Supplement of

Application and Evaluation of CRACMM V1.0 Mechanism in $PM_{2.5}$ Simulation Over China

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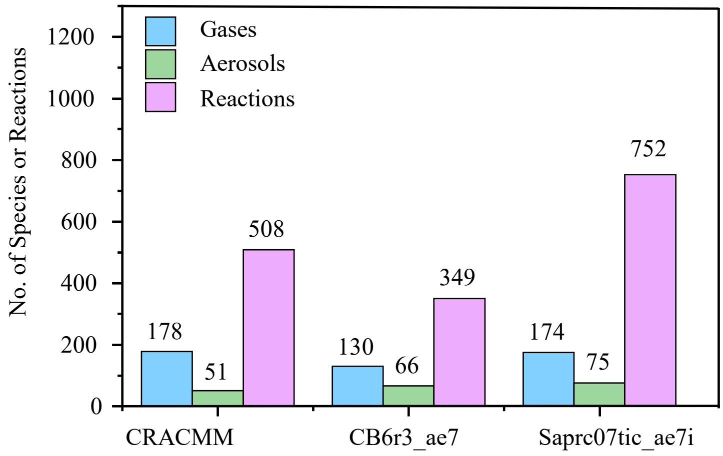

Figure S1. Number of chemical reactions, gas-phase species, and particle-phase species in three chemical mechanisms implemented in CMAQ.

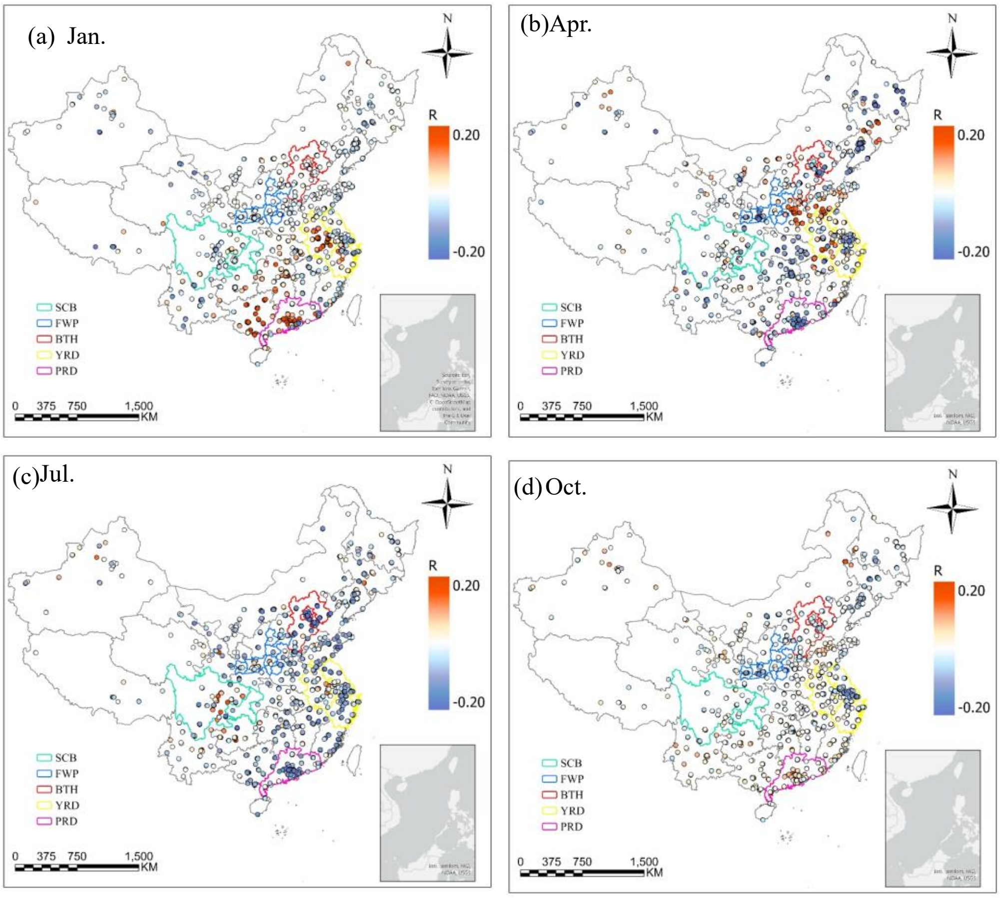

Figure S2. Differences in the R values of $PM_{2.5}$ between CRACMM（full volatile inventory）and CB6r3_ae7, evaluated for January, April, July, and October of 2021.

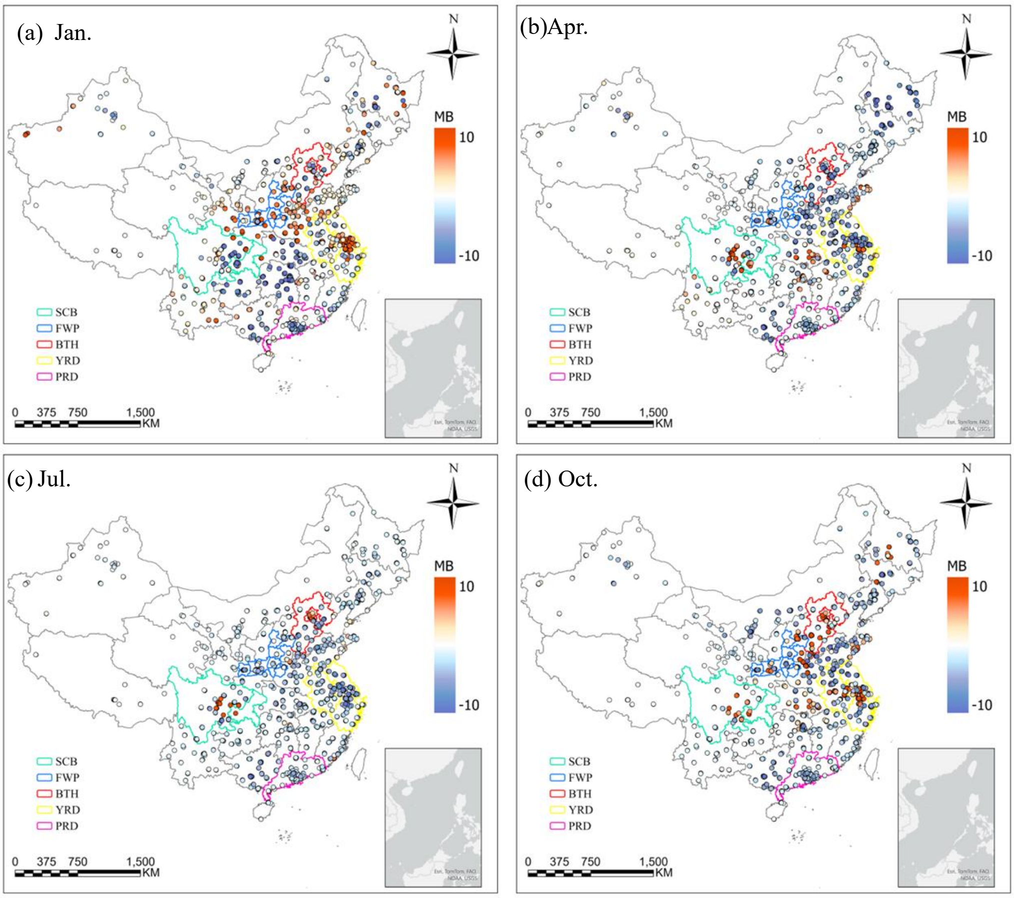

Figure S3. Differences in the MB values of $PM_{2.5}$ between CRACMM（full volatile inventory） and CB6r3_ae7, evaluated for January, April, July, and October of 2021.

