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Current status of model predictions of volatile organic compounds and impacts on surface ozone predictions during summer in China

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S.1 VOCs measurements

In the ATMSYC project, sampling was conducted in both winter and summer. The VOC measurements from 6 June to 24 August 2018 were employed in this study. Table S1 shows the locations of 28 sites, along with sampling time and the number of VOC samples. The methods for sampling and analyses were consistent across sites. Non-methane hydrocarbons (NMHCs) were collected in 2L stainless steel canisters, and all canisters were cleaned and evacuated at least three times with zero air before sampling. During the sampling, flow restrictors were used to guarantee that each sample lasted for one hour (Lyu et al., 2019; Lyu et al., 2020). Oxygenated VOCs (OVOCs) were sampled with 2,4-dinitrophenylhydrazine (DNPH) cartridges with O_3 scrubbers installed in front of them to remove airborne O_3. The sampling duration of OVOC was 2 h and the sampling flow rate was fixed at 0.5 L/min. All the DNPH cartridges were stored in a refrigerator at 4 ℃ before the chemical analyses (Lyu et al., 2019; Lyu et al., 2020).

The NMHC species were identified and quantified by gas chromatography coupled with a mass spectrometry detector, electron capture detector, and flame ionization detector at Hong Kong Polytechnic University (Lyu et al., 2020). The detection limit, accuracy, and precision for each NMHC were given in (Zhou et al., 2023), following the U.S. Environmental Protection Agency (U.S. EPA) TO-15 method (Agency, 1999). With outliers removed, 834 valid samples were obtained. The analyses for the 60 NMHCs were in good agreement with those analyzed by Prof. Donald Blake's laboratory at the University of California, Irvine (Blake, 2003; Simpson et al., 2010), with goodness-of-fit (R2) values ranging from 0.85-0.97 and slopes ranging from 0.85-1.24. In addition, HCHO was analyzed by high-performance liquid chromatography (Lyu et al., 2020). One calibration standard was run for every ten samples to ensure instrument stability, following a previous study (Cheng et al., 2014).

S.2 Supplement figures and tables

Table S1. List of sampling sites and periods in the field campaign of ATMSYC project.

Regions	Cities	Station code	Start time	End time	Novs	Latitude	Longitude
NCP	Beijing	BJ-B	2 August	24 August	57	40°24′28″N	116°40′26″E
		BJ-U	2 August	24 August	57	39°58′28″N	116°22′13″E
	Shijiazhuang	SJZ-B	29 June	4 July	18	37°59′52″N	114°30′56″E
		SJZ-U	29 June	4 July	17	38°02′35″N	114°30′15″E
	Ji’nan	JN-B	29 June	5 July	17	36°35'56″N	117°02'46″E
		JN-U	29 June	5 July	18	36°40′23″N	117°03′01″E
Northwest	Lanzhou	LZ-B	1 August	18 August	53	35°56′35″N	104°09′11″E
		LZ-U	1 August	18 August	52	36°06′11″N	103°37'48″E
YRD	Shanghai	SH-B	1 August	24 August	60	31°31′26″N	121°57′32″E
		SH-U	1 August	24 August	55	31°11'27″N	121°26'04″E
Central China	Wuhan	WH-B	1 August	11 August	42	30°21'40"N	114°20'10"E
		WH-U	1 August	11 August	39	30°31'50″N	114°18'28″E
	Zhengzhou	ZZ-B	29 June	4 July	17	34°51′35″N	113°24′24″E
		ZZ-U	29 June	4 July	17	34°45′12″N	113°36′48″E
Southwest	Chengdu	CD-B	6 August	20 August	55	30°33′47″N	104°16′18″E
		CD-U	6 August	20 August	58	30°37′45″N	104°03′50″E
	Guiyang	GY-B	29 June	4 July	18	26°38'28″N	106°36'60″E
		GY-U	29 June	4 July	17	26°34'02″N	106°41'60″E
PRD	Guangzhou	GZ-B	29 June	4 July	17	23°39′01″N	113°37′28″E
		GZ-U	29 June	4 July	17	23°08′58″N	113°21′28″E
	Shenzhen	SZ	6 June	14 June	18	22°35′47″N	113°58′22″E
	Huizhou	HZ	6 June	14 June	13	23°03'10″N	114°25'06″E
	Jiangmen	JM	7 June	13 June	17	22°35'01″N	113°04'23″E
	Dongguan	DG	6 June	13 June	15	23°03′13″N	113°46′55″E
	Foshan	FS	6 June	13 June	17	23°00′09″N	113°06′13″E
	Zhaoqing	ZQ	6 June	13 June	18	23°02'46″N	112°27'52″E
	Zhongshan	ZS	6 June	13 June	18	22°30′40″N	113°24′27″E
	Zhuhai	ZH	6 June	13 June	17	22°14′19″N	113°29′44″E

Nos: Number of VOC samples. For the sites, B representing the background, and U representing the urban, Sites in the PRD except GZ-B belong to urban.

