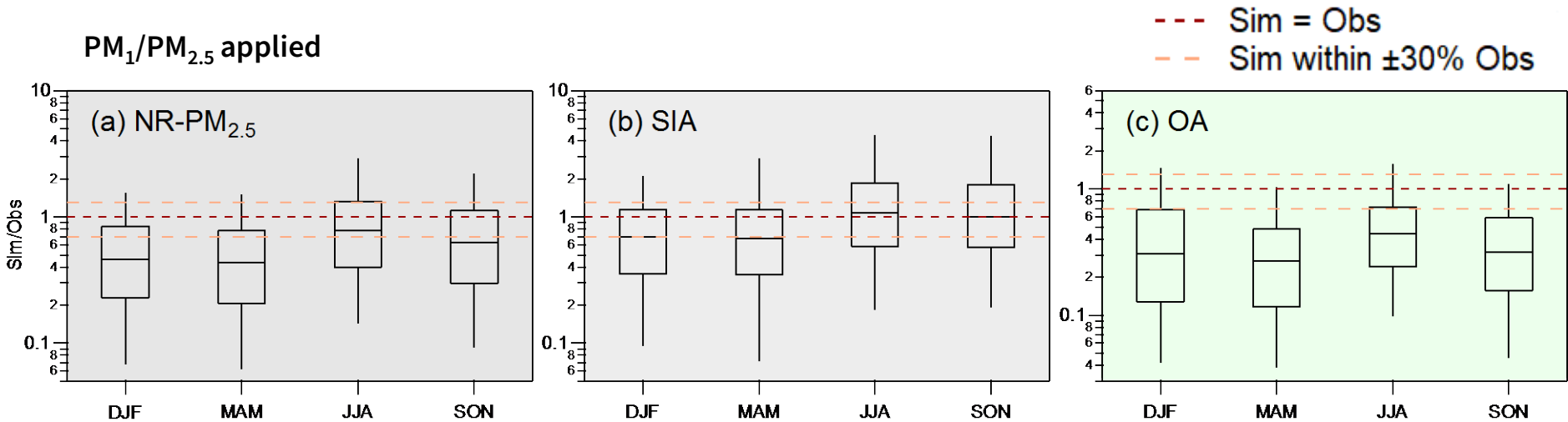
HNO₃

Unit: ppbv	Obs	Sim	Sim/Obs
20 Oct – 14 Nov 2008	1.07	3.74	3.5

- SO₂ comparisons show a clear seasonal trend, similar to sulfate.
- NH₃ is largely underestimated while HNO₃ is largely overestimated.
- Concentrations of aromatics are underestimated (mostly within a factor of 2).

Major chemical components of PM_{2.5}

PM₁/PM_{2.5} applied



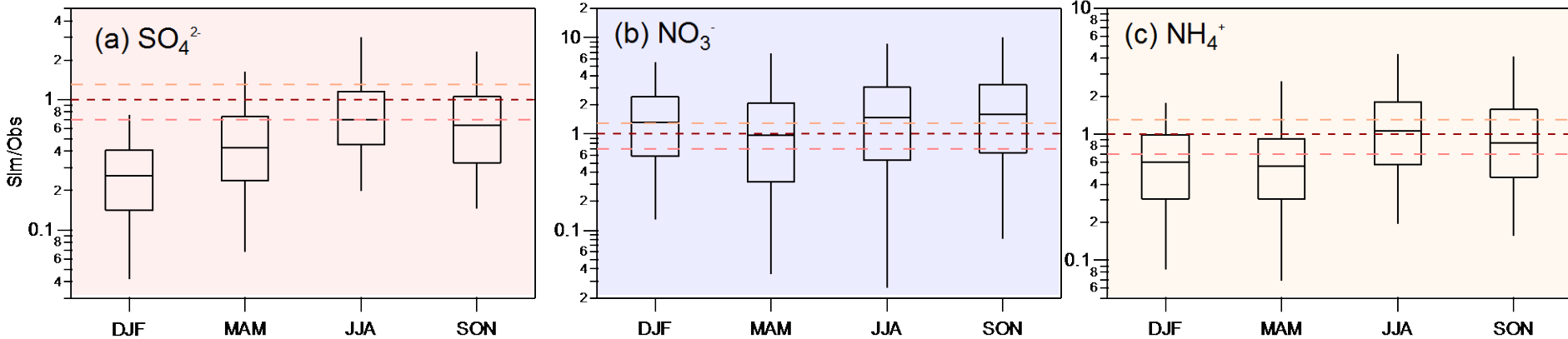
Sim/Obs	NR-PM _{2.5}				SIA				OA			
Percentile	DJF	MAM	JJA	SON	DJF	MAM	JJA	SON	DJF	MAM	JJA	SON
25	0.23	0.21	0.39	0.30	0.35	0.35	0.58	0.57	0.13	0.12	0.24	0.16
50	0.46	0.43	0.82	0.63	0.69	0.67	1.07	1.00	0.31	0.27	0.44	0.32
75	0.85	0.78	1.40	1.12	1.14	1.14	1.85	1.81	0.69	0.48	0.72	0.59
0.7×Obs < Percent of data	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