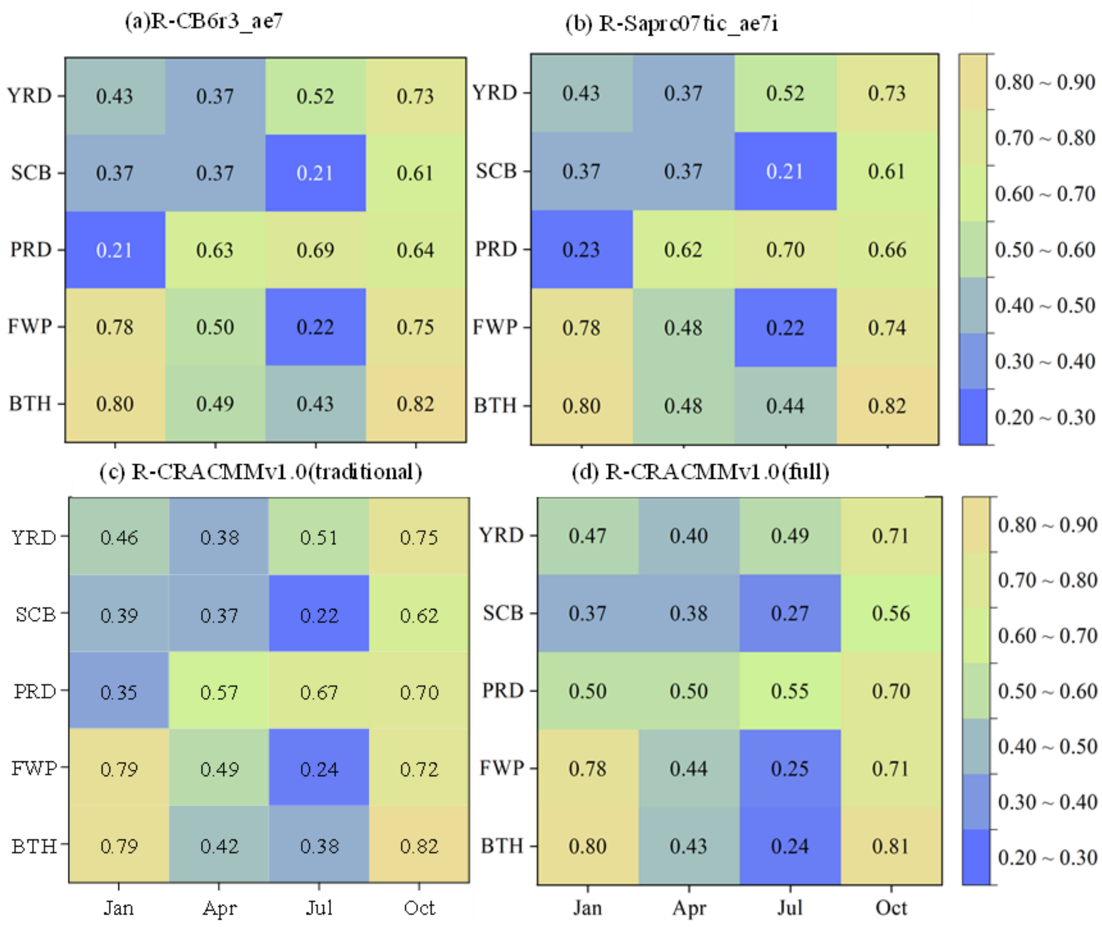

Figure S4. R values across five regions (YRD, SCB, PRD, FWP, BTH) and four months (January, April, July, October) for $PM_{2.5}$ estimated using (a) CB6r3_ae7, (b) Saprc07tic_ae7i, (c) CRACMM with traditional POA inventory and (d) CRACMM with full volatile inventory.

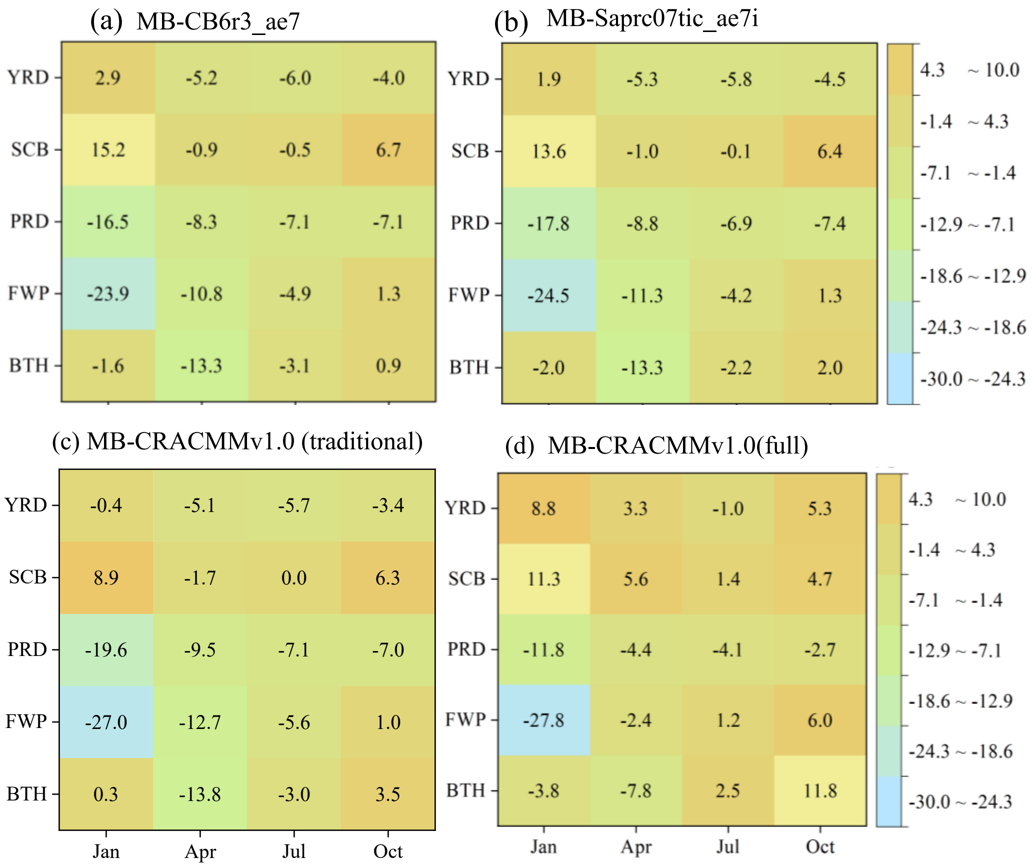

Figure S5. MB (μg/m³) across five regions (YRD, SCB, PRD, FWP, BTH) and four months (January, April, July, October) for $PM_{2.5}$ using (a) Cb6r3_ae7, (b) Saprc07tic_ae7i, (c) CRACMM with traditional POA inventory and (d) CRACMM with full volatile inventory.

