Supplement of Atmos. Chem. Phys., 24, 3029–3042, 2024
https://doi.org/10.5194/acp-24-3029-2024-supplement

Atmospheric Chemistry and Physics
Open Access
EGU

Supplement of

Spatial disparities of ozone pollution in the Sichuan Basin spurred by extreme, hot weather

Nan Wang et al.

Correspondence to: Nan Wang (nan.wang@scu.edu.cn) and Fumo Yang (fmyang@scu.edu.cn)

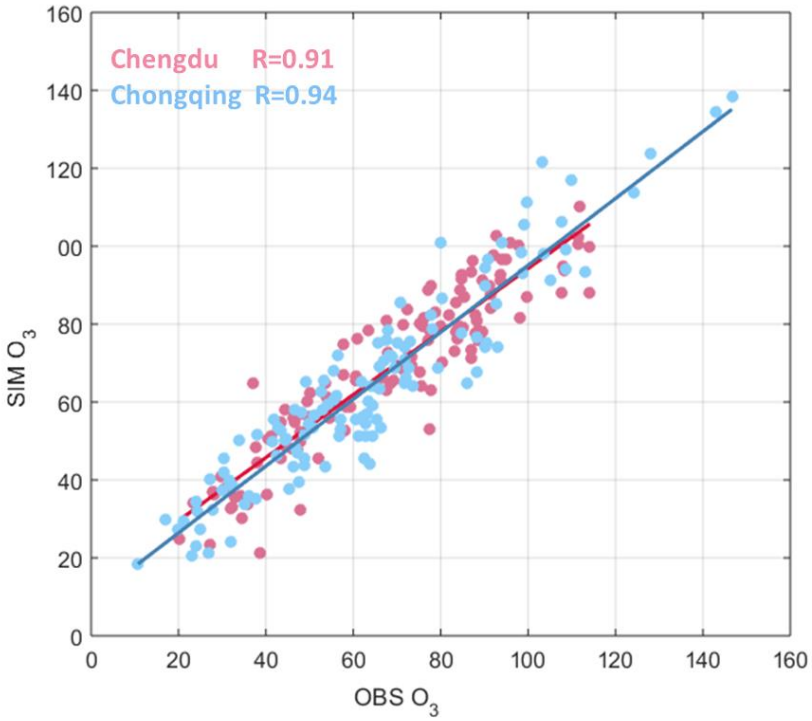

Fig S1 Comparision of machine learning simulated O_3 with observations in Chengdu and Chongqing

