Supplement of

Estimating emissions of biogenic volatile organic compounds from urban green spaces and their contributions to secondary pollution

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Table S1 The sources of satellite datasets

Datasets	Year	Temporal Resolution	Spatial Resolution	Source
			Leaf Area Index Datasets	
GLASS	2000-2021	8 days	500 m	Available at http://www.glass.umd.edu/LAI/MODIS/, last access: 11 April 2022
			Land Cover Datasets	
MODIS MCD12Q1	2001-2021	Yearly	500 m	Available at https://search.earthdata.nasa.gov/, last access: 10 April 2022
C3S LC	1992-2021	Yearly	300 m	Available at https://cds.climate.copernicus.eu/cdsapp#!/dataset/satellite-land-cover?tab=form, last access: 21 March 2022
CGLS LC	2015-2019	Yearly	100 m	Available at https://land.copernicus.eu/global/products/lc, last access: 15 April 2022
FROM-GLC10	2017	Yearly	10 m	Available at https://data-starcloud.pcl.ac.cn/zh/resource/1

Table S2 WRF model physics schemes used in this study

Physical mechanism	Scheme	Reference
Microphysics	Thompson scheme	Thompson et al.[1]
Long-wave radiation	RRTM scheme	Iacono et al.[2]
Short-wave radiation	Goddard short wave	Chou and Suarez[3]
Land Surface	Thermal diffusion scheme	Dudhia[4]
PBL Scheme	YSU scheme	Hong; Hong et al.[5, 6]
Cumulus parameter	Grell-Freitas ensemble scheme	Grell and Freitas[7]

20   **Table S3** The area of urban tree area in each district in Beijing, unit is km^2

Number	District	Official data	C3S	CGLS	MCD12Q1	FROM-GLC10	FROM-GLC10-U
1	Dongcheng District	8.8	2.2	0.7	0.0	2.3	7.0
2	Xicheng District	7.3	1.7	0.5	0.0	1.9	6.1
3	Chaoyang District	114.0	19.6	17.6	0.0	15.3	81.8
4	Haidian District	110.2	25.7	28.8	9.4	44.3	84.5
5	Fengtai District	52.0	15.1	20.1	2.0	20.2	41.4
6	Shijingshan District	33.3	7.2	13.4	4.6	16.8	23.9
7	Mentougou District	11.4	14.7	21.2	10.5	28.7	8.2
8	Fangshan District	66.2	32.9	70.7	17.4	61.5	58.9
9	Tongzhou District	40.4	11.9	23.7	0.0	2.8	26.4
10	Shunyi District	40.4	8.0	12.9	0.5	15.9	30.2
11	Changping District	51.0	23.5	46.7	30.7	60.7	42.8
12	Daxing District	46.3	11.7	23.4	0.0	3.0	30.5
13	Huairou District	15.0	4.7	12.0	8.7	12.9	12.8
14	Pinggu District	8.8	1.4	3.6	1.4	5.4	7.9
15	Miyun District	13.2	4.6	13.1	7.4	14.5	11.3
16	Yanqing District	14.6	1.8	6.4	3.1	9.4	13.4
	Total	632.9	186.7	314.8	95.7	315.6	487.1

Table S4 The area of urban green spaces in each district in Beijing, unit is km^2

