Supplementary Materials for "Spatial Disparities of Ozone Pollution in the Sichuan Basin Spurred by An Extreme Heatwave"

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Supporting Information

Supporting Information includes 9 pages, 6 figures and 3 tables

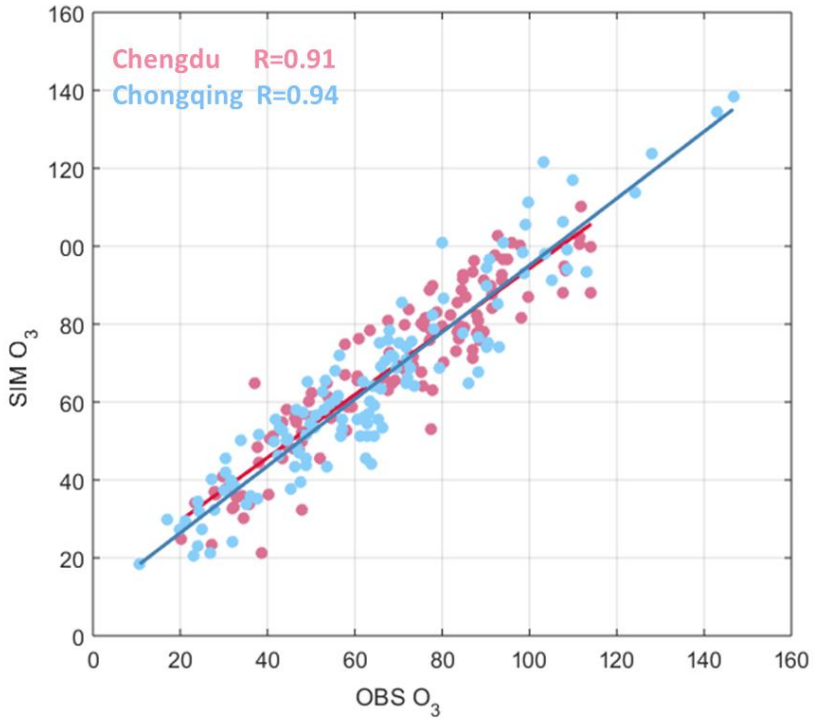

Fig S1 Comparision of machine learning simulated O_3 with observations in Chengdu and Chongqing