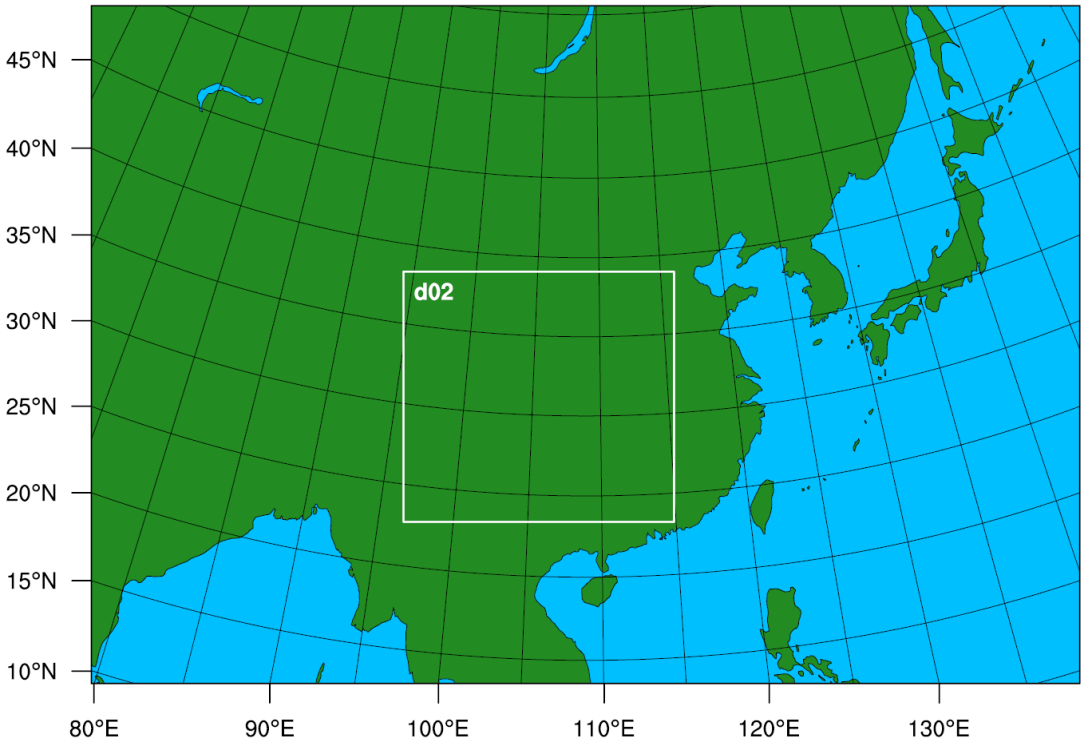

Fig S2 Domain coverage of the WRF-CMAQ model. The outer box shows the domain of d01 and the inner box shows the domain of d02.

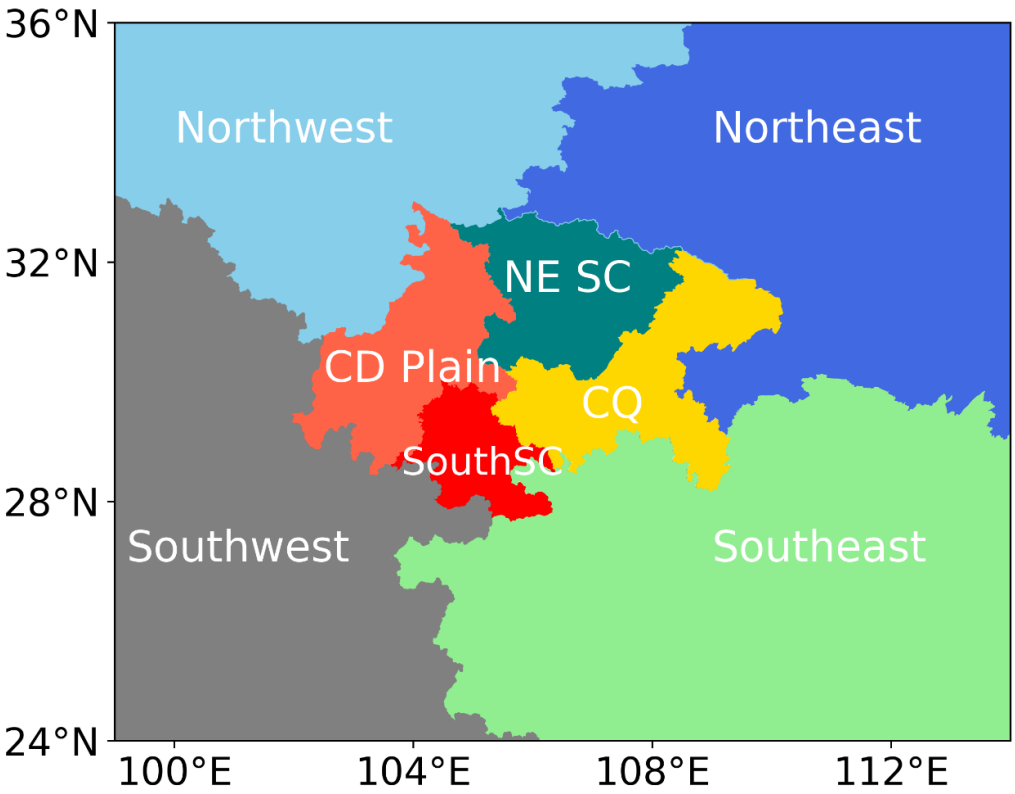

Fig S3 The map showing the tracked source regions in CMAQ-ISAM model.