Table S2. The specific classification of VOCs in this study

Species groups	Species types in saprc07tic	Species included both in observation and simulation	Remarks
Alkanes	ALK1	ethane	kOH between 2 and 5 × 10^2 ppm^{-1} min^{-1}
	ALK2	n-propane	kOH between 5 × 10^2 and 2.5 × 10^3 ppm^{-1} min^{-1}
	ALK3	1-/i-butene, n-butane, isobutane, 2,2-dimethylbutane, 2,2,4-trimehylpentane	kOH between 2.5 × 10^3 and 5 x 10^3 ppm^{-1} min^{-1}
	ALK4	i-pentane, n-pentane, 2-methylpentane, 3-methylpentane, cyclopentane, n-hexane, n-heptane, methylcyclopentane, 2,4-dimethylpentane, 2,3-dimethylpentane, 2,3,4-trimethylpentane, 2,3-dimethylbutane	kOH between 5 × 10^3 and 1 × 10^4 ppm^{-1} min^{-1}
	ALK5	cyclohexane, methylcyclohexane, 2-methylhexane, 3-methylhexane, 2-methylheptane, 3-methylheptane, n-octane, n-nonane, n-decane	kOH > 1 × 10^4 ppm^{-1} min^{-1}
Aromatics	ARO1	ethylbenzene, isopropylbenzene, n-propylbenzene	kOH < 2 × 10^4 ppm^{-1} min^{-1}
	ARO2MN	1,2,3-trimethylbenzene, 1,3,5-trimetylbenzene, o-ethyltoluene, 3-ethyltoluene, 4-ethyltoluene, 1,2,4-trimethylbenzene (0.5)	kOH > 2 × 10^4 ppm^{-1} min^{-1}, minus naphthalene
	TOLU	toluene	
	BENZ	benzene	
	XYL	o-xylene, m/p-xylene	
	B124	1,2,4-trimethylbenzene (0.5)	
Alkenes	OLE1	1-butene, 1-pentene, 3-methyl-1-butene, 4-methyl-1-pentene	kOH < 7 × 10^4 ppm^{-1} min^{-1}, other than ethene
	OLE2	trans-2-butene, cis-2-butene, 2-methyl-1-butene, 2-methyl-2-butene, trans-2-pentene, cis-2-pentene, 2-methyl-1-pentene, cyclopentene, styrene	kOH > 7 × 10^4 ppm^{-1} min^{-1}
	ISOP	isoprene	
	ETHE	ethylene	
	PRPE	propene	
	APIN	a-pinene	
	BDE13	1,3-butadiene	
Alkynes	ACYE	acetylene	
HCHO	HCHO	formaldehyde	

kOH: The reaction rate constant between VOCs and Hydroxyl radical (OH).

Table S3. Model performance of MDA8 O_3 and NO_2 in the 28 sites from June 6th to August 24th, 2018

sites	MDA8 O_3 ($\mu g/m^3$)					NO_2 ($\mu g/m^3$)				
	OBS	PRE	NMB	NME	R	OBS	PRE	NMB	NME	R
BJ-B	162.84	165.43	0.02	0.20	0.72	24.45	15.49	-0.37	0.40	0.40
BJ-U	164.44	193.04	**0.17**	0.23	0.75	34.19	29.61	-0.13	0.31	0.11
SJZ-B	170.29	168.29	-0.01	0.21	0.66	25.20	39.46	0.57	0.63	0.19
SJZ-U	163.98	168.29	0.03	0.22	0.64	29.70	39.46	0.33	0.41	0.30
JN-B	175.43	161.04	-0.08	0.19	0.68	21.05	26.08	0.24	0.41	0.46
JN-U	167.26	161.04	-0.04	0.18	0.72	36.91	26.08	-0.29	0.34	0.46
LZ-B	118.63	116.73	-0.02	0.11	0.66	15.78	6.23	-0.61	0.61	0.22
LZ-U	165.22	135.31	**-0.18**	**0.25**	0.65	38.06	20.75	-0.46	0.46	0.18
SH-B	106.43	88.93	**-0.16**	**0.33**	0.57	21.04	1.43	-0.93	0.93	0.45
SH-U	113.56	136.59	**0.20**	**0.29**	0.80	23.01	32.99	0.43	0.47	0.70
WH-B	140.23	141.09	0.01	0.23	0.70	36.42	37.62	0.03	0.27	0.47
WH-U	126.62	141.09	0.11	0.25	0.72	35.46	37.62	0.06	0.22	0.51
ZZ-B	150.74	172.08	0.14	0.23	0.61	34.96	36.51	0.05	0.22	0.52
ZZ-U	147.25	158.44	0.08	0.24	0.66	39.16	34.23	-0.13	0.22	0.49
CD-B	114.06	119.92	0.05	0.25	0.62	43.09	30.80	-0.29	0.36	0.14
CD-U	140.56	133.25	-0.05	**0.28**	0.56	30.99	59.51	0.92	0.94	0.14
GY-B	89.98	95.00	0.06	0.15	0.82	16.76	18.54	0.11	0.34	0.44
GY-U	85.49	95.00	0.11	0.19	0.79	30.06	18.54	-0.38	0.39	0.67
GZ-B	106.09	121.60	0.15	**0.35**	**0.37**	21.72	12.24	-0.44	0.44	0.71
GZ-U	115.63	144.78	**0.25**	**0.34**	0.55	35.30	23.71	-0.33	0.36	0.56
SZ	80.73	112.05	**0.39**	**0.50**	0.71	20.97	31.38	0.50	0.52	0.67
HZ	97.19	111.21	0.15	**0.27**	0.75	21.99	19.57	-0.11	0.24	0.65
JM	104.73	118.35	0.13	**0.28**	0.82	28.08	19.39	-0.31	0.34	0.54
DG	118.77	139.30	**0.21**	**0.35**	0.64	32.25	24.93	-0.23	0.27	0.62
FS	113.21	148.99	**0.32**	**0.44**	0.64	33.31	27.79	-0.17	0.28	0.51
ZQ	109.02	117.98	0.08	0.23	0.76	30.94	12.00	-0.61	0.62	0.40
ZS	102.66	134.08	**0.31**	**0.42**	0.79	12.87	17.42	0.35	0.49	0.65
ZH	92.39	114.00	**0.23**	**0.38**	0.72	13.71	9.30	-0.32	0.52	0.49
Benchmarks			<=±0.15	<0.25	>0.5					

