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Recommendations on benchmarks for numerical air quality model applications in China – Part 2: Ozone and uncertainty analysis

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Contents

Table S1 4MDA8 and MDA8-90 in 74 Cities of China and 1151 Sites across the United States (2013–2019) (unit: μg/m3, adopted from China Blue Book for the Prevention and Control of Atmospheric Ozone Pollution 2020)

Statistical methods	Region	2013	2014	2015	2016	2017	2018	2019
Fourth-highest MDA8	74 cities in China	189	201	204	204	227	222	236
	US	142	141	143	144	143	145	—
MDA8-90	74 cities in China	139	145	150	154	167	168	181
	US	122	121	123	122	121	122	—

Table S2 Summary of studies complied in this work

Reference	Model	Chemical Mechanism	O_3 evaluated	Seasons	Regions
An et al. (2013)	CMAQ	CB4	O_3	Annual	BTH, Northeast, YRD
Ansari et al. (2019)	WRF-Chem	CBM-Z	O_3	Fall	BTH, NCP
Bei et al. (2016)	WRF-Chem	CBM-Z	O_3	Winter	PRD
Bei et al. (2018)	WRF-Chem	SAPRC-99	O_3	Summer	BTH
Bouarar et al. (2019)	WRF-Chem	MOZART	O_3	Winter, Summer	BTH, YRD, PRD
Campbell et al. (2017)	WRF-Chem	CBM-Z	O_3	Spring	PRD, Southeast
Chang et al. (2021)	WRF-Chem	RADM2	O_3	Spring	PRD
Che et al. (2011)	CMAQ	CB05	O_3	Fall	PRD
Chen et al. (2016)	WRF-Chem	CBM-Z	O_3	Fall	BTH
Chen et al. (2019)	WRF-Chem	RACM	O_3	Fall	PRD
Chen et al. (2020)	CMAQ	CB06	O_3	Annual	BTH+NCP+YRD+Central China+Northeast
Chen et al. (2021a)	WRF-Chem	Not mentioned	O_3	Winter	BTH
Chen et al. (2021b)	CMAQ	SAPRC-11	8-hr max O_3	Summer	BTH
Chen et al. (2021c)	CMAQ	SAPRC07	O_3	Fall	BTH, YRD, PRD, BTH+YRD+PRD+Southeast
Cheng et al. (2019)	CMAQ	CB05	O_3	Annual	BTH
Cui et al. (2015)	WRF-Chem	RACM	8-hr max O_3	Annual	PRD

Reference	Model	Chemical Mechanism	O_3 evaluated	Seasons	Regions
Dang and Liao (2019)	GEOS-Chem	default	O_3	Winter, Spring, Summer, Fall	Entire China
Dang et al. (2021)	GEOS-Chem	default	8-hr max O_3	Summer	YRD, NCP
Ding et al. (2022)	CMAQ	CB06	O_3	Winter, Spring, Summer, Fall	BTH, Central China, NCP
Dong et al. (2013)	CMAQ	CB05	O_3	Summer	YRD
Duan et al. (2021)	CMAQ	CB05	8-hr max O_3	Annual	BTH
Fan et al. (2014)	CMAQ	CB4	O_3	Fall	PRD
Fan et al. (2015)	CMAQ	Not mentioned	O_3	Spring	PRD
Fang et al. (2021)	CMAQ, CAMx	CB06	O_3	Fall	PRD
Feng et al. (2016a)	WRF-Chem	MOZART	O_3	Spring	Northwest
Feng et al. (2016b)	WRF-Chem	SAPRC-99	O_3	Summer	Northwest
Feng et al. (2018)	WRF-Chem	SAPRC-99	O_3	Winter	Northwest
Feng et al. (2019a)	CMAQ	CB05	8-hr max O_3	Winter+Spring+Fall	YRD
Feng et al. (2019b)	WRF-Chem	SAPRC-99	O_3	Fall	BTH
Feng et al. (2020)	WRF-Chem	SAPRC-99	O_3	Winter	Northwest
Feng et al. (2021a)	WRF-Chem	SAPRC-99	O_3	Fall	BTH
Feng et al. (2021b)	GEOS-Chem	default	O_3	Summer	Entire China
Fu et al. (2008)	CMAQ	CB4	O_3	Summer	Entire China, PRD + Southeast

