



1 **Land-surface forcing and anthropogenic heat modulate ozone by**  
2 **meteorology: A perspective from the Yangtze River Delta region**

3 Chenchao Zhan <sup>a</sup>, Min Xie <sup>a,\*</sup>

4 <sup>a</sup> School of Atmospheric Sciences, CMA-NJU Joint Laboratory for Climate Prediction Studies,  
5 Jiangsu Collaborative Innovation Center for Climate Change, Joint Center for Atmospheric Radar  
6 Research of CMA/NJU, Nanjing University, Nanjing 210023, China

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8 \* Corresponding author. minxie@nju.edu.cn (M. Xie)

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10 **Abstract:** With the rapid advance in urbanization, land-surface forcing related to the urban  
11 expansion and anthropogenic heat (AH) release from human activities significantly affect the urban  
12 climate and in turn the air quality. Focusing on the Yangtze River Delta (YRD) region, a highly  
13 urbanized place with severe ozone (O<sub>3</sub>) pollution and complex geography, we estimate the impacts  
14 of land-surface forcing and AH on meteorology (meteorological factors and local circulations) and  
15 O<sub>3</sub> using the WRF-chem model, which can enhance our understanding about the formation of O<sub>3</sub>  
16 pollution in those rapidly developing regions with unique geographical features as most of our  
17 results can be supported by previous studies conducted in other regions in the world. Regional O<sub>3</sub>  
18 pollution episodes occur frequently (26 times per year) in the YRD in recent years. These O<sub>3</sub>  
19 pollution episodes are usually under calm conditions characterized by high temperature (over 20 °C),  
20 low relative humidity (less than 80%), light wind (less than 3 m s<sup>-1</sup>) and shallow cloud cover (less  
21 than 5). In this case, high O<sub>3</sub> mainly appears during the daytime influenced by the local circulations  
22 (the sea and the lake breezes). The change in land-surface forcing can cause an increase in 2-m  
23 temperature (T<sub>2</sub>) by maximum 3 °C, an increase in planetary boundary layer height (PBLH) by  
24 maximum 500 m and a decrease in 10-m wind speed (WS<sub>10</sub>) by maximum 1.5 m s<sup>-1</sup>, and surface O<sub>3</sub>  
25 can increase by maximum 20 µg m<sup>-3</sup> eventually. Furthermore, the expansion of coastal cities  
26 enhances the sea-breeze below 500 m. During the advance of the sea-breeze front inland, the upward  
27 air flow induced by the front makes well vertical mixing of O<sub>3</sub>. However, once the sea-breeze is  
28 fully formed, further progression inland is stalled, thus the O<sub>3</sub> removal by the low sea-breeze will  
29 be weakened and surface O<sub>3</sub> can be 10 µg m<sup>-3</sup> higher in the case with cities than no-cities. The



30 expansion of lakeside cities can extend the lifetime of the lake-breeze from the noon to the afternoon.  
31 Since the net effect of the lake-breeze is to accelerate the vertical mixing in the boundary layer, the  
32 surface  $O_3$  can increase as much as  $30 \mu\text{g m}^{-3}$  in lakeside cities. Compared with the effects from  
33 land-surface forcing, the impacts of AH are relatively small. And the changes mainly appear in and  
34 around cities where AH emission is large. There are increases in  $T_2$ , PBLH,  $WS_{10}$  and surface  $O_3$   
35 when AH are taken into account, with the increment about  $0.2 \text{ }^\circ\text{C}$ , 75 m,  $0.3 \text{ m s}^{-1}$  and  $4 \mu\text{g m}^{-3}$ ,  
36 respectively. Additionally, AH can affect the urban-breeze circulations, meteorological factors and  
37  $O_3$  concentration, but its effect on local circulations, such as the sea and the lake breezes, seems to  
38 be limited.