SIA: compensating errors

PM₁/PM_{2.5} applied

--- Sim = Obs
 - - - Sim within ±30% Obs



Sim/Obs	SO ₄ ²⁻				NO ₃ ⁻				NH ₄ ⁺			
Percentile	DJF	MAM	JJA	SON	DJF	MAM	JJA	SON	DJF	MAM	JJA	SON
25	0.14	0.24	0.45	0.33	0.58	0.32	0.53	0.63	0.31	0.31	0.57	0.46
50	0.26	0.42	0.70	0.63	1.31	0.97	1.47	1.61	0.60	0.56	1.06	0.85
75	0.41	0.74	1.15	1.05	2.41	2.07	3.04	3.27	0.99	0.92	1.80	1.58

Driven factors (if corrected)

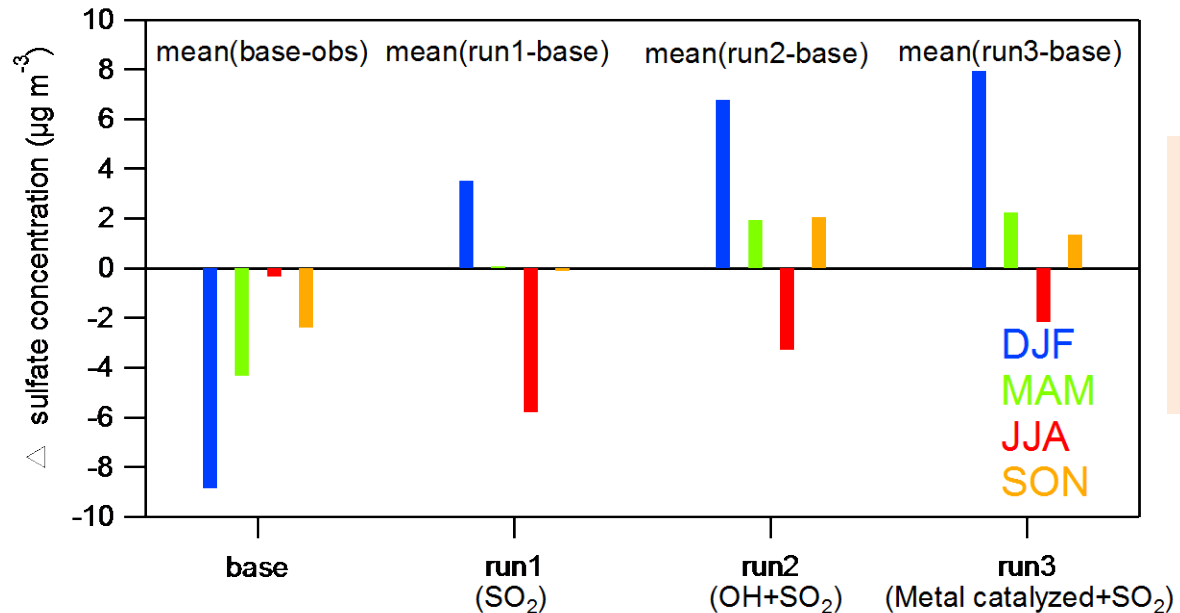
SO₂: better (seasonal error error)
 OH: better (overall underestimated)
 PBL: worse (smaller effect in effect in summer)

HNO₃: better (overestimated;

NH₃: better (underestimated)

Sensitivity runs for modeling sulfate

Simulation Names	Description
Sensitivity run1 - SO ₂	Anthropogenic SO ₂ emission are doubled in winter and reduced by 50% in summer
Sensitivity run2 – OH+SO ₂	Emissions are the same as Sensitivity run1. The rate of SO ₂ gas phase reaction is doubled.
Sensitivity run3- Metal catalyzed+ SO ₂	Emissions are the same as Sensitivity run1. Metal catalyzed oxidation of SO ₂ is implemented.



