Supplement of

Tighter Control of AVOCs/NOx atop Carbon Neutrality Mitigations for China to Meet WHO Ambient Ozone Standard

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Table S1 City abbreviations and geographic coordinates for the Beijing-Tianjin-Hebei (BTH) and Chengdu-Chongqing (CY) urban agglomerations.

Megalopolis	Province	City	City abbreviations	Latitude	Longitude
Beijing-Tianjin-Hebei Region (BTH)	municipal	Beijing	BJ	39.92	116.42
	municipal	Tianjing	TJ	39.13	117.20
	Hebei	Baoding	BD	38.51	115.3
		Cangzhou	CZ1	38.18	116.52
		Handan	HD	36.36	114.28
		Hengshui	HS1	37.44	115.42
		Langfang	LF	39.31	116.42
		Shijiazhuang	SJZ	38.02	114.3
		Tangshan	TS	39.36	118.11
		Xingtai	XT1	37.04	114.3
	Henan	Anyang	AY	36.06	114.21
		Hebi	HB	35.54	114.11
		Jiaozuo	JZ1	35.14	113.12
		Kaifeng	KF	34.47	114.21
		Puyang	PY	35.44	115.01
		Xinxiang	XX	35.18	113.52
		Zhengzhou	ZZ1	34.46	11340
	Shandong	Binzhou	BZ	37.22	118.02
		Dezhou	DZ1	37.26	116.17
		Heze	HZ1	35.14	115.26
		Jinan	JN1	36.65	117.12
		Jining	JN2	35.23	116.33
		Liaocheng	LC	36.26	115.57
		Zibo	ZB	36.48	118.03
		Changzhi	CZ2	36.11	113.06
		Jincheng	JC	35.49	112.85
		Taiyuan	TY	37.54	112.33
		Yangquan	YQ	37.51	113.34
Chengdu-Chongqing Region (CY)	municipal	Chongqing	CQ	29.35	106.33
	Sichuan	Chengdu	CD1	30.4	104.04
		Dazhou	DZ2	31.21	107.46
		Deyang	DY	31.09	104.22
		Guangan	GA	30.45	106.63
		Leshan	LS	29.36	103.44
		Luzhou	LZ	28.54	105.24
		Meishan	MS	30.07	103.84
		Mianyang	MY	31.3	104.42
		Nanchong	NC1	30.49	106.04
		Neijiang	NJ1	29.36	105.02
		Suining	SN	30.31	105.33
		Yaan	YA	29.59	102.59
		Yibin	YB	28.47	104.34
		Zigong	ZG	29.23	104.46
		Ziyang	ZY	30.09	104.38

Table S2 City abbreviations and geographic coordinates for the Middle Reaches of the Yangtze River (MYR) and Pearl River Delta (PRD) urban agglomerations.

Megalopolis	Province	City	City abbreviations	Latitude	Longitude
Yangtze River Midstream Region (MYR)	Hubei	Ezhou	EZ	30.23	114.52
		Huanggang	HG	30.45	114.87
		Huangshi	HS2	30.12	115.06
		Jinmen	JM2	31.02	112.12
		Jinzhou	JZ2	30.34	112.24
		Qianjiang	QJ	30.26	112.53
		Tianmen	TM	30.66	113.16
		Wuhan	WH1	30.35	114.17
		Xiangyang	XY1	32.01	112.12
		Xianning	XN	29.53	114.17
		Xiantao	XT	30.22	113.27
		Xiaogan	XG	30.56	113.54
		Yichang	YC1	30.42	111.17
	Hunan	Changde	CD2	29.02	111.51
		Changsha	CS	28.12	112.59
		Hengyang	HY2	26.89	112.57
		Loudi	LD	27.44	111.59
		Xiangtan	XT3	27.52	112.53
		Yiyang	YY1	28.55	112.35
		Yueyang	YY2	29.22	113.06
		Zhuzhou	ZZ2	27.51	113.09
	Jiangxi	Fuzhou	FZ	27.94	116.35
		Jian	JA	27.09	114.96
		Jindezheng	JDZ	29.27	117.18
		Jiujiang	JJ	29.66	115.95
		Nanchang	NC2	28.68	115.85
		Pingxiang	PX	27.65	113.88
		Shangrao	SR	28.45	117.94
		Xinyu	XY2	27.48	114.56
		Yichun	YC2	27.47	114.23
		Yingtan	YT	28.14	117.03
Pearl River Delta Region (PRD)	Guangdong	Dongguan	DG	23.02	113.45
		Foshan	FS	23.02	113.06
		Guangzhou	GZ	23.08	113.14
		Heyuan	HY1	23.43	114.41
		Huizhou	HZ2	23.05	114.22
		Jiangmen	JM1	22.35	113.04
		Qingyuan	QY	23.42	113.01
		Shaoguan	SG	24.48	113.37
		Shanwei	SW	22.47	115.21
		Shenzhen	SZ1	22.33	114.07
		Yunfu	YF	22.57	112.02
		Zhaoqin	ZQ	23.03	112.27
		Zhongshan	ZS1	22.31	113.22
		Zhuhai	ZH	22.17	113.34

