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Supplement of

Photochemical mechanism–dependent ozone formation and precursor sensitivity under varying NO_x conditions

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Supporting Information

Supporting Information includes 13 pages, 5 figure and 9 tables

SI Figures S1-S5, p3-p5

SI Tables S1-S9, p6-p13

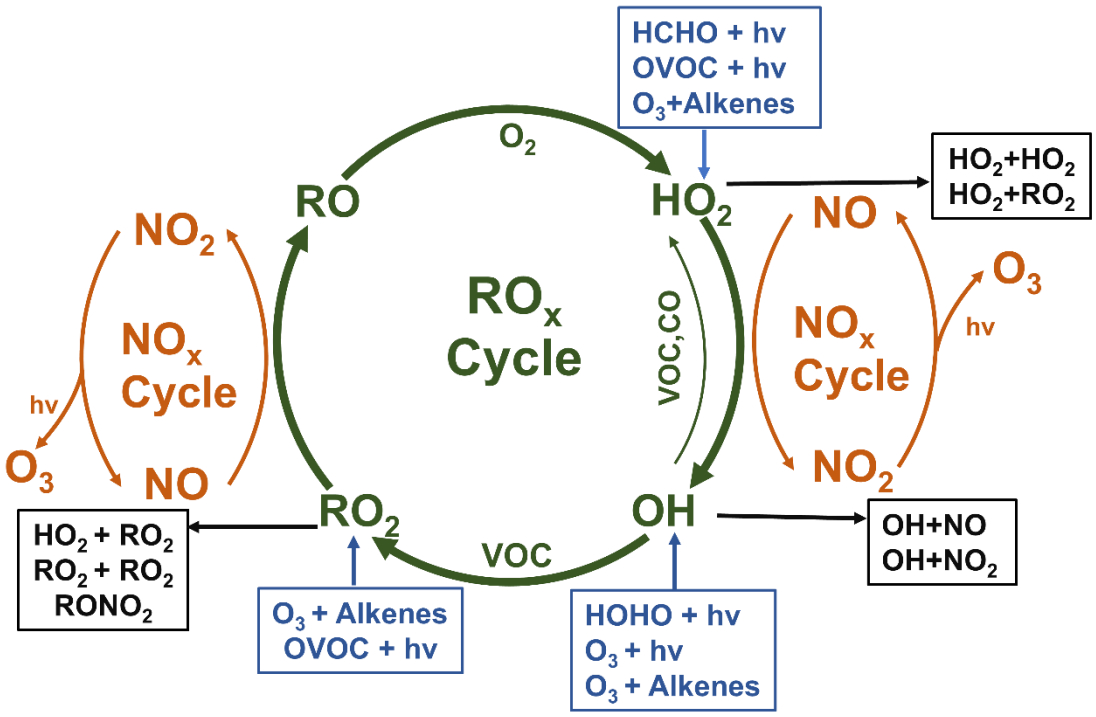


Figure S1 Schematic of simplified ozone formation mechanism and the coupling of the NO_x and RO_x radical cycle. The primary source reactions and the termination reactions of RO_x radicals were shown in blue and black, respectively.

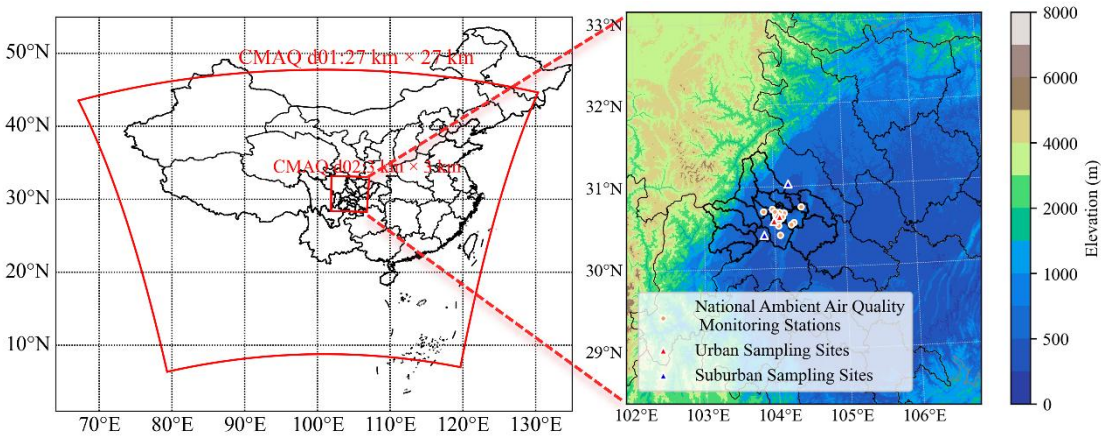


Figure S2 (a) Configuration of the nested domains used in the CMAQ simulations; (b) Topography of the simulation domain and distribution of Nation Ambient Air Quality Monitoring stations and in-situ field sites.

