Supplementary Materials: The WRF-CMAQ Simulation of a Complex Pollution Episode with High-level O₃ and PM₂.₅ over the North China Plain: Pollution Characteristics and Causes

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S1. Calculation Formula of the Statistical Metrics

The modeling results were compared with the observational data to evaluate the WRF-CMAQ simulation performances. Table S1 presents the statistical metrics, including mean bias (MB), mean error (ME), root mean square error (RMSE), and the index of agreement (IOA) for T2, RH2, WS10, and WD10 in Handan, Jining, Anyang, and Kaifeng. Additionally, normalized mean bias (NMB), normalized mean error (NME), and the Pearson's correlation coefficient (R) were added to assess the PM₂.₅ and O₃ simulations as shown in Table S2. The definitions of these statistical metrics are as follows:

$$\text{MB} = \overline{M} - \overline{O} \tag{S1}$$

$$\text{ME} = \frac{\sum_{i=1}^{N} |M_i - O_i|}{N} \tag{S2}$$

$$\text{RMSE} = \sqrt{\frac{\sum_{i=1}^{N} (M_i - O_i)^2}{N}} \tag{S3}$$

$$\text{IOA} = 1 - \frac{N \times \text{RMSE}^2}{\sum_{i=1}^{N} (|O_i - \overline{O}| + |M_i - \overline{O}|)^2} \tag{S4}$$

$$\text{NMB} = \frac{\overline{M}}{\overline{O}} - 1 \tag{S5}$$

$$\text{NME} = \frac{\sum_{i=1}^{N} |M_i - O_i|}{\sum_{i=1}^{N} O_i} \tag{S6}$$

$$R = \frac{\sum_{i=1}^{N} (M_i - \overline{M})(O_i - \overline{O})}{\sqrt{\sum_{i=1}^{N} (M_i - \overline{M})^2 \times \sum_{i=1}^{N} (O_i - \overline{O})^2}} \tag{S7}$$

where $\overline{M}$ and $\overline{O}$ are mean model-predicted and observed values, respectively. M_i and O_i are model-predicted and observed values, respectively, and N is the number of samples.

Table S1. Performance statistics of 2 m temperature (T2), 2 m relative humidity (RH2), 10 m wind speed (WS10), and 10 m wind direction (WD10) in the 4 cities from 00:00 LT March 30 to 00:00 LT April 10, 2019. Mean observations (Obs), mean simulations (Sim), MB, ME, RMSE, and IOA are given. Observation frequency is 3 hourly.

Meteorological elements	City	Obs	Sim	MB	ME	RMSE	IOA
T2 (°C)	Anyang	13.70	13.65	-0.06	1.61	2.19	0.95
	Handan	13.47	13.01	-0.46	1.60	2.18	0.95
	Jining	13.24	13.63	0.39	1.45	1.88	0.96
	Kaifeng	14.96	14.67	-0.29	1.11	1.40	0.98
RH2 (%)	Anyang	45.13	49.31	4.19	8.50	12.24	0.92
	Handan	44.31	46.02	1.72	8.16	11.54	0.93
	Jining	56.36	58.94	2.58	11.02	14.80	0.87
	Kaifeng	52.90	54.86	1.96	10.80	15.56	0.87
WS10 (m/s)	Anyang	3.52	4.19	0.67	1.78	2.14	0.73
	Handan	4.49	3.76	-0.73	1.84	2.36	0.71
	Jining	2.22	3.92	1.70	1.93	2.32	0.53
	Kaifeng	2.84	3.68	0.84	1.38	1.78	0.80
WD (°)	Anyang	189.85	170.59	-19.26	104.71	148.07	0.52
	Handan	207.89	180.64	-27.26	105.97	152.23	0.55
	Jining	192.58	173.49	-19.09	75.66	121.01	0.62
	Kaifeng	144.16	121.79	-22.37	45.72	87.99	0.79

Table S2. Performance statistics of $PM_{2.5}$ and O_3 in the 4 cities from 00:00 LT March 30 to 00:00 LT April 10, 2019. Obs, Sim, MB, ME, NMB, NME, and R are listed.

Pollutants	City	Obs	Sim	MB	ME	NMB	NME	R
O_3 (μg/m³)	Anyang	76.58	68.31	-8.27	23.64	-10.8%	30.9%	0.77
	Handan	81.28	60.64	-20.65	28.48	-25.4%	35.0%	0.79
	Jining	86.45	78.40	-8.05	26.84	-9.3%	31.1%	0.77
	Kaifeng	86.68	87.83	1.15	19.83	1.3%	22.9%	0.80
$PM_{2.5}$ (μg/m³)	Anyang	65.42	51.99	-13.43	23.41	-20.5%	35.8%	0.73
	Handan	56.64	50.58	-6.07	15.96	-10.7%	28.2%	0.74
	Jining	68.57	59.12	-9.44	17.82	-13.8%	26.0%	0.81
	Kaifeng	61.48	58.92	-2.56	21.64	-4.2%	35.2%	0.56