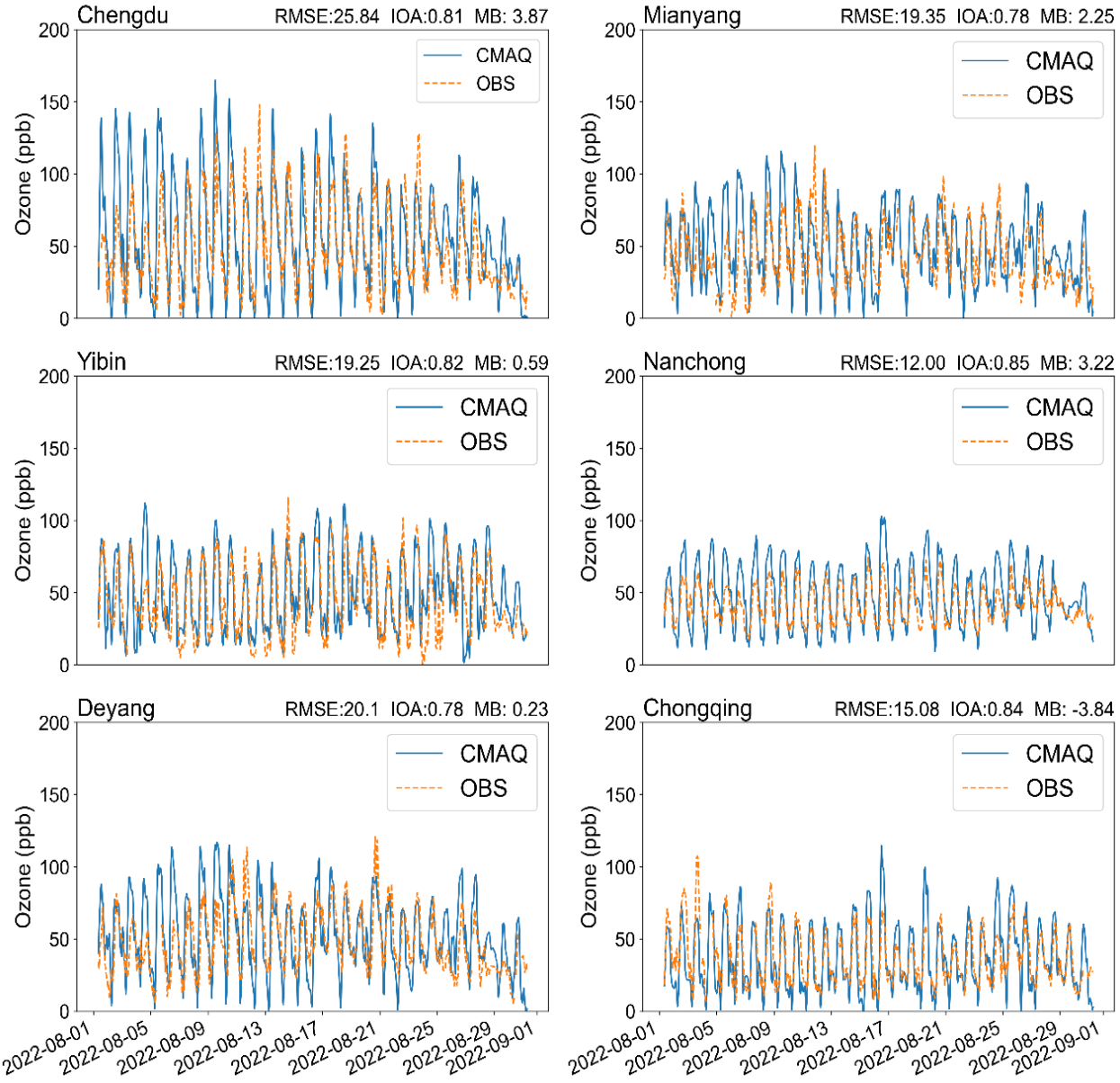

Fig S4 Comparison of the simulated and observed O_3 concentrations at different cities within the SCB regions.(RMSE stands for root mean square error; IOA stands for index of agreement and MB stands for mean bias)