OBS: mean observation; PRE: mean prediction; NMB: normalized mean bias; NME: normalized mean error; R: the correlation coefficient. The performance criteria for MDA8 O_3 were suggested by (Emery et al., 2017). The values that exceed the criteria were highlighted in bold.

Table S4. Comparison of mean values of O_3, NO_2 and TVOCs concentrations at 28 sites during the study period

sites	O_3 (μg/m^3)		NO_2 (μg/m^3)		TVOCs (ppbv)	
	OBS	PRE	OBS	PRE	OBS	PRE
BJ-B	139.32	150.78	14.85	8.35	23.19	18.36
BJ-U	140.94	188.26	23.65	20.62	33.24	30.45
SJZ-B	164.56	164.68	29.65	14.88	35.59	14.47
SJZ-U	150.50	161.58	29.19	15.09	35.47	14.67
JN-B	135.33	158.06	42.94	11.15	53.37	12.03
JN-U	144.75	161.99	41.82	11.13	61.93	12.07
LZ-B	97.59	107.96	13.49	3.19	33.16	5.16
LZ-U	129.04	117.69	30.92	11.16	52.21	8.92
SH-B	100.19	81.46	22.17	0.80	12.97	3.66
SH-U	111.04	120.69	21.59	28.62	18.79	29.72
WH-B	141.45	168.78	37.37	22.60	22.65	24.69
WH-U	118.03	166.14	34.38	22.70	30.48	25.10
ZZ-B	127.76	169.24	40.71	17.21	29.79	15.89
ZZ-U	131.35	161.50	46.06	14.93	28.13	13.71
CD-B	100.85	119.01	37.98	14.55	39.43	27.64
CD-U	130.86	131.87	25.09	43.52	34.72	62.36
GY-B	58.18	68.08	11.44	8.92	26.06	9.50
GY-U	53.82	66.69	25.59	8.77	22.83	9.41
GZ-B	78.29	140.98	19.38	7.20	15.92	12.84
GZ-U	88.29	137.19	24.12	12.75	24.19	17.05
SZ	89.23	106.51	36.27	38.40	34.09	33.41
HZ	66.31	62.82	22.62	21.40	26.86	24.84
JM	104.29	100.04	29.44	18.48	28.68	22.02
DG	66.71	102.58	40.43	29.02	32.08	25.06
FS	68.93	98.16	33.29	38.47	32.76	33.08
ZQ	80.24	89.25	30.06	12.92	31.98	22.44
ZS	95.78	118.94	18.83	23.21	27.29	23.18
ZH	103.82	147.99	24.00	17.99	28.53	20.26

Table S5. The mean, median, maximum (max), minimum (min), and standard deviation (SD) values of the ratios and differences (Diff) for 5 VOCs groups, ARO2MN and BENZ at 18 urban sites, accurate to two places of decimals

		Alkanes	Alkenes	Aromatics	ARO2MN (aromatics)	BENZ (aromatics)	Alkyne	HCHO
	mean	0.66	0.72	1.46	0.44	3.29	0.53	1.83
	median	0.59	0.69	1.41	0.32	2.75	0.42	1.19
Ratio(pre/obs)	max	1.87	2.46	3.29	1.96	9.01	1.50	8.70
	min	0.13	0.09	0.10	0.05	0.14	0.09	0.25
	SD	0.42	0.54	0.84	0.46	1.97	0.34	1.91
	mean	-5.78	-3.29	1.07	-0.26	0.42	-1.23	0.58
	median	-5.42	-2.17	1.61	-0.18	0.54	-1.35	0.54
Diff(pre-obs)	max	14.12	3.50	6.09	0.24	1.28	0.87	5.57
	min	-19.40	-15.50	-8.18	-0.74	-2.58	-2.64	-8.90
	SD	7.82	4.86	3.68	0.24	0.81	0.97	2.95