- Metal catalyzed oxidation is also an important pathway of sulfate formation that contributes roughly over $4 \mu\text{g m}^{-3}$ in winter

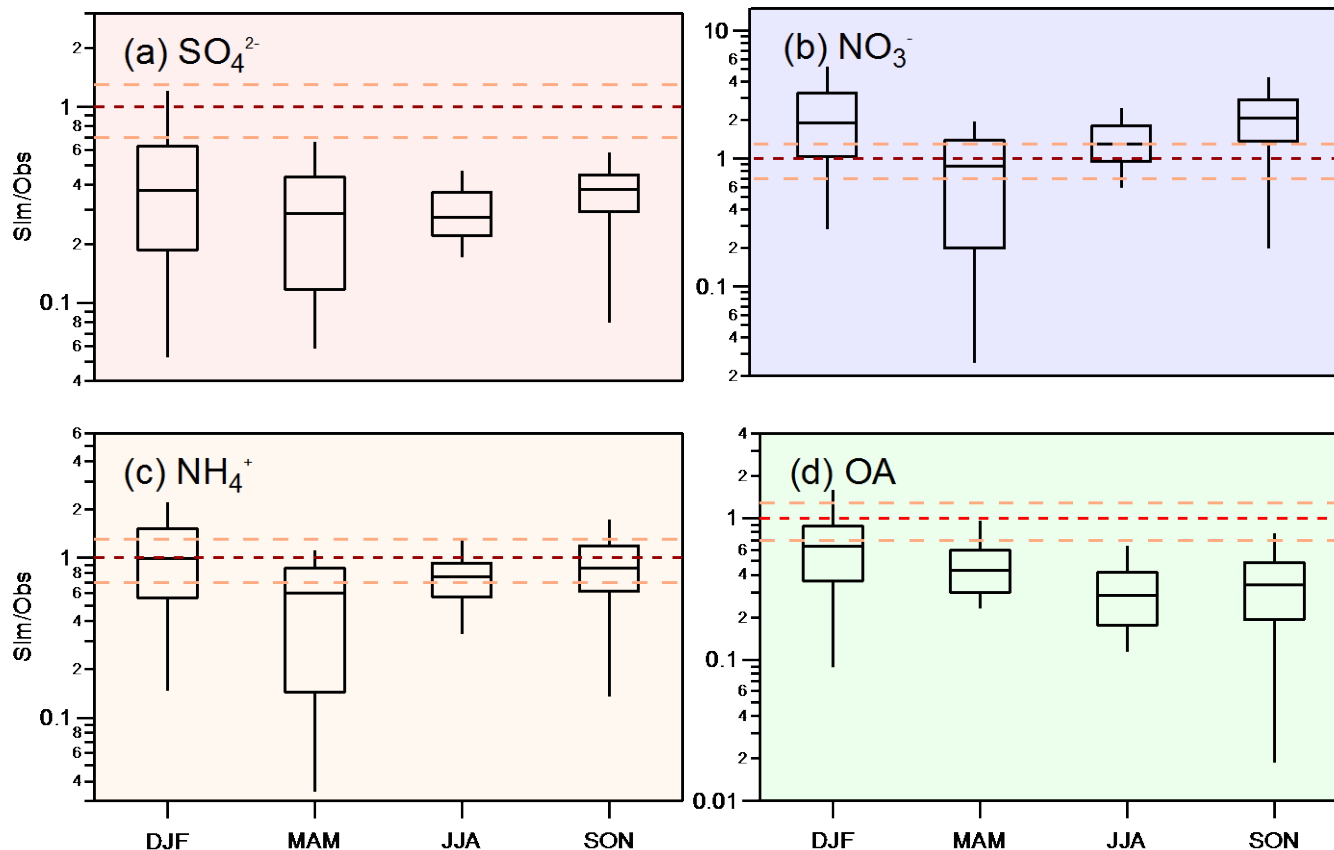
Summary

- $PM_{2.5}$ is underestimated, particularly in winter and spring, driven by OA underestimation that along with underestimated OH, VOC but mixed PBL effects
- Compensating errors make the SIA simulations looking fine.
- SO_2 drives the seasonal errors in sulfate simulations and metal catalyzed oxidation is an important pathway of sulfate formation.