39 **Key Words:** ozone; meteorology; local circulations; land-surface forcing; anthropogenic heat; the  
40 Yangtze River Delta;

41

## 42 **1 Introduction**

43 Ozone ( $O_3$ ) is a key constituent in the atmosphere, and is deeply relevant to climate (Worden  
44 et al., 2008), biosphere (Van Dingenen et al., 2009) and human health (Jerrett et al., 2009).  $O_3$  acts  
45 quite differently in different parts of the atmosphere, often described as being “good up high and  
46 bad nearby”.  $O_3$  in the stratosphere helps protect life on earth from strong ultraviolet radiation.  
47 However, high  $O_3$  in the troposphere is harmful to human respiratory system and the growth of  
48 vegetation, and thereby the tropospheric  $O_3$  has long been regarded as an important air pollutant  
49 (Young et al., 2013).

50 Tropospheric  $O_3$  is a secondary air pollutant, which is formed by a series of complex chemical  
51 reactions (Chameides and Walker, 1973; Xie et al., 2014) of precursor gases such as nitrogen oxides  
52 ( $\text{NO}_x = \text{NO} + \text{NO}_2$ ) and volatile organic compounds (VOCs) in combination with sunlight. The global  
53 average lifetime of tropospheric  $O_3$  is 20 to 25 days, and it will be reduced to 5 days in boundary  
54 layer (Young et al., 2013). The relatively long lifetime of tropospheric  $O_3$  favors regional/long-range  
55 transport, and brings huge challenges to its control (Shao et al., 2006).  $O_3$  levels considerably depend  
56 on the variations in weather conditions because weather conditions play an important role in  
57 determining the chemistry, dispersion and removal of  $O_3$  (Jacob and Winner, 2009). Generally,  
58 elevated  $O_3$  occurs under warm dry weather with strong sunlight, high temperature, low relative  
59 humidity and light wind speed (Zhang et al., 2015). Furthermore, weather conditions can have many



60 similarities in certain weather pattern (Buchholz et al., 2010; Zhan et al., 2019), and the main  
61 weather patterns associated with O<sub>3</sub> episodes in China are tropical cyclones and continental  
62 anticyclones (Wang et al., 2017).

63 O<sub>3</sub> levels as well as weather conditions in urban areas are of great concern simply because  
64 urban areas have huge populations. A report from the United Nations pointed out that 69.6% of the  
65 world's population will live in cities by 2050. The urbanization process has further increased urban  
66 environmental hazards (Zhang et al., 2011), particularly in the most rapidly developing countries  
67 like China (Liu and Tian, 2010). Because of historical and cultural factors, many cities have similar  
68 topography, usually along the coast, close to mountains or in basins. For these cities, the local  
69 circulations induced by thermal contrast of the topography, such as sea-land breezes, mountain-  
70 valley breezes and lake-land breezes, will have an important impact on air quality of the city,  
71 especially when the dominant background weather system is weak (Crosman and Horel, 2010).  
72 Examples can be found around the world. Ding et al. (2004) simulated the main features of the sea-  
73 land breezes during a multiday episode in the Pearl River Delta (PRD) region, and found that the  
74 sea-land breezes play a crucial role in transporting air pollutant between inland and coastal cities.  
75 Miao et al. (2015) studied the effects of mountain-valley breezes on boundary layer structure in the  
76 Beijing-Tianjin-Hebei (BTH) region, suggesting that the mountain-valley breezes are vital to the  
77 vertical transport and distribution of air pollutants in Beijing. Wentworth et al. (2015) identified a  
78 causal link between lake-breeze and O<sub>3</sub> in the Greater Toronto Area that the daytime O<sub>3</sub> maxima  
79 was 13.6-14.8 ppb higher on lake breeze days than no-lake breeze days.

