

Supplemental Materials

Text

Model validation

The model performance of the meteorological parameters in Nanjing is evaluated as shown in **Fig. S2** and **Table S3**. For temperature (T), the simulated level both in summer of 2015 and 2020 is highly consistent with the observed values, and the index of agreement (IOA) exceeds 0.9 with the lower values of Normalized Mean Bias (NMB) and Normalized Mean Error (NME) (less than 0.05). The daily variation of observed relative humidity (RH) is captured by prediction with the IOA more than 0.9 and 0.7 in 2015 and 2020, respectively. The overall underestimation of average simulated results for RH is mainly caused by the lower prediction in nighttime, which is more obvious in 2020. The good performance in simulating daytime RH can meet MDA8 O_3 analysis. For wind direction at 10 m (WD), the modeled results can well reproduce the variation trend during the study period with the low values of NMB (no more 0.1) and relatively high IOA (0.79 and 0.66 in 2015 and 2020, respectively). The time series of wind speed at 10 m (WS) shows that the simulations have a good ability to capture the peak value meeting the benchmark of Root Mean Square Error (RMSE) less than 2.0 during study period in 2020, although there is slightly overestimation in general.

The model performance of air pollutants of O_3 and NO_2 is also evaluated in this study (**Table S4**). As shown in **Figs. S3(a)** and **S3(b)**, the simulated results of MDA8 O_3 are in good agreement with the observed values. The predictions basically reproduce the daily variation trend and concentration level of O_3 , satisfying the criteria proposed by Boylan and Russell (2006) ($NMB \leq \pm 0.15$, $NME \leq \pm 0.25$, $R > 0.5$). Considering that there is a rainfall process on or around August 10 in these two years, the days with the observed concentration of MDA8 O_3 higher than $100 \mu\text{g}/\text{m}^3$ during study period are only analyzed in the following discussion. The prediction of NO_2 is also assessed in this study due to NO_2 participating in the calculation of ozone production efficiency (OPE). Overall, the statistical parameter NMB is guaranteed to be below 0.15, and **Figs. S3(c)** and **S3(d)** also show good capture in the concentration of diurnal variation, although the daily average NO_2 are overestimated about $4 \mu\text{g}/\text{m}^3$.

Tables and Figures

Table S1 Physics and corresponding parameterization options in the optimized scheme.

Physics category	Parameterization scheme
Microphysics	Thompson
Longwave Radiation	RRTMG
Shortwave Radiation	RRTMG
Land-Surface	Noah Land Surface Model
Surface Layer	Monin-Obukhov
Planetary Boundary Layer	MYJ
Cumulus Parameterization	Modified Tiedtke

Table S2 The assessment of attributions of MDA8 O₃ variations in Nanjing during study period of August (only the days that observed MDA8 O₃ is higher than 100 µg/m³ are considered) in 2020 relative to the 2015. Units are µg/m³ (the value in parentheses is the contribution fraction).

MDA8 O ₃	Total change	2015Base	S1	S2	Met _{tot}	Emis	Met _{dir}	Met _{indir}
	-19.1	156.1	147.7	138.7	-8.4	-10.7	-17.4	9

Table S3 Statistics of model performance metrics for hourly meteorological factors in Nanjing from 1 to 19 on August in 2015 and 2020.

	Year	OBS	PRE	MB	ME	NMB	NME	RMSE	IOA
<i>T</i> (°C)	2015	28.36	29	0.64	1.3	0.02	0.05	1.78	0.94
	2020	30.81	31.51	0.7	1.3	0.02	0.04	1.72	0.92
<i>RH</i> (%)	2015	74.08	71.35	-2.73	5.39	-0.04	0.07	7.2	0.94
	2020	80.84	68.88	-11.96	12.35	-0.15	0.15	15.2	0.78
<i>WD</i> (°)	2015	138.16	141.1	2.95	40.7	0.02	0.29	66.38	0.79
	2020	163.76	178.52	14.76	38.48	0.09	0.23	57.09	0.66
<i>WS</i> (m/s)	2015	3	4.27	1.27	1.56	0.42	0.52	1.85	0.79
	2020	2.89	3.98	1.09	1.45	0.38	0.5	1.85	0.67

Table S4 Model performance metrics for MDA8 O₃ and daily average NO₂ (24h NO₂) concentrations in Nanjing from 1 to 19 on August in 2015 and 2020. Units for observation and prediction are µg/m³.