Table S3 City abbreviations and geographic coordinates for the Yangtze River Delta (YRD) urban agglomeration.

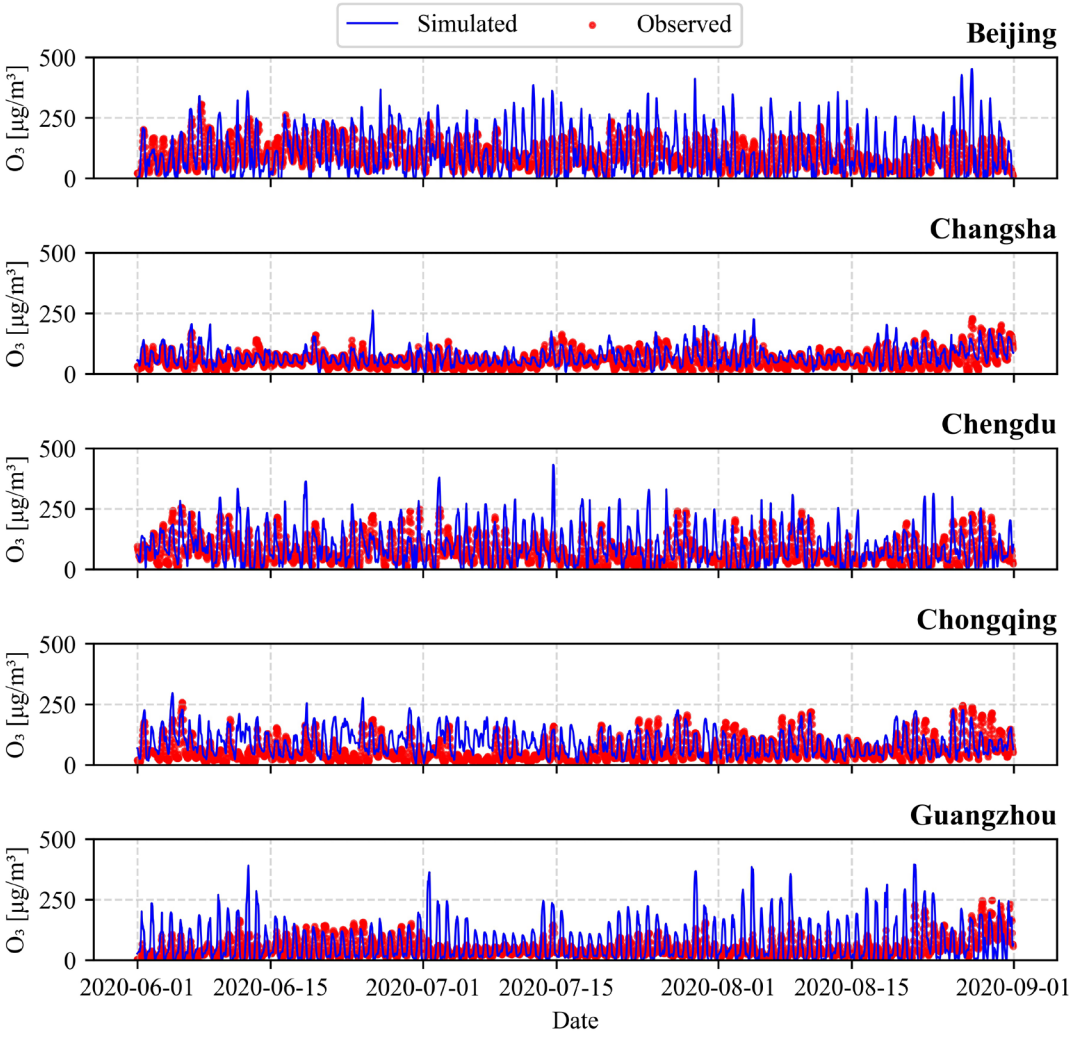
Megalopolis	Province	City	City abbreviations	Latitude	Longitude
Yangtze River Delta Region (YRD)	municipal	Shanghai	SH	31.23	121.47
	Anhui	Anqing	AQ	30.31	117.02
		Chizhou	CZ3	30.67	117.50
		Chuzhou	CZ4	32.18	118.18
		Hefei	HF	31.52	117.17
		Maanshan	MAS	31.43	118.28
		Tongling	TL	30.56	117.48
		Wuhu	WH2	31.19	118.22
		Xuancheng	XC	30.94	118.76
	Jiangsu	Changzhou	CZ5	31.47	119.58
		Nanjing	NJ2	32.03	118.46
		Nantong	NT	32.01	120.51
		Suzhou	SZ2	31.19	120.37
		Taizhou	TZ1	32.46	119.54
		Wuxi	WX	31.34	120.18
		Yancheng	YC3	33.22	120.08
		Yangzhou	YZ	32.23	119.26
	Jiangsu	Zhengjiang	ZJ2	32.11	119.27
		Hangzhou	HZ3	30.25	120.21
		Huzhou	HZ4	30.52	120.06
		Jiaxing	JX	30.46	120.45
		Jinhua	JH	29.07	119.39
		Ningbo	NB	29.52	121.33
		Shaoxing	SX	30.05	120.34
		Taizhou	TZ2	28.41	121.27
		Wenzhou	WZ	28.01	120.39
		Zhoushan	ZS3	30.01	122.06

