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Sources of organic aerosols in eastern China: a modeling study with high-resolution intermediate-volatility and semivolatile organic compound emissions

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Table S1. Gas-ratios for specific sources and emission profiles used in CMAQ simulations. The characters in brackets are the source codes in the SPECIATE 5.1 database.

	Source	G-ratios	Volatility (C* at 298 K, μg·m^{-3})										References
			IVOCP6	IVOCP5	IVOCP4	IVOCP3	SVOCP2	SVOCP1	SVOCP0	SVOCN1	IVOCP6ARO	IVOCP5ARO	
			10^6	10^5	10^4	10^3	10^2	10	1	10^{-1}	10^6	10^5	
Industrial process	Oil refinery	0.039	0.759	0.123	0.004	0.110	0.003	0.000	0.000	0.000	0.000	0.000	SPECIATE 5.1
	Chemical production	0.282	0.430	0.230	0.025	0.116	0.199	0.000	0.000	0.000	0.000	0.000	SPECIATE 5.1
	Pulp and paper	0.140	0.571	0.393	0.028	0.006	0.001	0.001	0.000	0.000	0.000	0.000	SPECIATE 5.1
Industrial solvent-use	Textile	2.473	0.041	0.448	0.182	0.268	0.040	0.002	0.019	0.000	0.000	0.000	SPECIATE 5.1
	Leather tanning	0.231	1.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	SPECIATE 5.1
	Timber processing	0.119	0.584	0.416	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	SPECIATE 5.1
	Furniture coating	0.021	0.888	0.112	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	SPECIATE 5.1
	Solvent-based coating	0.177	0.948	0.044	0.008	0.000	0.000	0.000	0.000	0.000	0.000	0.000	SPECIATE 5.1
	Water-based coating	0.504	0.096	0.893	0.011	0.000	0.000	0.000	0.000	0.000	0.000	0.000	SPECIATE 5.1
	Dry cleaning	0.004	0.885	0.115	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	SPECIATE 5.1
	Paint remover	0.072	0.987	0.010	0.004	0.000	0.000	0.000	0.000	0.000	0.000	0.000	SPECIATE 5.1
Mobile sources	Gasoline vehicle	0.265	0.206	0.056	0.113	0.098	0.000	0.000	0.000	0.000	0.406	0.121	SPECIATE 5.1
	Diesel vehicle	1.358	0.331	0.318	0.244	0.095	0.000	0.000	0.000	0.000	0.004	0.007	SPECIATE 5.1
	Fuel evaporation	0.002	0.841	0.159	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	SPECIATE 5.1
	Diesel machinery	0.400	0.282	0.279	0.264	0.102	0.057	0.012	0.003	0.000	0.000	0.000	Qi et al., 2019
	Marine vessel	0.300	0.230	0.375	0.193	0.097	0.029	0.000	0.000	0.000	0.077	0.000	Huang et al., 2018
	Aircraft	0.482	0.761	0.148	0.063	0.028	0.000	0.000	0.000	0.000	0.000	0.000	SPECIATE 5.1
Residential sources	Coal combustion	0.180	0.439	0.439	0.088	0.035	0.000	0.000	0.000	0.000	0.000	0.000	Cai et al., 2019
	Residential solvent-use	0.240	0.938	0.047	0.003	0.007	0.000	0.003	0.000	0.001	0.000	0.000	SPECIATE 5.1
	Cooking	0.036	0.554	0.374	0.052	0.015	0.003	0.001	0.000	0.000	0.000	0.000	SPECIATE 5.1
Agriculture sources	Biomass burning	0.064	0.337	0.330	0.215	0.118	0.000	0.000	0.000	0.000	0.000	0.000	SPECIATE 5.1

Table S2. P-ratios for specific sources and emission profiles used in CMAQ simulations.

