

## Supplementary Material:

# Causes investigation of PM<sub>2.5</sub> and O<sub>3</sub> complex pollution in a typical coastal city in the Bohai Bay region of China in autumn: Based on one-month continuous intensive observation and model simulation

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## 1. Figures

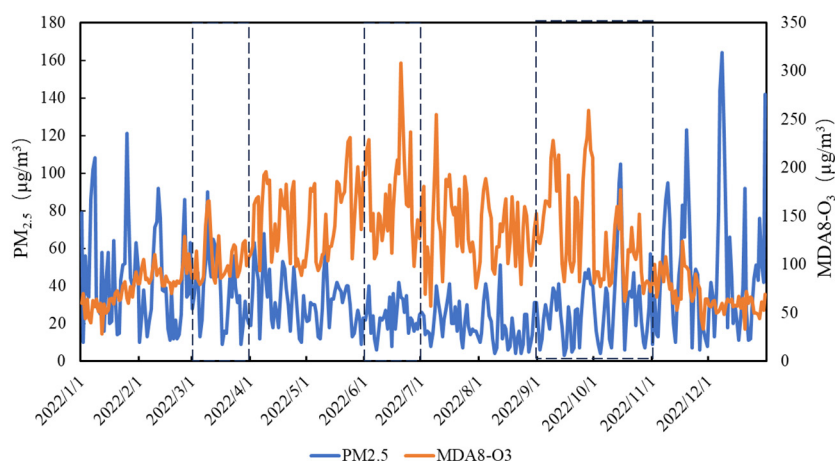
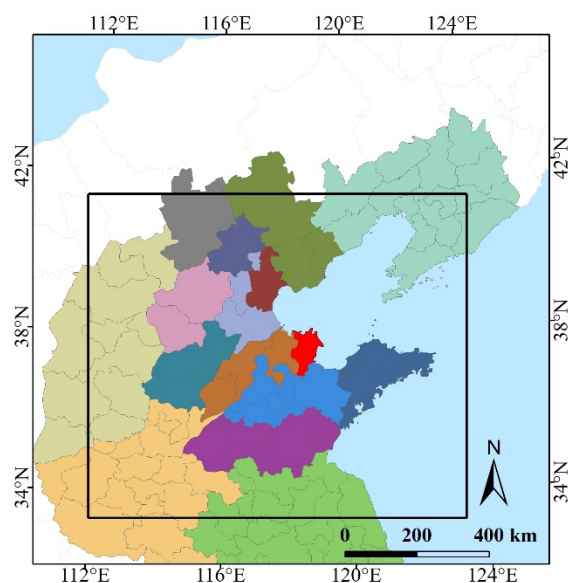
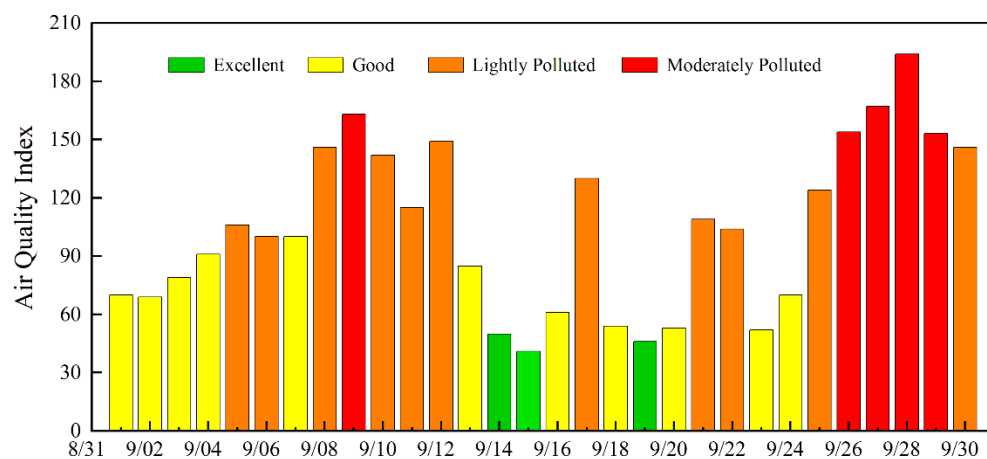