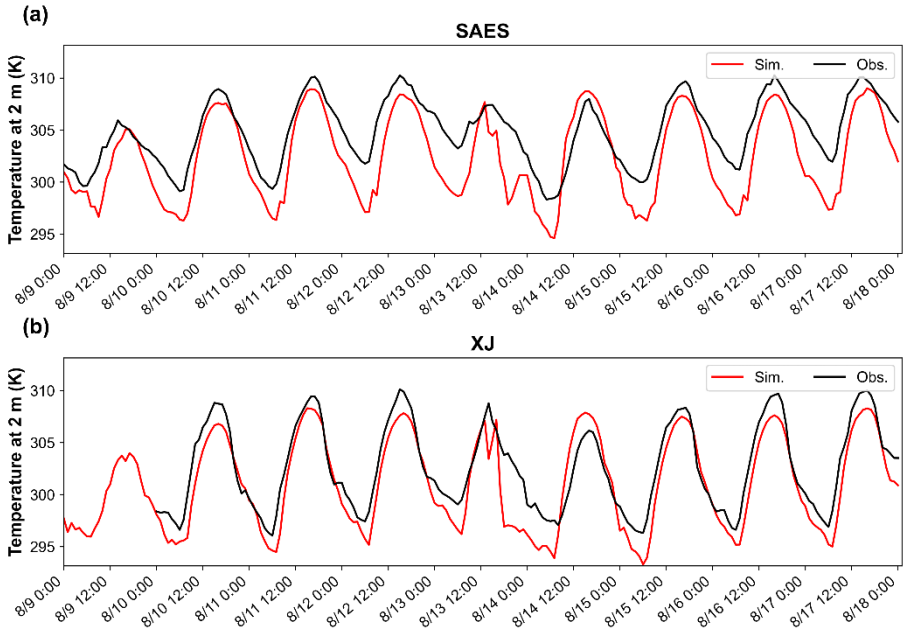


Figure S3 Time series of temperature (K) at 2 m simulation (red lines) and observation (black lines) at SEAS (a) and XJ (b) sites.

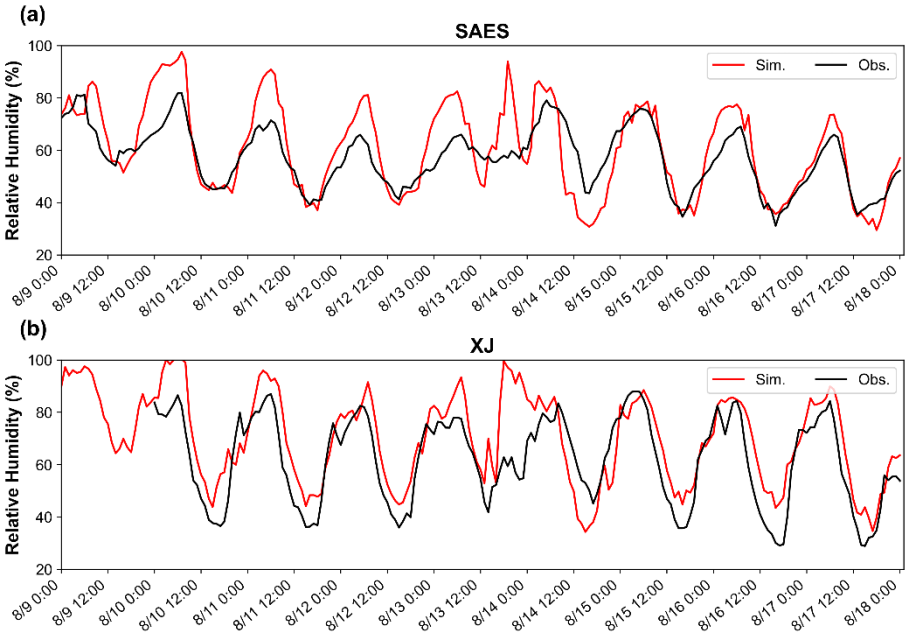


Figure S4 Time series of relative humidity (%) simulation (red lines) and observation (black lines) at SEAS (a) and XJ (b) sites.