Source		P-ratios	Volatility (C* at 298 K, μg·m^{-3})					References
			IVOCP3	SVOCP2	SVOCP1	SVOCP0	SVOCN1	
			10^3	10^2	10	1	10^{-1}	
Mobile sources	Gasoline vehicle	0.901	0.000	0.323	0.406	0.073	0.197	Lu et al., 2020
	Diesel vehicle	0.867	0.000	0.419	0.420	0.099	0.063	Lu et al., 2020
	Diesel machinery	0.420	0.455	0.204	0.123	0.131	0.087	Qi et al., 2019
	Marine vessel	0.469	0.305	0.140	0.185	0.166	0.204	Huang et al., 2018
Residential sources	Cooking	0.830	0.000	0.152	0.152	0.196	0.500	Louvaris et al., 2017
Agriculture sources	Biomass burning	0.150	0.500	0.250	0.125	0.125	0.000	May et al., 2013

Table S3. Source-specific emissions of VOCs and POA for the year 2017 in the Yangtze River Delta region.

Source		VOCs		POA	
		kt	%	kt	%
Industrial process	Oil refinery	146	3.50	1.49	0.74
	Chemical production	865	20.7	1.65	0.82
	Pulp and paper	0.80	0.02	0.01	0.00
Industrial solvent-use	Textile	92.9	2.22	0.11	0.06
	Leather tanning	16.6	0.40	0.02	0.01
	Timber processing	262	6.27	0.10	0.05
	Furniture coating	63.0	1.51	0.00	0.00
	Solvent-based coating	979	23.4	1.80	0.89
	Water-based coating	99.8	2.39	0.00	0.00
	Dry cleaning	5.49	0.13	0.00	0.00
	Paint remover	0.07	0.00	0.00	0.00
Mobile source	Gasoline vehicle	575	13.8	9.4	4.64
	Diesel vehicles	88.0	2.10	28.0	13.9
	Fuel evaporation	356	8.53	0.00	0.00
	Diesel machinery	112	2.68	11.7	5.78
	Marine vessel	7.77	0.19	10.2	5.07
	Aircraft	1.32	0.03	0.00	0.00
Residential source	Coal combustion	15.1	0.36	6.42	3.18
	Residential solvent-use	147	3.51	0.00	0.00
	Cooking	224	5.35	82.9	41.1
Agriculture source	Biomass burning	122	2.92	48.0	23.8
Total anthropogenic emissions		4179	100	202	100
Total biogenic emissions		2005	/	/	/

Table S4. Parameterization scheme and inputs for the WRF model.

Option	Configuration/Data source
Version	WRF-v3.9.1
IC/BC condition	NCEP FNL1°×1°
Microphysical Process	Purdue Lin Scheme
Cumulus Convective Scheme	Grell-3 Scheme
Road Process Scheme	Noah Scheme
Boundary Layer Scheme	Yonsei University (YSU) Scheme
Long-wave and Short-wave radiation scheme	RRTM and Goddard radiation Scheme

Table S5. The statistical results of model performance for the meteorological parameters in each season (MB: mean bias; MGE: mean gross error; RMSE: root-mean-square error; IOA: index of agreement).

Parameters*	Seasons	MB	Criteria	MGE	Criteria	RMSE	Criteria	IOA (-)	Criteria
Temperature (K)	Spr	0.2	≤ +0.5	1.46	≤ 2	2.0	-	0.96	≥ 0.8
	Sum	-1.5		2.26		2.9		0.80	
	Aut	0.5		1.49		2.4		0.89	
	Win	1.4		1.87		2.5		0.94	
Humidity (%)	Spr	-8.0	-	11.03	-	15.7	-	0.85	≥ 0.6
	Sum	-2.8		7.82		13.2		0.80	
	Aut	-10.9		11.79		16.9		0.82	
	Win	-12.2		13.71		19.6		0.73	
Wind speed ($m \cdot s^{-1}$)	Spr	0.5	≤ +0.5	1.28	-	1.7	≤ 2	0.77	≥ 0.6
	Sum	0.2		1.15		1.5		0.75	
	Aut	0.6		1.14		1.5		0.75	
	Win	0.9		1.50		1.9		0.75	
Wind direction (°)	Spr	2.6	≤ +10	31.52	≤ 30	46.7	-	0.93	-
	Sum	1.6		31.31		46.0		0.91	
	Aut	10.3		28.29		42.9		0.96	
	Win	8.1		26.65		41.2		0.97	

*The units in the brackets are only for MB, MGE and RMSE. IOA is unitless.