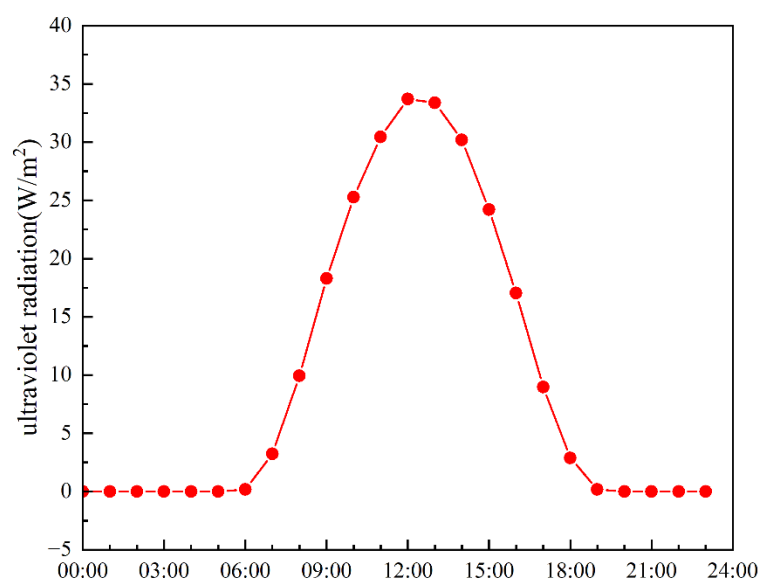
Figure S1. Daily variations of PM<sub>2.5</sub> and MDA8-O<sub>3</sub> in Dongying in 2022



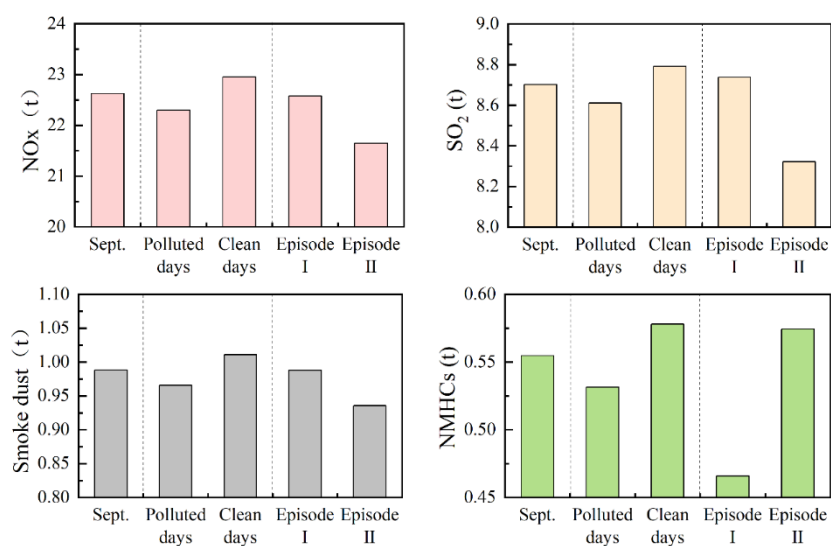
**Figure S2.** Simulated regions for source apportionment of O<sub>3</sub>.



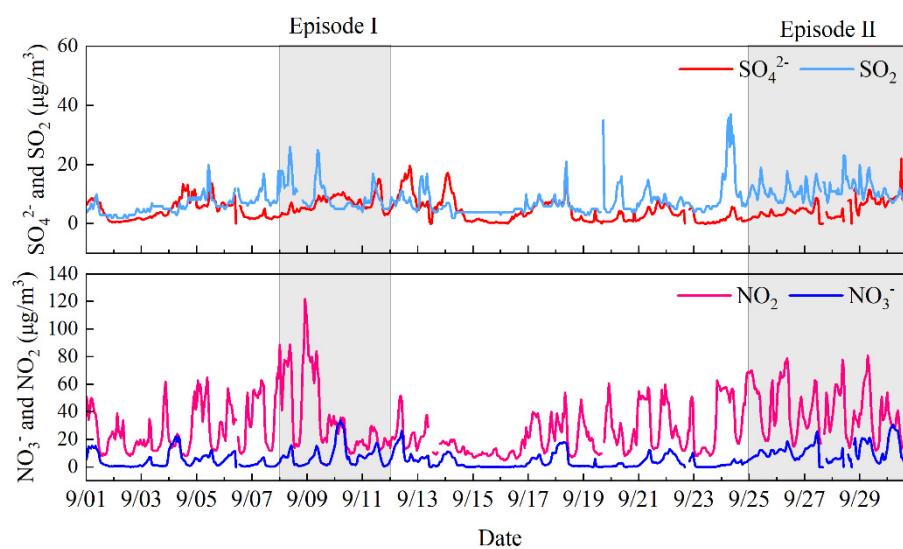
**Figure S3.** Daily variation of ambient air quality in Dongying City in September 2022.