Table S6. Impact of improvement of emission inventory. Median of ratio of predicted to observed values for each urban site after adjusting emission coefficients for individual species or both of them in MEIC

Cases in CMAQ	O_3	NO_2	ALK2	ARO2MN	BENZ	OLE1	PRPE	ACYE
Base case	1.240	0.623	0.270	0.325	2.541	0.340	0.445	0.468
case_NO_x	1.148	0.899						
case _ALK2	1.243		0.789					
case_ARO2MN	1.250			0.863				
case_BENZ	1.240				1.556			
case_OLE1	1.249					0.522		
case_PRPE	1.248						0.688	
case_ACYE	1.241							0.978
case_all	1.269	0.622	0.791	0.863	1.556	0.687	0.652	0.981

Table S7. The mean, median, max, min, and SD values of the ratios for predicted/observed TVOCs for 28 sites in base case and eight new cases, accurate to two places of decimals

	mean	median	max	min	SD
Base case	0.70	0.74	1.90	0.15	0.40
case_NOx	0.70	0.73	1.91	0.14	0.40
case _ALK2	0.75	0.79	2.04	0.16	0.42
case_ARO2MN	0.71	0.75	1.93	0.15	0.40
case_BENZ	0.69	0.73	1.87	0.14	0.39
case_OLE1	0.72	0.75	1.94	0.15	0.41
case_PRPE	0.71	0.75	1.94	0.15	0.40
case_ACYE	0.74	0.78	2.00	0.15	0.42
case_all	0.81	0.86	2.25	0.17	0.47

Table S8. The mean, median, max, min, and std values of O_3 changes were calculated for eight new cases relative to the base case for 28 sites, accurate to two places of decimals

	mean	median	max	min	SD
case_NOx	0.02%	1.01%	8.66%	-12.29%	5.69%
case _ALK2	0.30%	0.31%	0.54%	0.13%	0.10%
case_ARO2MN	0.82%	0.68%	2.41%	0.06%	0.54%
case_BENZ	0.01%	0.00%	0.09%	-0.07%	0.04%
case_OLE1	0.79%	0.76%	1.78%	0.19%	0.40%
case_PRPE	0.63%	0.55%	1.81%	0.14%	0.35%
case_ACYE	0.01%	0.02%	0.05%	-0.03%	0.02%
case_all	2.51%	2.32%	6.27%	0.62%	1.28%

Table S9. Model performance of temperature (T2) and relative humidity (RH) in the 28 sites from June 6th to August 24th, 2018

sites	T2 (℃)					RH (%)				
	OBS	PRE	MB	ME	RMSE	OBS	PRE	MB	ME	RMSE
BJ-B	26.51	26.63	0.12	1.27	1.61	74.99	61.60	-13.39	14.11	16.50
BJ-U	27.46	29.51	**2.05**	**2.09**	2.58	67.23	49.64	-17.59	17.66	19.27
SJZ-B	28.56	29.38	0.83	1.34	1.63	65.24	51.28	-13.96	14.09	16.03
SJZ-U	28.07	29.38	**1.32**	1.60	2.05	66.23	51.28	-14.95	14.97	17.32
JN-B	28.11	28.45	0.34	1.08	1.49	66.56	61.32	-5.23	7.32	9.75
JN-U	28.11	28.45	0.34	1.08	1.49	66.56	61.32	-5.23	7.32	9.75
LZ-B	19.41	19.00	-0.41	0.85	1.09	71.23	65.58	-5.66	7.64	9.14
LZ-U	23.36	22.24	**-1.13**	1.29	1.53	58.30	52.92	-5.37	6.45	8.15
SH-B	27.21	23.55	**-3.66**	**3.93**	4.62	85.48	92.74	7.26	8.92	10.62
SH-U	28.40	28.94	**0.54**	0.99	1.22	75.48	66.03	-9.46	9.75	10.83
WH-B	29.19	29.25	0.07	0.91	1.20	75.27	70.62	-4.65	6.25	8.04
WH-U	29.19	29.25	0.07	0.91	1.20	75.27	70.62	-4.65	6.25	8.04
ZZ-B	29.05	30.05	**1.00**	1.17	1.50	65.88	54.92	-10.96	11.24	13.04
ZZ-U	29.25	29.42	0.17	1.01	1.28	65.69	59.09	-6.60	9.56	11.06
CD-B	25.90	26.21	0.31	1.00	1.27	87.03	77.37	-9.66	9.95	12.23
CD-U	26.10	27.13	**1.03**	1.36	1.65	82.16	72.21	-9.94	10.53	12.48
GY-B	22.93	21.84	**-1.10**	1.12	1.32	76.95	86.56	9.61	9.61	10.56
GY-U	24.12	21.84	**-2.28**	**2.28**	2.42	75.85	86.56	10.71	10.71	11.69
GZ-B	27.74	27.20	-0.54	0.89	1.11	87.30	81.71	-5.59	6.25	7.98
GZ-U	28.12	31.27	**3.15**	**3.15**	3.38	84.48	62.21	-22.27	22.27	23.17
SZ	28.38	30.53	**2.15**	**2.20**	2.35	83.16	65.96	-17.20	17.20	17.84
HZ	27.95	28.00	0.05	0.89	1.12	83.42	79.16	-4.26	5.79	7.04
JM	28.74	28.52	-0.22	0.79	0.98	83.56	78.71	-4.85	6.23	7.55
DG	28.38	31.36	**2.98**	**2.98**	3.15	81.59	62.09	-19.50	19.50	20.42
FS	29.03	31.80	**2.77**	**2.77**	2.93	79.31	60.25	-19.06	19.06	19.74
ZQ	27.92	28.04	0.12	0.91	1.06	84.76	80.73	-4.04	5.65	6.86
ZS	28.63	30.86	**2.23**	**2.24**	2.41	86.39	65.91	-20.48	20.48	21.21
ZH	28.42	28.54	0.13	0.98	1.20	82.75	87.53	4.78	7.02	8.55
Benchmarks			≤±0.5	≤2.0						