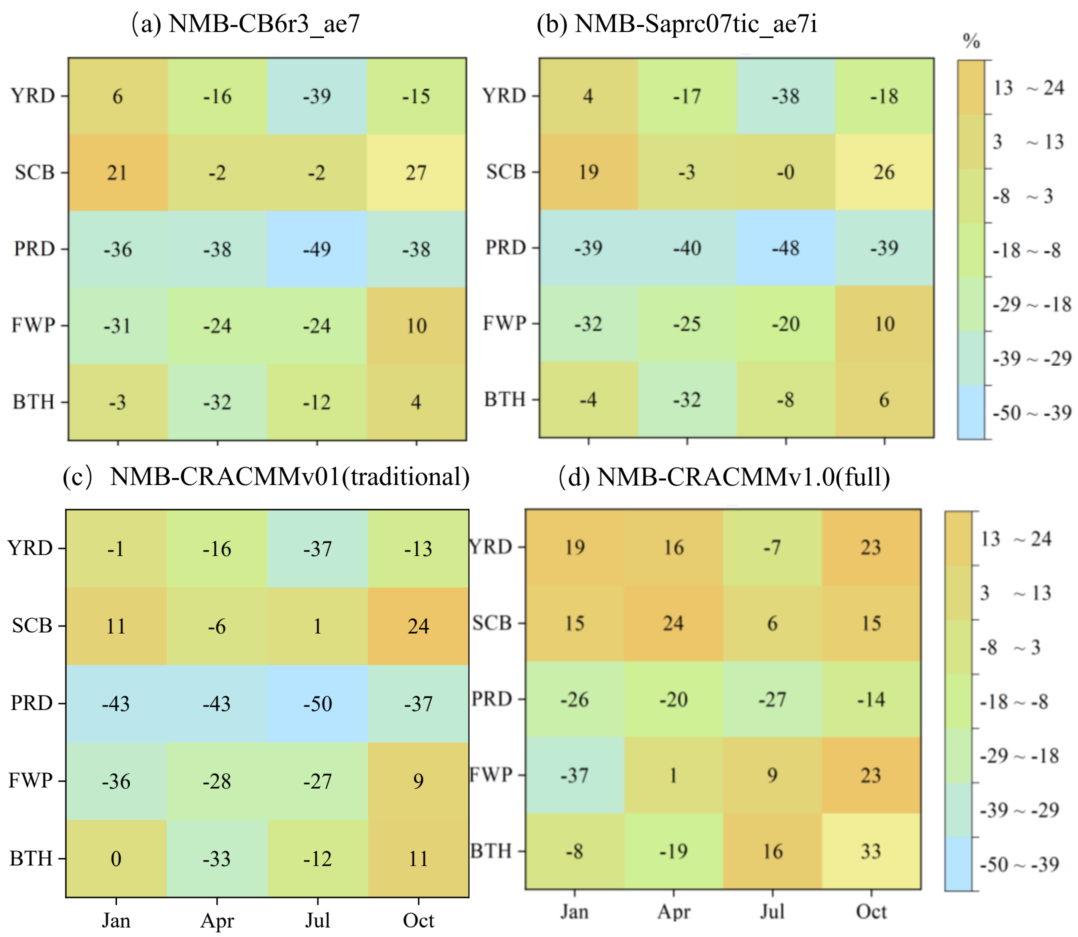

Figure S6. NMB (%) across five regions (YRD, SCB, PRD, FWP, BTH) and four months (January, April, July, and October) for (a) CB6r3_ae7, (b) Saprc07tic_ae7i, (c) CRACMM with traditional POA inventory, and (d) CRACMM with full volatile POA inventory.

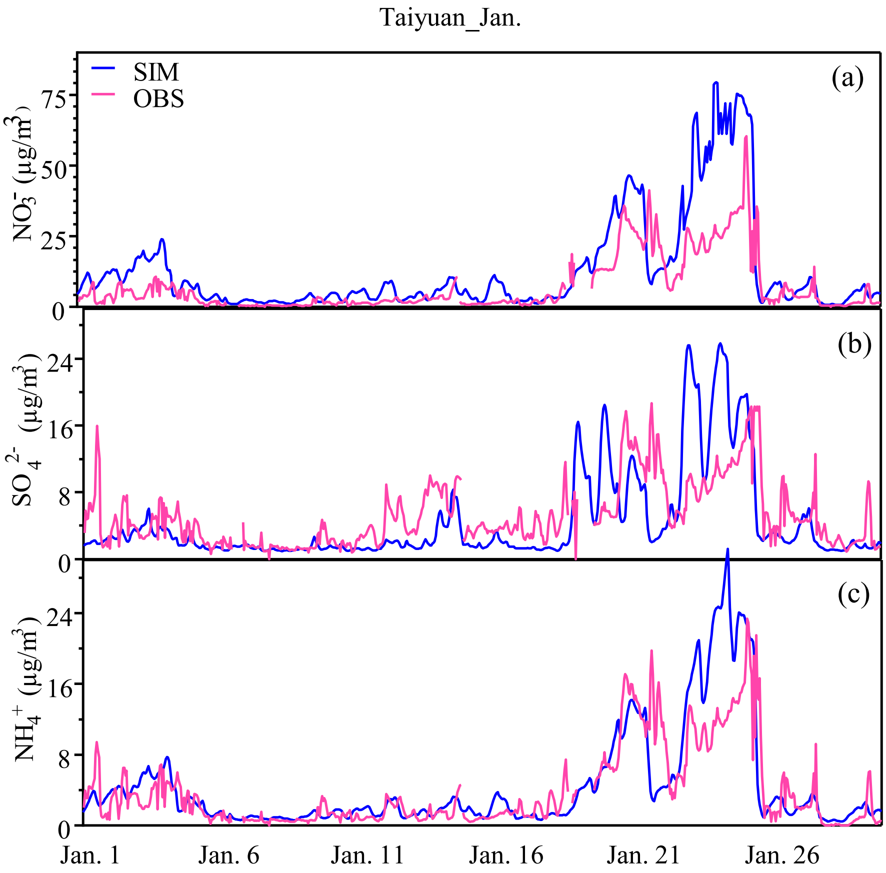

Figure S7. Comparison of hourly concentrations of (a) NO_3^-, (b) SO_4^{2-}, (c) NH_4^+ at Taiyuan in January 2021, based on ground-based observations (pink) and model simulations (blue).

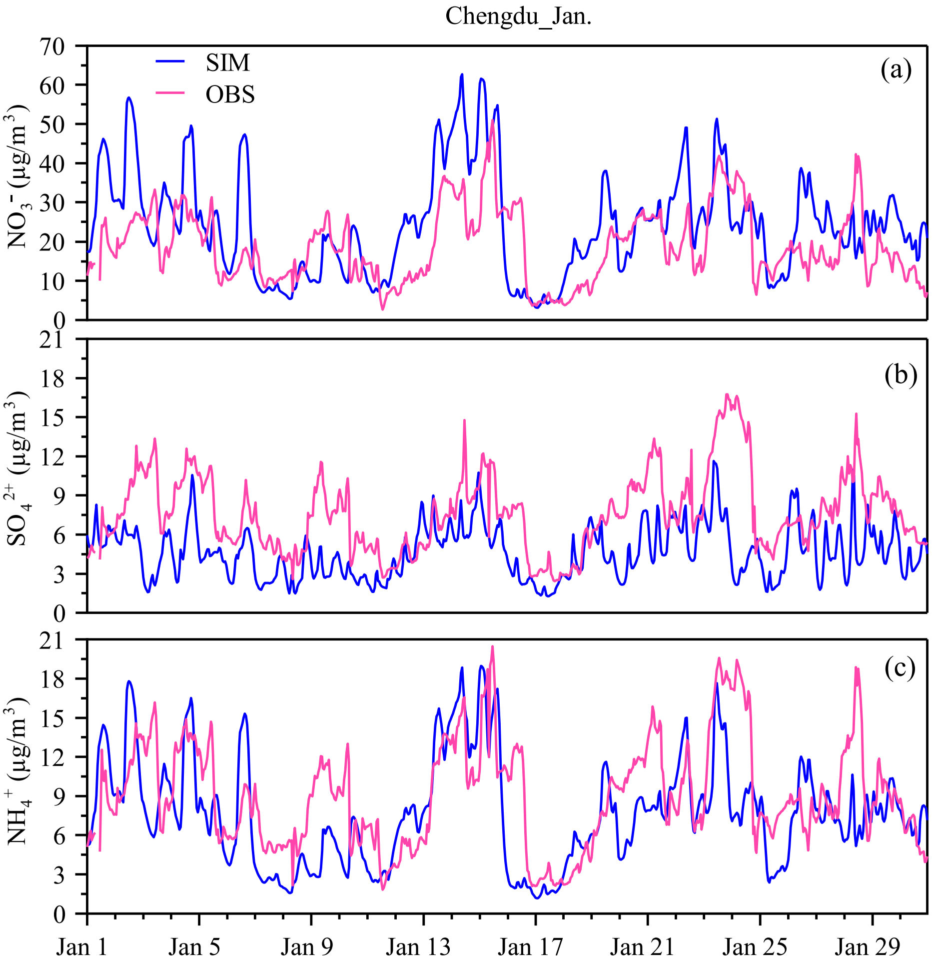

Figure S8. Comparison of hourly concentrations of (a) NO_3^-, (b) SO_4^{2-}, (c) NH_4^+ at Chengdu in January 2021, based on ground-based observations (pink) and model simulations (blue).