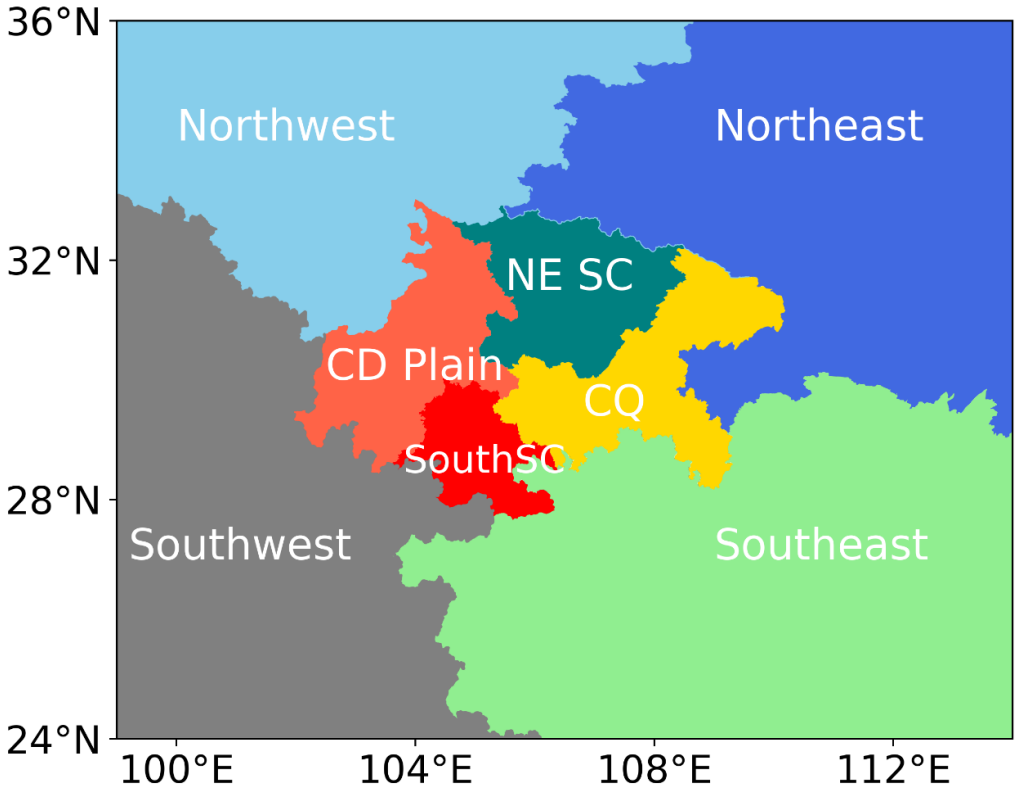

Fig S2 The map showing the tracked source regions in CMAQ-ISAM model.