Reference	Model	Chemical Mechanism	O_3 evaluated	Seasons	Regions
Fu et al. (2012)	CMAQ	CB05	O_3	summer	Southeast
Fu et al. (2019)	CMAQ	CB05	8-hr max O_3	Winter	PRD
Gao and Zhang (2012)	CMAQ	CB4	O_3	Summer	BTH
Gao et al. (2016)	WRF-Chem	CBM-Z	O_3	Spring	YRD
Gao et al. (2017)	WRF-Chem	CBM-Z	O_3	Summer	YRD
Gao et al. (2020a)	WRF-Chem	CBM-Z	O_3	fall	BTH+YRD+PRD+Southeast
Gao et al. (2020b)	WRF-Chem	CBM-Z	O_3	Annual	NCP, YRD, PRD
Gong and Liao (2019)	GEOS-Chem	default	8-hr max O_3	Summer	BTH
Gong et al. (2021)	GEOS-Chem	default	8-hr max O_3	Spring+Summer+Fall	BTH, YRD
Guo et al. (2016)	WRF-Chem	CBM-Z	O_3	Fall	BTH
Guo et al. (2019)	CMAQ	SAPRC-11	O_3	Summer	Entire China
Guo et al. (2020)	WRF-Chem	MOZART	O_3	Summer, Fall	BTH, YRD, PRD
H. et al. (2009)	CMAQ,WRF-Chem	SAPRC-99	O_3	Summer	BTH
Han et al. (2013)	CMAQ	CB05	O_3	Winter	BTH
Han et al. (2014)	CMAQ	CB05	O_3	Winter, Summer	BTH
Han et al. (2018)	CMAQ	CB05	O_3	Summer, Winter	BTH
He et al. (2012)	GEOS-Chem	default	O_3	Summer	Entire China
Hong et al. (2017)	two-way	CB05	O_3	Spring, Summer	Entire China

Reference	Model	Chemical Mechanism	O_3 evaluated	Seasons	Regions
Hong et al. (2020)	CMAQ	SAPRC07	O_3	Annual	Entire China
Hu et al. (2016)	CMAQ	SAPRC-11	1-hr max O_3, 8-hr max O_3	Annual	Entire China, NCP, YRD, PRD, SCB, Northeast, Central China, Northwest, Southwest
Hu et al. (2017)	CMAQ	SAPRC-11	O_3,1-hr max O_3	Annual	Entire China, Northeast, NCP, Northwest, YRD, Central China, SCB, PRD+Southwest
Hu et al. (2018)	WRF-Chem	RADM2	O_3	Summer	YRD
Huang et al. (2016)	CAMx	CB05	O_3	Spring, Fall	PRD
Huang et al. (2021)	CMAQ	CB06	O_3	Winter+Spring	Central china
Itahashi et al. (2015)	CAMx	SAPRC-99	O_3	Spring	Entire China
Jeong and Park (2013)	GEOS-Chem	default	O_3	Annual	Entire China
Jiang et al. (2008)	WRF-Chem	RADM2	O_3	Fall	PRD
Jiang et al. (2021)	GEOS-Chem	default	8-hr max O_3	Summer	Entire China
Kwok et al. (2010)	CMAQ	CB4	O_3	Winter, Spring, Summer, Fall	PRD
Leung et al. (2020)	CMAQ	SAPRC-99	1-hr max O_3	Winter, Summer	BTH+YRD+PRD+Central China+Southeast
Li et al. (2007)	NAQPMS	CBM-Z	O_3	Annual	YRD, NCP, Northwest

Reference	Model	Chemical Mechanism	O_3 evaluated	Seasons	Regions
Li et al. (2008)	NAQPMS	CBM-Z	O_3	Summer	NCP
Li et al. (2011a)	NAQPMS	CBM-Z	O_3	Summer	NCP
Li et al. (2011b)	WRF-Chem	CBM-Z	O_3	Summer	BTH
Li et al. (2012)	CMAQ	CB05	O_3	Summer	YRD
Li et al. (2013)	CAMx	CB05	O_3,Ox	Winter, Spring, Summer, Fall	PRD
Li et al. (2016a)	CAMx	CB05	O_3	Summer	YRD
Li et al. (2016b)	WRF-Chem	CBM-Z	O_3	Spring	PRD
Li et al. (2016c)	CMAQ	SAPRC-99	O_3	Annual	Southeast
Li et al. (2016d)	WRF-Chem	RACM	O_3,1-hr max O_3	Winter	PRD
Li et al. (2017a)	WRF-Chem	SAPRC-99	O_3	Spring	BTH, YRD, PRD, NCP, Northeast, Northwest, Central China, Southeast, Southwest
Li et al. (2017b)	WRF-Chem	CBM-Z	O_3	Spring	YRD
Li et al. (2017c)	two-way	CB05	O_3	Summer+Fall	YRD
Li et al. (2018a)	WRF-Chem	RADM2	O_3	Summer	Northwest
Li et al. (2018b)	WRF-Chem	SAPRC-99	O_3	Winter	BTH
Li et al. (2019)	CAMx	CB05	8-hr max O_3	Spring, Summer, Fall	YRD
Li et al. (2020a)	WRF-Chem	MOZART	O_3	Summer	Northwest