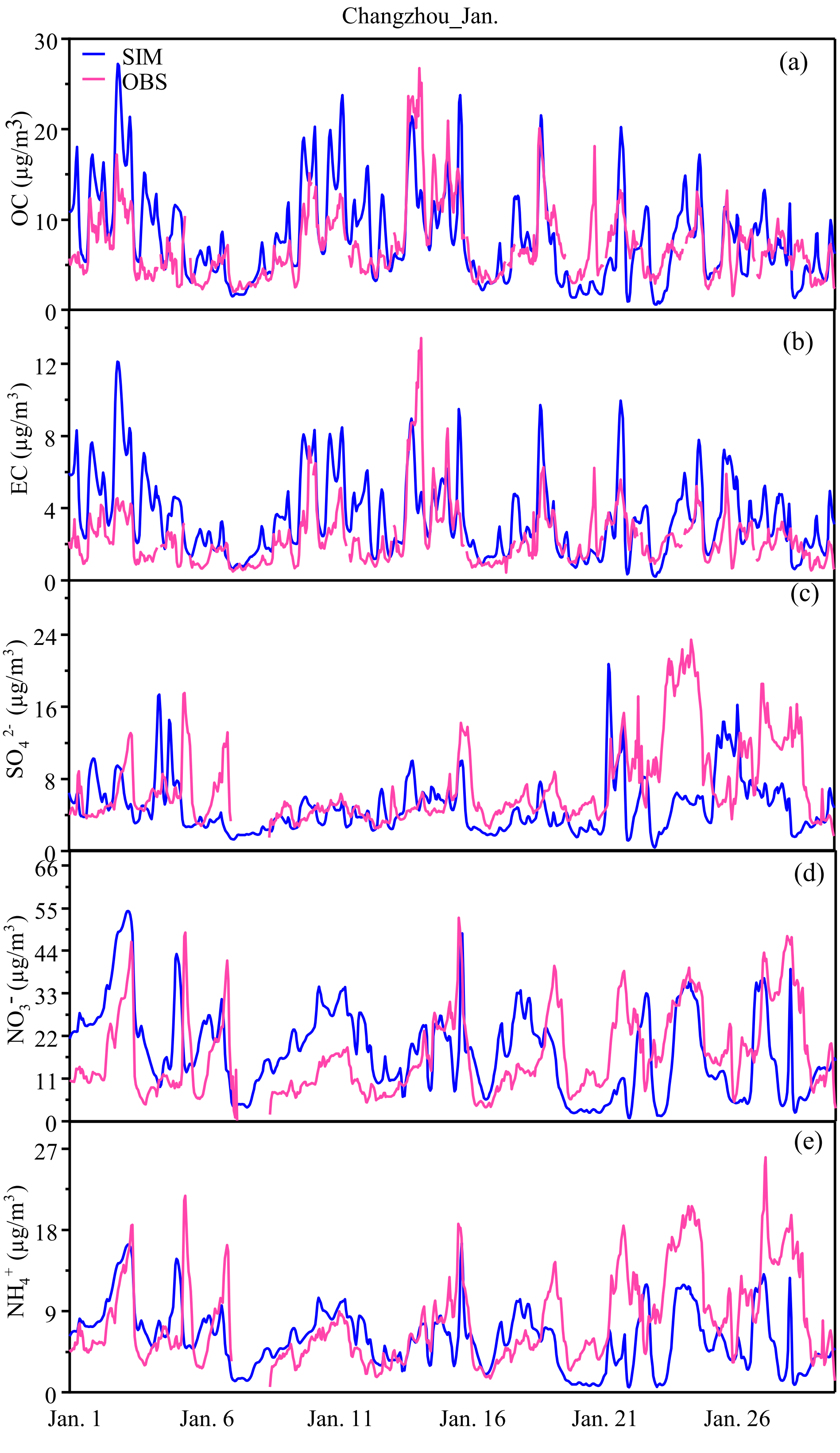

Figure S9. Comparison of hourly concentrations of (a) OC, (b) EC, (c) SO_4^{2-}, (d) NO_3^-, (e) NH_4^+ at Changzhou in January 2021, based on ground-based observations (pink) and model simulations (blue).