Table S4 Anthropogenic VOC species represented in the Carbon Bond 6 (CB6) mechanism

Model Species	Description	Molecular Weight	Type
AACD	acetic acid	60	E
ACET	acetone	58.1	E
ACRO_PRIMARY	acrolein from emissions only	56.1	E
ACROLEIN	acrolein	56.1	E
ALD2	acetaldehyde	44	E
ALD2_PRIMARY	acetaldehyde from emissions only	44	E
ALDX	aldehydes with 3 or more carbons	58.1	L
APIN	alpha pinene	136.2	E
BENZENE	benzene	78.1	E
BUTADIENE13	1,3-butadiene	54	E
DMS	dimethylsulfide	62	E
ECH4	methane	16	E
ETH	ethene (ethylene)	28	E
ETHA	ethane	30.1	E
ETHY	ethyne (acetylene)	26	E
ETOH	ethanol	46.1	E
FACD	formic acid	46	E
FORM	formaldehyde	30	E
FORM_PRIMARY	formaldehyde from emissions only	30	E
GLY	glyoxal	58	E
GLYD	glycoaldehyde (hydroxyacetaldehyde)	60	E
IOLE	internal alkene bond	56.1	L
ISOP	isoprene	68.1	E
KET	carbon-ketone bond	72.1	L
MEOH	methanol	32	E
NAPH	naphthalene	128.2	E
OLE	terminal alkene bond	42.1	L
PAR	paraffinic carbon bond	14	L
TOL	toluene and other monoalkyl aromatics	92.1	L
XYL	xylenes and other polyalkyl aromatics	106.2	L
NVOL	non-volatile organic compounds	–	L
UNR	unreactive carbon groups	–	L