		Obs	Pre	MB	ME	NMB	NME	RMSE	R	IOA
MDA8 O ₃	2015	138.2	137.3	-0.9	27.4	-0.01	0.2	34.55	0.75	0.86
	2020	123.73	134.14	10.41	22.39	0.08	0.18	26.16	0.8	0.84
24h NO ₂	2015	36.62	41.07	4.45	8.42	0.12	0.23	9.93	0.52	0.68
	2020	24.8	28.21	3.41	5.72	0.14	0.23	7.26	-0.3	0.26

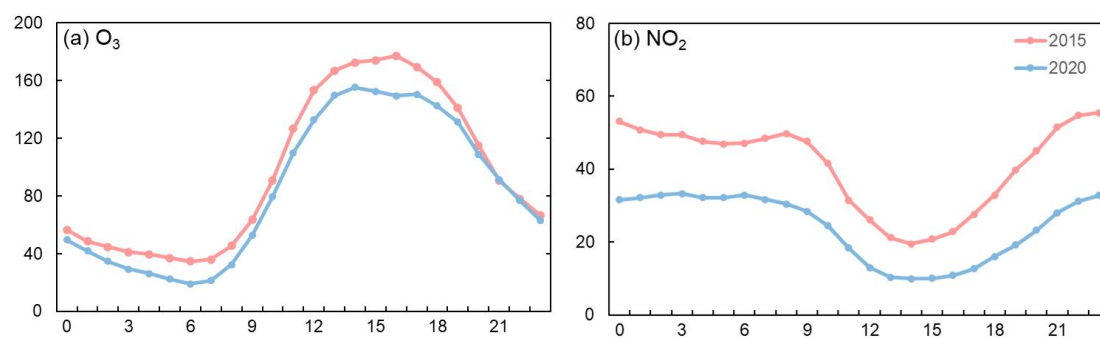


Fig. S1 Comparison of the diurnal variation of observed concentrations of (a) O₃ and (b) NO₂ in Nanjing during August in 2015 and 2020 (Unit: µg/m³).