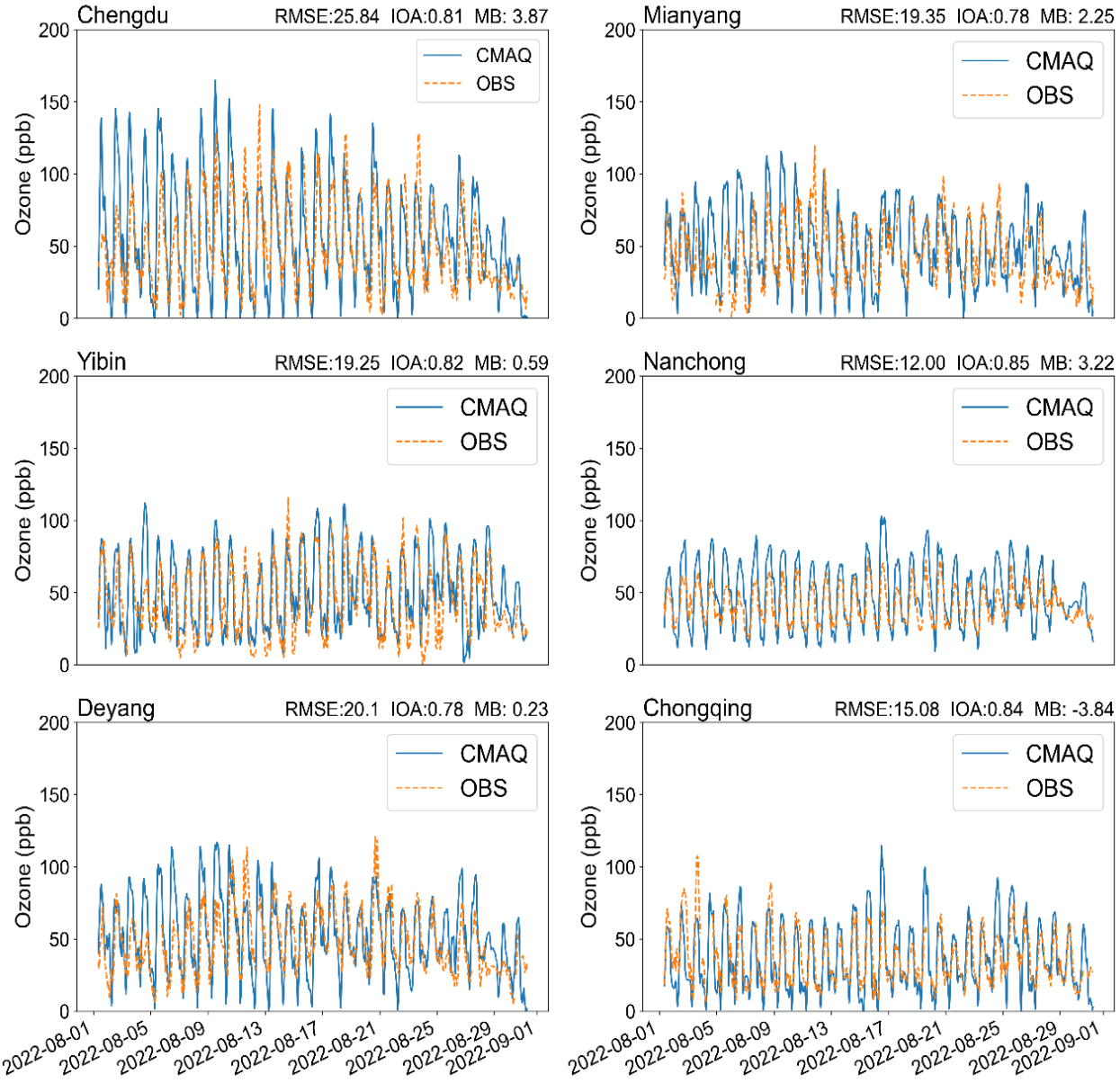

Fig S3 Comparison of the simulated and observed O_3 concentrations at different cities within the SCB regions.(RMSE stands for root mean square error; IOA stands for index of agreement and MB stands for mean bias)

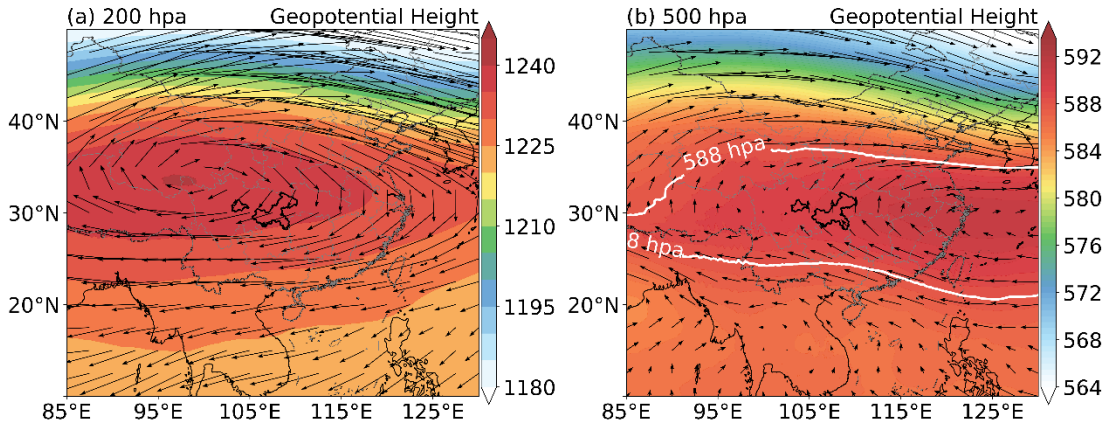

Fig S4 (a) Distributions of the South Asia High (200 hpa) and (b) the Western Pacific Subtropical High (500 hpa)