Table S6. The statistical results of model performance for major air pollutants in each season. (MB: mean bias; MGE: mean gross error; RMSE: root-mean-square error; MFB: mean fractional bias; MFE: mean fractional error; IOA: index of agreement)

Species	Scenario	Seasons	MB ($\mu g \cdot m^{-3}$)	MGE ($\mu g \cdot m^{-3}$)	RMSE ($\mu g \cdot m^{-3}$)	MFB (%)	MFE (%)
SO_2	IMPROVE	Spr	8.0	11.0	21.9	33	70
		Sum	5.9	9.6	20.5	15	80
		Aut	9.9	12.5	23.2	43	73
		Win	11.4	14.2	25.0	44	74
NO_2	IMPROVE	Spr	-8.3	18.4	26.2	-37	61
		Sum	5.1	13.7	21.9	7	57
		Aut	-7.1	17.0	23.1	-29	53
		Win	-10.1	19.1	25.5	-31	53
O_3	IMPROVE	Spr	39.8	45.5	55.0	27	34
		Sum	29.8	43.7	54.3	17	33
		Aut	30.0	35.4	43.1	23	29
		Win	19.1	32.5	43.4	14	31
$PM_{2.5}$	BASE	Spr	6.9	21.3	30.3	14	47
		Sum	9.4	15.3	22.5	28	54
		Aut	14.0	23.8	34.8	27	52
		Win	4.5	25.9	38.7	8	47
	IMPROVE	Spr	9.2	22.3	31.5	18	49
		Sum	11.6	16.5	24.1	34	56
		Aut	19.0	26.7	37.8	36	55
		Win	7.6	27.0	40.4	12	47

Table S7. The statistical results of model performance for organic carbon (OC) in each season.

Seasons	Sites	MB (μg·m^{-3})		MGE (μg·m^{-3})		RMSE (μg·m^{-3})		MFB (%)		MFE (%)	
		BASE	IMPROVE	BASE	IMPROVE	BASE	IMPROVE	BASE	IMPROVE	BASE	IMPROVE
Spring	SAES	-4.5	-3.2	4.5	3.3	23.7	14.4	-67	-48	67	48
	Changzhou	-5.3	-3.6	5.3	3.6	30.8	16.6	-74	-47	74	47
	Dianshan Lake	-2.3	-0.8	2.3	1.7	6.7	4.0	-57	-25	57	37
	Chongming Dongtan	-2.2	-1.1	2.2	1.3	5.9	2.6	-71	-41	71	45
	Hefei	-4.5	-3.5	4.5	3.5	23.7	16.2	-83	-60	83	61
	Jinhua	-4.7	-3.7	4.8	4.0	28.7	20.2	-100	-71	102	76
	Qiandao Lake	-2.3	-1.5	2.4	1.6	6.9	4.2	-82	-48	82	52
	Jiaxing	-3.3	-1.6	3.3	1.7	13.9	5.5	-63	-28	63	31
Summer	SAES	-0.3	0.3	1.0	1.0	2.0	1.6	1	12	26	24
	Changzhou	-4.4	-3.2	4.4	3.3	22.9	14.3	-75	-53	75	53
	Chongming Dongtan	0.1	0.7	1.2	1.5	2.8	6.0	-31	-12	93	98
	Jinhua	-2.0	-1.4	2.2	1.9	6.0	5.2	-61	-44	63	52
	Qiandao Lake	-1.1	-0.6	1.5	1.5	3.2	3.2	-49	-31	62	57
	Suzhou	-1.4	-0.6	1.4	1.0	3.0	1.5	-32	-15	32	23
	Jiaxing	-1.7	-0.8	1.7	1.0	4.4	1.5	-50	-24	50	27
Autumn	SAES	-2.6	-1.9	2.9	2.4	12.4	8.8	-43	-31	46	37
	Changzhou	-2.9	-1.5	3.2	2.3	12.9	7.7	-50	-27	53	35
	Dianshan Lake	-1.5	-0.6	1.6	1.1	3.6	2.0	-45	-21	47	31
	Chongming Dongtan	-1.5	-1.0	1.5	1.0	2.5	1.4	-97	-61	97	63
	Hefei	-2.6	-1.2	2.6	1.8	8.4	4.2	-54	-29	54	37
	Jinhua	-4.2	-2.9	4.3	3.5	28.4	21.3	-71	-47	72	54
	Nanjing	0.4	1.5	1.0	1.7	2.0	6.1	6	21	18	27
	Qiandao Lake	-0.4	0.8	1.5	2.0	3.2	6.2	-26	5	54	54
	Suzhou	-0.6	0.3	1.0	0.8	1.7	2.0	-16	2	24	18
	Jiaxing	-3.1	-1.9	3.1	2.2	11.8	6.7	-64	-40	65	44
Winter	SAES	-0.9	-0.1	4.7	5.6	34.3	46.8	-16	-9	68	73
	Changzhou	-3.7	-2.5	3.7	2.7	19.3	12.1	-50	-34	50	35
	Chongming	-2.5	-2.1	2.5	2.2	8.7	6.5	-117	-105	117	107
	Hefei	-3.4	-2.5	3.4	2.5	15	9.1	-58	-43	58	43
	Qiandao Lake	-2.5	-1.5	2.5	1.8	9.4	5.5	-86	-57	86	63
	Suzhou	-2.2	-1.5	2.3	1.6	7.9	5.0	-41	-35	43	38
	Jiaxing	-3.9	-2.7	3.9	2.8	22.3	11.8	-75	-57	75	58