Thanks for your attention!

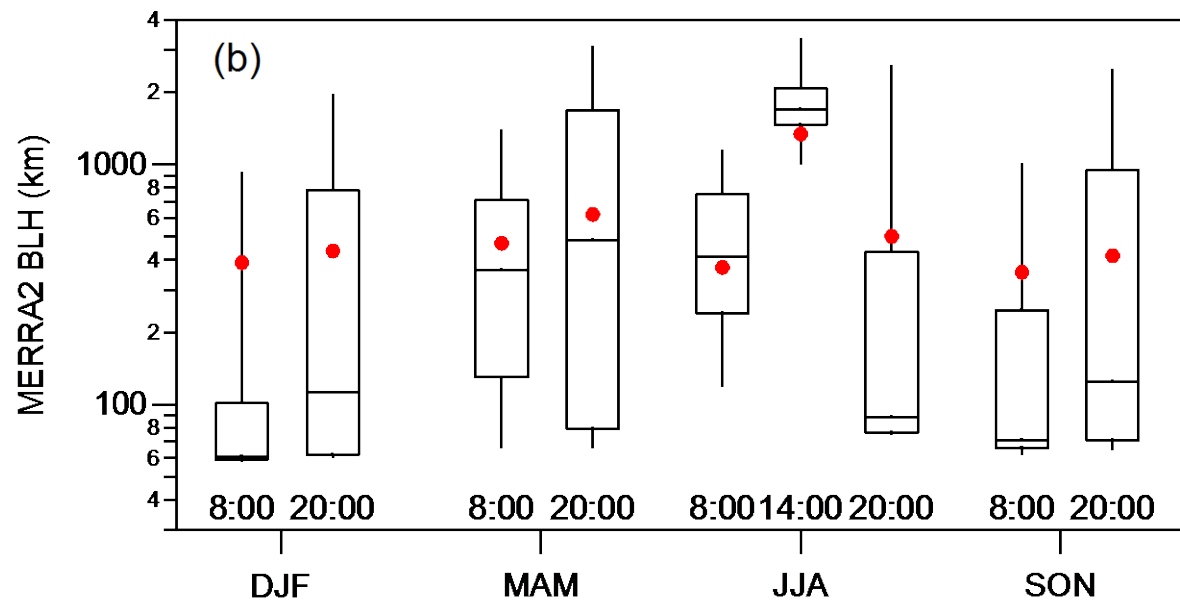
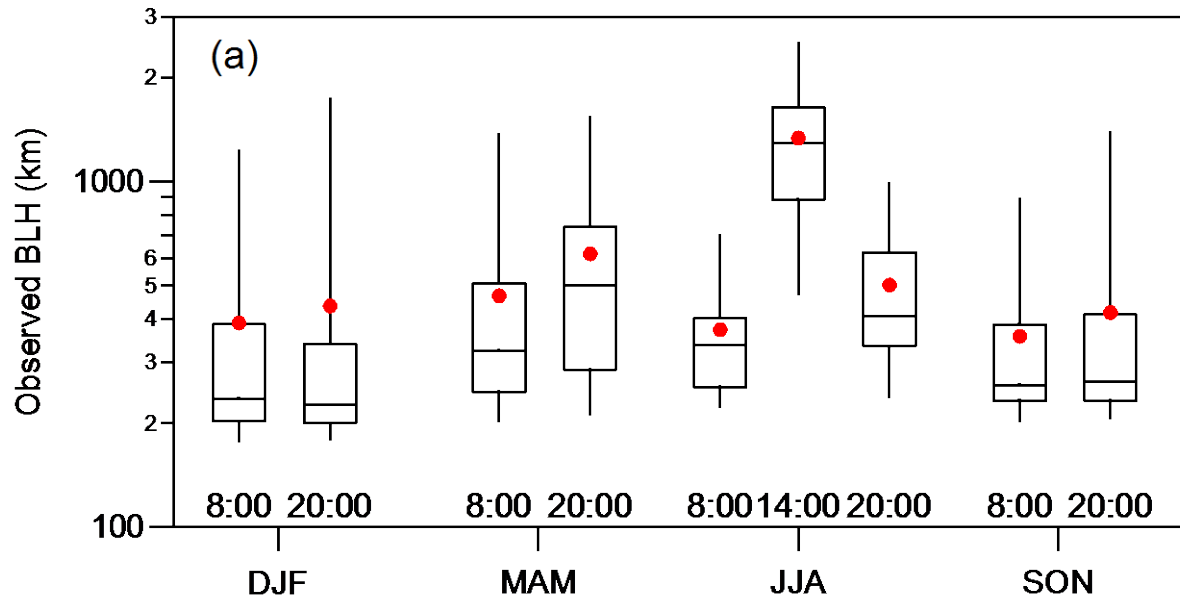
Model performance of Sensitivity run1 during severe haze events