Number	District	Official data	C3S	CGLS	MCD12Q1	FROM-GLC10	FROM-GLC10-U
1	Dongcheng District	11.0	9.0	1.4	0.0	10.8	9.2
2	Xicheng District	10.6	7.0	1.1	0.0	8.7	9.4
3	Chaoyang District	148.8	80.0	26.3	1.0	134.3	116.6
4	Haidian District	121.5	65.3	40.3	31.5	97.2	95.8
5	Fengtai District	60.3	52.7	33.5	16.8	84.8	49.7
6	Shijingshan District	43.0	17.4	19.0	15.2	25.6	33.7
7	Mentougou District	15.9	26.9	32.3	30.9	31.9	12.7
8	Fangshan District	80.1	91.4	111.1	81.7	113.2	72.7
9	Tongzhou District	56.5	50.7	35.0	6.6	61.3	42.5
10	Shunyi District	73.6	32.2	20.0	18.3	56.6	63.4
11	Changping District	64.6	73.5	64.2	70.2	116.4	56.2
12	Daxing District	79.5	47.2	28.5	10.0	83.3	63.7
13	Huairou District	22.6	9.7	14.5	22.9	16.2	20.4
14	Pinggu District	15.6	3.6	4.7	5.2	5.9	14.7
15	Miyun District	15.6	10.4	16.4	22.3	15.5	13.8
16	Yanqing District	15.7	6.5	9.5	12.3	10.4	14.5
	Total	835.0	583.5	457.8	344.9	872.1	688.8

Table S5 Indices used to evaluate model performance

Index	Definition*	Remarks
Mean bias (MB)	$\frac{1}{N}\sum_{i=1}^{N}(M_i - O_i)$	
Root mean square error (RMSE)	$\sqrt{\frac{1}{N}\sum_{i=1}^{N}(M_i - O_i)^2}$	Reported as %
Gross Error (GE)	$\frac{1}{N}\sum_{i=1}^{N}\frac{\lvert M_i - O_i\rvert}{O_i}$	Reported as %
Mean normalized bias (MNB)	$\frac{1}{N}\sum_{i=1}^{N}\frac{M_i - O_i}{O_i}$	Reported as %
Mean normalized error (MNE)	$\frac{1}{N}\sum_{i=1}^{N}\frac{\lvert M_i - O_i\rvert}{O_i}$	Reported as %
Mean fractional bias (MFB)	$\frac{2}{N}\sum_{i=1}^{N}\frac{(M_i - O_i)}{(M_i + O_i)}$	Reported as %
Mean fractional error (MFE)	$\frac{2}{N}\sum_{i=1}^{N}\frac{\lvert M_i - O_i\rvert}{(M_i + O_i)}$	Reported as %

25   Note: * i represents the pairing of N observations O and predictions M by site and time.

Table S6 Model performance of meteorological parameters temperature (T2), wind speed (WS), wind direction and relative humidity (RH) in summer in Beijing. The values without meeting the benchmarks are bolded. (PRE is prediction; OBS is observation; MB is bias; GE is gross error; and RMSE is root mean square error)

	Statistics		Benchmarks*
T2 (K)	OBS	297.3	
	PRE	298.4	
	MB	**1.1**	≤±0.5
	GE	**2.2**	≤2.0
	RMSE	3.0	
WS (ms^{-1})	OBS	3.3	
	PRE	3.2	
	MB	-0.05	≤±0.5
	GE	1.3	≤2.0
	RMSE	1.7	≤2.0
WD (°)	OBS	152.9	
	PRE	150.5	
	MB	-2.4	≤±10
	GE	**44.6**	≤±30
	RMSE	60.9	
RH (%)	OBS	49.5	
	PRE	35.6	
	MB	-14.0	
	GE	14.8	
	RMSE	18.7	

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Note: * are benchmarks suggested by Emery *et al.*[8].

Table S7 Model performance on maximum daily average 1h (MDA1) O_3, maximum daily average 8h (MDA8) O_3, $PM_{2.5}$, NO_2, and SO_2 in different cases in Beijing. The values without meeting the criteria are bolded. (OBS is mean observation; PRE is mean prediction; MNB: mean normalized bias; MNE: mean normalized error; MFB: mean fractional bias; and MFE: mean fractional error).