Reference	Model	Chemical Mechanism	O_3 evaluated	Seasons	Regions
Li et al. (2020b)	CMAQ	CB05	O_3	Annual	YRD
Li et al. (2021a)	CMAQ	SAPRC-99	O_3	Spring	NCP
Li et al. (2021b)	GEOS-Chem	default	8-hr max O_3	Winter	BTH
Li et al. (2021c)	WRF-Chem	SAPRC-99	O_3	Winter	BTH
Liao et al. (2014)	WRF-Chem	CBM-Z	O_3	Winter, Summer	YRD
Liao et al. (2015)	WRF-Chem	CBM-Z	O_3	Winter, Summer	YRD
Lin et al. (2009)	CMAQ	CB4	O_3	spring+Summer	BTH, YRD, NCP, Northwest
Lin et al. (2016)	CAMx	SAPRC-99	O_3	Summer	BTH
Liu and Wang (2020)	CMAQ	SAPRC07	8-hr max O_3	Annual	entire china
Liu et al. (2010)	CMAQ	Not mentioned	1-hr max O_3	Spring, Summer, Fall, Winter	BTH+YRD+PRD+Southeast
Liu et al. (2018a)	CMAQ	CB05	1-hr max O_3, 8-hr max O_3	Annual	Entire China
Liu et al. (2018b)	CMAQ	CB05	O_3	Summer	YRD
Liu et al. (2019a)	CMAQ	CB05	O_3	Summer	BTH
Liu et al. (2019b)	WRF-Chem	SAPRC-99	O_3	Winter	BTH
Liu et al. (2019c)	WRF-Chem	SAPRC-99	O_3	Summer	BTH
Liu et al. (2020)	CMAQ	SAPRC-11	O_3	Annual	YRD
Liu et al. (2021)	WRF-Chem	CBM-Z	O_3	Winter	YRD

Reference	Model	Chemical Mechanism	O_3 evaluated	Seasons	Regions
Long et al. (2016)	WRF-Chem	RADM2	O_3	Fall	BTH, NCP
Lou et al. (2014)	GEOS-Chem	default	O_3	Annual	BTH+YRD+PRD+SCB
Lou et al. (2015)	GEOS-Chem	default	O_3	Annual	PRD, Southwest
Lu et al. (2016)	CAMx	CB05	O_3	Winter, Spring, Summer, Fall	PRD
Lu et al. (2019a)	CAMx	CB05	O_3	Annual	PRD
Lu et al. (2019b)	GEOS-Chem	default	8-hr max O_3	Annual	BTH, Central China, NCP, YRD, Northwest, SCB, PRD, Southwest
Ma et al. (2018)	WRF-Chem	RADM2	O_3	Fall	BTH
Ma et al. (2021)	CAMx	CB05	O_3	Summer	NCP
Ni et al. (2018)	GEOS-Chem	default	8-hr max O_3, O_3	Spring	BTH, YRD, PRD, NCP, Northeast, Southwest
Ni et al. (2019)	WRF-Chem	CBM-Z	8-hr max O_3	Summer+Fall	Entire China
Ni et al. (2020)	WRF-Chem	CBM-Z	8-hr max O_3, O_3	Summer+Fall	YRD
Peng et al. (2011)	CAMx	Not mentioned	O_3	Summer, Fall, Winter, Spring	Southeast
Peng et al. (2018)	WRF-Chem	RACM	O_3	Fall	BTH
Qiao et al. (2019a)	CMAQ	SAPRC-11	O_3	Annual	Entire China
Qiao et al. (2019b)	CMAQ	SAPRC-11	8-hr max O_3, 1-	Winter, Summer	SCB

Reference	Model	Chemical Mechanism	O_3 evaluated	Seasons	Regions
			hr max O_3		
Qiao et al. (2021)	CMAQ	SAPRC-99	8-hr max O_3	Summer	SCB
Qin et al. (2015)	CMAQ	SAPRC-99	8-hr max O_3	Winter, Spring, Summer, Fall	PRD
Qiu et al. (2017)	WRF-Chem	CBM-Z	O_3	Winter	BTH+NCP
Qiu et al. (2019a)	CMAQ	CB05	O_3	Summer	BTH
Qiu et al. (2019b)	CMAQ	SAPRC-11	O_3	Summer	BTH
Qiu et al. (2019c)	WRF-Chem	RADM2	O_3	Winter	BTH
Qiu et al. (2020)	GEOS-Chem	default	Ox(1-hr max)	Winter	BTH
Qu et al. (2014)	CAMx	CB05	O_3	Summer	BTH
Qu et al. (2020)	WRF-Chem	Not mentioned	O_3	spring	YRD
Qu et al. (2021)	CMAQ	SAPRC07	8-hr max O_3	Fall, Summer	PRD
Sahu et al. (2021)	CMAQ	CB06	O_3	Annual	Entire China
Shen et al. (2021)	CMAQ	CB05	8-hr max O_3	Spring+Summer+Fall	Entire China
Shi et al. (2021)	CAMx	CB06	O_3	Summer, Fall	YRD
Shu et al. (2016)	CMAQ	CB05	O_3	Summer	YRD
Sicard et al. (2021)	WRF-Chem	MOZART	O_3	Annual	Entire China
Su et al. (2017)	WRF-Chem	RADM2	O_3	Fall	BTH
Su et al. (2021)	CMAQ	SAPRC-99	8-hr max O_3	Summer+Fall	BTH

