Supplementary file for "Photochemical mechanism–dependent ozone formation and precursor sensitivity under varying NO_x conditions"

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Supporting Information

Supporting Information includes 5 pages, 1 figure and 4 tables

SI Figures S1, p3

SI Tables S1-S4, p4-p7

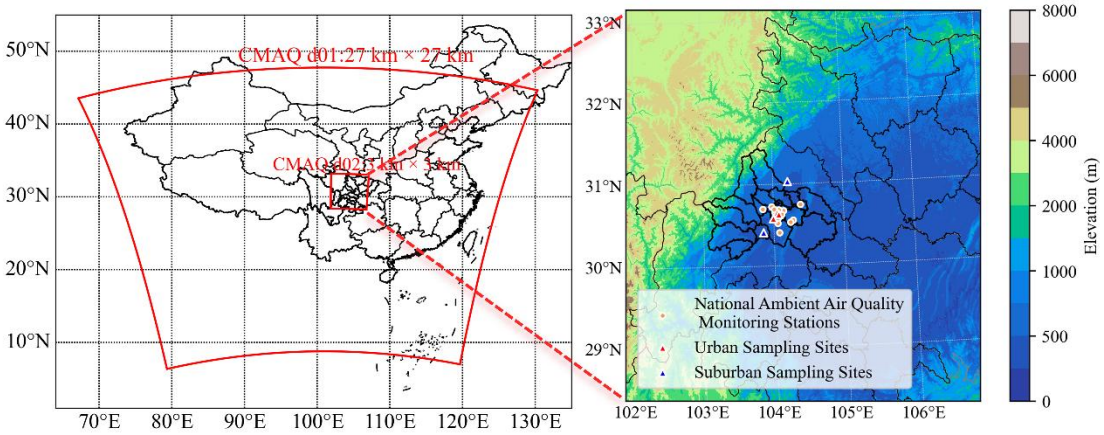

Figure S1 (a) Configuration of the nested domains used in the CMAQ simulations; (b) Topography of the simulation domain and distribution of Nation Ambient Air Quality Monitoring stations and in-situ field sites.

Table S1 Location information of the China National Environmental Monitoring stations in Chengdu and in-situ field sites.

Type	Station ID	Station Name	Longitude	Latitude
China National Environmental Monitoring stations	1431A	JinQuanLiangHe	103.97275°E	30.72358333°N
	1432A	ShiLiDian	104.176°E	30.6872°N
	1433A	SanWaYao	104.079°E	30.5706°N
	1434A	ShaHePu	104.1113889°E	30.63°N
	1437A	JunPingJie	104.054°E	30.6578°N
	2880A	DaShiXiLu	104.0238889°E	30.65638889°N
	3136A	LongQuanYiQuQuZhengFu	104.2725°E	30.5589°N
in-situ field sites	/	Xinjin (XJ)	103.81°E	30.41°N
	/	Sichuan Academy of Environmental Sciences (SAES)	104.07°E	30.63°N

Table S2 Major Physics Options for WRF Simulations.

Physics parameterization	Option	Meaning of the option
Microphysics	mp_physics=28	Thompson Aerosol scheme
Planetary boundary layer	bl_pbl_physics=2	Mellor-Yamada-Janjic scheme
Long wave radiation	ra_lw_physics=4	RRTMG scheme
Shortwave radiation	ra_sw_physics=4	RRTMG scheme
Cumulus Parameterization	cu_physics=6	Tiedtke scheme
Land surface	sf_surface_physics=2	Noah scheme
Surface layer	sf_sfclay_physics=2	Eta Similarity scheme
Urban Surface	sf_urban_physics=1	Urban Canopy Model
Pressure top (in Pa) to use in the model	5000	The pressure top is 50 hPa

Table S3 The VOC emission species input into the CMAQ model under three photochemical mechanisms: CB06, SAPRC07 and RACM2.

	CB06	SAPRC07	RACM2
VOCs Emission	AACD	AACD	ACD
	ACET	ACET	ACE
	ALD2	ACYE	ALD
	ALDX	ALK1	API
	BENZENE	ALK2	BALD
	CRES	ALK3	BENZENE
	ETHA	ALK4	CSL
	ETH	ALK5	EOH
	ETOH	ARO1	ETE
	ETHY	ARO2	ETH
	FACD	BACL	GLY
	FORM	BALD	HC3
	GLY	BENZENE	HC5
	IOLE	CCHO	HC8
	ISOP	CRES	HCHO
	KET	ETHE	ISO
	MEOH	FACD	KET
	MGLY	GLY	MACR
	OLE	HCHO	MEK
	PAR	IPRD	MGLY
	TERP	ISOP	MOH
	TOL	MACR	MVK
	XYLMN	MEK	OLI
	PRPA	MEOH	OLT
		MGLY	ORA1
		MVK	ORA2
		OLE1	PHEN
		OLE2	TOL
		PACD	UALD
		PRD2	XYM
		RCHO	XYO
		TERP	XYP

Table S4 Statistical metrics for photochemical mechanisms performance evaluation discussed in this study.

Statistic/abbreviation	Definition	Notes
Correlation coefficient (R)	$\frac{\sum[(S_i - \bar{S}) \times (O_i - \bar{O})]}{\sqrt{\sum(S_i - \bar{S})^2 \times \sum(O_i - \bar{O})^2}}$	-1≤R≤1
Index of Agreement (IOA)	$1 - \frac{\sum(S_i - O_i)^2}{\sum(\lvert S_i - \bar{O}\rvert + \lvert O_i - \bar{O}\rvert)^2}$	0≤IOA≤1
Mean Fractional Bias (MFB)	$\frac{2}{N}\sum\frac{(S_i - O_i)}{(S_i + O_i)} \times 100$	-200%≤MFB≤＋200%
Mean Fractional Error (MFE)	$\frac{2}{N}\sum\frac{\lvert S_i - O_i\rvert}{(S_i + O_i)} \times 100$	0≤MFE≤＋200%

Note. Subscript i represents the pairing of N observations O and simulations S by site and time.

Overbars signify means over site and/or time.