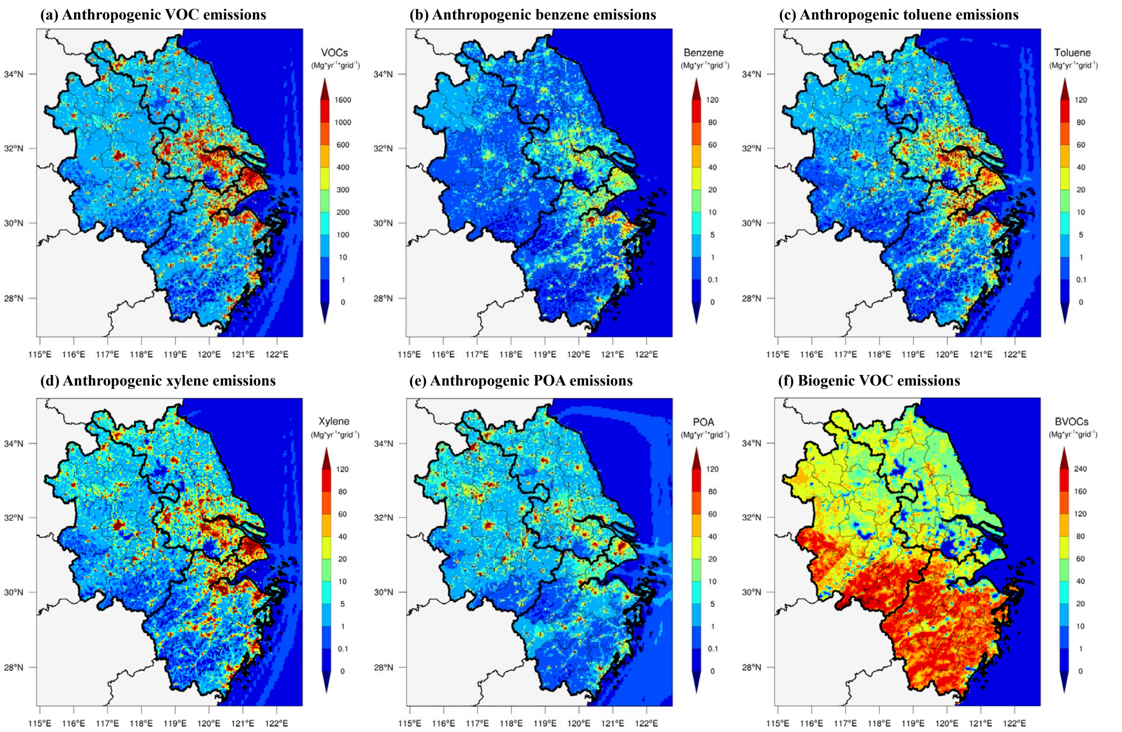

Figure S1. Spatial distribution of I/SVOC, POA, anthropogenic VOC (including benzene, toluene, and xylene), and biogenic VOC emissions in the YRD region for the year 2017.