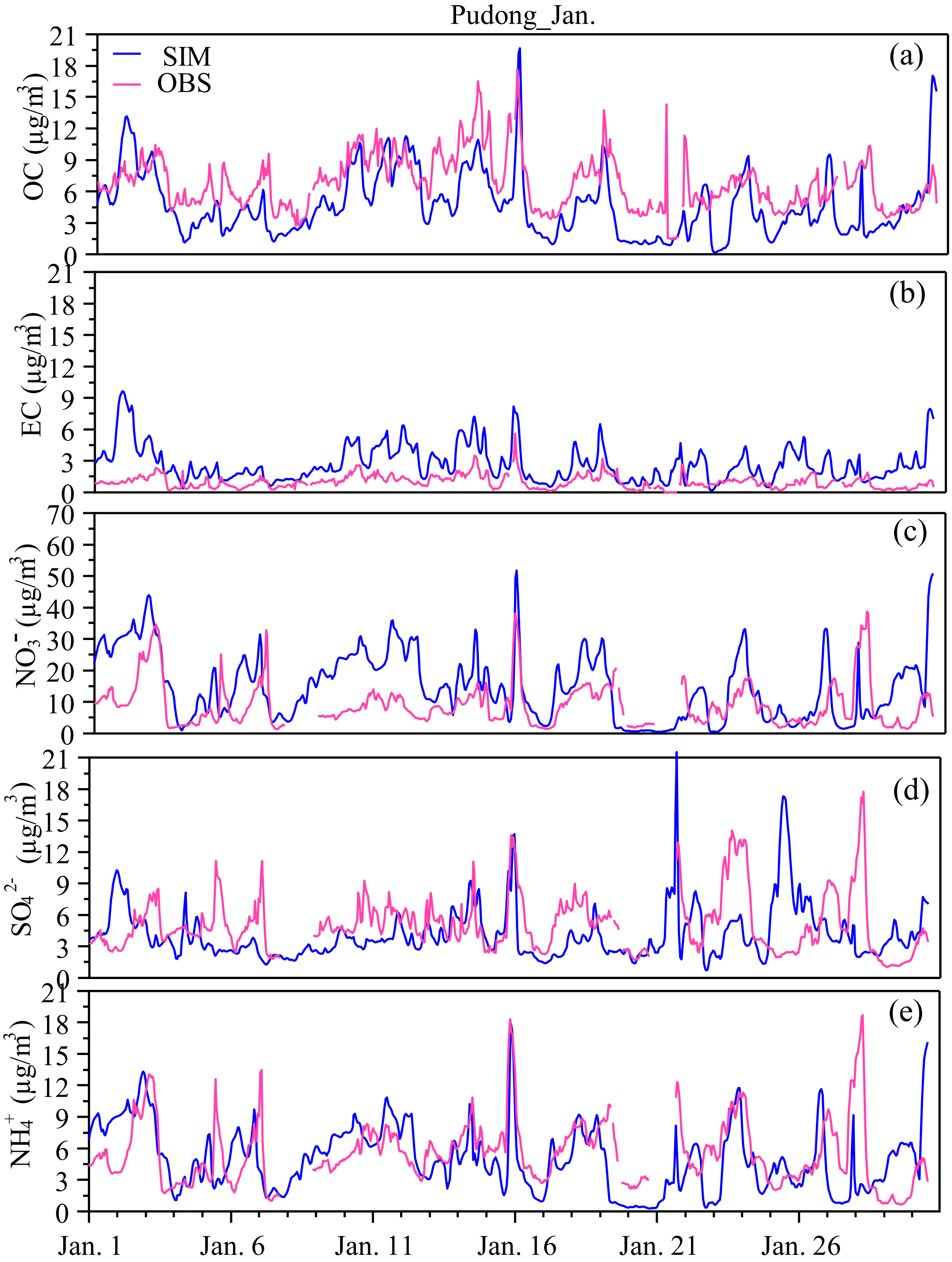

Figure S10. Comparison of hourly concentrations of (a) OC, (b) EC, (c) SO_4^{2-}, (d) NO_3^-, (e) NH_4^+ at Pudong in January 2021, based on ground-based observations (pink) and model simulations (blue).

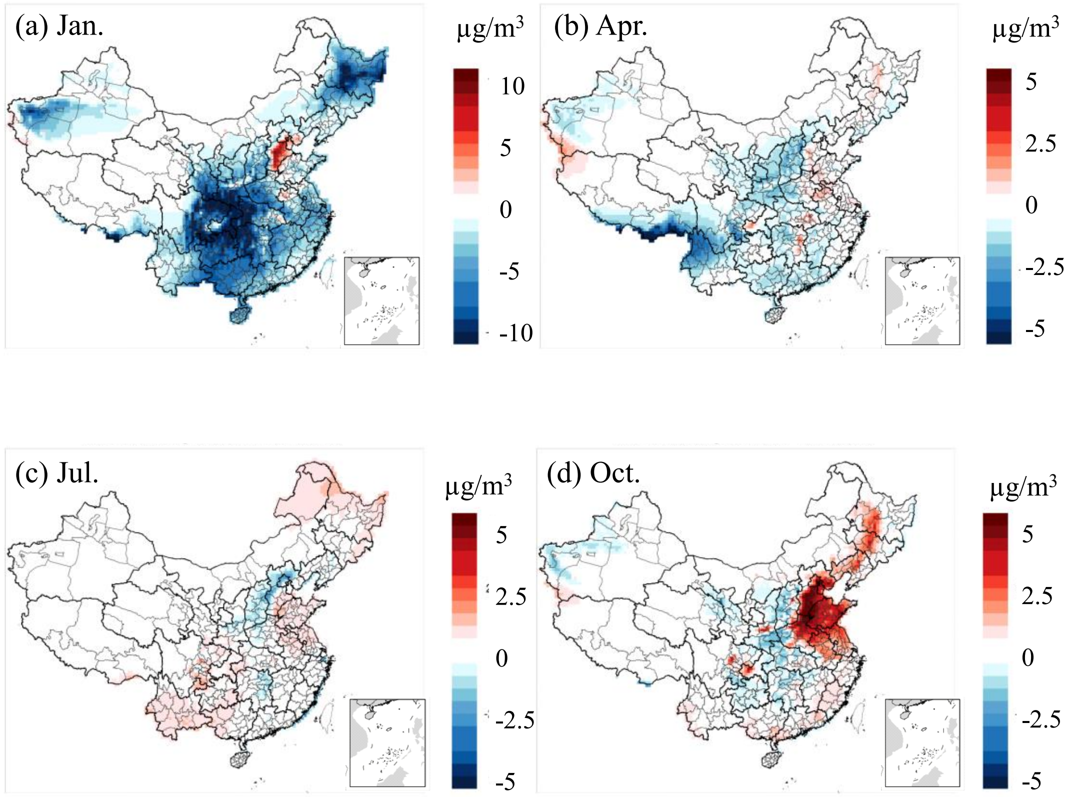

Figure S11. Differences in model-predicted $PM_{2.5}$ concentrations between CRACMM（traditional POA inventory) and CB6r3_ae7.

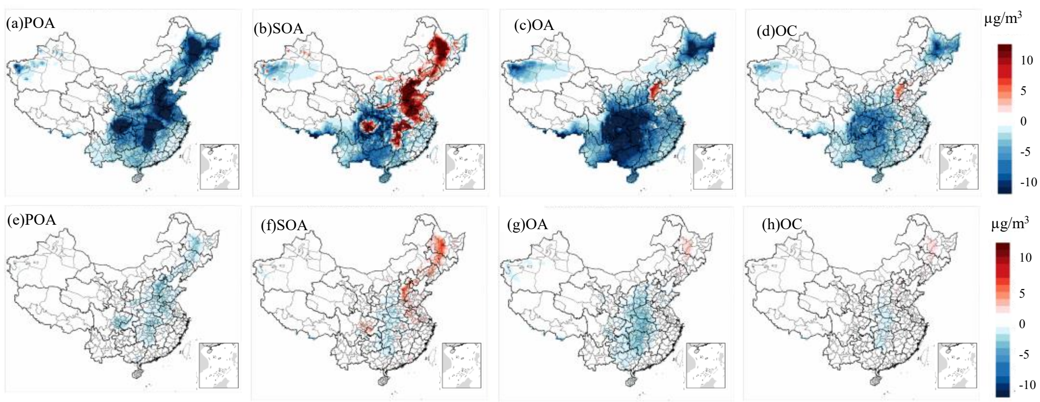

Figure S12. Differences in model-predicted $PM_{2.5}$ components—(a) POA, (b) SOA, (c) OA, and (d) OC for January, and (e) POA, (f) SOA, (g) OA, and (h) OC for October—between CRACMM (with the traditional POA inventory) and CB6r3_ae7. Figures (a–d) share the same scale, as do figures (e–h).

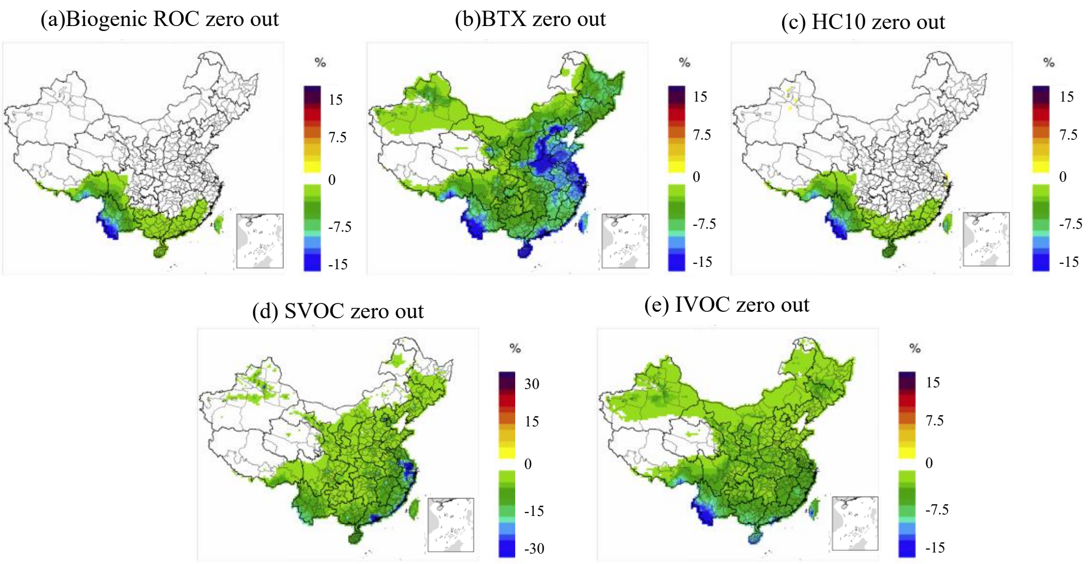

Figure S13. Percent changes in $PM_{2.5}$ concentrations between each zero-out scenario and its corresponding base simulation: (a)biogenic emissions, (b) BTX, (c) HC10, (d) SVOC, and (e) IVOC.