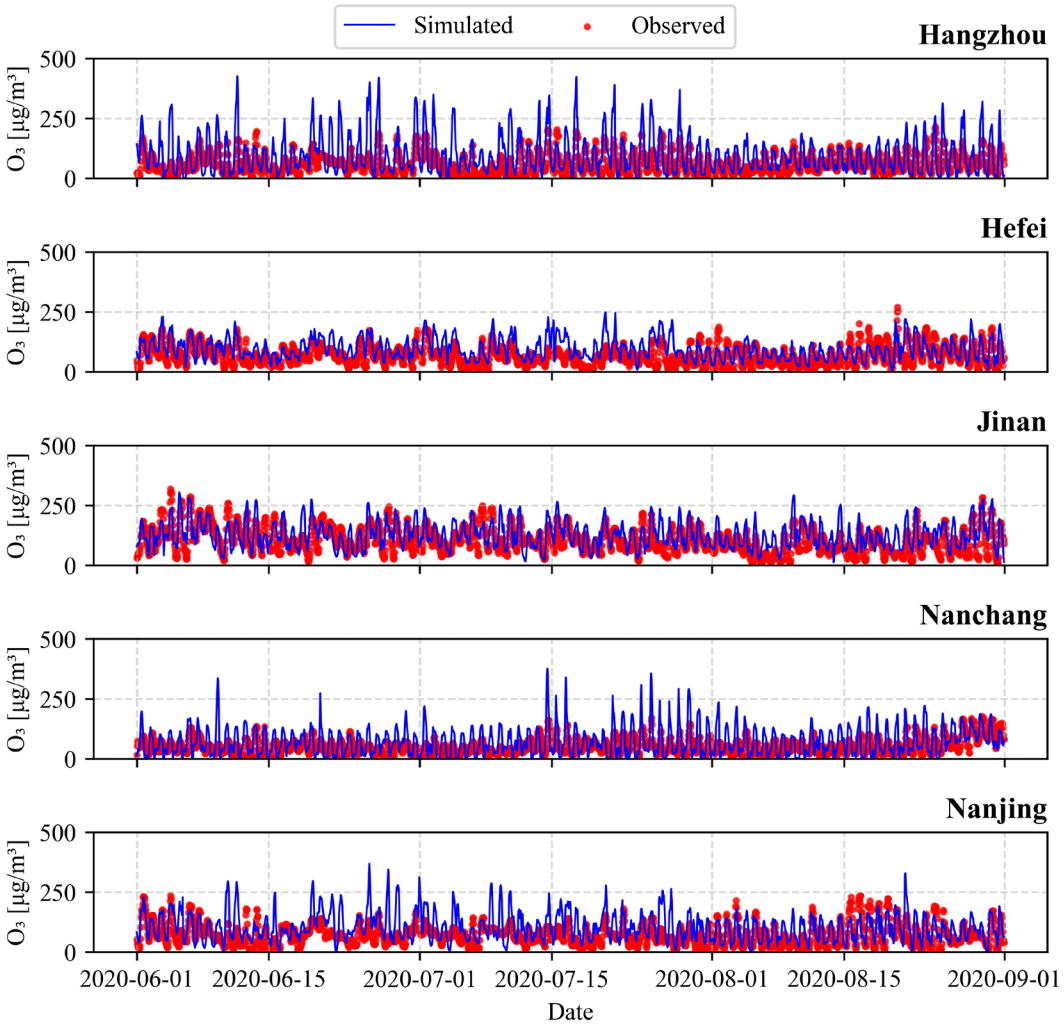
Notes:
(1) "E" denotes explicit species (individually tracked), while "L" denotes lumped species (representing a group of chemically similar compounds). Molecular weights are in g mol^{-1}.
(2) This table is based on the cb6r3_ae7_aq mechanism and may vary slightly across different CMAQ versions.
(3) NVOL (non-volatile organic compounds) and UNR (unreactive carbon groups) are lumped species that do not participate in gas-phase photochemistry.
(4) Some species (e.g., APIN, DMS) may be partially biogenic in origin but are included here as they are also represented in anthropogenic emission inventories.
(5) Molecular weights of lumped species represent the carbon bond group and may vary depending on the specific CB6 version used.

Figure S1. Hourly O_3 concentrations in five provincial-level cities during summer 2020.