Reference	Model	Chemical Mechanism	O_3 evaluated	Seasons	Regions
Sun et al. (2019)	GEOS-Chem	default	O_3	Summer	BTH+YRD+Sichuan Basin+NCP+Northwest+Southwest+Central China
Sun et al. (2021a)	WRF-Chem	SAPRC-99	O_3	Summer, Summer	Central China, NCP
Sun et al. (2021b)	GEOS-Chem	UCX(universal tropospheric–stratospheric chemistry extension mechanism)	O_3	Annual	Entire China
Tang et al. (2015)	WRF-Chem	CBM-Z	O_3	Summer	BTH, PRD
Tang et al. (2017a)	CMAQ	Not mentioned	O_3	Summer+Fall	BTH
Tang et al. (2017b)	CMAQ	RADM2	1-hr max O_3	Summer	BTH
Tao et al. (2015)	WRF-Chem	RADM2	O_3	Spring+Summer+Fall	YRD
Tao et al. (2018)	CMAQ	CB06	O_3	Summer, Winter	BTH
Tie et al. (2013)	WRF-Chem	RADM2	O_3	Fall	YRD
Wai and Tanner (2014)	CMAQ	CB05	1-hr max O_3, 8-hr max O_3	Spring, Summer, Fall, Winter	Entire China
Wang et al. (2006)	NAQPMS	CB4	O_3	Spring	BTH, PRD, NCP, Central China, Southeast

Reference	Model	Chemical Mechanism	O_3 evaluated	Seasons	Regions
Wang et al. (2010)	CMAQ	SAPRC-99	O_3	Fall	PRD
Wang et al. (2011a)	CMAQ	CB05,CB4	O_3	Fall	PRD
Wang et al. (2011b)	CMAQ	SAPRC-99	O_3	Fall	PRD
Wang et al. (2014)	WRF-Chem	CBM-Z	O_3	Summer	BTH
Wang et al. (2015)	CMAQ	CB05	O_3	Fall	PRD
Wang et al. (2016a)	WRF-Chem	CBM-Z	O_3	Spring	Entire China
Wang et al. (2016b)	CMAQ	CB05	O_3	Annual	PRD
Wang et al. (2019a)	NAQPMS	CBM-Z	O_3	Summer	BTH, NCP, Central China
Wang et al. (2019b)	CMAQ	CB4	O_3	Summer	BTH, YRD, PRD, SCB, Southwest, Northwest, Central China, Northeast, NCP
Wang et al. (2019c)	CMAQ	CB05	O_3	Annual	BTH, YRD, PRD
Wang et al. (2019d)	CMAQ	SAPRC-11	O_3	Summer	BTH, YRD, PRD, SCB
Wang et al. (2019e)	WRF-Chem	SAPRC-99	O_3	Fall	YRD
Wang et al. (2020)	WRF-Chem	RADM2	8-hr max O_3	Winter, Summer	SCB
Wang et al. (2021a)	WRF-Chem	CBM-Z	O_3	Summer	PRD
Wang et al. (2021b)	CMAQ	CB05	O_3	Annual	BTH
Wang et al. (2021c)	CMAQ	SAPRC-11	8-hr max O_3	Summer	Entire China
Wang et al. (2021d)	WRF-Chem	CBM-Z	O_3	Winter+Spring+Summer	Central China
Wang et al. (2021e)	CMAQ	SAPRC-11	O_3	Spring+Summer	YRD