RMSE: root mean square error. The performance criteria for T2 were suggested by (Emery et al., 2001). The values that exceed the criteria were highlighted in bold.

Table S10. Model performance of wind speed (WS) and wind direction (WD) in the 28 sites from June 6th to August 24th, 2018

sites	WS (m/s)					WD (°)				
	OBS	PRE	MB	ME	RMSE	OBS	PRE	MB	ME	RMSE
BJ-B	1.75	2.67	**0.92**	0.97	1.19	192.45	129.46	**-62.99**	**67.84**	80.15
BJ-U	1.82	2.43	**0.61**	0.74	0.95	130.57	144.46	**13.88**	**38.27**	51.37
SJZ-B	1.73	2.83	**1.10**	1.15	1.34	165.69	155.74	-9.95	**37.99**	52.44
SJZ-U	2.31	2.83	**0.53**	0.70	0.88	180.14	155.74	**-24.40**	**45.03**	60.91
JN-B	3.22	3.76	**0.54**	0.82	0.99	142.89	146.54	3.65	19.84	25.48
JN-U	3.22	3.76	**0.54**	0.82	0.99	142.89	146.54	3.65	19.84	25.48
LZ-B	2.59	3.24	**0.65**	0.79	0.92	183.44	147.74	**-35.71**	**45.89**	66.64
LZ-U	1.47	2.70	**1.23**	1.23	1.39	124.15	130.88	6.74	**42.11**	53.33
SH-B	3.99	6.14	**2.15**	**2.16**	**2.59**	124.58	122.10	-2.48	18.50	27.98
SH-U	0.39	3.69	**3.30**	**3.30**	**3.52**	66.66	129.84	**63.18**	**65.19**	77.48
WH-B	3.01	2.54	-0.47	0.65	0.81	157.99	142.73	**-15.26**	**46.70**	67.92
WH-U	3.01	2.54	-0.47	0.65	0.81	157.99	142.73	**-15.26**	**46.70**	67.92
ZZ-B	1.99	3.04	**1.05**	1.11	1.46	144.26	135.84	-8.42	**30.04**	38.62
ZZ-U	2.58	3.22	**0.65**	0.81	1.14	141.91	136.46	-5.45	29.11	42.43
CD-B	2.03	2.21	0.18	0.53	0.71	142.02	117.14	**-24.87**	**49.27**	60.78
CD-U	1.40	2.02	**0.62**	0.73	0.83	163.73	149.16	**-14.57**	**41.82**	52.33
GY-B	2.66	3.34	**0.68**	0.87	1.15	141.62	154.37	**12.75**	**30.86**	42.07
GY-U	2.00	3.34	**1.34**	1.45	1.85	151.02	154.37	3.36	**32.10**	45.16
GZ-B	1.61	2.63	**1.03**	1.10	1.39	126.01	139.07	**13.07**	**47.50**	61.43
GZ-U	1.93	2.74	**0.81**	0.91	1.13	147.31	139.80	-6.96	**44.63**	58.13
SZ	2.35	3.37	**1.02**	1.13	1.35	155.20	159.66	4.46	24.36	32.15
HZ	2.48	3.00	**0.52**	0.70	0.93	146.88	137.97	-8.91	26.70	34.97
JM	3.04	3.04	0.00	0.68	0.81	155.96	163.82	7.87	27.65	39.23
DG	3.00	3.18	0.18	0.56	0.67	136.78	149.56	**12.79**	23.61	31.29
FS	2.75	3.02	0.27	0.62	0.74	149.55	153.86	4.32	**32.81**	42.51
ZQ	1.60	2.64	**1.04**	1.06	1.23	122.24	156.20	**33.97**	**56.66**	65.52
ZS	2.53	3.29	**0.76**	0.80	0.96	144.01	158.70	**14.69**	20.44	29.20
ZH	3.74	4.96	**1.22**	1.27	1.53	159.18	156.30	-2.88	22.25	31.82
Benchmarks			⩽±0.5	⩽2.0	⩽2.0			⩽±10	⩽±30	

The performance criteria for WS and WD were suggested by (Emery et al., 2001). The values that exceed the criteria were highlighted in bold.