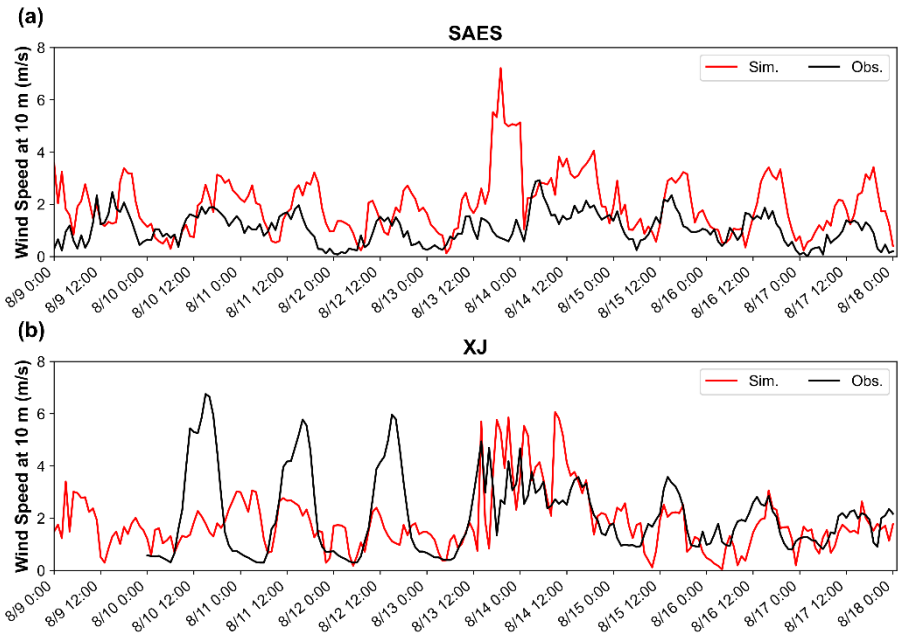


Figure S5 Time series of wind speed (m/s) at 10 m simulation (red lines) and observation (black lines) at SEAS (a) and XJ (b) sites.

Table S1 The representative reactions involved in NO_2 photolysis and initiation, chain propagation, and termination of RO_x radical cycle for ozone formation.

Reactions	**No.**
$NO_2 + hv\ (< 424\ nm) \rightarrow O(^3P) + NO$	(R1)
$O(^3P) + O_2 + M \rightarrow O_3 + M$	(R2)
$O_3 + NO \rightarrow NO_2 + O_2$	(R3)
Initiation reactions of the RO_x cycle	
$O_3 + hv\ (<\ 340\ nm) \rightarrow O(^1D) + O_2$ $O(^1D) + H_2O \rightarrow OH + OH$	(R4)
$HONO + hv\ (<\ 400\ nm) \rightarrow OH + NO$	(R5)
$HCHO + hv\ (<\ 335\ nm) + 2O_2 \rightarrow 2HO_2\ +\ CO$	(R6)
$Alkenes + O_3 \rightarrow OH + HO_2/RO_2\ + products$	(R7)
Chain propagation reactions of the RO_x cycle	
$OH + VOCs + O_2 \rightarrow RO_2 + products$	(R8)
$HCHO + OH + O_2 \rightarrow CO + H_2O + HO_2$	(R9)
$CO + OH + O_2 \rightarrow CO_2 + HO_2$	(R10)
$RO_2 + NO \rightarrow RO + NO_2$ $RO + O_2 \rightarrow RCHO + HO_2$	(R11)
$HO_2 + NO \rightarrow OH + NO_2$	(R12)
$HO_2 + O_3 \rightarrow OH + 2O_2$	(R13)
Termination reactions of the RO_x cycle	
$OH + NO_2 \rightarrow HNO_3$	(R14)
$OH + NO \rightarrow HONO$	(R15)
$RO_2 + NO \rightarrow RONO_2$	(R16)
$RO_2 + RO_2 \rightarrow products$	(R17)
$RO_2 + HO_2 \rightarrow ROOH + O_2$	(R18)
$HO_2 + HO_2 \rightarrow H_2O_2 + O_2$	(R19)
$HO_2 + HO_2 + H_2O \rightarrow H_2O_2 + H_2O + O_2$	(R20)

Note. The reactions highlighted in orange are related to NO_x cycle.

Table S2 The details of instruments for measuring trace gases in this study.