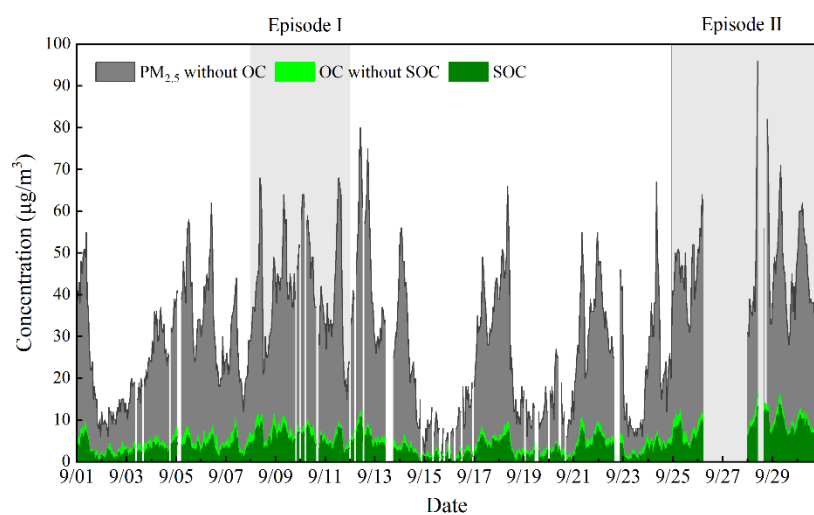
**Figure S4.** Diurnal variation of ultraviolet radiation in Dongying City in September 2022.



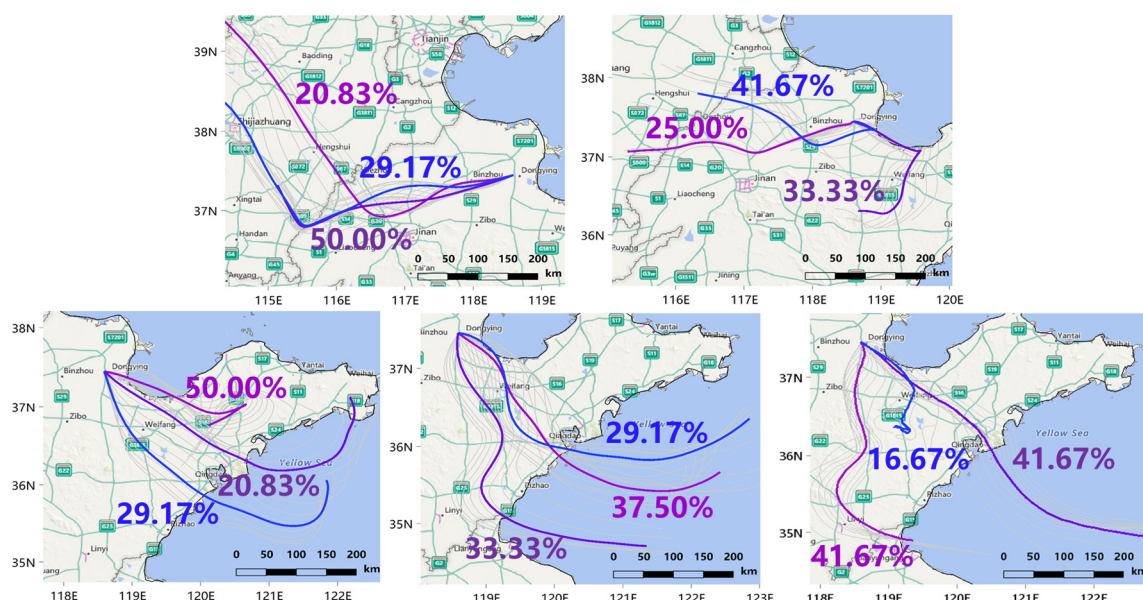
**Figure S5.** Comparison of pollution source emissions in Dongying in September 2022.