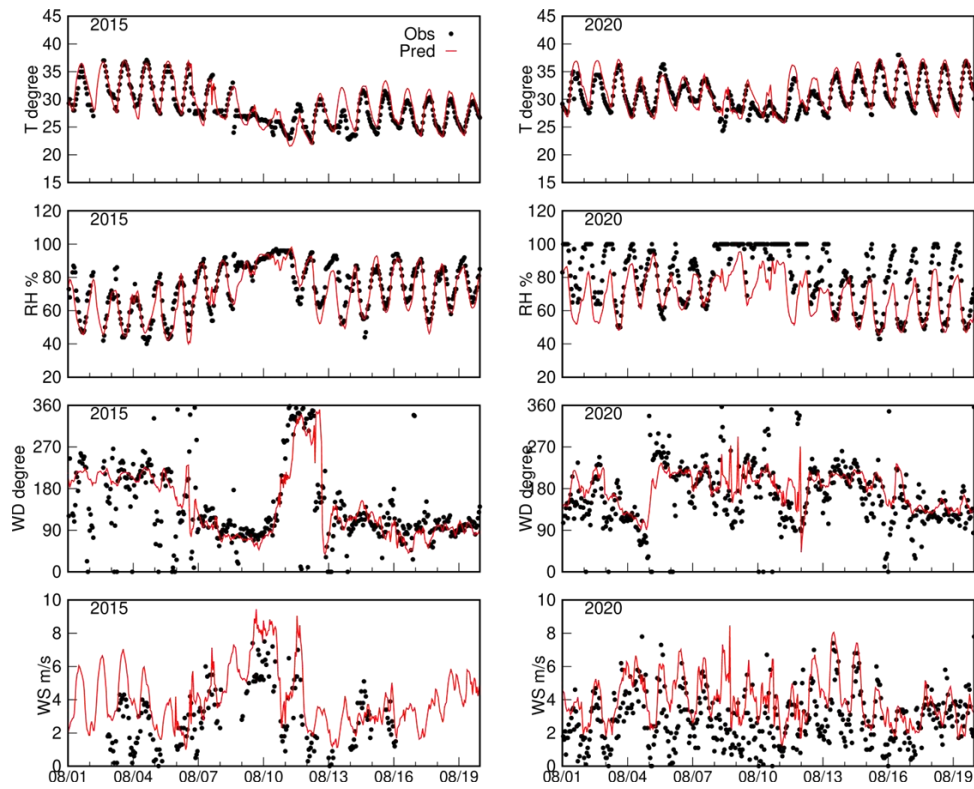


Fig. S2 Time series of meteorological parameters in Nanjing from 1 to 19 on August in 2015 and 2020 (black dots denote observations, and red line denotes CMAQ simulated result).

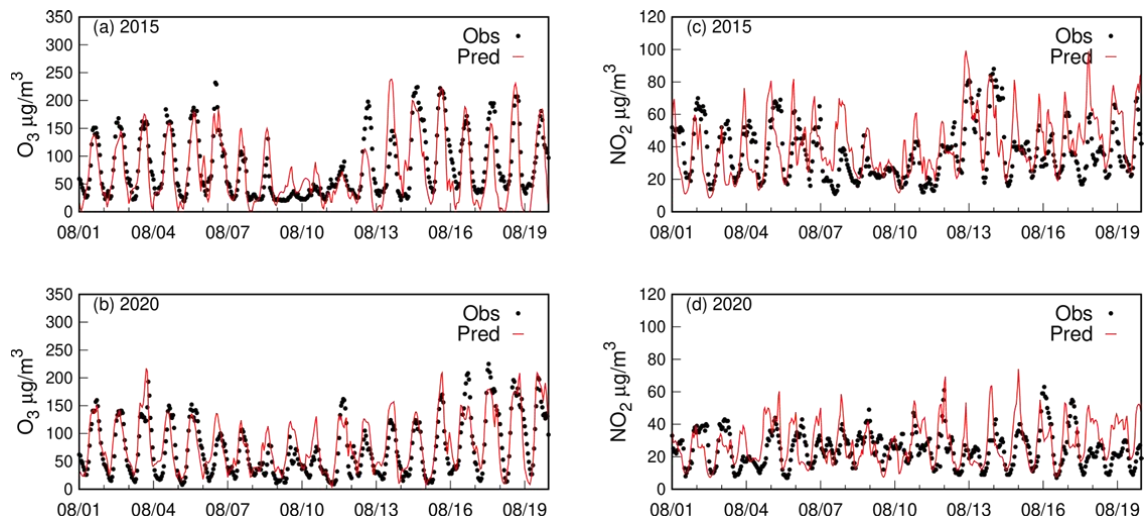


Fig. S3 Time series of pollutants concentrations in Nanjing during August 1-19 in 2015 and 2020 (black dots denote observations, and red line denotes CMAQ simulated result). (a) and (b) are O_3 levels in 2015 and 2020, respectively. (c) and (d) are NO_2 levels in 2015 and 2020, respectively.

References

Boylan J W, Russell A G (2006). PM and light extinction model performance metrics, goals, and criteria for three-dimensional air quality models. *Atmospheric Environment*, 40(26): 4946-495