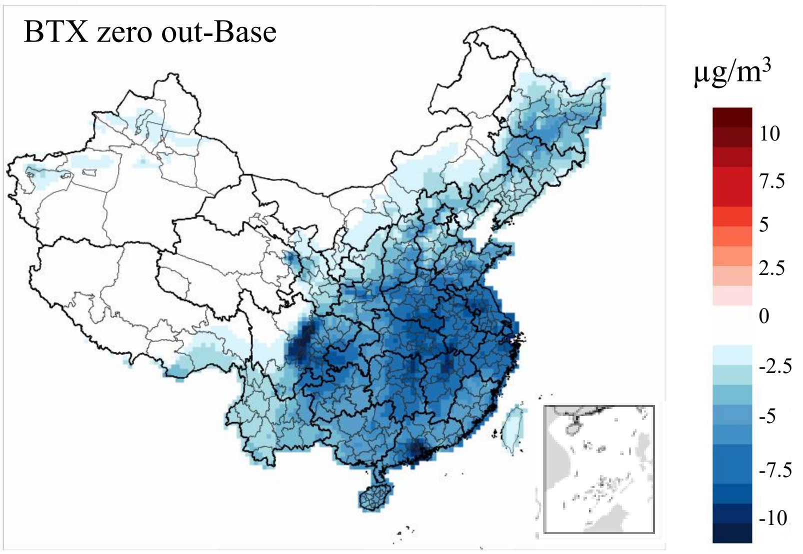

Figure S14. Difference in average O_3 concentrations between the BTX zero-out scenario and the base CRACMM simulation using the full volatile inventory.

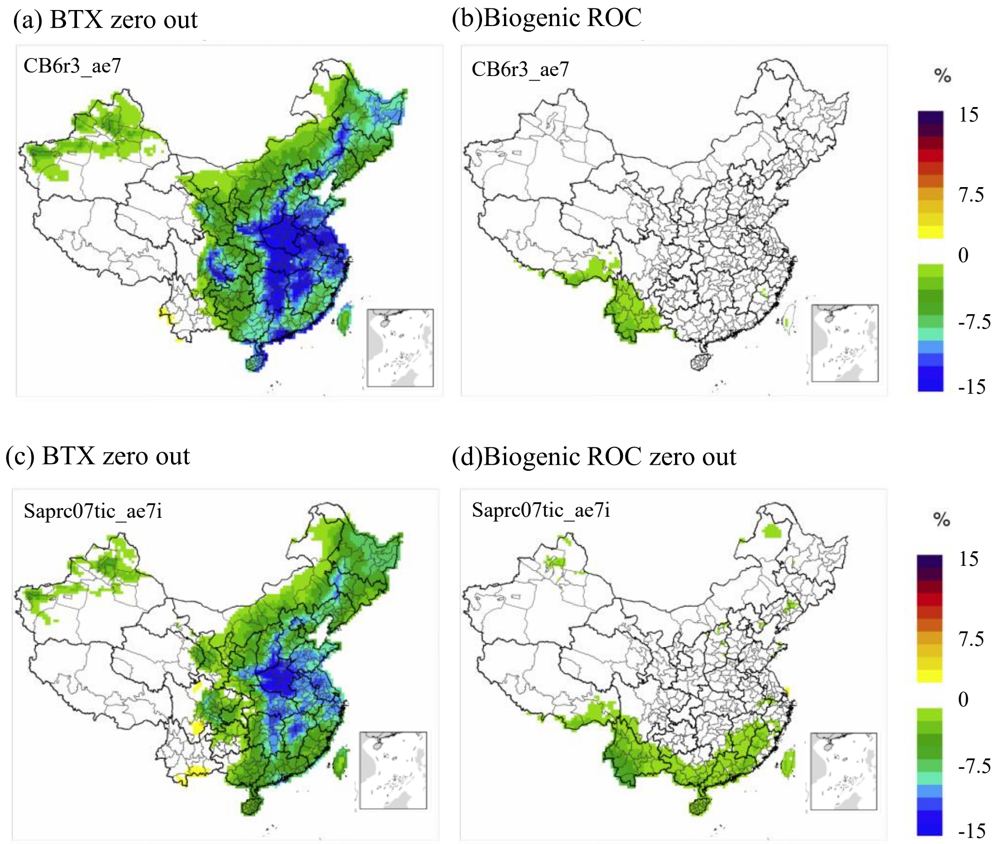

Figure S15. Percent changes in $PM_{2.5}$ concentrations between each zero-out scenario and its corresponding base simulation: (a) BTX, (b) biogenic ROC for CB6r3_ae7, (c) BTX, and (d) biogenic ROC for Saprc07tic_ae7i.

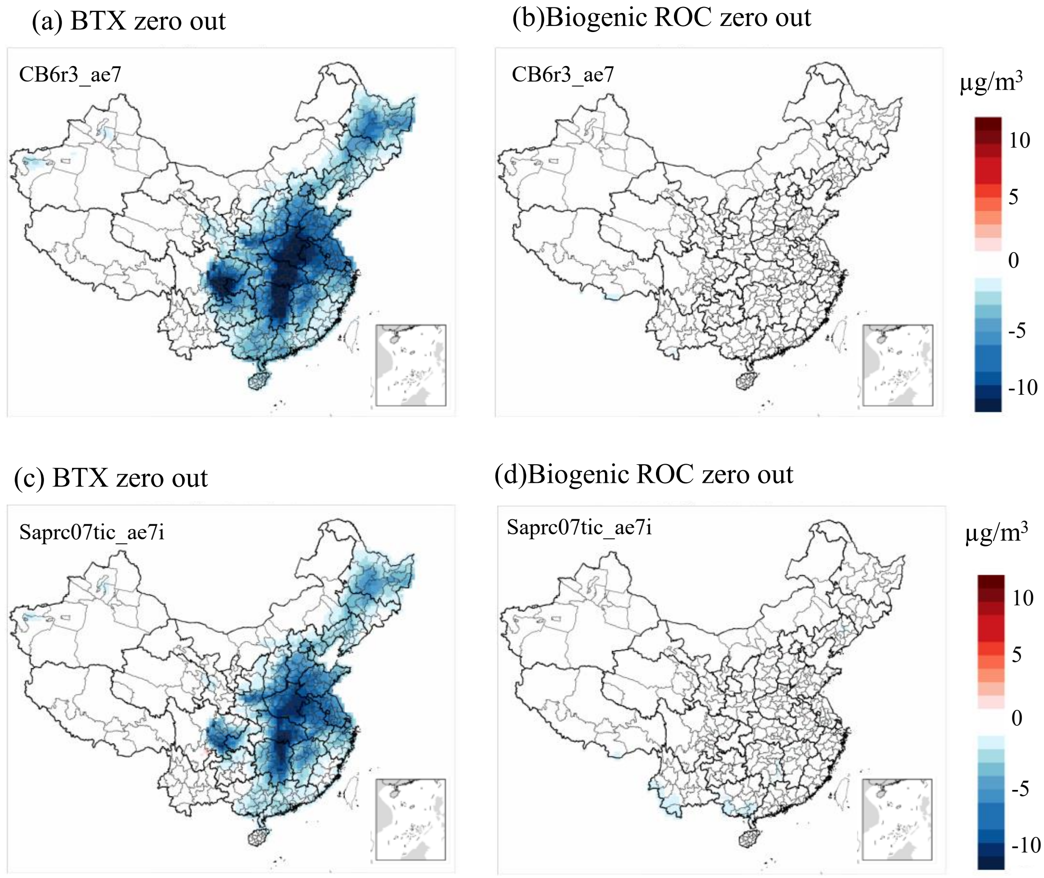

Figure S16. Changes in $PM_{2.5}$ concentrations between each zero-out scenario and its corresponding base simulation: (a) BTX and (b) biogenic ROC for CB6r3_ae7, and (c) BTX and (d) biogenic ROC for Saprc07tic_ae7i.