Parameters	Method	Time resolution	Accuracy (%)	Limit of detection
O_3	UV absorption	1 min	± 5	0.5 ppbv
NO,	Chemiluminescence	1 min	± 20	0.5 ppbv
NO_2				300 ppbv
VOC	GC–MS/FID[1]	1 h	± (15-20)	20–300 pptv
Formaldehyde	Hantzsch fluorimetry	1 min	±5	25 pptv
HNO_3	GAC-IC[2]	1 h	±5	0.13 μg/m³
HONO	Long-path absorption photometry	300 s	300 s ±20	10 pptv 10 pptv ±20%

Note. [1] GC–MS/FID is Gas Chromatography with Mass Spectrometry/with Flame Ionization Detection. [2] Gas and Aerosol Collector coupled with Ion Chromatography.

Table S3 Location information of the China National Environmental Monitoring stations in Chengdu and in-situ field sites.

Type	Station ID	Station Name	Longitude	Latitude	Urban/Suburban Category
China National Environmental Monitoring stations	1431A	JinQuanLiangHe	103.97275°E	30.72358333°N	Urban
	1432A	ShiLiDian	104.176°E	30.6872°N	Urban
	1433A	SanWaYao	104.079°E	30.5706°N	Urban
	1434A	ShaHePu	104.1113889°E	30.63°N	Urban
	1437A	JunPingJie	104.054°E	30.6578°N	Urban
	2880A	DaShiXiLu	104.0238889°E	30.65638889°N	Urban
	3136A	LongQuanYiQuQuZhengFu	104.2725°E	30.5589°N	Urban
in-situ field sites	/	Xinjin (XJ)	103.81°E	30.41°N	Suburban
	/	Sichuan Academy of Environmental Sciences (SAES)	104.07°E	30.63°N	Urban
	/	Guanghan	104.21°E	31.03°N	Suburban
	/	Chengdu University of Information Technology	103.99°E	30.58°N	Urban
	/	Chengdu Academy of Environmental Sciences	104.05°E	30.65°N	Urban

Table S4 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 S5 The anthropogenic VOC emission species input into the CB06 mechanism in the CMAQ model.

Mechanism	Category	Model Species	Definition
CB06	Alkanes	ETHA	ethane
		PRPA	propane
		PAR	carbon-carbon single bond
	Alkenes	ETH	ethene (ethylene)
		OLE	terminal alkene bond
		IOLE	internal alkene bond
		ISOP	isoprene
		TERP	monoterpenes
	Aromatics	BENZENE	benzene
		TOL	toluene and other monoalkyl aromatics
		XYLMN	xylene and other polyalkyl aromatics except naphthalene
		CRES	cresol and higher molecular weight phenols
	Aldehydes	FORM	formaldehyde
		ALD2	acetaldehyde
		ALDX	aldehydes with 3 or more carbons
		GLY	glyoxal
		MGLY	methyl glyoxal
	Acids	FACD	formic acid
		AACD	acetic acid
	Others	ETHY	ethyne (acetylene)
		ACET	acetone
		ISPD	isoprene reaction products (methacrolein, methylvinyl ketone, others)
		MEOH	methanol
		ETOH	ethanol
		KET	carbon-ketone bond

Table S6 The anthropogenic VOC emission species input into the SAPRC07 mechanism in the CMAQ model.