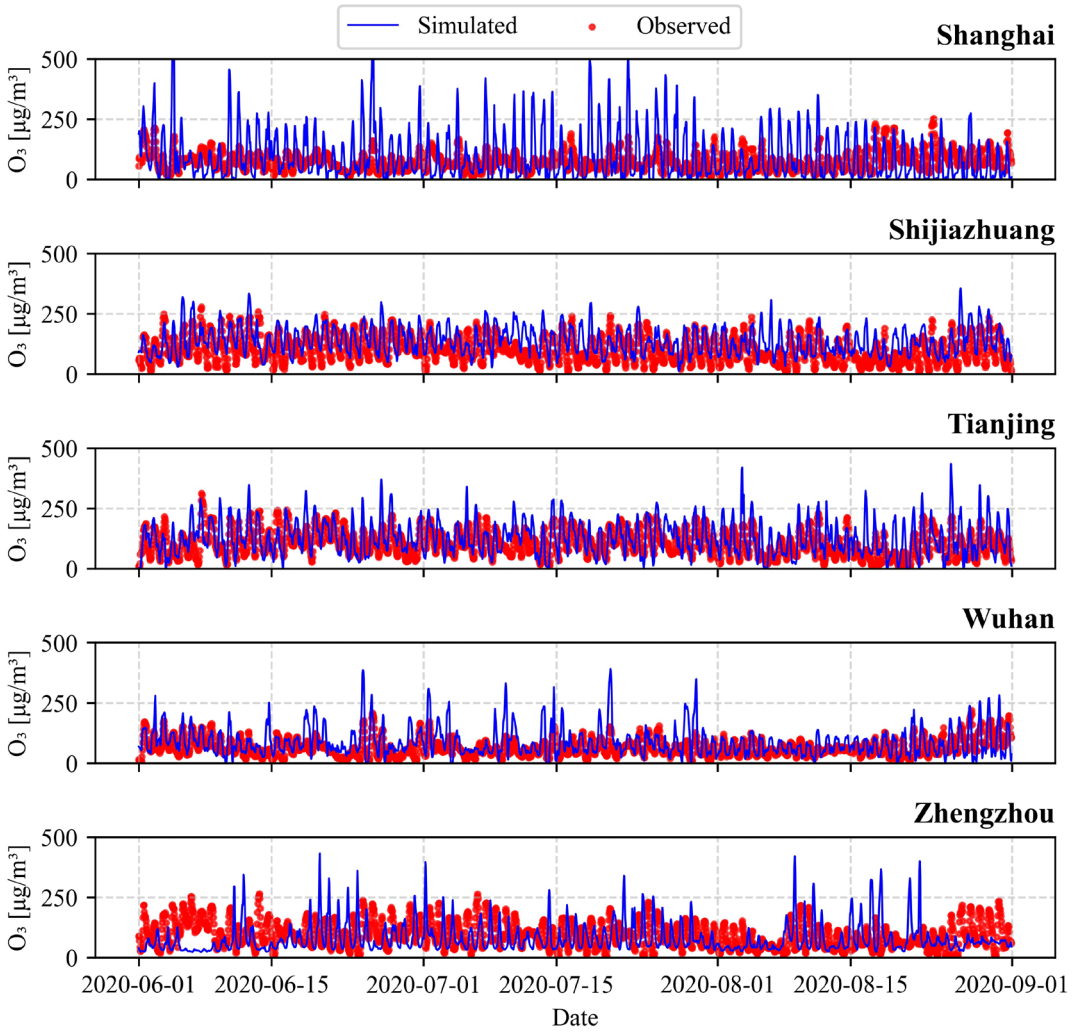
Note: Data are derived from the baseline 2020 CMAQ simulation (hourly output). The selected dates represent typical summer conditions across June–August. The selected cities represent the following urban agglomerations: Beijing (BTH), Changsha (MYR), Chengdu (CY), Chongqing (CY), and Guangzhou (PRD). Data are derived from the baseline 2020 simulation.

Figure S2. Hourly O_3 concentrations in five provincial-level cities during summer 2020.



Note: Data are derived from the baseline 2020 CMAQ simulation (hourly output). The selected dates represent typical summer conditions across June–August. The selected cities represent the following urban agglomerations: Hangzhou (YRD), Hefei (YRD), Jinan (BTH/Shandong), Nanchang (MYR), and Nanjing (YRD).

Figure S3. Hourly O_3 concentrations in five provincial-level cities during summer 2020.