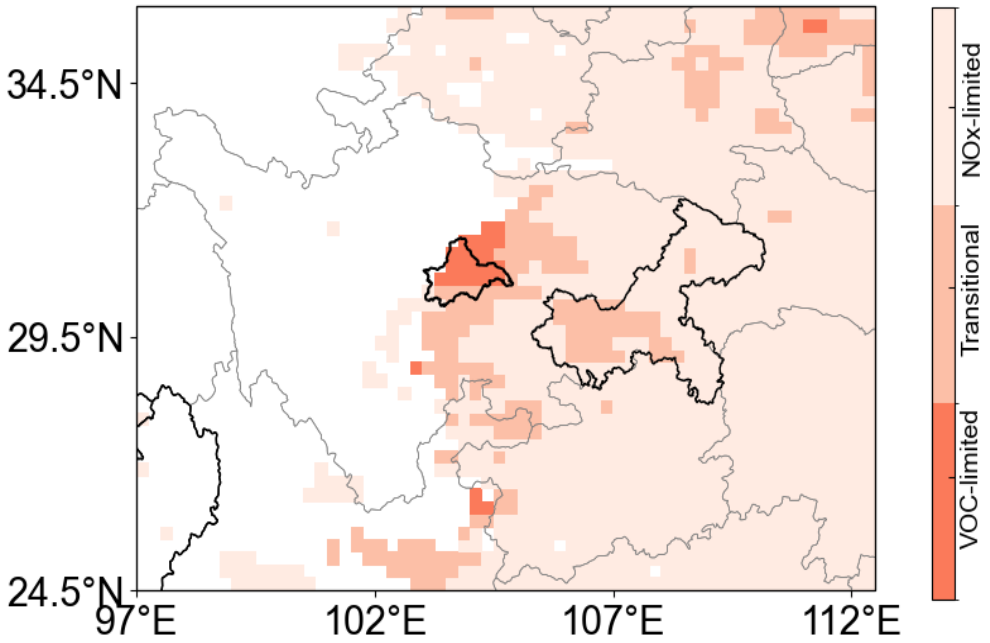

Fig S5 Spatial distribution of satellite diagnosed O_3-NO_x-VOCs sensitivity in the SCB. (The regime was identified based on the ration of HCHO and NO_2)

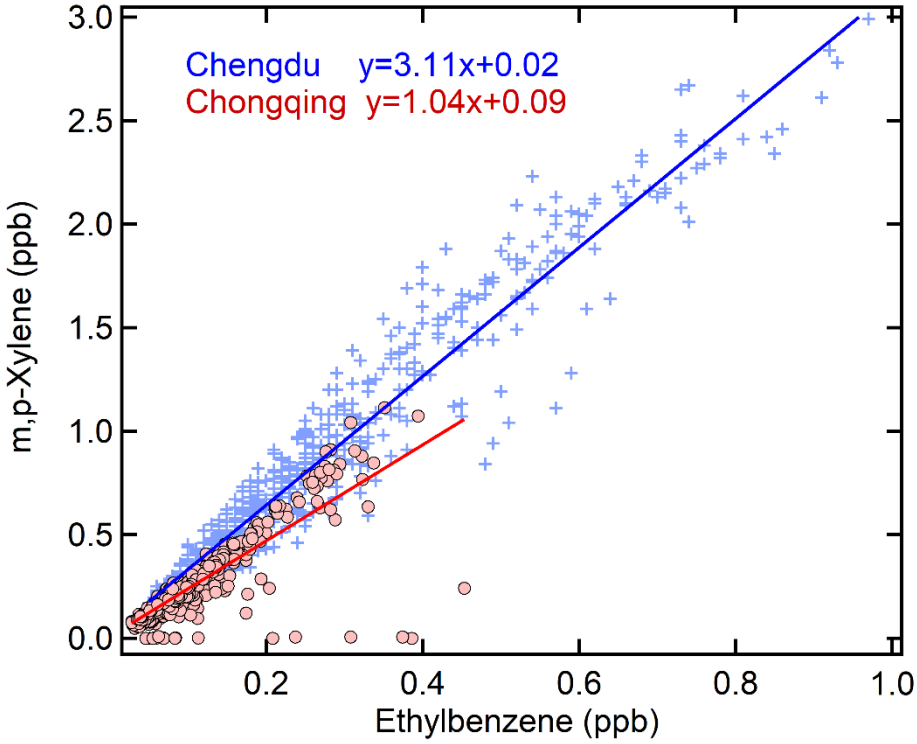

Fig S6 Scatter plot of m,p-Xylene and ethylbenzene in Chengdu and Chongqing

Table S1 Introduction of monitoring instruments used in this work

Parameter	Manufacture	model	resolution
O3	Thermo Scientific	49i-D1NAA	5min
NOx	Thermo Scientific	42i-DNMSDAA	5min
CO	Thermo Scientific	48i-DNSAA	5min
SO2	Thermo Scientific	43i-DNSAA	5min
VOC	Synspec	GC955-611/811	1h
Meteorology	Lufft	Chengdu: WS600-UMB Chongqing: WS502-WTB100	

Tables S2. Statistics of VOC mixing ratios measured in Chengdu and Chongqing. The S.D. denotes the standard deviation of the mixing ratios of VOC species (Unit: ppbv).