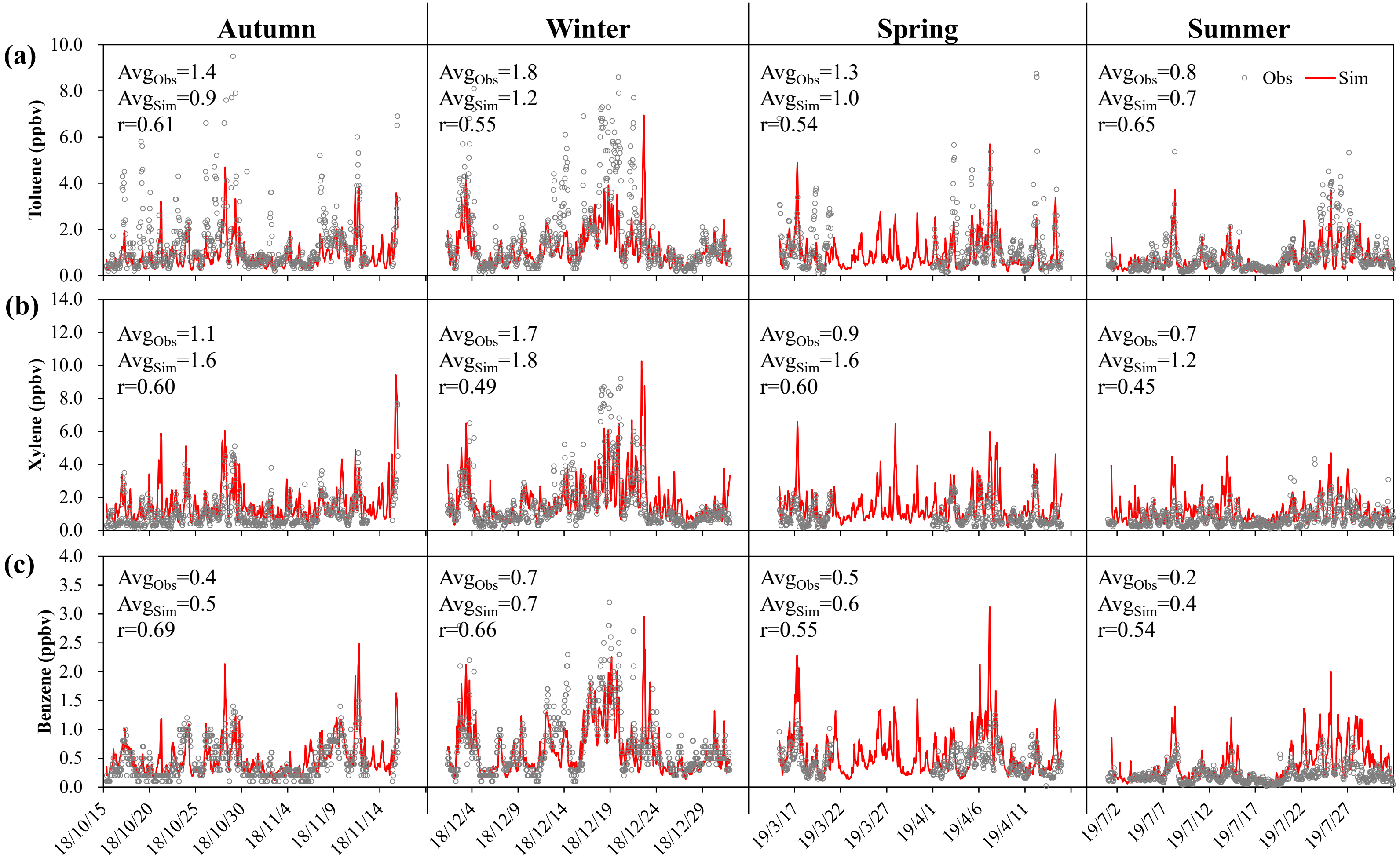

Figure S2. Comparisons of measured (black dots) and modeled (red lines) concentrations of (a) toluene, (b) xylene, and (c) benzene in different seasons at the SAES supersite in Shanghai.

