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Characteristics of Ozone Pollution in Tai'an and Topographic Effects of Mount Tai

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Abstract: Through the analyses of the observed concentrations of ozone (O_3) in Tai'an from 2016 to 2021, the results show that O_3 pollution was relatively serious, with the mean concentrations of the 90th percentile of daily maximum 8-h O_3 (O_3-8h-90per) above 180 μg/m^3. O_3 pollution in Tai'an mainly occurred from May to September, accounting for 69%~100% of the total O_3 pollution days, of which the most serious pollution occurred in June. Combined with the analyses of temperature, humidity, and wind speeds, the probability of O_3 exceedances in Tai'an increased significantly under the conditions with the temperatures higher than 30 °C, the relative humidity of 20%~40%, and the wind speeds of 1~3 m/s. The dominant wind directions on O_3 pollution days in Tai'an were southerly winds, based on the analyses of wind directions and their clustering trajectories. Based on the results at three monitoring stations at different distances from Mount Tai from May to September in 2021, the average O_3 concentrations at the Renkou School station near the mountain was about 13~15 μg/m^3 higher than those at the other two stations (Dianli College and Shandong First Medical University) which are far away from the mountain, indicating that the Renkou School site was more affected by the obstruction of the mountain. In addition, the WRF-CMAQ model was used to simulate ten O_3 pollution events in 2021, showing that the average O_3 concentrations in Tai'an were reduced by 1.7~7.5 μg/m^3 after changing the topographic height of Mount Tai.

Keywords: ozone; pollution characteristics; terrain; mount tai; WRF-CMAQ

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1. Introduction

In recent years, ozone (O_3) has gradually become the primary pollutant affecting air quality in China, and it has shown a rapid growth and deterioration trend in vast areas of China [1–5]. Ground-level O_3 is generated due to complex photochemical reactions of volatile organic compounds (VOCs) and nitrogen oxides (NOx) under sunlight [6–9]. The surface O_3 can stimulate the respiratory tract and cause changes in lung function and respiratory inflammation and asthma, seriously threatening human health [10–13]. In order to improve the regional air quality and reduce the serious harm of O_3 pollution to the human body, effectively reducing the concentrations of surface O_3 has become an arduous task for local environmental protection departments.

Since 2016, O_3 pollution in Tai'an has been serious. In 2016, the 90% percentile of annual O_3 concentrations ranked 168th among 168 key cities specially selected by the Ministry of Ecology and Environment for the national urban air quality ranking in China.

In 2021, it ranked 166th among 168 cities, showing that O_3 has become the primary pollutant affecting air quality in Tai'an [14,15]. Tai'an city has a special geographical environment, with the terrain high in the north and low in the south. It is located at the foot of Mount Tai, with the Taishan Mountains in the north and the Culai Mountain in the east, being favorable for pollutants to accumulate at the foot of the mountain and the downtown area [15]. VOCs and NOx are transported northward by the southerly winds, providing precursors for the photochemical reactions of O_3. In addition, Mount Tai is rich in vegetation, thus VOCs emitted by vegetation can provide certain precursors to O_3 generations in Tai'an. This study analyzed the characteristics of O_3 pollution in Tai'an from 2016 to 2021, and explored the effects of Mount Tai on O_3 concentrations. It may provide scientific basis and technical support for the causes of O_3 pollution and air pollution prevention and control measures in Tai'an.

2. Materials and Methods

2.1. Observation Data

The observation data of O_3, CO, SO_2, NO_2, $PM_{2.5}$, and PM_{10} at six air quality stations of Tai'an, as shown in Figure 1, from 2016 to 2021 were obtained from the Tai'an ambient air quality automatic monitoring system. The daily data were obtained from the average of observations at these six air quality observation stations, and the monthly and annual average O_3 concentrations were taken as the 90th percentile of the maximum 8 h average concentration of O_3 (O_3-8h-90per). The O_3 observation data of other cities were from China National Environmental Monitoring Centre. The observational data of temperatures, relative humidity, and wind speeds in Tai'an were provided by the Tai'an ambient air quality automatic monitoring system, and the wind direction data were obtained from the weather post report website (http://tianqihoubao.com/weather/top/taian.html) (accessed on 1 January 2022).