80 The land-surface forcing and anthropogenic heat (AH) of a city also affect the atmospheric  
81 state and compositions above it (Yu et al., 2012; Oke et al., 2017). The land-surface forcing changes  
82 chiefly come from the urban expansion (typically from vegetation to impervious surface), which  
83 directly changes the surface physical properties (e.g., albedo, surface moisture and roughness) and  
84 thereby significantly affects the meteorology and in turn the air quality. Li et al. (2019) found that  
85 increases in thermal inertia, surface roughness and evapotranspiration due to urban expansion can  
86 lead to an increase in O<sub>3</sub> by up to 5.6 ppb in Southern California. AH is an important waste by-  
87 product of urban metabolism. Nearly all energy consumed by human activities will be dissipated as  
88 heat within Earth's land-atmosphere system (Flanner, 2009; Sailor, 2011) that is then "injected" into  
89 the energy balance processes. Ryu et al. (2013a) reported that AH affects the



90 characteristics/structures of boundary layer and local circulations, resulting in an increase of O<sub>3</sub> by  
91 3.8 ppb in the Seoul metropolitan area.

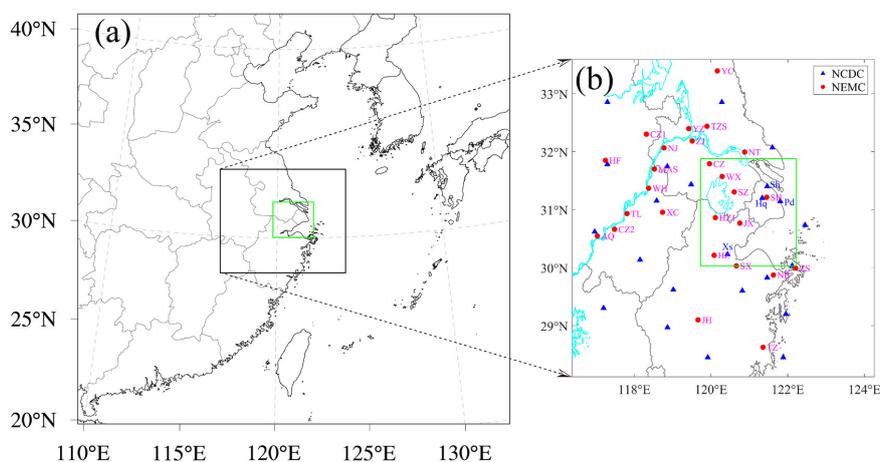
92 These previous studies separately investigated the impact of local circulations, land-surface  
93 forcing and AH on meteorology and air quality, usually focusing on a specific megacity. However,  
94 local circulations, land-surface forcing and AH can work together in near-calm conditions. And the  
95 role of multi-scale atmospheric circulations associated with the abovementioned factors in regional  
96 meteorology and air quality of city clusters is unclear. Actually, complex interactions exist widely  
97 among these thermally-driven circulations and the effects can even spread from one city to nearby  
98 areas. For example, Zhu et al. (2015) demonstrated that the meteorological conditions and air quality  
99 over Kunshan are significantly affected by Shanghai urban land surface forcing (Kunshan is located  
100 downstream of Shanghai, with a straight-line distance of about 50 km). Therefore, assessing the  
101 effects of land-surface forcing and AH (The topography rarely changes.) in the city cluster is  
102 meaningful, which helps understand the connection between urban development, local meteorology  
103 and regional air quality.

104 The Yangtze River Delta (YRD) region, located on the western coast of the Pacific Ocean  
105 (Figure 1a), has undergone accelerated urbanization process and rapid economic development over  
106 the past decades, and is now one of the largest economic zones in the world. It includes the areas of  
107 the southern part of Jiangsu Province, the northern part of Zhejiang Province and the eastern part of  
108 Anhui Province, with 26 mega/large cities such as Shanghai, Hangzhou and Nanjing (Figure 1b).  
109 With dense population and huge energy consumption, this area is now suffering from air quality  
110 deterioration (Ding et al., 2013; Xie et al., 2017), especially severe O<sub>3</sub> pollution in recent years  
111 (Zhan et al., 2020, 2021). It was reported that 16 out of the 26 typical cities in the YRD failed to  
112 meet the urban national standard for O<sub>3</sub> in 2017 (Bulletin on the state of China's ecological  
113 environment in 2018, <http://www.cleanairechina.org/product/9943.html>), and to make matters worse,  
114 O<sub>3</sub> concentration has been rising in this region during the past few years (Li et al., 2020; Wang et  
115 al., 2020). The YRD region is deeply affected by the East Asian monsoon, and has complex weather  
116 like other mid-latitude regions in the world. Sever air pollution and unique geography make this  
117 area an ideal place for studying the complex interactions between the atmosphere and human  
118 activities.