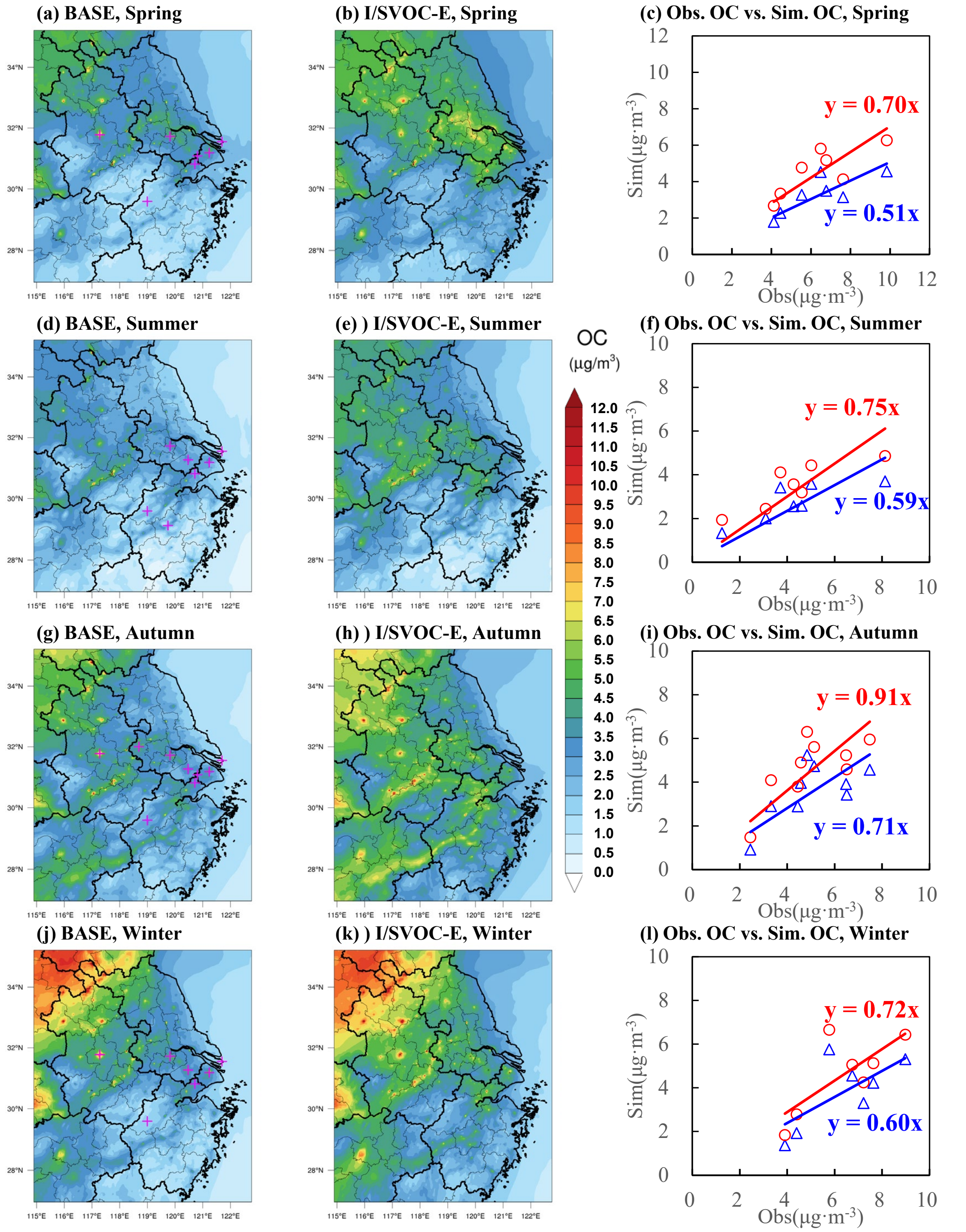

Figure S3. Spatial distributions of modeled OC concentrations in different seasons in BASE and I/SVOC-E simulations and their comparisons with OC observations. The blue triangle points represent the correlation between the modeled and observed OC in the BASE simulation, and the red dots represent the correlation between the modeled and observed OC in the I/SVOC-E simulation. The purple crosses in the left figures represent the observation sites of OC.