**Figure S6.** Time series of SO<sub>2</sub>, NO<sub>2</sub>, NO<sub>3</sub><sup>-</sup> and SO<sub>4</sub><sup>2-</sup> in Dongying in September 2022



**Figure S7.** Time series diagram of SOC, OC and PM<sub>2.5</sub> concentrations in Dongying in September 2022.



**Figure S8.** Results of backward trajectory cluster analysis during Sep. 8<sup>th</sup> to 12<sup>th</sup>.

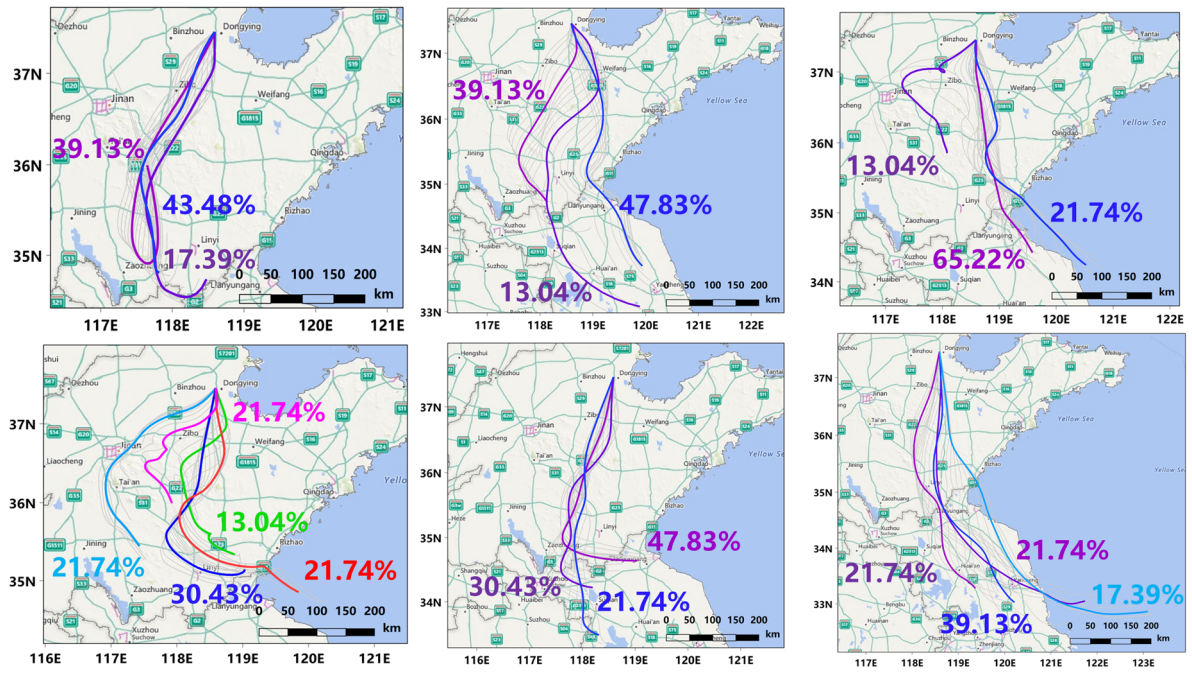


Figure S9. Results of backward trajectory cluster analysis during 25th to 30th, September.