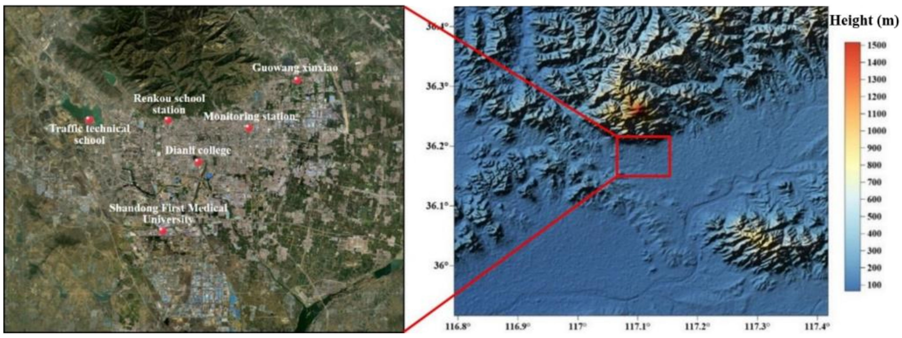


Figure 1. Map of Tai'an and distributions of six air quality monitoring stations in Tai'an.Map data © 2022, Gaode Map.

2.2. Analytical Method

According to the relevant regulations of the "Ambient Air Quality Standards" in China (GB 3095-2012), this study defined an O_3 pollution day when the maximum 8 h average concentration of O_3 (O_3-8h) exceeded 160 μg/m^3, and then conducted monthly and annual compliance evaluations based on the "Ambient Air Quality Assessment Technical Specifications (Trial)" (HJ 663-2013). According to the relevant requirements of the "Ambient Air Quality Index (AQI) Technical Regulations (Trial)" (HJ 633-2012), the air quality was divided into five levels depending on the concentrations of O_3-8h: excellent (0–100 μg/m^3), good (101–160 μg/m^3), mild (161–215 μg/m^3), moderate (216–265 μg/m^3), and heavy pollutions (266–800 μg/m^3).

2.3. Model Settings

The Community Multiscale Air Quality model (CMAQ) was applied to simulate the O_3 concentrations in Tai'an (https://www.epa.gov/cmaq) (accessed on 9 August 2022). The model meteorological field was provided by the Weather Research and Forecasting Model (WRF) (https://www.mmm.ucar.edu/weather-research-and-forecasting-model) (accessed on 9 August 2022). The input data for the WRF model were obtained from the Meteorological Reanalysis Data (FNL) of the US National Center of Environmental Prediction (NCEP). The CMAQ model adopted the CB05 carbon bond chemistry mechanism and the AERO6 aerosol chemistry mechanism [16,17]. The model had a horizontal resolution of 36 km and covered central and eastern China, as shown in Figure 2. Figure 2b,c show the terrain heights in the baseline simulation and the sensitivity simulation scenario, respectively, and the difference in the height of Mount Tai, as can be seen in Figure 2d. The anthropogenic emission sources were provided by the Multi-resolution Emission Inventory for China (MEIC) developed by Tsinghua University, and the biological sources were calculated by the online Biogenic Emission Inventory System version 3.14 (BEISv3.14).