Table S1. The species mapping from Sarprc07tic_ae7i and CB6r3_ae7 to CRACMM used in CMAQ.

Saprc07/CB06	CRACMM	E/L	Saprc07/CB06	CRACMM	E/L
ACYE	ACE	E	ALDX	ALD	E
ACET	ACT	E	ETHA	ETH	E
CH4	ECH4	E	ETH	ETE	E
ETOH	EOH	E	MGLY	MGLY	L
HCHO	HCHO	E	GLY+CCHO*0.25	GLY	L
ETOH	EOH	E	MEK*0.001	HKET	L
HCHO	HCHO	E	CCHO*0.75	ACD	E
ISOP	ISO	E	TERP*0.65	LIM	L
MEOH	MOH	E	TERP*0.35	API	L
FACD	ORA1	E	ALK4*0.1	ROH	L
ACRO	ACRO	E	ALK5*0.03	PROG	L
ETOH	EOH	E	ALK4*0.9	HC5	L
BENZ	BEN	E	ALK5*0.97	HC10	L
MVK	MVK	L	MEK*0.75	MEK	L
ETH	ALK1	L	XYM*0.3	XYE	L
RNO3	ONIT	L	XYM*0.7	XYM	L
OLE1	OLI	L	MEK*0.25+PRD2	KET	L
OLE2	OLT	L	AACD+PACD	ORA2	L
CRES*0.25	CSL	L	ALK2+ALK3	HC3	L
CRES*0.75	PHEN	L	MACR+IPRD	MACR	L

Table S2. Emissions of VOCs by mechanism for January, April, July, and October. Units are in thousand tons per year.

Mechanisms	January	April	July	October
Cb6r3_ae7	227.1	202.4	203.1	215.8
Saprc07tic_ae7i	237.6	211.3	211.1	220
CRACMM	221.1	205.1	202	212.8

Table S3. Properties of semi-volatile POA species as defined in CB6r3_ae7, Saprc07tic_ae7i, and CRACMM.

Species name	MW	C^*	O:C	Hvap	Mechanisms
ALVPO1/VLVPO1	218	0.1	0.185	89	
ASVPO1/VSVPO1	230	1	0.123	85	
ASVPO2/VSVPO2	241	10	0.073	81	
ASVPO3/VSVPO3	253	100	0.032	77	
AIVPO1/VIVPO1	266	1000	0	73	CB6r3_ae7/
ALVOO1/VLVOO1	136	0.01	0.886	93	Saprc07tic_ae7i
ALVOO2/VLVOO2	136	0.1	0.711	89	
ASVOO1/VSVOO1	135	1	0.567	85	
ASVOO2/VSVOO2	135	10	0.447	81	
ASVOO3/VSVOO3	134	100	0.345	77	
VROCN2OXY2/AROCN2OXY2	282	0.01	0.2	93	
VROCP0OXY2/AROCP0OXY2	242	1	0.2	85	
VROCP1OXY1/AROCP1OXY1	270	10	0.1	81	
VROCP2OXY2/AROCP2OXY2	200	100	0.2	77	
VROCP3OXY2/VROCP3OXY2	186	1000	0.2	73	
AROCN2ALK	422	0.01	0	104	CRACMM
AROCN1ALK	408	0.1	0	96	
AROCP0ALK	394	1	0	85	
AROCP1ALK	380	10	0	81	
AROCP2ALK	338	100	0	77	
AROCP3ALK	296	1000	0	73	

A: aerosol; **V**: vapor; **LV**: low volatility; **SV**: semi-volatile; **OO**: oxidized organic; **ROC**: reactive organic carbon; **OXY**: oxygen; **ALK**: alkene; **P**: positive; **N**: negative; **MW**: molecular weight ($g \cdot mol^{-1}$); **Hvap**: enthalpy of vaporization ($kJ \cdot mol^{-1}$).

Table S4. Locations of monitoring sites with observations of $PM_{2.5}$ components in each region.

Site	Region	Longitude (°)	Latitude (°)
Chengdu	SCB	104.079	30.636
Changzhou	YRD	119.891	38.011
Taiyuan	FWP	112.434	38.011
Pudong	YRD	121.533	31.228
Chongming	YRD	121.972	31.524
Dianshanhu	YRD	120.978	31.094

Table S5. Evaluation of $PM_{2.5}$ components simulations using CRACMM in selected cities during January 2021.

Month	Region	$PM_{2.5}$ components	NMB	MB	RMSE	NME	IOA	OBS	SIM
Jan.	Chengdu	NO_3^-	29.5	5.5	12.4	52.8	0.7	18.8	24.3
		SO_4^{2-}	-39.4	-3	4.2	42.1	0.6	7.7	4.6
		NH_4^+	-15.2	-1.4	4.1	35.4	0.7	9.1	7.7
	Chongming	OC	14.7	0.6	2.6	44.0	0.7	4.2	4.8
		EC	212.0	1.9	2.5	215.8	0.3	0.9	2.8
		NO_3^-	85.6	6.7	12.3	120.7	0.6	7.9	14.6
		SO_4^{2-}	19.9	0.8	5.5	74.1	0.2	3.9	4.6
		NH_4^+	37.0	1.4	3.8	75.3	0.7	3.8	5.2
	Dianshanhu	OC	15.9	0.4	2.8	47.1	0.7	5.1	5.5
		EC	99.2	0.7	1.5	117.2	0.7	2.0	2.7
		NO_3^-	81.9	3.4	12.5	120.0	0.5	12.3	15.7
		SO_4^{2-}	-0.4	-1.3	4.9	48.6	0.4	5.4	4.0
		NH_4^+	24.2	-0.7	4.6	68.9	0.6	6.0	5.3
	Pudong	OC	-25.4	-1.6	3.0	39.4	0.7	6.5	4.9
		EC	145.9	1.3	2.1	154.2	0.5	1.5	2.8
		NO_3^-	126.5	6.3	12.0	153.1	0.5	9.1	15.3
		SO_4^{2-}	17.3	-0.5	5.5	69.9	0.3	5.1	4.7
		NH_4^+	25.0	-0.3	3.7	70.0	0.6	5.6	5.3
	Changzhou	OC	0.1	1.3	13.5	64	0.5	17.3	18.6
		EC	-0.3	-2.1	5.6	52	0.4	7.1	5.1
		NO_3^-	-0.2	-1.6	5.3	49	0.6	7.9	6.2
		SO_4^{2-}	0	-0.2	3.5	0.5	0.8	4.6	4.3
		NH_4^+	-0.1	-0.5	4	0.5	0.8	5.6	5
	Taiyuan	NO_3^-	0.9	6.4	14.2	1.1	0.8	7	13.4
		SO_4^{2-}	-0.2	-1	5.9	0.6	0.6	5.3	4.2
		NH_4^+	0.1	0.5	4	0.6	0.9	3.9	4.4

Table S6. Evaluation of $PM_{2.5}$ components simulations using CRACMM in selected cities during April 2021.