Reference	Model	Chemical Mechanism	O_3 evaluated	Seasons	Regions
Wang et al. (2021f)	GEOS-Chem	default	8-hr max O_3	Summer	BTH
Wang et al. (2021g)	CMAQ	SAPRC-11	1-hr max O_3, 8-hr max O_3, O_3	Winter	YRD
Wei et al. (2018)	WRF-Chem	SAPRC-99	8-hr max O_3	Summer	BTH
Wei et al. (2019)	WRF-Chem	SAPRC-99	O_3	Summer	BTH
Wen et al. (2020)	WRF-Chem	CBM-Z	O_3	Winter	BTH
Wu et al. (2011)	NAQPMS	CBM-Z	O_3	Summer	BTH
Wu et al. (2017)	WRF-Chem	SAPRC-99	O_3	Summer	BTH
Wu et al. (2018)	WRF-Chem	SAPRC-99	O_3	Spring	NCP
Wu et al. (2020)	CMAQ	CB05	1-hr max O_3	Summer	Entire China, BTH, YRD, PRD, SCB, Entire China except BTH+YRD+PRD+SCB
Wu et al. (2021)	WRF-Chem	SAPRC-99	O_3	Winter	Northwest
Xie et al. (2016a)	WRF-Chem	CBM-Z	O_3	Winter, Summer	YRD
Xie et al. (2016b)	WRF-Chem	RADM2	O_3	Winter, Summer	PRD, Southwest
Xing et al. (2011a)	CMAQ	CB05	1-hr max O_3	Summer	BTH, YRD, PRD, BTH+YRD+PRD+Southeast
Xing et al. (2011b)	CMAQ	CB05	O_3	Summer	BTH
Xing et al. (2017)	CMAQ	CB05	1-hr max O_3	Winter, Summer	Entire China, BTH, YRD, PRD, Central

Reference	Model	Chemical Mechanism	O_3 evaluated	Seasons	Regions
					China, SCB
Xing et al. (2018)	CMAQ	SAPRC-99	O_3	Winter, Summer	BTH
Xu et al. (2019)	WRF-Chem	RADM2	O_3	Fall	YRD
Xu et al. (2020)	WRF-Chem	CBM-Z	O_3	Summer	BTH
Yamaji et al. (2010)	CMAQ	SAPRC-99	O_3	Summer	NCP
Yan et al. (2021)	GEOS-Chem	Not mentioned	8-hr max O_3	Spring+Summer	Central China
Yang et al. (2014)	GEOS-Chem	default	O_3	Summer	PRD
Yang et al. (2018)	CMAQ	CB05	O_3	Summer	BTH
Yang et al. (2019a)	WRF-Chem	CBM-Z	8-hr max O_3	Annual	Northwest, SCB, NCP, Southwest
Yang et al. (2019b)	NAQPMS	CBM-Z	O_3	Winter, Spring, Summer, Fall	PRD
Yang et al. (2020a)	WRF-Chem	CBM-Z	O_3	Annual	Northwest+Southwest
Yang et al. (2020b)	CMAQ	CB06	O_3	Summer	scb
Yang et al. (2021a)	CMAQ	CB06	O_3	Spring	SCB
Yang et al. (2021b)	CMAQ	CB05	O_3,8-hr max O_3	Winter, Spring, Summer, Fall	YRD
Yao et al. (2021)	CMAQ	CB06	8-hr max O_3	Summer	BTH
Ye et al. (2016)	WRF-Chem	Not mentioned	O_3	Fall	PRD
Yin et al. (2018)	CAMx	CB05	O_3	Spring, Fall	PRD

Reference	Model	Chemical Mechanism	O_3 evaluated	Seasons	Regions
Yin et al. (2021)	GEOS-Chem	default	O_3	Spring+Summer	Entire China
You et al. (2017)	CMAQ	CB05	O_3	Summer	PRD
Yu et al. (2012)	WRF-Chem	CBM-Z	O_3	Spring	BTH, YRD
Yu et al. (2014a)	WRF-Chem	CBM-Z	O_3	Summer	BTH
Yu et al. (2014b)	CMAQ	Not mentioned	O_3	Summer	PRD
Yu et al. (2019)	CMAQ	CB06	O_3	Winter, Spring, Summer, Fall	PRD
Zeren et al. (2019)	WRF-Chem	RADM2	O_3	Fall	PRD
Zhang et al. (2013)	CMAQ	CB05	O_3	Fall	PRD
Zhang et al. (2015)	WRF-Chem	CBM-Z	O_3	Summer	YRD
Zhang et al. (2016)	CMAQ,WRF-Chem	CB05	O_3	Winter, Spring, Summer, Fall	PRD, Southeast, Southeast
Zhang et al. (2017a)	WRF-Chem	RADM2	O_3	Spring	YRD
Zhang et al. (2017b)	WRF-Chem	CBM-Z	O_3	Summer	Entire China, YRD, PRD, BTH+NCP
Zhang et al. (2018)	WRF-Chem	CBM-Z	O_3	Winter	YRD
Zhang et al. (2020)	NAQPMS	CBM-Z	O_3,Ox	Summer	BTH
Zhang et al. (2021a)	WRF-Chem	CBM-Z	O_3	Winter, Spring, Summer, Fall	Entire China
Zhang et al. (2021b)	CMAQ	Not mentioned	O_3	Fall, Summer, Winter	BTH+YRD+PRD+SCB