Select the periods whose hourly averaged NR-PM₁ concentration larger than 75 μg m⁻³ and duration over 36 hours as the haze periods; then define the moments that NR-PM₁ concentration larger than 150 μg m⁻³ in haze periods as severe haze



	SO ₄ ²⁻				NO ₃ ⁻				NH ₄ ⁺				OA			
Median	DJF	MAM	JJA	SON	DJF	MAM	JJA	SON	DJF	MAM	JJA	SON	DJF	MAM	JJA	SON
General	0.61	0.63	0.54	0.88	1.77	1.38	2.31	2.30	0.96	0.80	1.29	1.21	0.44	0.38	0.63	0.45

PBL: observation and simulation



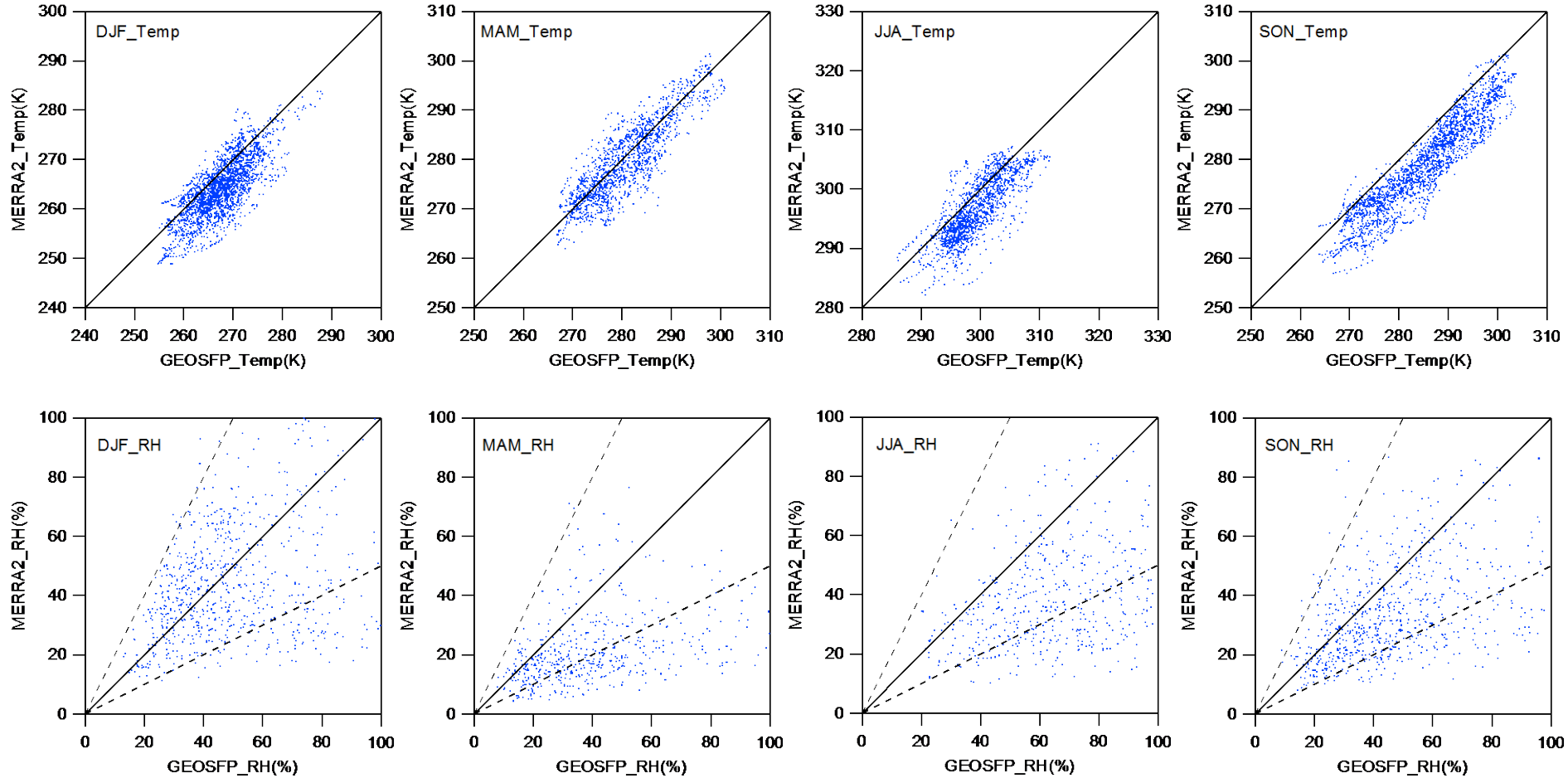
Model performance statistics of MERRA2

		DJF	MAM	JJA	SON
T (K)	OBS	270.9639	286.4200	300.4637	289.3845
	SIM	263.3404	280.0753	296.3330	281.2050
	NMB	-2.8134	-2.2152	-1.3748	-2.8264
	NME	2.8811	2.4056	1.6515	2.8524
	RMSE	8.6469	8.0734	5.8750	8.9956
RH (%)	OBS	32.5698	34.0036	61.9143	46.1532
	SIM	41.9572	23.0102	35.1229	34.3734
	NMB	28.8223	-32.3303	-43.2717	-25.5233
	NME	60.3485	54.3405	47.0566	39.2439
	RMSE	23.5048	24.0147	34.2125	23.2616
WS (m s ⁻¹)	OBS	1.5264	2.2338	1.7102	1.8204
	SIM	4.3314	5.1309	4.2245	4.3624
	NMB	183.7561	129.6942	147.0132	139.6440
	NME	207.7873	147.7744	155.3253	163.4271
	RMSE	3.8589	4.1587	3.2450	3.7078
WD (°)	OBS	322.6251	291.4940	231.8174	304.8270
	SIM	84.5445	111.6363	298.1649	82.9301
	NMB	5.8463	1.0849	1.5704	6.4906
	NME	35.2705	39.5037	37.2289	33.9944
	RMSE	108.1112	102.3086	99.0717	102.9257