Note: Data are derived from the baseline 2020 CMAQ simulation (hourly output). The selected dates represent typical summer conditions across June–August. The selected cities represent the following urban agglomerations: Shanghai (YRD) , Shijiazhuang (BTH), Tianjin (BTH), Wuhan (MYR), and Zhengzhou (BTH).

Table S5. Model performance statistics for summertime daytime O_3 concentrations across cities in the Beijing-Tianjin-Hebei (BTH) and Chengdu-Chongqing (CY) urban agglomerations.

Megalopolis	City	Obs_Mean	Mod_Mean	MB	NMB (%)	RMSE	IOA	R
BTH	Beijing	99.13	109.81	10.69	10.78	74.64	0.70	0.60
	Tianjing	105.67	127.06	21.39	20.24	56.55	0.78	0.68
	Baoding	104.12	131.10	26.97	25.90	48.13	0.79	0.71
	Cangzhou	106.84	125.68	18.84	17.64	43.89	0.80	0.69
	Handan	102.05	132.10	30.05	29.45	51.29	0.77	0.69
	Hengshui	107.78	127.67	19.89	18.46	41.61	0.80	0.70
	Langfang	104.64	130.14	25.50	24.36	54.55	0.78	0.67
	Shijiazhuan	102.93	136.84	33.92	32.95	56.32	0.75	0.68
	Tangshan	101.72	132.44	30.72	30.21	57.59	0.76	0.66
	Xingtai	103.04	135.76	32.72	31.75	52.79	0.78	0.73
	Anyang	106.11	130.29	24.18	22.78	47.38	0.79	0.70
	Hebi	99.37	130.76	31.39	31.59	49.95	0.75	0.70
	Jiaozuo	101.69	128.65	26.96	26.51	50.89	0.78	0.68
	Kaifeng	92.98	114.61	21.64	23.27	40.94	0.77	0.66
	Puyang	96.53	120.07	23.54	24.39	43.79	0.77	0.68
	Xinxiang	95.50	124.40	28.90	30.26	48.52	0.77	0.70
	Zhengzhou	96.17	39.79	36.38	58.62	89.75	0.75	0.64
	Binzhou	101.38	117.84	16.46	16.23	44.12	0.86	0.77
	Dezhou	110.43	126.86	16.43	14.87	41.45	0.81	0.71
	Heze	94.98	116.44	21.47	22.60	41.30	0.77	0.67
	Jinan	105.87	127.18	21.31	20.13	49.43	0.79	0.68
	Jining	101.07	114.34	13.27	13.13	41.22	0.83	0.72
	Liaocheng	100.12	123.32	23.20	23.17	45.21	0.80	0.72
	Zibo	103.01	119.61	16.60	16.11	49.85	0.77	0.64
	Changzhi	105.26	128.41	23.16	22.00	44.65	0.76	0.66
	Jincheng	104.48	130.94	26.46	25.33	49.42	0.73	0.64
	Taiyuan	96.70	122.46	25.76	26.64	54.57	0.73	0.64
	Yangquan	102.55	133.23	30.68	29.92	60.19	0.60	0.44
CY	Chongqing	60.50	91.25	30.75	50.82	55.90	0.71	0.57
	Chengdu	74.69	97.05	22.36	29.94	66.83	0.69	0.56
	Dazhou	53.85	77.44	23.59	43.81	32.36	0.70	0.66
	Deyang	74.69	99.46	24.77	33.16	48.38	0.77	0.67
	Guangan	68.86	83.66	14.80	21.49	34.23	0.74	0.60
	Leshan	69.06	104.97	35.91	51.99	51.96	0.59	0.48
	Luzhou	69.13	81.89	12.77	18.47	40.47	0.62	0.44
	Meishan	72.76	99.07	26.31	36.16	53.02	0.64	0.47
	Mianyang	67.44	96.71	29.27	43.40	50.70	0.67	0.54
	Nanchong	55.34	82.06	26.72	48.28	37.16	0.66	0.61
	Neijiang	70.45	91.49	21.03	29.86	41.16	0.70	0.56
	Suining	64.54	84.21	19.67	30.48	37.05	0.71	0.59
	Yaan	62.29	86.93	24.64	39.56	44.10	0.51	0.28
	Yibin	68.02	84.88	16.86	24.79	43.67	0.51	0.33
	Zigong	73.22	91.94	18.72	25.56	37.59	0.73	0.63
	Ziyang	76.93	88.49	11.56	15.03	35.96	0.70	0.52

Notes:

(1) Obs_Mean and Mod_Mean are in $\mu g/m^3$.