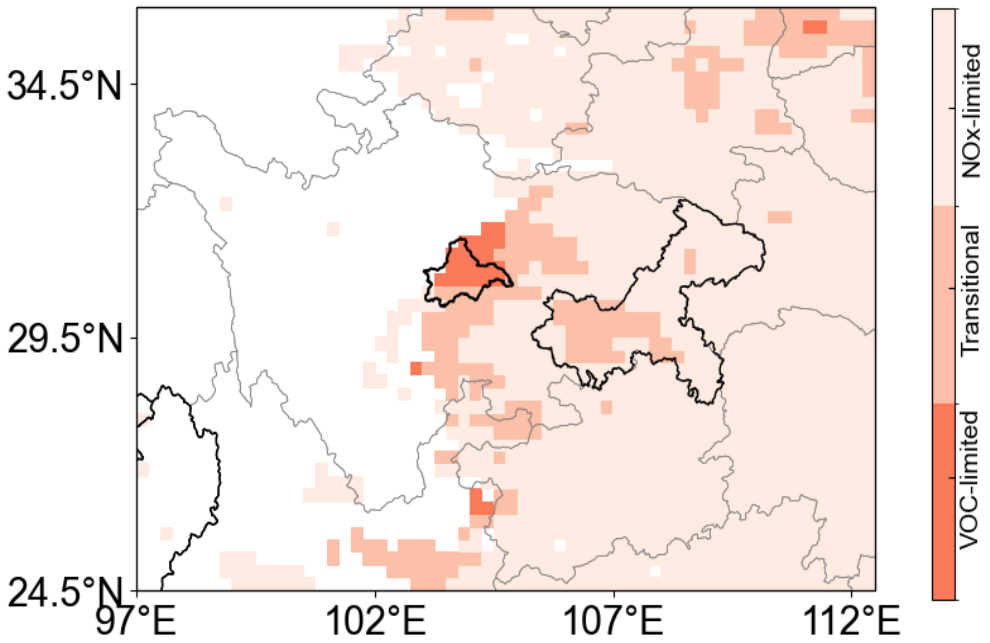

Fig S5 Spatial distribution of satellite diagnosed O_3-NO_x-VOCs sensitivity in the SCB. (The regime was identified based on the ration of HCHO and NO_2)