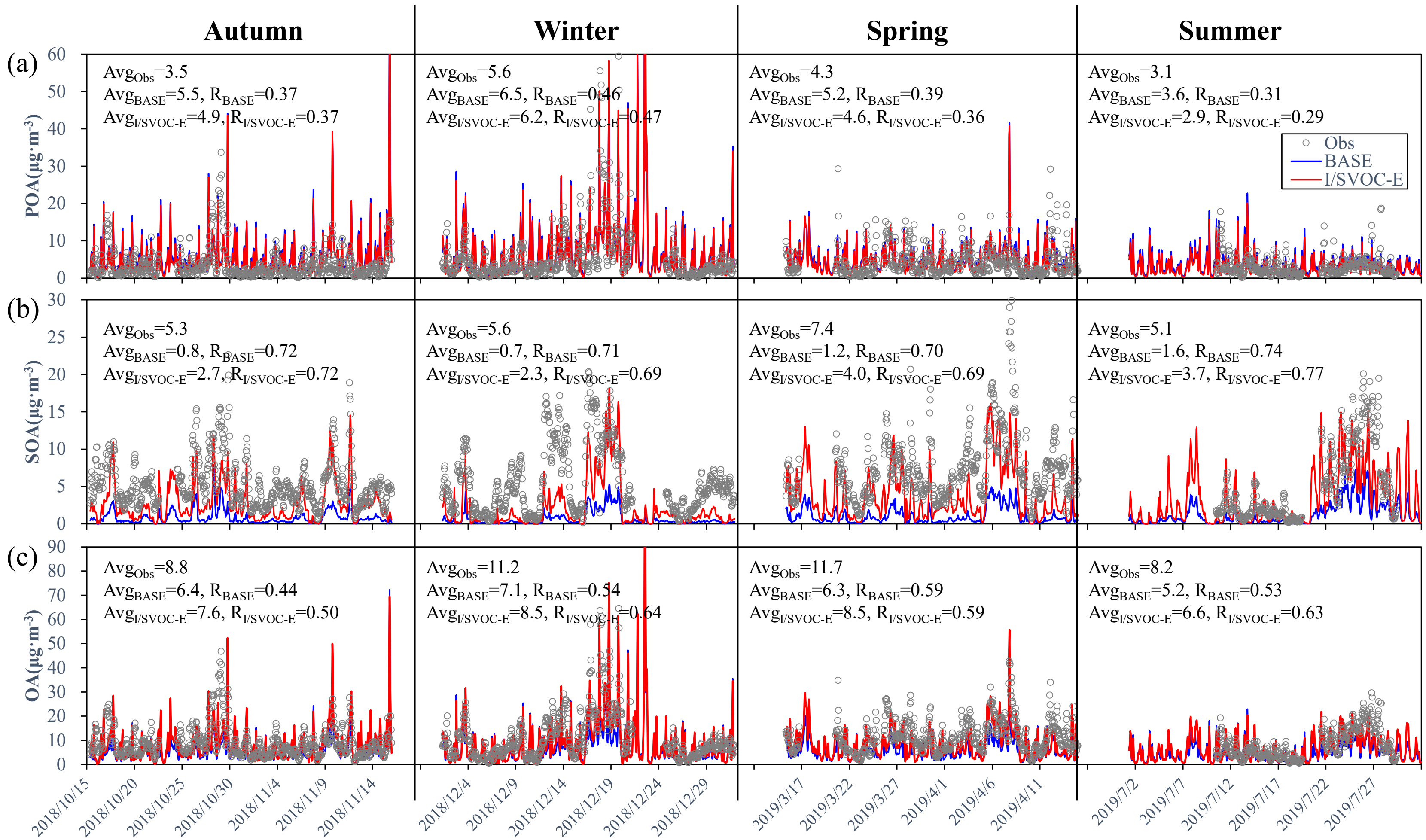

Figure S4. Comparisons of measured (grey dots) and modeled concentrations of (a) POA, (b) SOA, and (c) OA in different seasons in the BASE (bule lines) and I/SVOC-E (red lines) simulation cases at the SAES supersite in Shanghai.