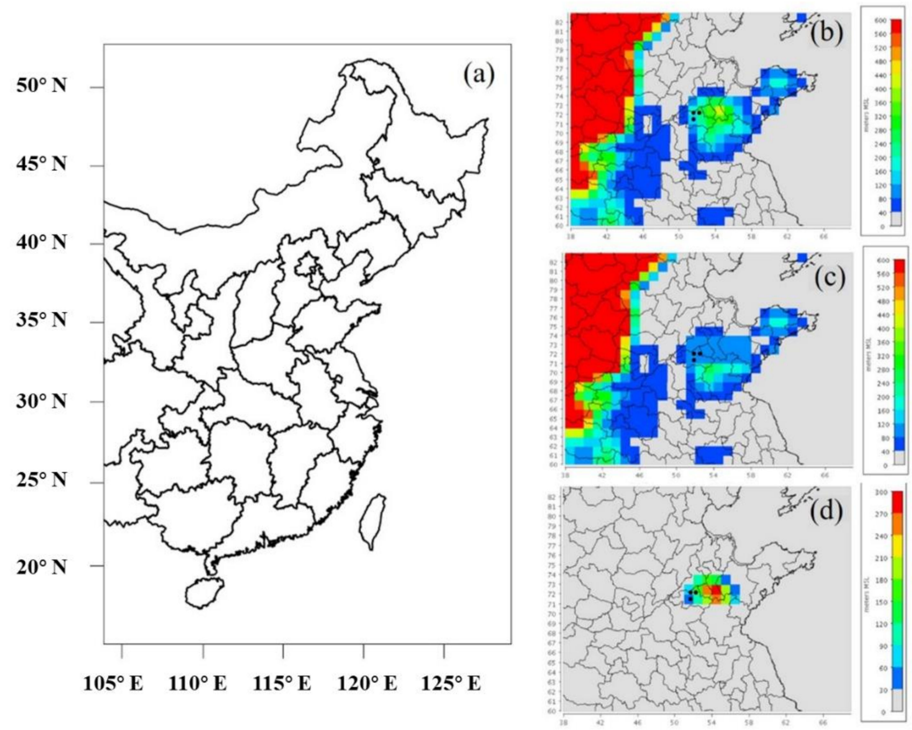


Figure 2. Map of (**a**) the model domain; (**b**) default terrain height (m); (**c**) modified terrain height (m); and (**d**) the terrain height difference between (**b**) and (**c**) in the model.

3. Results and Discussion

3.1. Overview of Ozone Pollutions in Tai'an

The annual average concentrations of O_3-8h in Tai'an from 2016 to 2021 were selected to analyze the interannual variation characteristics of O_3 pollution. As shown in Table 1, the annual average concentrations of O_3-8h-90per in Tai'an from 2016 to 2021 were above 180 μg/m^3 (except in 2018), suggesting that the O_3 pollution in Tai'an has been very serious in recent years. Among them, the highest annual average concentration of O_3-8h occurred in 2019, reaching 195 μg/m^3, while the lowest concentration was in 2018. From 2019 to 2020, the O_3 concentrations in Tai'an showed a decreasing trend with the reduction of 12 μg/m^3, while O_3 concentrations in 2021 were similar to those in 2020, indicating that the O_3 pollution situation in Tai'an was still relatively severe.

Table 1. Annual average concentrations of pollutants from 2016 to 2021 and O_3 pollution days for different wind directions in Tai'an during May–September from 2016 to 2021. The quantities in parenthesis represent the proportion of polluted days in a certain wind direction to the total polluted days.

Year	**Pollutants (μg/m³)**						**O_3 Pollution Days (%) with Different Wind Directions**		
	O_3-8h-90per	**CO-95per**	**SO_2**	**NO_2**	**$PM_{2.5}$**	**PM_{10}**	**Southerly**	**Northerly**	**Easterly**
2016	180	2.0	34	35	61	108	46 (74)	15 (24)	1 (2)
2017	193	1.6	23	36	53	97	58 (82)	12 (17)	1 (1)
2018	178	1.6	17	33	48	96	37 (74)	9 (18)	4 (8)
2019	195	1.5	15	34	53	98	62 (79)	16 (20)	1 (1)
2020	183	1.5	14	30	47	83	46 (78)	13 (22)	0 (0)
2021	182	1.3	12	28	42	76	52 (80)	12 (18)	1 (2)

Ground-level O_3 is mainly produced due to complex photochemical reactions of volatile organic compounds (VOCs) and nitrogen oxides (NOx) under the conditions of strong light, high temperature, and low humidity [18–21]. In view of the strong solar radiation, high temperature, and low humidity from May to September in Tai'an (Figure S1), these meteorological factors are favorable for generation of near-surface O_3. Therefore, this study selected the period of May–September to conduct a statistical analysis of the O_3 pollution in Tai'an from 2016 to 2021 (Figure 3a).