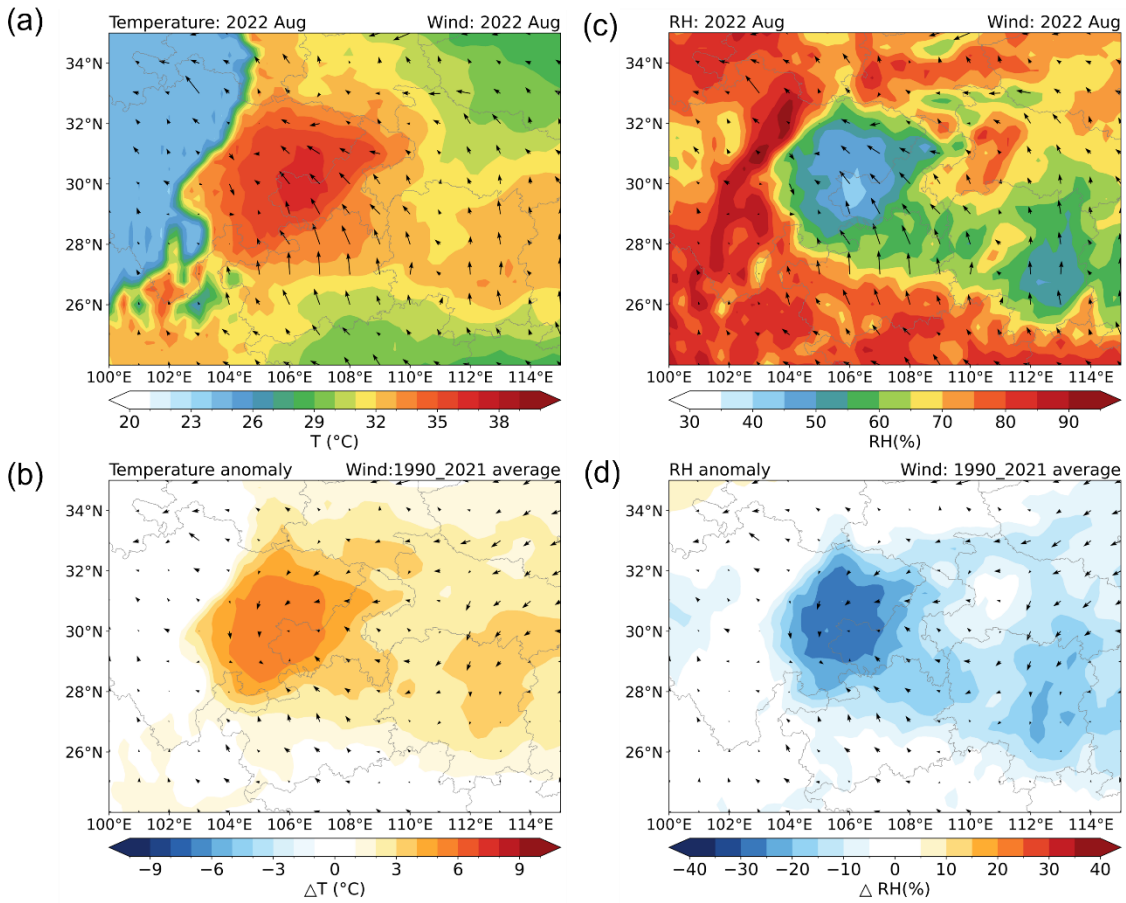

Fig S6 (a) Spatial distribution of temperature and winds at 1000 hPa during 2022 Aug; (b) Spatial distribution of temperature anomaly (2022 – climate average) and the averaged wind between 1990 and 2021; (c) Same as (a) but for relative humidity (RH); (d) Same as (b) but for RH.

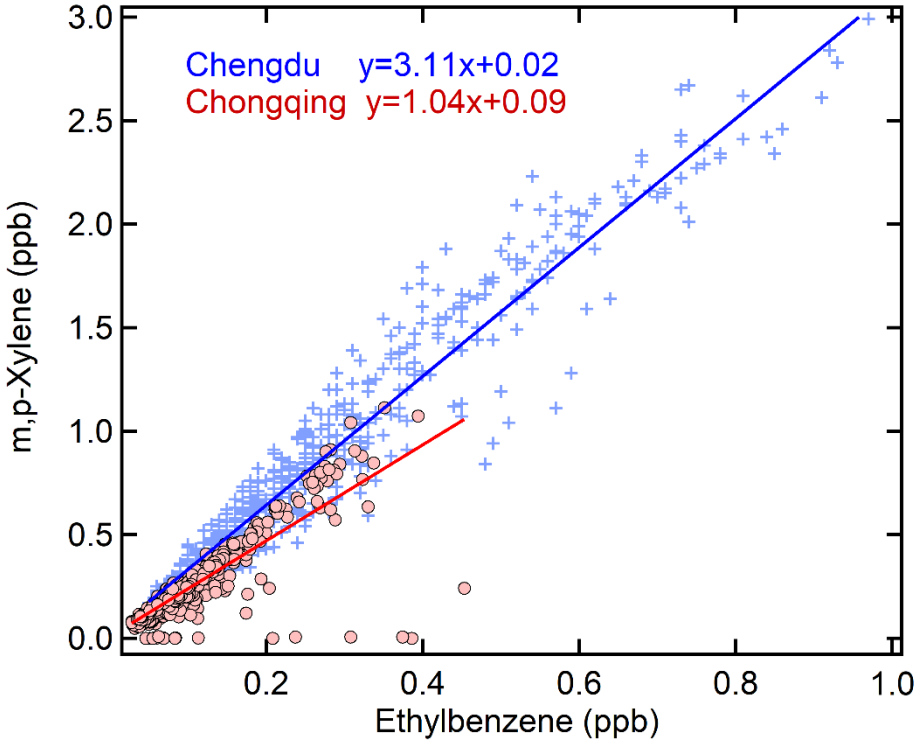

Fig S7 Scatter plot of m,p-Xylene and ethylbenzene in Chengdu and Chongqing

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
J_{NO2}	MetCon	UF-CCD	1min
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)

Table S4 Statistical validation of WRF simulated meteorological parameters.

	MB	RMSE	R
Temperature (℃)	-0.6	2.1	0.91
Relative humidity (%)	-4.5	8.6	0.86
Wind speed (m/s)	1.6	1.8	0.45