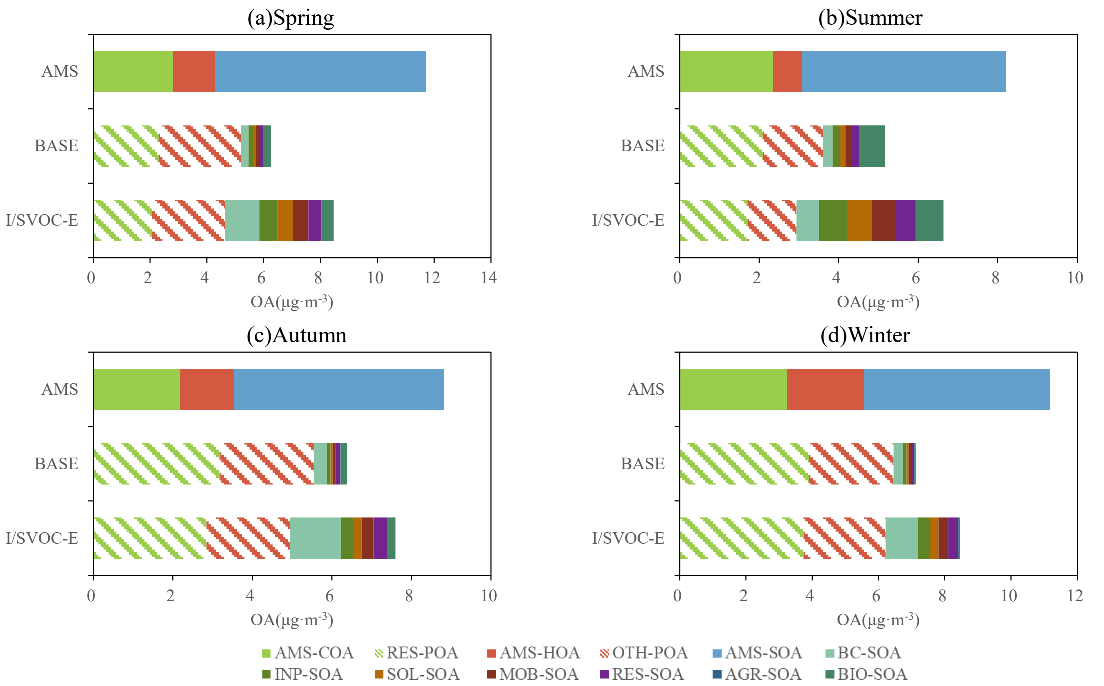

Figure S5. Comparisons of modeled POA and SOA source contributions with PMF results by AMS in different seasons in the BASE and I/SVOC-E simulations at the SAES supersite in Shanghai.