Month	Region	$PM_{2.5}$ components	NMB	MB	RMSE	NME	IOA	OBS	SIM
Apr.	Chengdu	OC	-60.5	-6.6	8.1	61.9	0.4	10.8	4.3
		EC	45.4	0.7	1.7	87.2	0.5	1.5	2.2
		NO_3^-	37.9	2.5	8.1	83.7	0.6	6.7	9.2
		SO_4^{2-}	-10.4	-0.4	2.4	50.2	0.6	3.5	3.1
		NH_4^+	-13.6	-0.5	2.7	56.3	0.7	3.6	3.1
	Chongming	NO_3^-	6.8	0.3	6.8	102.9	0.5	3.9	4.1
		SO_4^{2-}	53.7	1.7	3.8	82.6	0.4	3.2	4.9
		NH_4^+	2.9	0.1	3.0	96.5	0.5	2.0	2.1
	Dianshanhu	NO_3^-	-25.9	-6.1	12.1	82.2	0.6	11.6	5.5
		SO_4^{2-}	-3.5	-1.3	3.6	39.4	0.7	5.5	4.2
		NH_4^+	-25.3	-2.6	4.8	67.4	0.6	5.0	2.4
	Pudong	NO_3^-	-21.9	-4.5	10.0	79.5	0.5	8.6	4.1
		SO_4^{2-}	35.4	0.2	3.4	60.8	0.7	4.7	4.9
		NH_4^+	-25.4	-2.1	4.1	59.2	0.5	4.2	2.1

Table S7. Evaluation of $PM_{2.5}$ components simulations using CRACMM in selected cities during July 2021.

Month	Region	$PM_{2.5}$ components	NMB	MB	RMSE	NME	IOA	OBS	SIM
Jul.	Chengdu	OC	-52.1	-5.6	6.5	53.3	0.3	10.8	5.2
		EC	15.5	0.3	1.4	68.1	0.6	1.6	1.9
		NO_3^-	54.1	2.2	8.9	138.8	0.4	4.1	6.3
		SO_4^{2-}	-10.3	-0.4	2.4	49.7	0.5	3.6	3.2
		NH_4^+	-19.3	-0.6	3	72.6	0.5	3	2.4
	Chongming	NO_3^-	-39.6	-0.5	2.8	102.4	0.3	1.2	0.7
		SO_4^{2-}	-2.8	-0.1	2.0	60.1	0.5	2.3	2.3
		NH_4^+	-36.7	-0.3	1.3	99.4	0.4	0.7	0.4
	Dianshanhu	NO_3^-	-38.4	-1.6	3.9	80.6	0.5	2.7	1.1
		SO_4^{2-}	-36.8	-2.0	2.8	60.3	0.5	3.6	1.6
		NH_4^+	-69.7	-1.7	2.3	87.3	0.5	2.2	0.5
	Pudong	NO_3^-	-47.0	-1.6	3.4	84.0	0.4	2.3	0.7
		SO_4^{2-}	-4.8	-1.1	2.3	58.9	0.6	3.4	2.3
		NH_4^+	-69.2	-1.4	2.0	81.9	0.5	1.8	0.4
	Taiyuan	NO_3^-	-0.2	-0.9	7.9	1	0.4	5	4.1
		SO_4^{2-}	0	-0.1	4.5	0.6	0.5	6.4	6.3
		NH_4^+	-0.5	-1.9	3.5	0.6	0.5	4.1	2.1

Table S8. Evaluation of $PM_{2.5}$ components simulations using CRACMM in selected cities during October 2021.

Month	Region	$PM_{2.5}$ components	NMB	MB	RMSE	NME	IOA	OBS	SIM
Oct.	Chengdu	OC	-30.1	-2.8	4.5	39.8	0.5	9.4	6.6
		EC	59.9	1.3	2.5	89.7	0.3	2.2	3.5
		NO_3^-	127.9	8.3	12.7	138.5	0.5	6.5	14.9
		SO_4^{2-}	51.4	1.5	3.2	72.9	0.5	3	4.5
		NH_4^+	61.1	1.9	3.3	79.7	0.7	3	4.9
	Chongming	NO_3^-	-14.7	-0.3	3.3	77.7	0.8	1.7	1.5
		SO_4^{2-}	23.1	0.6	1.7	48.7	0.6	2.5	3.0
		NH_4^+	-41.4	-0.6	1.5	63.7	0.8	1.3	0.8
	Dianshanhu	NO_3^-	-36.5	-2.2	6.2	85.9	0.8	4.7	2.5
		SO_4^{2-}	34.8	0.1	1.6	54.0	0.8	2.8	2.9
		NH_4^+	-19.1	-0.9	2.5	85.7	0.7	2.0	1.1
	Pudong	NO_3^-	-66.3	-2.0	4.3	73.3	0.8	3.5	1.5
		SO_4^{2-}	3.5	-0.4	1.7	41.4	0.7	3.4	3.0
		NH_4^+	-65.9	-1.2	1.9	70.3	0.8	2.0	0.8
	Taiyuan	NO_3^-	0.6	4.9	10.7	0.9	0.8	8.2	13.2
		SO_4^{2-}	0.4	2	5.2	0.8	0.5	4.8	6.8
		NH_4^+	0	-0.2	3.6	0.5	0.7	4.7	4.5

Table S9. Averaged $PM_{2.5}$ evaluation metrics and the number of monitoring sites in five regions of China in January, 2021.

January	R	IOA	NMB	NME	No.
BTH	0.79	0.87	0.03%	37.87%	73
FWP	0.78	0.78	-35.80%	41.52%	50
PRD	0.35	0.45	-43.40%	46.23%	44
SCB	0.39	0.55	14.95%	49.24%	98
YRD	0.46	0.65	-0.84%	35.90%	199
Recommend Benchmark	>0.60	>0.70	<±45%	<±55%	/

Table S10. Averaged $PM_{2.5}$ evaluation metrics and the number of monitoring sites in five regions of China in April, 2021.

April	R	IOA	NMB	NME	No.
BTH	0.42	0.59	-33.18%	41.73%	74
FWP	0.49	0.58	-28.49%	41.08%	52
PRD	0.57	0.55	-43.26%	44.86%	45
SCB	0.37	0.53	-4.67%	43.04%	102
YRD	0.38	0.57	-15.59%	37.15%	202
Recommend Benchmark	>0.60	>0.70	<±45%	<±55%	/

Table S11. Averaged $PM_{2.5}$ evaluation metrics and the number of monitoring sites in five regions of China in July, 2021.

July	R	IOA	NMB	NME	No.
BTH	0.38	0.49	-11.95%	42.59%	72
FWP	0.24	0.47	-27.05%	42.11%	51
PRD	0.67	0.55	-49.75%	52.89%	41
SCB	0.21	0.39	13.30%	59.59%	99
YRD	0.51	0.59	-37.47%	50.33%	175
Recommend Benchmark	>0.60	>0.70	<±45%	<±55%	/

Table S12. Averaged $PM_{2.5}$ evaluation metrics and the number of monitoring sites in five regions of China in October, 2021.

October	R	IOA	NMB	NME	No.
BTH	0.81	0.87	10.73%	39.28	72
FWP	0.71	0.74	9.28%	48	52
PRD	0.7	0.66	-37.34%	43.93	44
SCB	0.61	0.57	50.26%	72.8	99
YRD	0.74	0.81	-13.15%	37.24	200
Recommend Benchmark	>0.60	>0.70	<±45%	<±55%	/

Table S13. List of emission reductions relative to the base simulations in CB6r3_ae7 and Saprc07tic_ae7i.

Chemical Mechanism	Emission Reduction
CB6r3_ae7	Biogenic-ROC emissions set to zero
CB6r3_ae7	Benzene-, toluene-, and xylene-like emissions set to zero
Saprc07tic_ae7i	Biogenic-ROC emissions set to zero
Saprc07tic_ae7i	Benzene-, toluene-, and xylene-like emissions set to zero