Model performance statistics of GEOS-FP

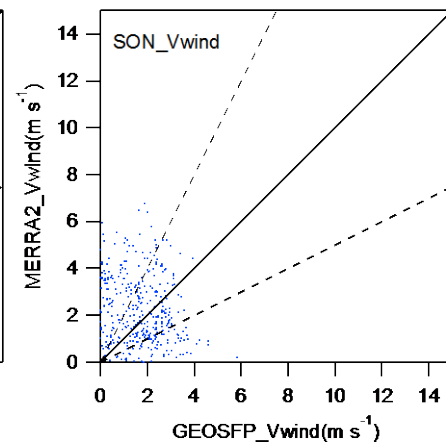
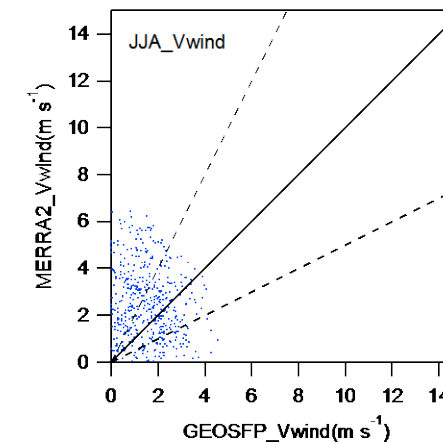
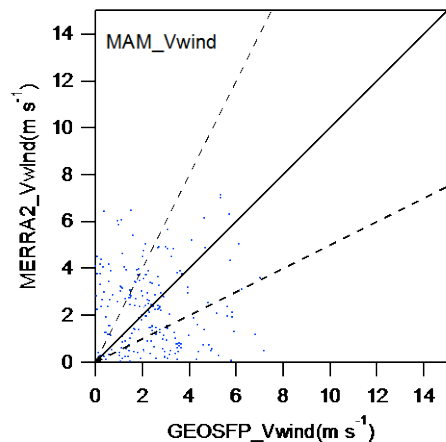
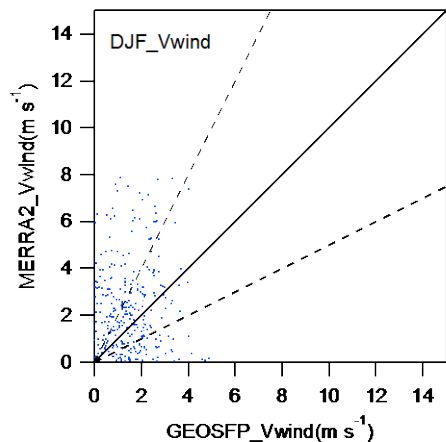
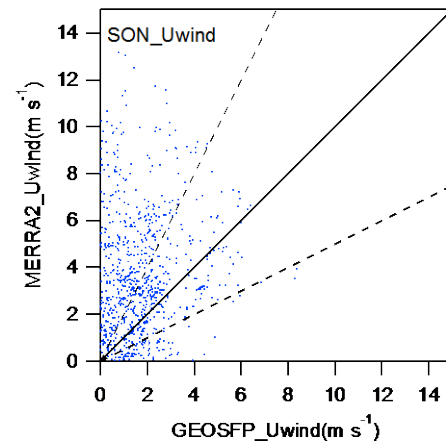
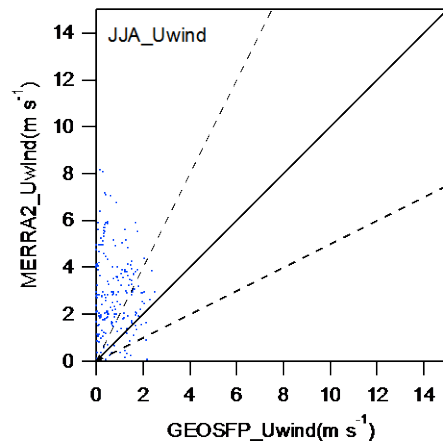
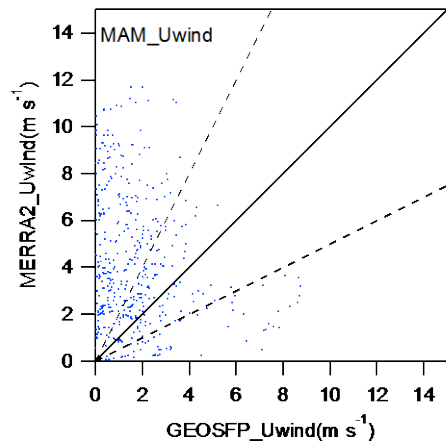
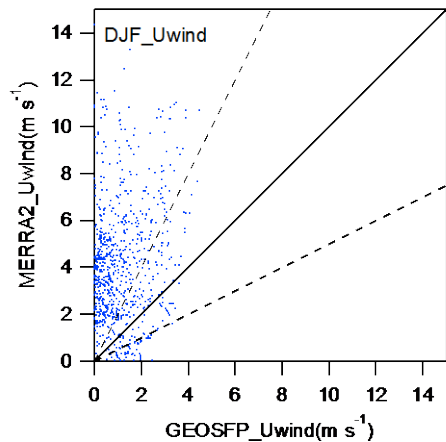
		DJF	MAM	JJA	SON
T (K)	OBS	270.6282	284.1636	300.9024	287.5518
	SIM	267.0708	280.2162	298.7724	284.4671
	NMB	-1.3145	-1.3891	-0.7079	-1.0728
	NME	1.3775	1.4871	0.8736	1.1742
	RMSE	4.3298	5.0896	3.1184	4.0284
RH (%)	OBS	36.9565	32.3894	61.7067	43.6553
	SIM	47.8338	38.9327	62.1406	45.3162
	NMB	29.4328	20.2020	0.7032	3.8046
	NME	36.3829	32.2330	14.8768	22.4389
	RMSE	15.7428	13.4552	11.4025	12.4083
WS (m s ⁻¹)	OBS	1.5579	2.1967	1.8838	1.9450
	SIM	2.2194	3.1879	5.4600	2.5403
	NMB	42.4666	45.1194	5.4600	30.6083
	NME	76.1664	66.1562	57.7792	62.7569
	RMSE	1.6014	1.9127	1.3594	1.5896
WD (°)	OBS	320.4910	303.6890	233.7796	313.9186
	SIM	168.6228	167.7513	303.3011	162.0450
	NMB	-10.1168	8.8202	-0.9087	-6.5421
	NME	44.5717	61.3368	49.3646	47.0601
	RMSE	130.5859	132.2074	125.5794	133.9619