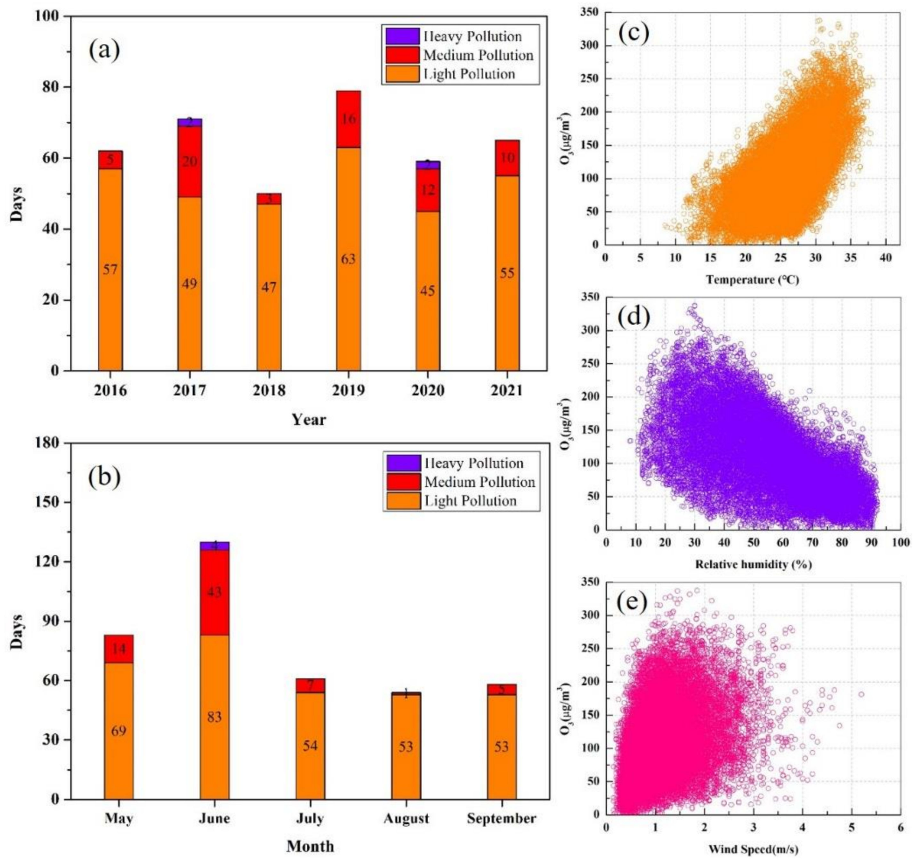


Figure 3. The number of days of O_3 pollution in different levels in Tai'an for (**a**) the annual values from 2016 to 2021 and (**b**) monthly values during May–September from 2016 to 2021, scatter plots between hourly O_3 concentrations and temperature (**c**); relative humidity (**d**); and wind speeds (**e**) in Tai'an during May–September from 2016 to 2021.

As seen from Figure 3a, the number of O_3 pollution days in Tai'an from May to September was in the range of 50~79 days from 2016 to 2021 for the annual values, accounting for 32.7% to 51.6% of the total days from May to September every year. Among them, the number of pollution days in 2019 was the most (79 days), and in 2021 it was 65 days, indicating that the O_3 pollution in Tai'an was still relatively severe. From the perspective of pollution extent, O_3 pollution in Tai'an was mainly mild pollution, accounting for 69.0%~94.0% of the total pollution days from 2016 to 2021. The number of days with moderate and above O_3 pollution gradually decreased from 16 days in 2019 to 14 days in 2020, and then to 10 days in 2021 (Table 2). The O_3-8h-90per concentrations also decreased year by year in the recent three years. This shows that Tai'an achieved certain improvements in O_3 controls in recent years.

Table 2. Monthly mean concentrations of maximum 8 h O_3 and NO_2 ($\mu g/m^3$) in Tai'an during May–September from 2016 to 2021.

Year	May		June		July		August		September		Average	
	O_3	NO_2	O_3	NO_2	O_3	NO_2	O_3	NO_2	O_3	NO_2	O_3	NO_2
2016	185	31	208	24	183	19	167	23	203	35	193	26
2017	240	30	236	31	177	22	190	21	182	28	225	26
2018	186	26	212	22	182	16	189	15	148	32	192	22
2019	186	27	225	22	211	22	169	22	211	31	216	25
2020	211	23	244	22	186	19	183	19	183	31	214	23
2021	206	19	239	20	188	14	190	17	188	17	200	17

Table 2 shows the statistical results of O_3-8h-90per in Tai'an during May–September from 2016 to 2021. The concentrations of O_3-8h-90per in May from 2020 to 2021 were both above 200 $\mu g/m^3$, indicating that the occurrence times of O_3 pollution in Tai'an had a tendency to advance. June was the most polluted month, with the most days of pollution exceedance, the concentrations of O_3-8h-90per ranging from 208–244 $\mu g/m^3$ and a total of 130 pollution days from 2016 to 2021, accounting for 34.7% of the total pollution days (Figure 3b). In addition, the moderate and above pollution in Tai'an occurred most frequently in June, with 43 days of O_3 moderate pollution, accounting for 61.4% of the total days of O_3 moderate pollution from 2016 to 2021. Notably, the four heavy pollution processes from 2016 to 2021 all occurred in June, which may be attributed to the relatively strong solar radiation and high temperature in June, resulting in strong photochemical reactions of O_3 in the atmosphere and high concentrations of ground-level O_3 [17].