119 In this study, the impacts of land-surface forcing and AH on meteorology in the central YRD



120 region, and how these impacts further modulate O<sub>3</sub> are investigated using the Weather Research and  
121 Forecasting model coupled to Chemistry (WRF-Chem). These results fill the knowledge gap about  
122 the formation of O<sub>3</sub> pollution in this region and provide valuable insight for other rapidly developing  
123 regions with complex geography in the world. The remainder of this paper is organized as follows.  
124 Sect. 2 gives a detailed description about the observation data, the model setup and experimental  
125 design. The main results, including the characteristics of O<sub>3</sub> pollution episodes, the model evaluation  
126 and the response of O<sub>3</sub> to land-surface forcing and AH, are presented in Sect. 3. Summary and  
127 conclusions are given in Sect. 4.  
128



129  
130 **Figure 1.** (a) Three nested WRF-Chem domains, (b) the locations of 26 cities (red dots) and weather  
131 stations (blue triangles) in the YRD. The green rectangular regions represent the innermost domain  
132 and also the central YRD region. These cities in (b) include: the megacity Shanghai (SH); Hangzhou  
133 (HZ), Ningbo (NB), Jiaxing (JX), Huzhou (HZ1), Shaoxing (SX), Jinhua (JH), Zhoushan (ZS) and  
134 Taizhou (TZ) located in Zhejiang Province; Nanjing (NJ), Wuxi (WX), Changzhou (CZ), Suzhou  
135 (SZ), Nantong (NT), Yancheng (YC), Yangzhou (YZ), Zhenjiang (ZJ) and Taizhoushi (TZS) located  
136 in Jiangsu Province; and Hefei (HF), Wuhu (WH), Maanshan (MAS), Tongling (TL), Anqing (AQ),  
137 Chuzhou (CZ1), Chizhou (CZ2) and Xuancheng (XC) located in Anhui Province.

138

## 139 2 Materials and methods



## 140 2.1 Surface observations

141 Hourly O<sub>3</sub> concentrations monitored by the National Environmental Monitoring Center  
142 (NEMC) of China are used in this study. These data strictly follow the national monitoring standards  
143 HJ 654-2013 and HJ 193-2013 (<http://www.cnemc.cn/jcgf/dqjh/>), and can be available at  
144 <https://quotsoft.net/air/>, a mirror of data from the official NEMC real-time publishing platform  
145 (<http://106.37.208.233:20035/>). The nationwide observation network initially operated in 74 major  
146 cities in 2013, and it has grown to more than 1,500 stations covering 454 cities by 2017 (Lu et al.,  
147 2018). The urban hourly O<sub>3</sub> concentrations are average results of measurements at all monitoring  
148 sites for each city. The maximum daily 8-h running average (MDA8) O<sub>3</sub> concentrations are then  
149 calculated based on the hourly O<sub>3</sub> concentration with more than 18-h measurements in the day (Liao  
150 et al., 2017).