	Statistics	B1	B2	B3	B4	B5	Benchmarks*
O_3-1h (ppb)	OBS	71.68	71.68	71.68	71.68	71.68	
	PRE	81.9	82.28	81.55	81.34	80.93	
	MNB	**0.16**	**0.16**	0.15	0.15	0.14	$\leq\pm0.15$
	MNE	0.22	0.22	0.21	0.21	0.2	≤0.3
	MFB	0.12	0.12	0.11	0.11	0.1	
	MFE	0.19	0.19	0.18	0.18	0.17	
O_3-8h (ppb)	OBS	68.16	68.16	68.16	68.16	68.16	
	PRE	77.68	77.94	76.92	76.74	76.33	
	MNB	0.13	0.13	0.12	0.11	0.11	$\leq\pm0.15$
	MNE	0.19	0.19	0.18	0.17	0.16	≤0.3
	MFB	0.11	0.11	0.1	0.09	0.08	
	MFE	0.17	0.17	0.16	0.15	0.14	
$PM_{2.5}$ ($\mu g\ m^{-3}$)	OBS	37.33	37.33	37.33	37.33	37.33	
	PRE	38.59	39.01	38.24	38.02	37.88	
	MNB	0.15	0.16	0.15	0.14	0.14	
	MNE	0.58	0.59	0.58	0.57	0.57	
	MFB	-0.11	-0.12	-0.11	-0.1	-0.1	$\leq\pm0.6$
	MFE	0.51	0.52	0.51	0.5	0.5	≤0.75
NO_2 (ppb)	OBS	15.56	15.56	15.56	15.56	15.56	
	PRE	16.08	16.15	16.03	15.92	15.83	
	MNB	0.24	0.25	0.24	0.23	0.22	
	MNE	0.55	0.56	0.55	0.54	0.53	
	MFB	0.01	0.02	0.01	0.01	0	
	MFE	0.43	0.44	0.43	0.42	0.41	
SO_2 (ppb)	OBS	2.37	2.37	2.37	2.37	2.37	
	PRE	4.75	4.76	4.75	4.74	4.72	
	MNB	1.80	1.81	1.80	1.80	1.79	
	MNE	2.0	2.01	2.0	1.99	1.98	
	MFB	0.46	0.47	0.46	0.45	0.44	
	MFE	0.76	0.77	0.76	0.75	0.74	

Note: * are criteria suggested by EPA. [9]

Table S8 The area of main plant function types (PFTs) in references and each land cover dataset in Beijing, unit is km^2

Plant function types	Official data	C3S	CGLS	MCD12Q1	FROM-GLC10
Needleleaf tree	1626.0	1016.0	1232.7	452.4	361.1
Broadleaf tree	5542.3	3249.0	5043.4	2877.9	6733.9
Shrub	2651.2	894.4	1003.1	1782.1	535.9
Grass	1046.9	2871.7	1706.7	4384.0	1366.9
Crop	2137.1	4854.1	3771.0	3175.4	4090.3

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Table S9 The mean fractional bias (MFB) and mean fractional error (MFE) between different cases with observations

Case	Name	Statics	
B1	CCI GLASS	MFB	-0.78
		MFE	1.42
B2	CGLS GLASS	MFB	-1.59
		MFE	1.66
B3	MODIS GLASS	MFB	-2.00
		MFE	2.00
B4	FROM-GLC10	MFB	-0.52
		MFE	1.40
B5	FROM-GLC10-Up	MFB	-0.21
		MFE	1.37