Reference	Model	Chemical Mechanism	O_3 evaluated	Seasons	Regions
Zhang et al. (2021c)	WRF-Chem	Not mentioned	O_3	Fall	YRD
Zhang et al. (2021d)	CMAQ	RACM	O_3,1-hr max O_3	Spring+Summer	YRD
Zhao et al. (2017)	CMAQ	SAPRC-99	1-hr max O_3	Winter, Spring, Summer, Fall	YRD
Zhao et al. (2021a)	CMAQ	CB05	O_3	Fall	PRD
Zhao et al. (2021b)	WRF-Chem	Not mentioned	O_3	Annual	NCP
Zheng et al. (2019)	CMAQ	CB05	O_3,1-hr max O_3, 8-hr max O_3	Summer, Winter	BTH
Zheng et al. (2021)	CMAQ	CB05	O_3	Summer+Fall	PRD, Southeast
Zhou et al. (2010)	CMAQ	Not mentioned	8-hr max O_3, O_3	Summer	YRD
Zhou et al. (2017a)	WRF-Chem	RADM2	8-hr max O_3	Annual	BTH+YRD+NCP+Central China+Southeast
Zhou et al. (2017b)	CMAQ	CB05	O_3	Fall	YRD
Zhu and Liao (2016)	GEOS-Chem	default	O_3	Annual	BTH, Northwest, YRD, PRD, SCB, Southwest, Northeast

Table S3 List of statistical metrics used in studies complied in this study

No.	Abbreviation	Metric	No. of studies used
1	R(R2)	Correlation coefficient	135
2	MB	Mean bias	112
3	NMB	Normalized mean bias	123
4	RMSE	Root mean square error	89
5	NME	Normalized mean error	78
6	IOA	Index of agreement	53
7	FB	Fractional bias	33
8	FE	Fractional error	30
9	ME	Mean error	14
10	MNB	Mean normalized bias	9
11	MNE	Mean normalized error	7
12	FAC2	Fraction of prediction within a factor of two of the observations	5
13	MAGE	Mean absolute gross error	2
14	NB	Normalized bias	2
15	UPPA	Unpaired peak prediction accuracy	1
16	AUP	Accuracy of Unpaired Peak	1
17	Bias Factor	No definition given	1
18	FAC5	Fraction of prediction within a factor of five of the observations	1
19	FRA	Fraction	1
20	MAD	Mean absolute deviation	1
21	NMAD	Normalized mean absolute difference	1
22	NMGE	Normalized mean gross error	1
23	RB	Relative bias	1

Table S4 Definition of regions

No.	Region	Provinces included
1	BTH(Beijing-Tianjin-Hebei)	Beijing, Tianjin, Hebei
2	Central China	Shanxi, Henan, Hubei, Hunan, Jiangxi
3	NCP(North China Plain)	Inner Mongolia, Shandong
4	Northeast	Liaoning, Heilongjiang, Jilin
5	Northwest	Xinjiang, Qinghai, Gansu, Ningxia, Shanxi
6	PRD(Pearl River Delta)	Guangdong, Hong Kong, Macau
7	SCB(Sichuan Basin)	Sichuan, Chongqing
8	Southeast	Fujian, Taiwan
9	Southwest	Tibet, Yunnan, Guizhou, Hainan, Guangxi
10	YRD(Yangtze River Delta)	Jiangsu, Zhejiang, Shanghai, Anhui

Table S5 Definition of statistical metrics used in more than ten studies complied in this work