Comparison of MERRA2 and GOES-FP



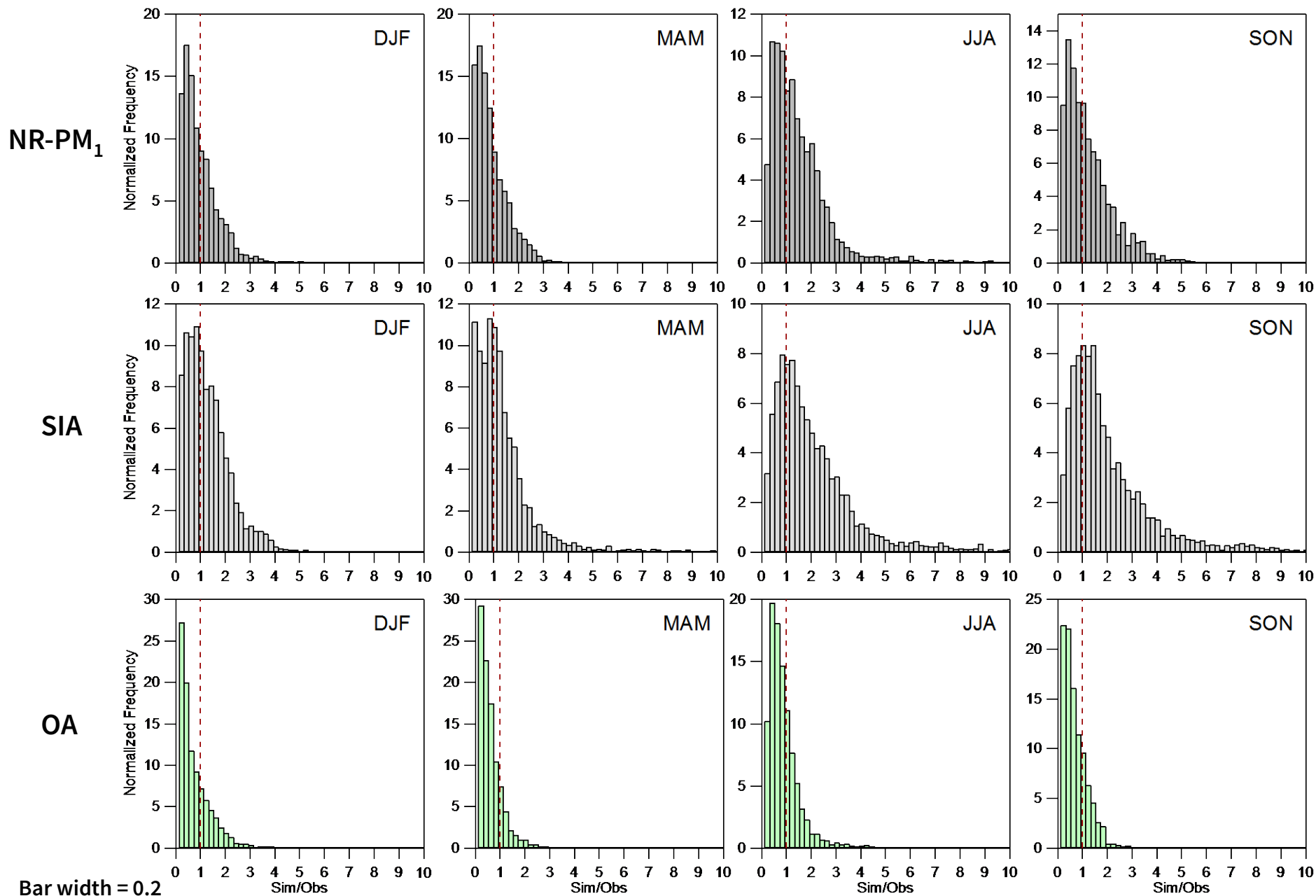
The solid line is 1:1
The dash line is 1:2 and 2:1

Comparison of MERRA2 and GOES-FP



The solid line is 1:1
The dash line is 1:2 and 2:1

Normalized frequency of model performance of NR-PM₁, SIA and OA



Normalized frequency of model performance of sulfate, nitrate and ammonium