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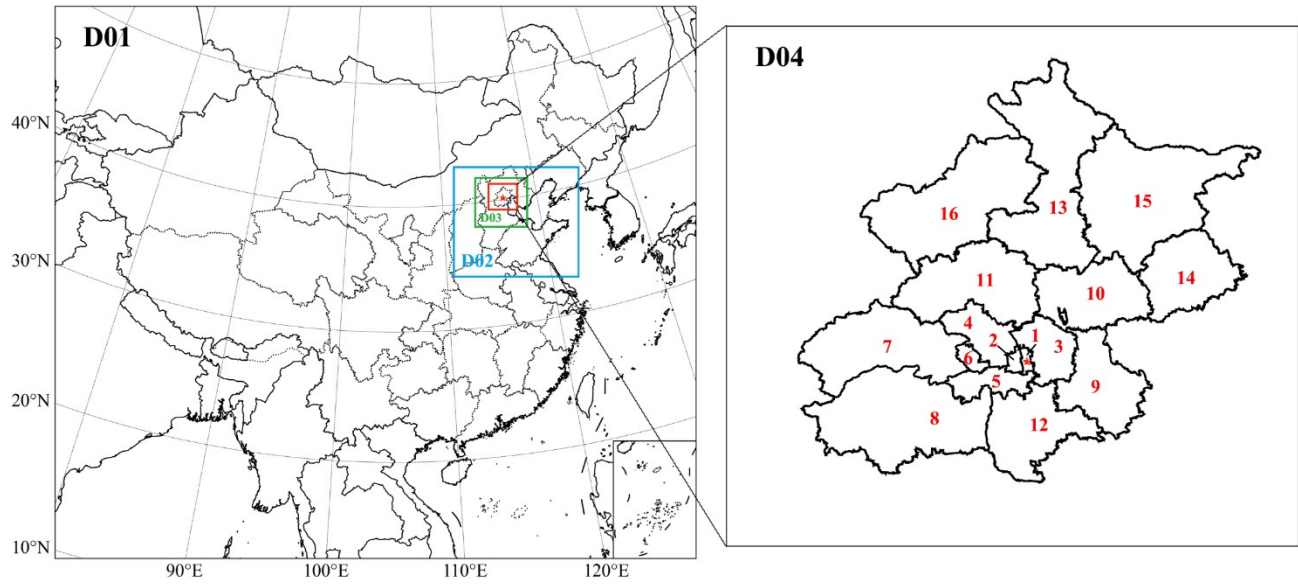
Fig. S1 Model domain (D01:36km, D02: 12km, D03:4km, and D04:1km) with numbers of district in Beijing (according to numbers in Table S2).
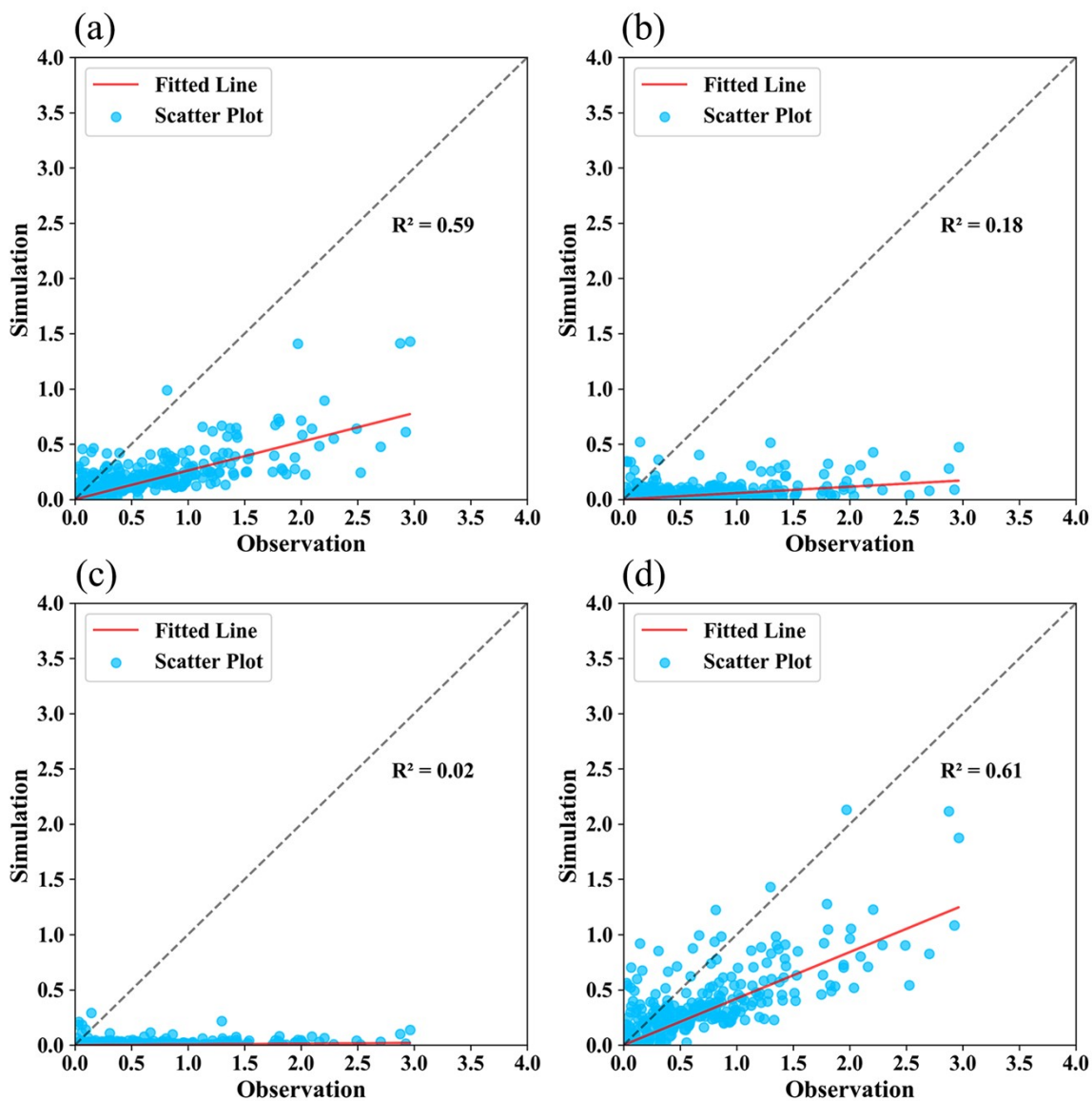
Fig. S2 Evaluation of isoprene concentrations