No.	Statistics (abbreviation)	Definition	Note
1	Correlation coefficient (R)	$\frac{\sum[(\boldsymbol{P_j}-\bar{\boldsymbol{P}})\times(\boldsymbol{O_j}-\bar{\boldsymbol{O}})]}{\sqrt{\sum(\boldsymbol{P_j}-\bar{\boldsymbol{P}})^2\times\sum(\boldsymbol{O_j}-\bar{\boldsymbol{O}})^2}}$	Unitless, -1≤R≤1
2	Index of agreement (IOA/*d*)	$\boldsymbol{1}-\frac{\sum(\boldsymbol{P_j}-\boldsymbol{O_j})^2}{\sum(\lvert\boldsymbol{P_j}-\bar{\boldsymbol{O}}\rvert+\lvert\boldsymbol{O_j}-\bar{\boldsymbol{O}}\rvert)^2}$	Unitless, 0≤*d*≤1
3	Normalize mean bias (NMB)	$\frac{\sum(\boldsymbol{P_j}-\boldsymbol{O_j})}{\sum\boldsymbol{O_j}}\times\boldsymbol{100}$	-100%≤NMB≤+∞
4	Normalize mean error (NME)	$\frac{\sum\lvert\boldsymbol{P_j}-\boldsymbol{O_j}\rvert}{\sum\boldsymbol{O_j}}\times\boldsymbol{100}$	0%≤NME≤+∞
5	Fractional bias (FB)	$\frac{\boldsymbol{2}}{\boldsymbol{N}}\frac{\sum(\boldsymbol{P_j}-\boldsymbol{O_j})}{(\boldsymbol{P_j}+\boldsymbol{O_j})}\times\boldsymbol{100}$	-200%≤FB≤+200%
6	Fractional error (FE)	$\frac{\boldsymbol{2}}{\boldsymbol{N}}\frac{\sum\lvert\boldsymbol{P_j}-\boldsymbol{O_j}\rvert}{(\boldsymbol{P_j}+\boldsymbol{O_j})}\times\boldsymbol{100}$	0%≤FE≤+200%
7	Root mean square error (RMSE)	$\sqrt{\frac{\sum(\boldsymbol{P_j}-\boldsymbol{O_j})^2}{\boldsymbol{N}}}$	concentration unit
8	Mean bias (MB)	$\frac{\sum(\mathbf{P_j}-\mathbf{O_j})}{\mathbf{N}}$	concentration unit
9	Mean error (ME)	$\frac{\sum\lvert\boldsymbol{P_j}-\boldsymbol{O_j}\rvert}{\boldsymbol{N}}$	concentration unit

Table S6 Major parameterizations used in WRF

Model input	Uncertainty factor	Reference
Microphysics scheme	Purdue Lin scheme	Lin et al. (1983)
Cumulus physics option	Grell 3D ensemble scheme	Grell (1993)
Land surface option	Noah land-surface model	Chen and Dudhia (2001)
Boundary layer scheme	Yonsei University (YSU) scheme	Hong et al. (2006)
Long wave radiation option	RRTM scheme	Mlawer et al. (1997)
Short wave radiation option	Goddard short scheme	Chou and Suarez (1994)

Table S7 Estimated uncertainties in emissions, dry deposition velocities and boundary concentrations

Model input	Uncertainty factor	Reference
Anthropogenic NO_x emissions	1.36	(Cheng et al., 2019; Zheng et al., 2021; Zhao et al., 2011)
Anthropogenic VOCs emissions	1.97	(Cheng et al., 2019; Zhao et al., 2013)
Soil NO_x emissions	2	(Dunker et al., 2020; Liu et al., 2017)
Biogenic VOCs emissions	1.71	(Wang et al., 2021; Wang et al., 2023)
Dry deposition velocity of O_3	2	(Dunker et al., 2020; Derwent et al., 2018)
Boundary concentrations of O_3	1.25	(Dunker et al., 2020; Beddows et al., 2017)

*The multiplicative factor represents 2σ of the lognormal uncertainty distribution. Estimates are subjective but based on a review of recent work

Table S8 Quantile values of selected statistical metrics for O_3, 1-hr max O_3 and 8-hr max O_3