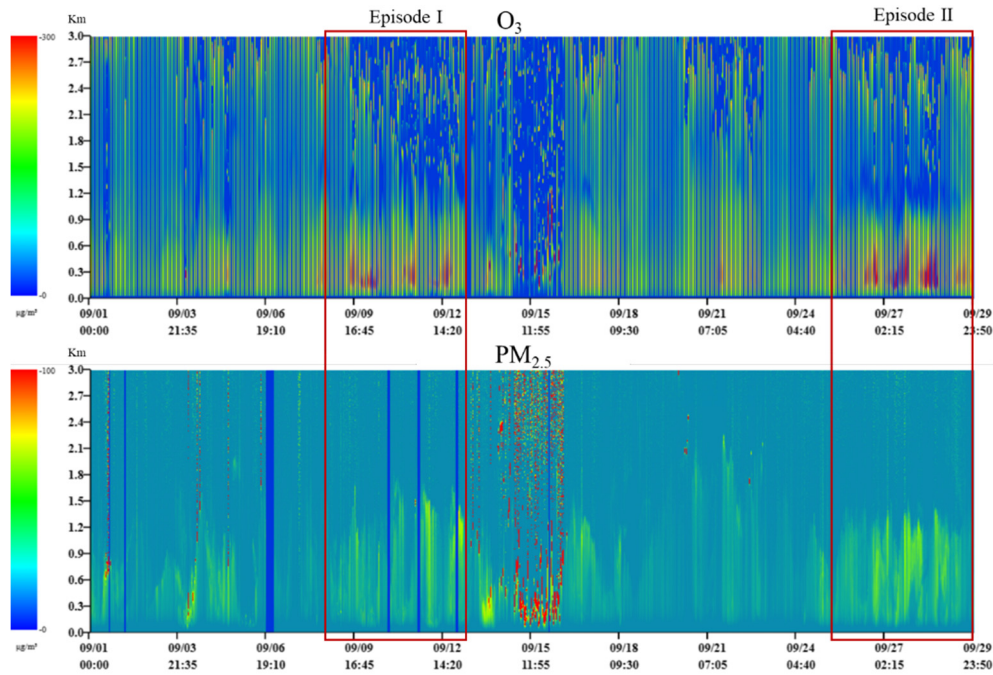


Figure S10. Vertical distribution characteristics of O<sub>3</sub> and PM<sub>2.5</sub> in Dongying in September 2022.

## 2. Definition and calculation of AQI

According to the requirements in the Technical Regulation on Ambient Air Quality Index (on trial) (HJ 633-2012), air quality index (AQI) is a dimensionless index that quantitatively describes air quality conditions. The following is the formula for calculate AQI.

$$AQI = \max \{IAQI_1, IAQI_2, IAQI_3, \dots, IAQI_n\}$$

Where, IAQI is an air quality sub-index, i.e., an air quality index for a single pollutant, and  $n$  is a pollutant. The IAQI and the corresponding pollutant concentration limits are as follows.

**Table S1.** Air quality sub-index (IAQI) and the corresponding pollutant concentration limits.

IAQI	Pollutant concentration limits									
	SO <sub>2</sub> 24-hour average (µg/m <sup>3</sup> )	SO <sub>2</sub> 1-hour average (µg/m <sup>3</sup> )	NO <sub>2</sub> 24-hour average (µg/m <sup>3</sup> )	NO <sub>2</sub> 1-hour average (µg/m <sup>3</sup> )	PM <sub>10</sub> 24-hour average (µg/m <sup>3</sup> )	CO 24-hour average (mg/m <sup>3</sup> )	CO 1-hour average (mg/m <sup>3</sup> )	O <sub>3</sub> 1-hour average (µg/m <sup>3</sup> )	O <sub>3</sub> 8-hour moving average (µg/m <sup>3</sup> )	PM <sub>2.5</sub> 24-hour average (µg/m <sup>3</sup> )
0	0	0	0	0	0	0	0	0	0	0
50	50	150	40	100	50	2	5	160	100	35
100	150	500	80	200	150	4	10	200	160	75
150	475	650	180	700	250	14	35	300	215	115
200	800	800	280	1200	350	24	60	400	265	150
300	1600	(1)	565	2340	420	36	90	800	800	250
400	2100	(1)	750	3090	500	48	120	1000	(2)	350
500	2620	(1)	940	3840	600	60	150	1200	(2)	500

Note: SO<sub>2</sub> and O<sub>3</sub> 1-hour average concentrations greater than 800 µg/m<sup>3</sup> are not subject to IAQI calculations.

The IAQI for pollutant P is calculated using the following equation.

$$IAQI_P = \frac{IAQI_{Hi} - IAQI_{Lo}}{BP_{Hi} - BP_{Lo}} (C_P - BP_{Lo}) + IAQI_{Lo}$$

Where, IAQI<sub>P</sub> is the IAQI of pollutant P, C<sub>P</sub> is the mass concentration of pollutant P, BP<sub>Hi</sub> and BP<sub>Lo</sub> are higher and lower values of pollutant concentration limits in Table 1 that are similar to C<sub>P</sub> respectively, IAQI<sub>Hi</sub> and IAQI<sub>Lo</sub> are IAQI in Table 1 corresponding to BP<sub>Hi</sub> and BP<sub>Lo</sub> respectively.