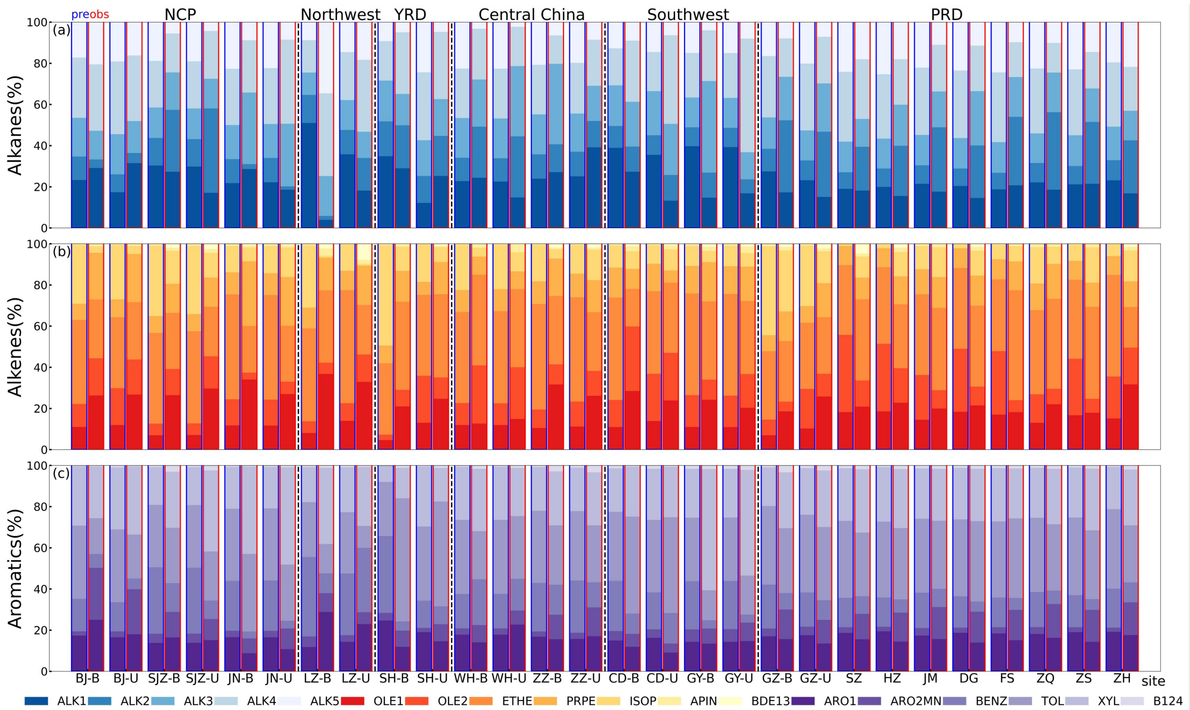

Figure S1. Percentage of predicted and observed VOCs of specific species at 28 sites during the study period. For each site, on the left are prediction values with blue edge, and on the right are observation values with red edge (a) Alkanes, (b) Alkenes, (c) Aromatics.

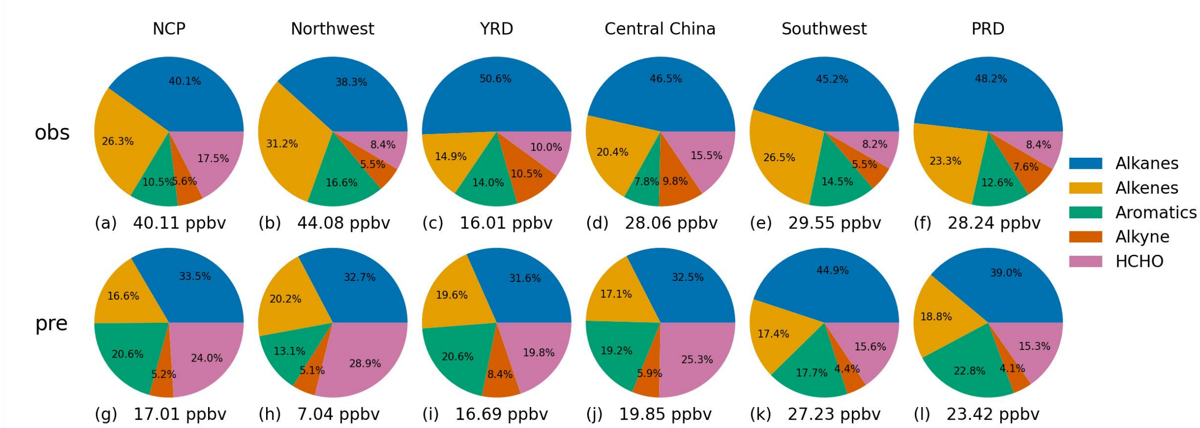

Figure S2. Observed (a-f) and predicted (g-l) values of different VOCs species groups by regional average. TVOCs concentration of each region is shown at the bottom.