(2) MB = Mod_Mean − Obs_Mean.

(3) NMB (%) = $(\Sigma(Mod-Obs)/\Sigma Obs)\times 100$.

(4) RMSE in $\mu g/m^3$.

(5) IOA = Willmott's index of agreement.

(6) R = Pearson correlation coefficient.

Table S6. Model performance statistics for summertime daytime O_3 concentrations across cities in the Middle Reaches of the Yangtze River (MYR) and Pearl River Delta (PRD) urban agglomerations.

Megalopolis	City	Obs_Mean	Mod_Mean	MB	NMB (%)	RMSE	IOA	R
MYR	Ezhou	68.12	101.46	33.34	48.95	57.40	0.68	0.64
	Huanggang	74.61	89.99	15.38	20.61	39.61	0.76	0.63
	Huangshi	68.19	86.22	18.03	26.44	38.05	0.75	0.63
	Jinmen	74.98	92.66	17.68	23.58	35.85	0.69	0.53
	Jinzhou	70.59	89.02	18.44	26.12	36.69	0.74	0.62
	Qianjiang	\	80.40	\	\	\	\	\
	Tianmen	\	80.73	\	\	\	\	\
	Wuhan	65.61	87.66	22.05	33.61	52.26	0.68	0.60
	Xiangyang	77.62	97.64	20.02	25.79	40.41	0.70	0.58
	Xianning	57.78	77.69	19.92	34.47	37.95	0.65	0.50
	Xiantao	\	83.66	\	\	\	\	\
	Xiaogan	67.23	86.83	19.60	29.15	48.23	0.67	0.51
	Yichang	62.74	90.77	28.03	44.67	45.08	0.64	0.54
	Changde	59.04	72.22	13.17	22.31	34.69	0.67	0.50
	Changsha	59.22	73.93	14.71	24.84	32.71	0.79	0.68
	Hengyang	59.92	69.95	10.03	16.73	26.34	0.81	0.70
	Loudi	64.74	69.75	5.01	7.73	30.23	0.69	0.53
	Xiangtan	63.80	66.35	2.55	4.00	27.88	0.74	0.61
	Yiyang	61.57	78.37	16.80	27.29	33.19	0.73	0.63
	Yueyang	66.29	82.19	15.90	23.99	33.12	0.75	0.64
	Zhuzhou	51.90	69.41	17.51	33.74	32.28	0.68	0.56
	Fuzhou	66.22	64.40	-1.81	-2.74	27.89	0.73	0.57
	Jian	61.04	65.84	4.80	7.86	31.59	0.68	0.52
	Jindezheng	53.80	70.02	16.21	30.13	33.44	0.67	0.55
	Jiujiang	55.33	84.66	29.33	53.00	44.57	0.58	0.45
	Nanchang	51.55	71.97	20.42	39.61	52.94	0.64	0.57
	Pingxiang	53.05	71.97	18.92	35.66	33.05	0.73	0.64
	Shangrao	56.18	65.45	9.27	16.50	28.62	0.73	0.57
	Xinyu	51.77	65.61	13.84	26.72	42.34	0.57	0.48
	Yichun	54.44	69.25	14.81	27.19	42.62	0.51	0.34
	Yingtan	53.98	65.76	11.78	21.83	43.36	0.58	0.54
PRD	Dongguan	47.69	71.38	23.69	49.67	58.53	0.69	0.66
	Foshan	46.22	71.07	24.85	53.75	59.07	0.67	0.62
	Guangzhou	49.65	74.42	24.77	49.88	68.80	0.62	0.57
	Heyuan	54.48	69.55	15.08	27.68	43.91	0.76	0.63
	Huizhou	46.34	69.87	23.53	50.78	58.71	0.53	0.53
	Jiangmen	40.75	52.72	11.97	29.38	32.12	0.72	0.57
	Qingyuan	43.39	69.96	26.57	61.23	59.92	0.53	0.49
	Shanwei	44.21	46.23	2.02	4.56	35.81	0.57	0.32
	Shaoguan	66.14	72.20	6.06	9.16	37.91	0.66	0.45
	Shenzhen	43.24	48.55	5.31	12.28	31.54	0.78	0.63
	Yunfu	43.21	57.21	14.00	32.40	25.81	0.73	0.62
	Zhaoqin	57.19	58.08	0.89	1.56	36.38	0.66	0.46
	Zhongshan	54.55	52.87	-1.68	-3.08	42.64	0.53	0.29
	Zhuhai	64.91	51.91	-13.00	-20.02	37.84	0.64	0.42