Class	VOC species	Chengdu		Chongqing	
		Mean	S.D.	Mean	S.D.
Alkanes	Ethane	4.1	0.6	1.6	0.2
	Propane	2.8	0.7	0.6	0.1
	2-Methylpropane	1.0	0.2	0.3	0.1
	Butane	1.5	0.4	0.7	0.2
	2-Methylbutane	1.3	0.3	1.0	0.1
	n-Pentane	0.3	0.1	0.3	0.1
	Cyclohexane	-	-	0.1	0.0
	2,2-Dimethylbutane	0.1	0.0	0.0	0.0
	2,3-Dimethylbutane	0.0	0.0	0.3	0.0
	2-Methylpentane	0.6	0.1	0.2	0.0
	3-Methylpentane	0.2	0.0	0.1	0.0
	n-Hexane	0.6	0.2	0.1	0.0
	2-Methylhexane	-	-	0.0	0.0
	3-Methylhexane	0.1	0.0	0.1	0.0
	Heptane	0.1	0.0	0.1	0.0
	Octane	0.2	0.0	0.0	0.0
	n-Nonane	0.0	0.0	0.1	0.0

	n-Decane	-	-	0.0	0.0
	Undecane	0.0	0.0	0.0	0.0
	n-Dodecane	-	-	0.0	0.0
Alkenes	Ethene	0.9	0.3	0.4	0.1
	Propene	0.1	0.1	0.2	0.0
	1,3-Butadiene	-	-	0.0	0.0
	1-Butene	0.1	0.0	0.1	0.0
	Cis-2-BUTENE	0.1	0.0	0.1	0.0
	Trans-2-Butene	0.1	0.0	0.1	0.0
	Isoprene	0.3	0.3	0.6	0.5
	Cis-2-Pentene	0.0	0.0	0.0	0.0
	1-Pentene	0.1	0.0	0.1	0.0
	Trans-2-Pentene	0.0	0.0	0.0	0.0
	1-Hexene	0.1	0.0	0.0	0.0
Alkyne	Ethyne	-	-	1.2	0.3
Aromatics	Benzene	0.4	0.1	0.3	0.1
	Toluene	1.0	0.2	0.5	0.1
	Ethenylbenzene	0.1	0.0	0.0	0.0
	Ethylbenzene	0.3	0.1	0.1	0.1
	m-Xylene	1.0	0.3	0.4	0.2
	o-Xylene	0.4	0.1	0.2	0.1
	Isopropylbenzene	0.0	0.0	0.0	0.0
	Propylbenzene	0.0	0.0	0.0	0.0
	3-Ethyltoluene	0.0	0.0	0.0	0.0
	4-Ethyltoluene	0.0	0.0	0.0	0.0
	1,3,5-Trimethylbenzene	0.0	0.0	0.0	0.0
	2-Ethyltoluene	0.0	0.0	0.0	0.0
	1,2,4-Trimethylbenzene	0.1	0.0	0.1	0.0
	1,2,3-Trimethylbenzene	0.0	0.0	0.0	0.0

Table S3 Configuration and settings of WRF-CMAQ modeling system

Item	Scheme
Grid resolution	outer: 36k×36km; inner: 12×12 km
Initial/boundary conditions	WRF: ECMWF reanalysis data CMAQ-outer: profile CMAQ-inner: CMAQ-outer
Microphysics	WRF single-moment 5-class microphysics
Short-wave radiation	Goddard
Long-Wave radiation	RRTM
WRF nudging	Yes
Boundary Layer	ACM2
Gas-phase Chemistry	CB6
Aerosol option	AERO6
Dry deposition	M3DRY
Anthropogenic emissions	MEIC+MIX
Natural emissions	MEGAN(version 2.10)