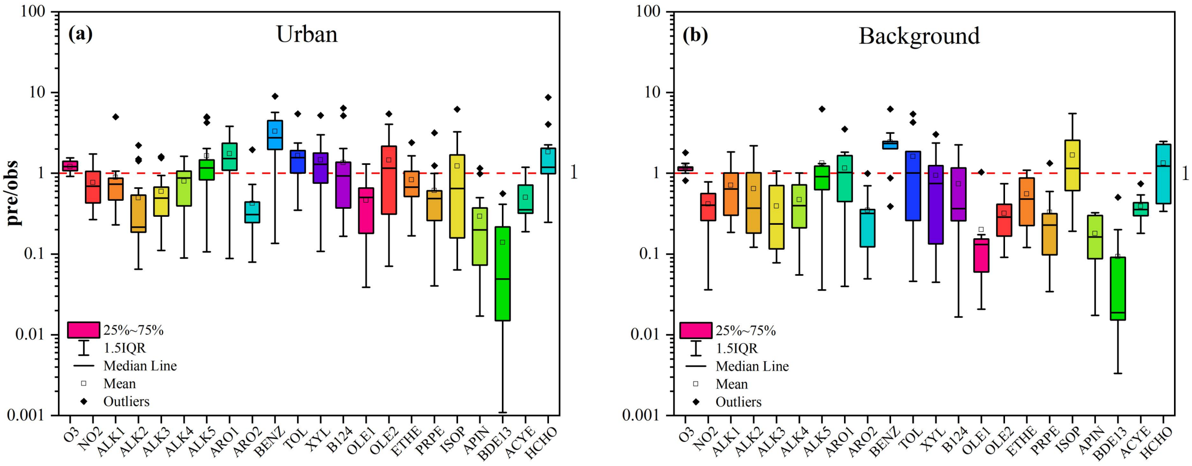

Figure S3. Ratio (pre/obs) of O_3, NO_2 and different VOCs species at (a) urban sites (18 sites) and (b) backgound sites (10 sites).