3.2. Analyses of Ozone Precursors and Meteorology

Based on the analyses of NO_2 concentrations in Tai'an from 2016 to 2021, it was found that the overall NO_2 concentrations showed a downward trend, as shown in Table 2 and Figure S2. The average NO_2 concentration during May–September in 2021 was 17 $\mu g/m^3$, while the NO_2 concentration in 2018 was relatively low, which might be caused by meteorological conditions such as typhoons. The NO_2 concentrations were relatively high from May to June in 2017, being consistent with the high levels of O_3 concentrations. From 2018 to 2020, the NO_2 concentrations were the highest in September, followed by May, while the highest NO_2 concentration occurred in June (20 $\mu g/m^3$) and May (19 $\mu g/m^3$) in 2021, being consistent with the months with high O_3 levels.

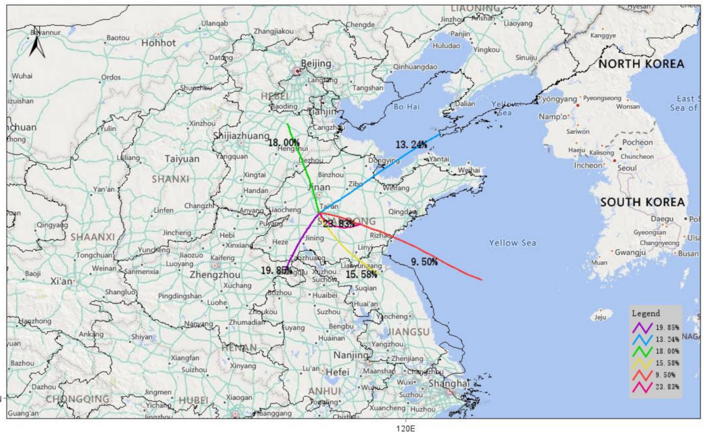
According to the analysis of temperature, humidity, and wind speed during the high-O_3 period (May–September) in Tai'an from 2016 to 2021, the probability of O_3 exceedances rose sharply under the conditions with the temperature higher than 30 °C, relative humidity of 20–40%, and wind speeds of 1–3 m/s, as shown in Figure 3c–e.

According to the statistical analysis of the wind directions during the O_3 pollution periods in Tai'an from 2016 to 2021, the dominant wind directions leading to O_3 pollution days were southerly (southwest, south, and southeast), accounting for 65%~100% of the total number of pollution days each year (see Table 1). The pollution days dominated by the northerly winds accounted for 17%~24%, and those dominated by easterly winds accounted for 0%~8%. In 2021, number of the O_3 pollution days in Tai'an dominated by southerly winds were 52 days, accounting for 80% of the total pollution days from May to September.