Mechanism	Category	Model Species	Definition
SAPRC07	Alkanes	ALK1	alkanes and other non-aromatic compounds that react only with OH, and have k_{OH} between 2 and 5×10^2 ppm^{-1} min^{-1}. (Primarily ethane)
		ALK2	alkanes and other non-aromatic compounds that react only with OH, and have k_{OH} between 5×10^2 and 2.5×10^3 ppm^{-1} min^{-1}. (Primarily propane and acetylene)
		ALK3	alkanes and other non-aromatic compounds that react only with OH, and have k_{OH} between 2.5×10^3 and 5×10^3 ppm^{-1} min^{-1}.
		ALK4	alkanes and other non-aromatic compounds that react only with OH, and have k_{OH} between 5×10^3 and 1×10^4 ppm^{-1} min^{-1}.
		ALK5	alkanes and other non-aromatic compounds that react only with OH, and have k_{OH} greater than 1×10^4 ppm^{-1} min^{-1}.
	Alkenes	ETHE	Ethene
		OLE1	alkenes (other than ethene) with $k_{OH} < 7 \times 10^4$ ppm^{-1} min^{-1}.
		OLE2	Alkenes with $k_{OH} > 7 \times 10^4$ ppm^{-1} min^{-1}.
		ISOP	isoprene
		TERP	terpenes
	Aromatics	ARO1	aromatics with $k_{OH} < 2 \times 10^4$ ppm^{-1} min^{-1}.
		ARO2MN	ARO2 minus naphthalene
		BENZENE	benzene
		CRES	phenols and cresols
	Aldehydes	HCHO	formaldehyde
		CCHO	acetaldehyde
		RCHO	lumped C3+ aldehydes (mechanism based on propionaldehyde)
		BALD	aromatic aldehydes (e.g., benzaldehyde)
		GLY	glyoxal
		MGLY	methyl glyoxal
		MACR	methacrolein
	Acids	FACD	formic acid
		CCOOH	acetic acid
		RCOOH	higher organic acids and, in Carter, peroxy acids (mechanism based on propionic acid).
	Other	ACYE	acetylene
		ACETONE	acetone
		MEK	ketones and other non-aldehyde oxygenated products which react with OH radicals faster than $5 < 10^{-13}$ but slower than 5×10^{-12} cm^3 $molec^{-2}$ sec^{-1}. (Based on mechanism for methyl ethyl ketone).
		PRD2	ketones and other non-aldehyde oxygenated products which react with OH radicals faster than 5×10^{-12} cm^3 $molec^{-2}$ sec^{-1}.
		BACL	Biacetyl
		MVK	Methyl Vinyl Ketone
		MEOH	Methanol
		IPRD	Lumped isoprene product species

Table S7 The anthropogenic VOC emission species input into the RACM2 mechanism in the CMAQ model.

Mechanism	Category	Model Species	Definition
RACM2	Alkanes	ETH	ethane
		HC3	alkanes, esters and alkynes with OH rate constant (298 K, 1 atm) less than 3.4×10^{-12}
		HC3	alkanes, esters and alkynes with OH rate constant (298 K, 1 atm) less than 3.4×10^{-12}
		HC5	alkanes, esters and alkynes with OH rate constant (298 K, 1 atm) between 3.4×10^{-13} and 6.8×10^{-12}
		HC8	alkanes, esters and alkynes with OH rate constant (298 K, 1 atm) greater than 6.8×10^{-12}
	Alkenes	ETE	ethene
		API	alpha-pinenes and other cyclic terpenes with one double bond
		ISO	isoprene
		OLI	internal alkenes
		OLT	terminal alkenes
	Aromatics	BEN	benzene
		CSL	cresol and other hydroxy substituted aromatics
		PHEN	phenol
		TOL	toluene and less reactive aromatics
		XYM	m-xylene
		XYP	p-xylene
		XYO	o-xylene
	Aldehydes	ACD	acetaldehyde
		ALD	C3 and higher aldehydes
		BALD	benzaldehyde and other aromatic aldehydes
		GLY	glyoxal
		HCHO	formaldehyde
		MACR	methacrolein
		MGLY	methylglyoxal and other alpha-carbonyl aldehydes
		UALD	unsaturated aldehydes
	Acids	ORA1	formic acid
		ORA2	acetic acid and higher acids
	Other	ACE	acetylene
		ACT	Acetone
		EOH	ethanol
		KET	ketones
		MEK	methyl ethyl ketone
		MVK	methyl vinyl ketone
		MOH	methanol

Table S8 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%
Root Mean Square Error (RMSE)	$\frac{\sqrt{\frac{1}{N}\sum(S_i-O_{i)}{}^2}}{\sqrt{\frac{1}{N}\sum[(S_i-\bar{S})-(O_i-\bar{O})]^2}}$	/
Gross Error (GE)	$\frac{2}{N}\sum\lvert S_i-O_i\rvert$	/

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.

Table S9 The WRF model performance for temperature (°C) at 2 m, relative humidity (%) at 2 m, wind speed (m/s) at SAES and XJ site.

	Obs.	**Sim.**	**R**	**MB**	**RMSE**	**GE**
2-m Temperature (K)						
SAES	302.4	304.8	0.9	-2.4	3.1	2.7
XJ	301.0	302.7	0.93	-1.5	2.2	1.8
Relative Humidity (%)						
SAES	60.7	57.0	0.84	3.7	10.6	8.1
XJ	70.5	61.7	0.81	7.2	12.6	10.3
10-m Wind Speed (m/s)						
SAES	2.0	1.1	0.32	0.9	1.4	1.0
XJ	1.9	2.1	0.32	-0.3	1.6	1.2

Note. R is correlation coefficient; MB is mean bias; RMSE is root mean square error; GE is gross error. The equations of R, MB, RMSE and GE can be found in Table S8.