between observations and the simulations in the IAP in different cases ((a) B1, (b) B2, (c) B3, (d) B4 during June 1-25, 2017 (unit: ppb).
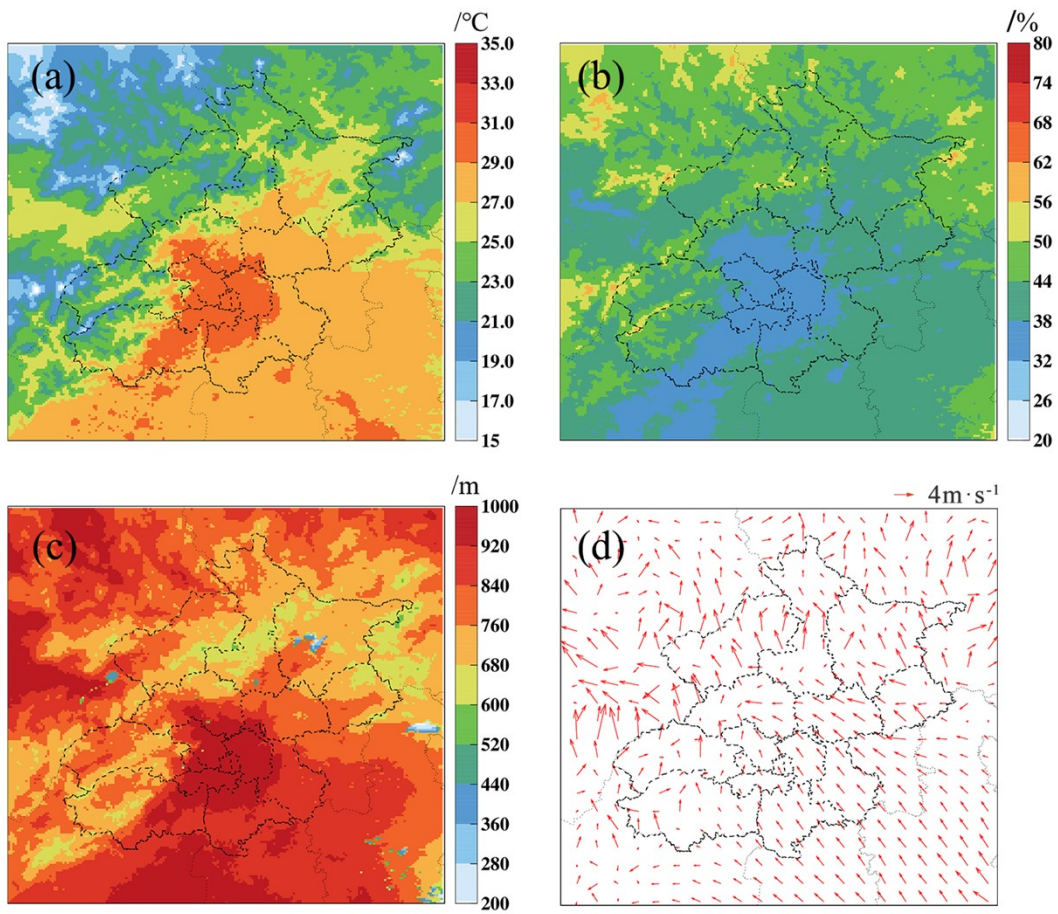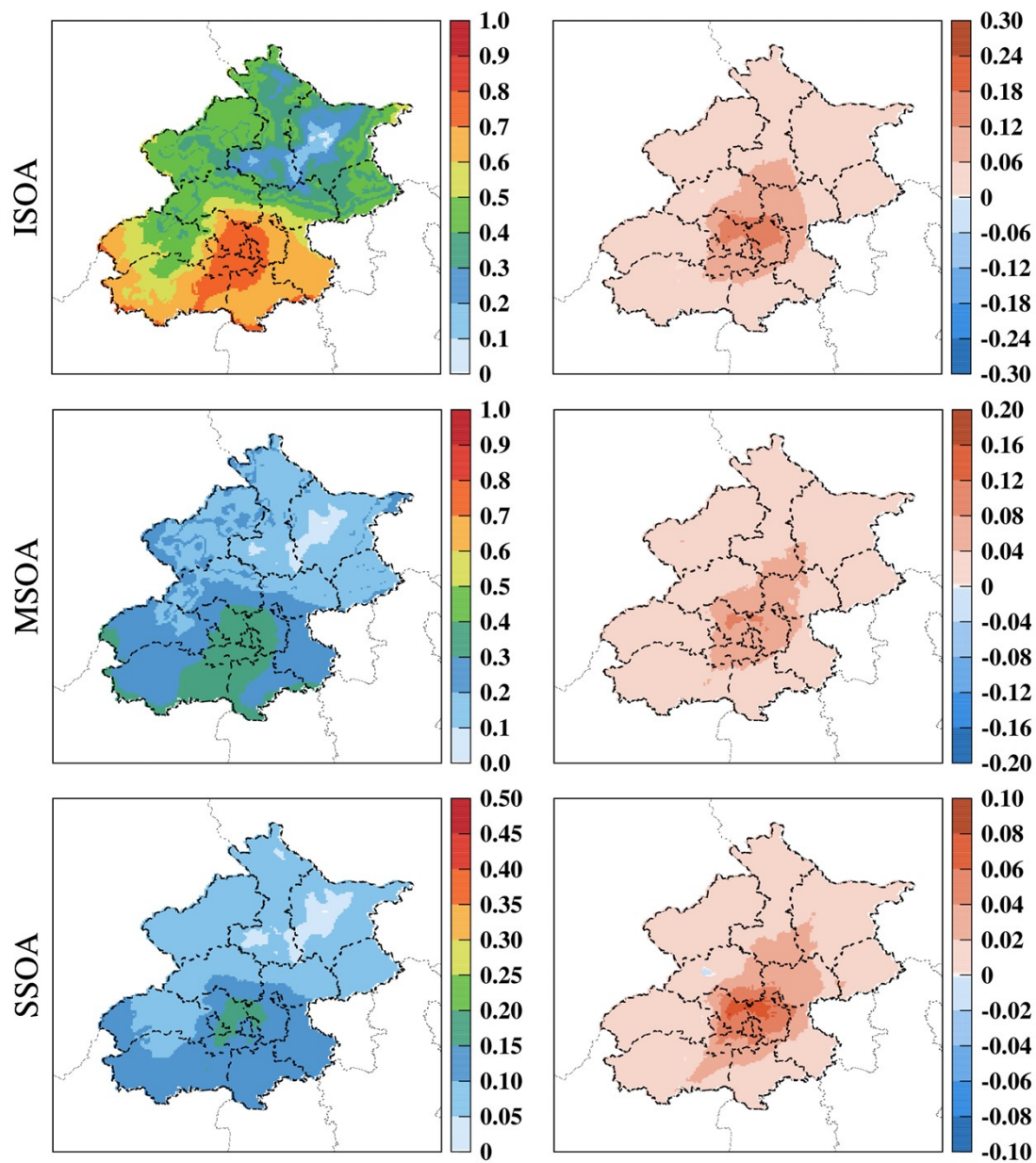
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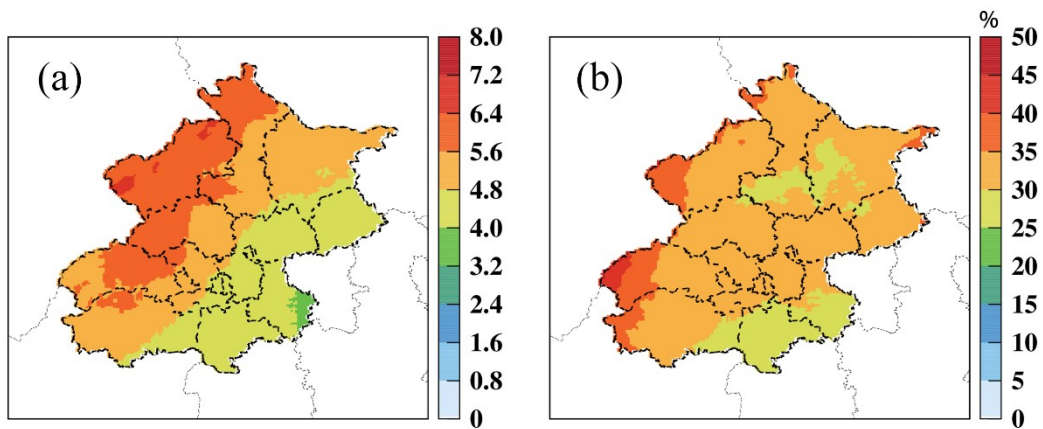
Fig. S3 (a) The spatial distributions of the biogenic SOA (BSOA) formed from total BVOCs (unit: μg m^{-3}) and (b) the contribution of BVOC emissions from areas outside Beijing to BSOA in B4 (unit: %).

Fig. S4 The regional meteorological conditions of (a) temperature, (b) humidity, (c) planetary boundary layer height, (d) wind speed.

65   **Fig. S5** The regional distributions of SOA formed by the three main BVOC species from urban green spaces of Beijing (isoprene: ISOA, monoterpenes: MSOA, and sesquiterpenes: SSOA) and their difference between the B5 case and the B4 case, unit is μg m^{-3}.

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