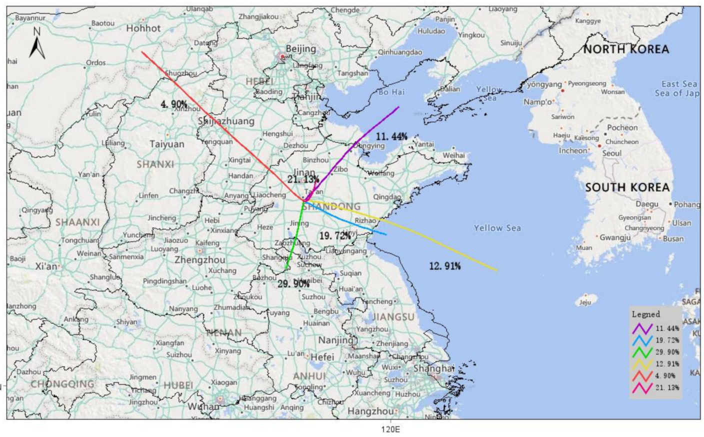
In order to study the effects of air flow trajectory differences on O_3 concentrations in Tai'an, cluster analysis was performed on the hourly backward trajectory during May–September from 2020 to 2021. Results show that the summer winds were dominated by southwesterly, northeasterly, and southeasterly winds, and the proportion of trajectory sources varied slightly between different years (see Table 3). Moreover, combining the hourly O_3 observation values in Tai'an with the backward trajectories, the trajectory pollution characteristics were explored. Referring to the secondary standard of O_3-8h (160 $\mu g/m^3$) in "Ambient Air Quality Standards" (GB 3095-2012), the backward trajectories were divided into clean and polluted trajectories: the polluted trajectory was defined as the one with the corresponding O_3 concentrations greater than 160 $\mu g/m^3$, otherwise as the clean trajectory [22]. The statistical results of various trajectories are shown in Figure 4 and Table 3. Results show that there were significant differences in the O_3 concentrations corresponding to different airflow trajectories and the proportions of pollution trajectories. In summer, the pollution trajectories in the southwesterly wind direction accounted for the highest proportion. The above analysis shows that due to the effects of southern transport and local topography, the proportion of O_3 pollution in Tai'an increased significantly under the southerly winds. The transports of ozone and its precursors were considered in the all simulation cases. Since Tai'an is located in the south of Mount Tai, O_3 concentrations in the other eight cases decreased after reducing the height of Mount Tai, indicating that the existence of Mount Tai led to the accumulation of pollutants blown from the south and east in Tai'an. A typical O_3 pollution event on 21 June 2021 was selected to compare the O_3 concentrations in Tai'an, Jinan, and Jining, and analyze the O_3 and NO_2 data in Tai'an. On 21 June 2021, the maximum concentration of O_3-8h in Tai'an was 254 $\mu g/m^3$ (corresponding to AQI of 189), which reached a moderate pollution level, significantly higher than that those in Jining (219 $\mu g/m^3$) and Jinan (230 $\mu g/m^3$) (Figure 5a). For the hourly variations of O_3 concentrations in Tai'an (Figure 5b), the O_3 concentrations gradually decreased from 0:00 to 7:00 (stage 1) due to the titration of nitrogen oxides (NOx) on O_3 [23,24]. From 7:00 to 13:00, the O_3 concentrations gradually increased and reached a peak at 13:00, and O_3 and NO_2 showed a significant negative correlation during the hours of 7:00–15:00 (stage 2), indicating that the near-surface O_3 during this period was mainly generated from the photochemical reactions [22]. From 13:00 to 20:00, the NO_2 concentrations gradually increased, which may be affected by the upwind transports and local effects. From 13:00 to 18:00, the O_3 concentrations remained above 250 $\mu g/m^3$ for 6 consecutive hours, significantly higher than that those in Jining and Jinan. Considering that the dominant wind direction in Tai'an was southerly with the wind power of 2~3 during this period, the persistent high O_3 in Tai'an was caused by the mountain blocking effects, and then the O_3 concentrations gradually decreased due to the titration of NOx.

Table 3. Statistics of occurrence frequencies of O_3 trajectories and their corresponding mean O_3 concentrations in Tai'an during May–September in 2020 and 2021.

Year	Type	Through Regions	All Trajectories		Pollution Trajectories		
			Percentage (%)	O_3 ($\mu g/m^3$)	O_3 ($\mu g/m^3$)	The Class Percentage (%)	The Year Percentage (%)
2021	1	Bohai Sea, Dongying, Binzhou, Zibo, Jinan, Tai'an	11.4	97	183	9.8	6.8
	2	Rizhao, Linyi, Tai'an	19.7	111	199	16.3	19.7
	3	Huaibei, Xuzhou, Jining, Taian	29.9	121	187	23.1	42.4
	4	Yellow Sea, Rizhao, Linyi, Jinan, Tai'an	12.9	93	198	6.8	5.3
	5	Inner Mongolia, North of Shanxi, Center of Hebei, Dezhou, Jinan, Tai'an	4.9	104	175	8.3	2.50
	6	Jinan, Tai'an	21.1	107	192	17.9	23.2
2020	1	Cangzhou, Dezhou, Jinan, Tai'an	18.0	94	196	9.1	10.6
	2	Bohai Sea, Dongying, Zibo, Jinan, Tai'an	13.2	102	196	13.8	11.8
	3	Heze, Jining, Tai'an	19.9	111	201	20.9	26.9
	4	Linyi, Tai'an	23.8	99	191	14.3	22.1
	5	Yellow Sea, Rizhao, Linyi, Jinan, Tai'an	9.5	102	194	10.9	6.7
	6	Lianyungang, Linyi, Jining, Tai'an	15.6	123	196	21.7	21.9



(**a**)



(**b**)

Figure 4. Clusters of average trajectory pathways of O_3 in Tai'an during May–September in 2020 (**a**) and 2021 (**b**).