Notes:
(1) Obs_Mean and Mod_Mean are in μg/m³.
(2) MB = Mod_Mean − Obs_Mean.
(3) NMB (%) = (Σ(Mod−Obs)/ΣObs)×100.
(4) RMSE in μg/m³.
(5) IOA = Willmott's index of agreement.
(6) R = Pearson correlation coefficient.

Table S7. Model performance statistics for summertime daytime O_3 concentrations across cities in the Yangtze River Delta (YRD) urban agglomeration.

Megalopolis	City	Obs_Mean	Mod_Mean	MB	NMB (%)	RMSE	IOA	R
YRD	Shanghai	76.60	94.22	17.61	22.99	94.42	0.47	0.38
	Anqing	67.66	83.85	16.19	23.93	38.38	0.68	0.52
	Chizhou	72.31	87.75	15.44	21.35	42.37	0.70	0.53
	Chuzhou	64.01	104.96	40.95	63.99	60.39	0.57	0.51
	Hefei	68.18	95.28	27.10	39.75	47.34	0.69	0.59
	Maanshan	64.58	96.37	31.80	49.24	57.37	0.60	0.55
	Tongling	71.05	84.48	13.43	18.90	47.05	0.61	0.42
	Wuhu	72.16	97.92	25.76	35.70	50.49	0.70	0.59
	Xuancheng	66.48	84.97	18.49	27.80	48.77	0.62	0.44
	Changzhou	74.42	103.95	29.53	39.67	60.10	0.70	0.60
	Nanjing	72.73	105.54	32.81	45.12	62.61	0.63	0.51
	Nantong	76.27	102.97	26.70	35.01	66.54	0.74	0.68
	Suzhou	77.72	115.67	37.95	48.83	82.53	0.53	0.48
	Taizhou	75.90	105.01	29.12	38.36	59.55	0.74	0.67
	Wuxi	76.16	121.82	45.66	59.96	86.95	0.57	0.52
	Yancheng	67.20	86.71	19.50	29.02	52.52	0.71	0.55
	Yangzhou	72.04	110.62	38.59	53.56	67.92	0.72	0.66
	Zhengjiang	67.11	110.45	43.34	64.58	76.07	0.63	0.56
	Hangzhou	61.61	98.74	37.13	60.26	72.71	0.65	0.63
	Huzhou	62.95	96.08	33.13	52.63	76.53	0.53	0.44
	Jiaxing	61.39	97.41	36.02	58.68	68.45	0.60	0.55
	Jinhua	61.92	75.27	13.35	21.57	35.79	0.68	0.51
	Ningbo	56.59	74.13	17.54	30.99	39.66	0.71	0.57
	Shaoxing	58.67	94.18	35.51	60.53	74.08	0.50	0.46
	Taizhou	52.35	88.90	36.56	69.84	54.16	0.65	0.57
	Wenzhou	65.69	70.91	5.22	7.95	40.35	0.50	0.73
	Zhoushan	68.83	102.97	34.14	49.60	66.89	0.41	0.69

Notes:
(1) Obs_Mean and Mod_Mean are in $\mu g/m^3$.
(2) MB = Mod_Mean − Obs_Mean.
(3) NMB (%) = $(\Sigma(Mod-Obs)/\Sigma Obs)\times 100$.
(4) RMSE in $\mu g/m^3$.
(5) IOA = Willmott's index of agreement.
(6) R = Pearson correlation coefficient.