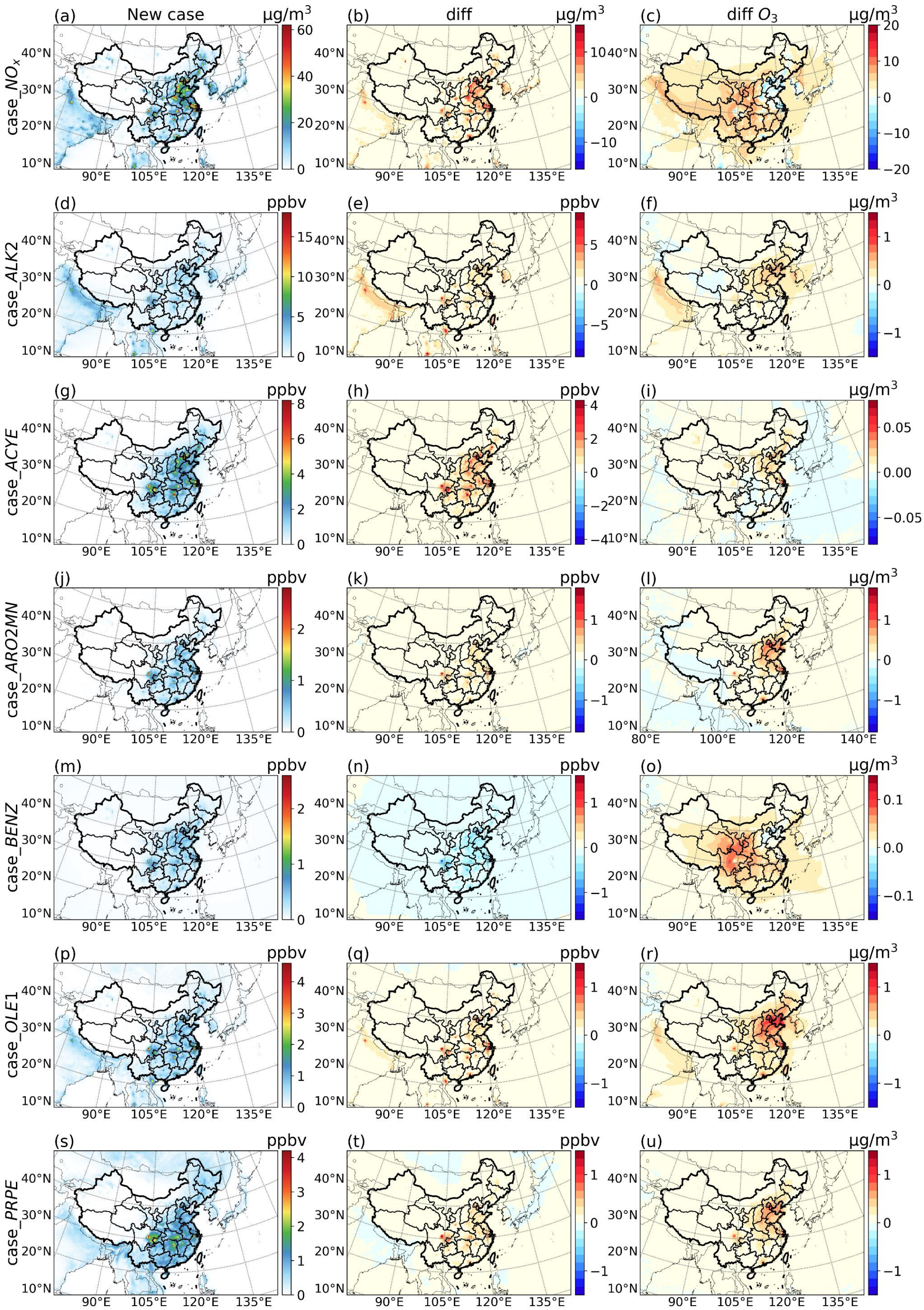

Figure S4. The difference between the predicted concentration of seven new cases and base case, and the impact on O_3 concentration from June 6th to August 24th in 2018. Concentration of NO_2 is shown in case_NO_x.

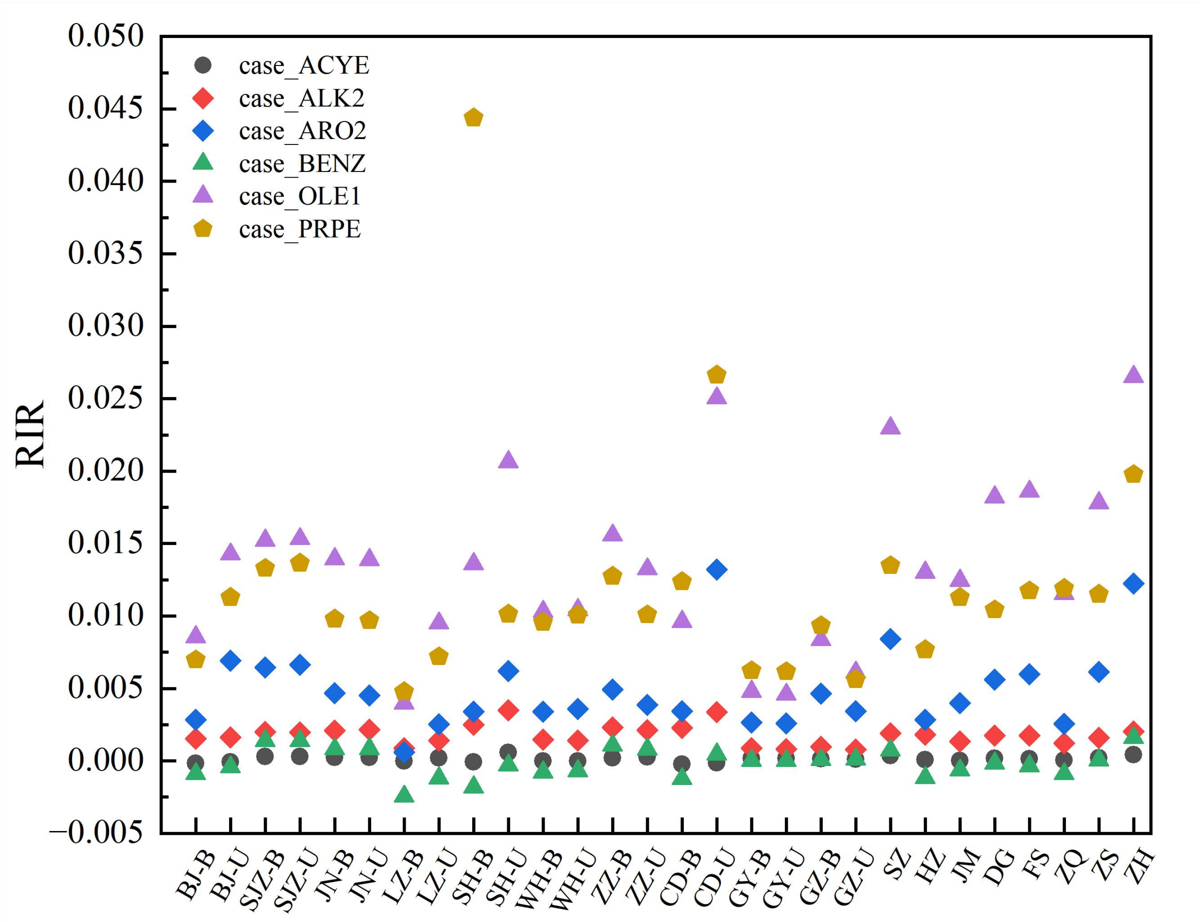

Figure S5. Relative Incremental Reactivity (RIR) of 6 VOCs at 28 sites during the study period. Each dot represents the RIR of the specific VOCs corresponding to the case at that site.

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