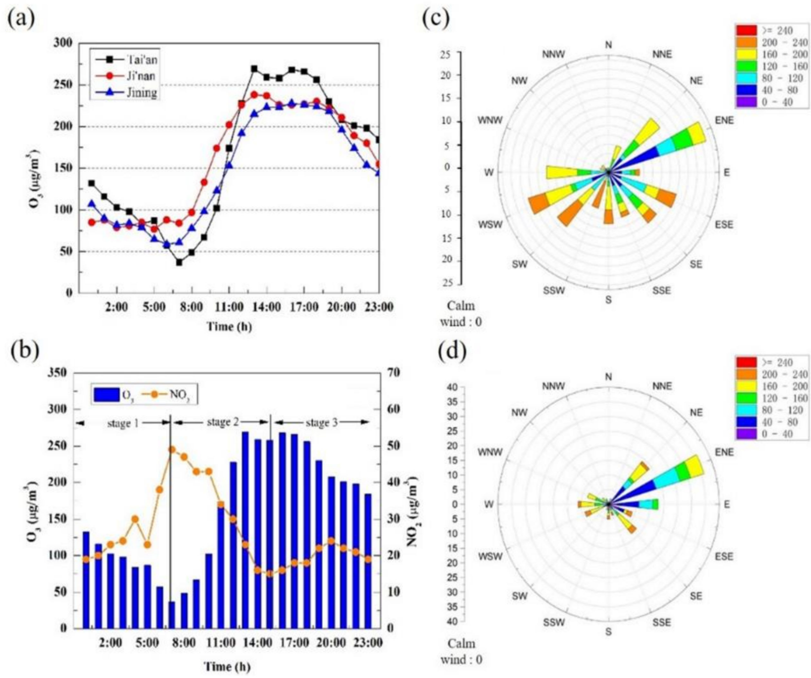


Figure 5. Comparisons of (**a**) diurnal variations of O_3 among Tai'an and surrounding cities and (**b**) diurnal variations of hourly O_3 and NO_2 concentrations in Tai'an on 21 June 2021; wind rise of observed O_3 concentrations in Tai'an during (**c**) 3–9 July and (**d**) 7–12 August 2021.

3.3. The Effects of Mount Tai on O_3

Three air quality stations in Tai'an, namely, Renkou School, Dianli College, and Shandong First Medical University, were selected to analyze the effects of the mountain on O_3 (see Table 4). The Renkou School, Dianli College, and the Shandong First Medical University stations are about 0.5, 3.5, and 8 km away from the mountain, respectively. The specific distributions of the three stations are shown in Figure 1. Based on the comparisons of monthly average concentrations of O_3 at the three stations from May to October 2021, the average O_3 concentration at the Renkou School station closer to the mountain was 118 $\mu g/m^3$, significantly higher than that at the Dianli College and Shandong First Medical University stations, which were relatively far away from the mountain. For different months from May to October 2021, the O_3 concentrations at the Renkou School station were 8~19 $\mu g/m^3$ higher than those at the Dianli College station, and 10~20 $\mu g/m^3$ higher than those at the Shandong First Medical University station. In summary, the Renkou School station was relatively more affected by the blocking of the mountain due to being closer to the mountain, leading to the significantly higher O_3 concentrations relative to those of other stations.

Table 4. Comparison of mean O_3-8h-90per concentrations ($\mu g/m^3$) at three monitoring stations in Tai'an from May to September 2021.

Stations	May	June	July	August	September	Average
Renkou School	120	144	104	120	102	118
Dianli College	112	125	91	105	84	103
Medical University	109	130	94	100	90	105

By setting the baseline simulations and sensitivity simulation scenarios of reducing the Mount Tai terrain heights to 150 m (Tai'an terrain height) (see Figure 2), the WRF-CMAQ air quality model was applied to simulate the changes of O_3 concentrations in Tai'an through the adjustment of topographic heights of Mount Tai. Note that biogenic VOCs in Mount Tai were not removed in the sensitivity simulations. A total of 10 O_3 pollution events that occurred in Tai'an from May to September 2021 were selected to compare the changes of O_3 concentrations between the baseline and sensitivity simulations. Results show that after changing the terrain height of Mount Tai in the 10 selected pollution events, the simulated O_3 concentrations in eight pollution events decreased by 1.7~7.5 μg/m^3 relative to the baseline simulations, suggesting the positive contributions of the topography of Mount Tai to the occurrences of ozone pollutions in Tai'an (see Table 5). The simulated O_3 concentrations after reducing the height of Mount Tai in another two pollution events increased relative to the base simulations. Among the three monitoring stations, the reductions of O_3 concentrations caused by reducing terrain height were 2.4~8.8, 2.4~8.8, and 0.3~6.3 μg/m^3 for the Renkou School, Dianli College, and Shandong First Medical University stations, respectively. In the simulations, Renkou School and Dianli College were on the same grid, so the reductions of O_3 concentrations were the same. Through the analyses of the wind directions in the two pollution events in which the O_3 concentrations increased (3–9 July 2021 and 7–12 August 2021), it was found that the prevailing wind directions in Tai'an were northeasterly during the two pollution events (see Figure 5c,d). This might affect the transports of ozone and precursors from the upwind areas and result in an increase in O_3 concentrations after reducing the terrain heights of Mount Tai.