Pollutant	Metric	Unit	n	10%	25%	33%	50%	67%	75%	90%
O_3	R	-	891	0.87	0.78	0.74	0.69	0.63	0.6	0.51
O_3	IOA	-	251	0.91	0.88	0.85	0.8	0.73	0.68	0.57
O_3	MB	$\mu g/m^3$	476	32.9	15.4	9.3	1.2	-4.8	-9.5	-22.6
O_3	ME	$\mu g/m^3$	41	49.2	44.0	41.5	35.5	30.9	26.1	17.9
O_3	NMB	%	593	40.8	18.2	10.2	-1.0	-12.7	-18.5	-33.0
O_3	NME	%	341	60.7	49.2	43.5	34.1	26.1	22.6	1.0
O_3	FB	%	439	31.2	8	-1	-15	-25	-31	-56
O_3	FE	%	440	90.1	73	65	56	47	44	1.375
O_3	RMSE	$\mu g/m^3$	331	69.5	56.3	49.4	37.5	27.8	23.4	16.1
1-hr max O_3	R	-	19	0.88	0.84	0.80	0.66	0.60	0.51	0.16
1-hr max O_3	IOA	-	0	—	—	—	—	—	—	—
1-hr max O_3	MB	$\mu g/m^3$	12	8.1	5.4	3.5	-4.4	-12.5	-13.3	-14.6
1-hr max O_3	ME	$\mu g/m^3$	6	22.7	17.8	17.2	16.5	15.6	14.9	12.3
1-hr max O_3	NMB	%	150	53.1	29.9	18.9	3.1	-20.8	-25.0	-32.1
1-hr max O_3	NME	%	71	55.0	36.5	32.9	29.0	21.9	17.8	14.0
1-hr max O_3	FB	%	35	12.0	8.0	5.8	1.0	-1.0	-3.0	-9.0
1-hr max O_3	FE	%	35	31.6	30.0	29.0	28.0	27.0	27.0	24.9
1-hr max O_3	RMSE	$\mu g/m^3$	9	55.5	49.0	42.7	37.0	31.3	28.2	23.8
8-hr max O_3	R	-	119	0.81	0.75	0.72	0.63	0.57	0.47	-0.40
8-hr max O_3	IOA	-	36	0.95	0.88	0.82	0.80	0.73	0.67	0.55
8-hr max O_3	MB	$\mu g/m^3$	36	25.9	10.1	8.4	4.5	-0.2	-0.3	-7.2
8-hr max O_3	ME	$\mu g/m^3$	12	44.6	27.8	16.1	0.4	0.3	0.3	0.3
8-hr max O_3	NMB	%	170	33.6	17.9	13.0	5.4	-2.0	-5.0	-14.0
8-hr max O_3	NME	%	140	47.2	37.3	31.0	26.6	20.0	17.0	11.9
8-hr max O_3	FB	%	180	73.3	24.3	10.0	4.0	-2.0	-6.0	-21.2
8-hr max O_3	FE	%	180	76.2	43.0	38.0	28.0	25.0	23.0	14.0
8-hr max O_3	RMSE	$\mu g/m^3$	11	57.4	49.5	39.5	21.3	19.1	17.3	16.2

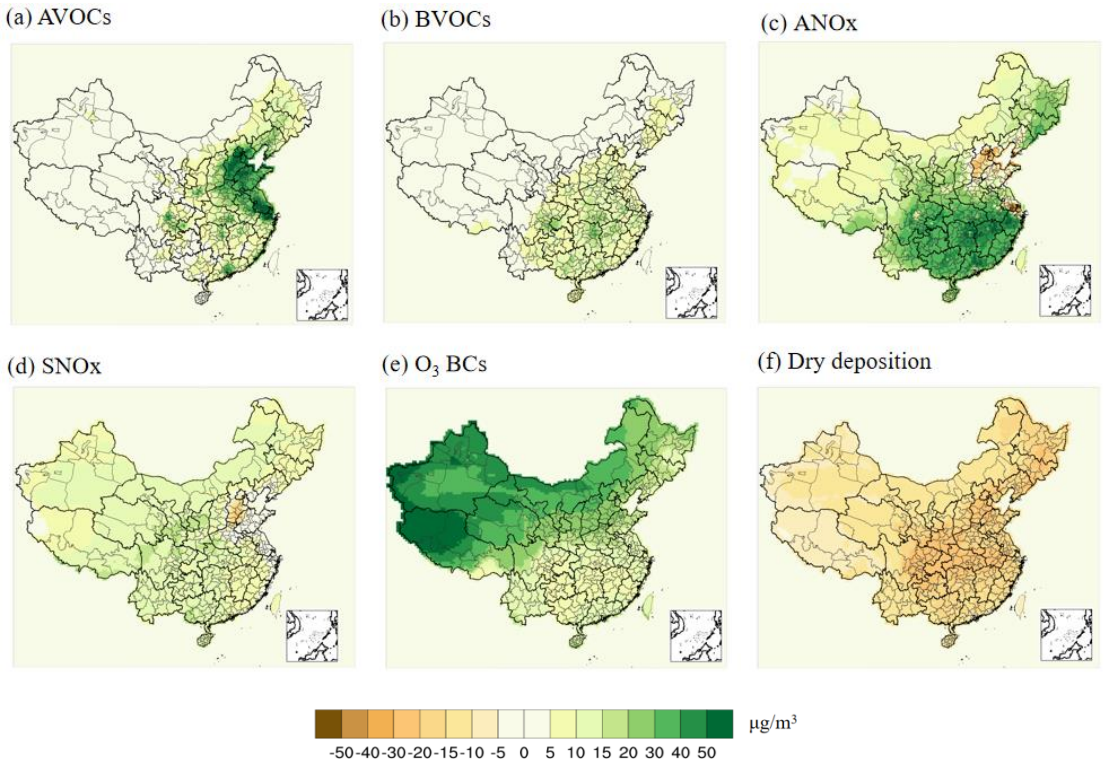

Figure S1 First-order sensitivities of MDA8 O_3 to (a) AVOCs, (b) BVOCs, (c) ANO_x, (d) SNO_x, (e) O_3 BCs and (f) Dry Deposition in $\mu g/m^3$. Results are averages over all days in June 2021.

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