Table 5. Comparisons of O_3 concentrations between the baseline and scenario simulations by reducing the Mount Tai terrain heights for ten O_3 pollution events in 2021 in Tai'an (μg/m^3).

Pollution Events	Average			$O_3 \geq 160$ (μg/m^3)			$O_3 \geq 200$ (μg/m^3)		
	Observation	Base	Scenario	Observation	Base	Scenario	Observation	Base	Scenario
2021.5.9–5.12	119.1	122.7	115.3	189.5	167.6	163.6	213.9	197.9	193.9
2021.5.18–5.21	125.8	130.9	129.2	169.6	180.2	177.4	/	/	/
2021.5.29–6.2	155.2	146.1	143.0	198.9	180.6	176.0	220.2	199.2	193.1
2021.6.4–6.13	151.6	138.1	136.1	212.3	180.7	176.6	233.8	195.2	190.9
2021.6.18–7.1	137.4	138.5	136.6	205.4	189.9	185.5	235.8	209.3	197.9
2021.7.3–7.9	124.2	132.3	142.0	188.0	185.0	195.0	207.2	209.9	214.6
2021.8.2–8.4	131.3	110.0	102.6	180.5	161.8	154.9	206.9	197.4	183.7
2021.8.7–8.12	119.6	128.9	124.8	187.5	168.5	172.2	218.4	190.5	186.4
2021.8.15–8.21	122.8	111.8	105.3	183.1	175.6	173.1	211.5	199.7	199.7
2021.9.3–9.6	84.3	69.1	63.8	/	/	/	/	/	/

4. Conclusions

In recent years, Tai'an has suffered from serious O_3 pollution, with the annual average concentrations of O_3-8h-90per above 180 μg/m^3 from 2016 to 2021. In this study, we analyzed the O_3 pollution situation in Tai'an from May to September, and found that the pollution during this period was mainly light pollution, accounting for 69% to 100% of the total polluted days, with June being the most polluted month. High temperature (>30 °C), low relative humidity (20%~40%), and low wind speed (1~3 m/s) provided favorable meteorological conditions for the generation of O_3, especially with prevailing southerly wind, resulting in light and above pollution in Tai'an. The results of backward trajectory analysis showed that in the summer pollution trajectories, the pollution trajectories in the southwest direction accounted for the highest proportion of all kinds of trajectories. When the southerly winds dominated, the accumulated O_3 concentrations were significantly higher than those of the surrounding cities due to the blocking of the northern mountains. Comparing the three monitoring stations in Tai'an, the average O_3 concentrations from May to September 2021 at the Renkou School station closer to the mountain were 13~15 μg/m^3 higher than those at the Dianli College and the Shandong First Medical University stations, which are relatively far away from the mountains, indicating that the Renkou School station was more affected by the obstructions of the mountains. The WRF-CMAQ was applied in this study to quantify the blocking effect of mountains, and results indicated that the average O_3 concentrations in Tai'an decreased about 1.7~7.5 μg/m^3 after reducing the terrain height of Mount Tai in the model. Our results are of great significance for guiding

Tai'an to control O_3 in the future, and measures can be formulated in advance based on our conclusions.

Supplementary Materials: The following supporting information can be downloaded at: https://www.mdpi.com/article/10.3390/atmos13081299/s1. Figure S1: The variations of average monthly concentrations of temperature, relative humidity, precipitation, and wind speed in Tai'an from 2016 to 2021; Figure S2: The monthly mean concentrations of maximum 8-h O_3 (a) and NO_2 (b) in Tai'an during May-September from 2016 to 2021.

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