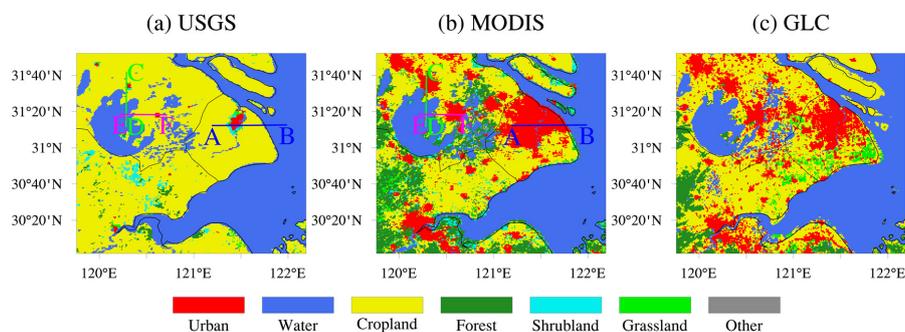
151 Meteorological data are provided by the National Climatic Data Center (NCDC), including  
152 temperature, wind speed and direction, and relative humidity, etc. These data as well as the technical  
153 documents recording the quality control, data collection and archive can be available at  
154 <ftp://ftp.ncdc.noaa.gov/pub/data/noaa/isd-lite/>. Locations of surface observation stations are shown  
155 in Figure 1b. Specifically, the meteorological stations in the innermost domain include Pudong (Pd),  
156 Shanghai (Sh), Hongqiao (Hq) and Xiaoshan (Xs).

## 157 2.2 MODIS-based and USGS land use classifications

158 To investigate the impact of land-surface forcing on regional meteorology and O<sub>3</sub> evolution in  
159 the YRD, the two land use categories defaulted in WRF (MODIS-based and USGS land use  
160 classifications) are used to set up the first two sensitivity simulations (Table 2). The MODIS-based  
161 land cover product was created from 500-m MODIS Terra and Aqua satellite imagery (Friedl et al.,  
162 2010), and replaced USGS as the default settings in WRF since version 3.8. The USGS data  
163 primarily derived from the Advanced Very High Resolution Radiometer (AVHRR) from 1992 to  
164 1993 at 1-km spatial resolution (Loveland et al., 2000), which is much earlier than the MODIS data.  
165 Figure 2 presents the land cover maps in the innermost domain. Apparently, urban fraction with  
166 MODIS is much higher than USGS, indicating rapid urbanization in recent decades in the YRD.  
167 The differences in urban land-surface forcing between USGS and MODIS mainly depend on urban  
168 expansion. Additionally, the Finer Resolution Observation and Monitoring-Global Land Cover in  
169 2015 (From-GLC\_2015), which can be considered as one of the latest (2015) and finest (30-m) land



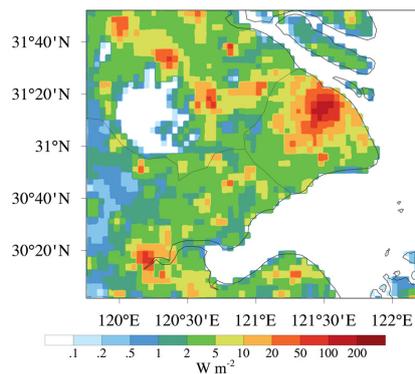
170 cover datasets (Gong et al., 2019), is quite consistent with the performance of MODIS in this region.  
171 This further confirms that urban fraction with MODIS is close to the reality.  
172



173  
174 **Figure 2.** Land cover maps in the innermost domain, including the result of (a) USGS, (b) MODIS,  
175 and (c) From-GLC\_2015.

### 177 2.3 Anthropogenic heat flux modeling

178 Another simulation involved the urban canopy model with the gridded AH fluxes is conducted  
179 to estimate AH release in the central YRD. The AH fluxes are mainly the result of chemical energy  
180 or electrical energy that are converted to heat, thereby they can be quantified using the top-down  
181 energy inventory method. Based on the statistics data of energy consumption in 2016, the AH fluxes  
182 were calculated, and then were gridded as 144 rows and 144 columns with a resolution at 2.5 arcmin  
183 using population density in China. Details on the calculation as well as the distribution of AH fluxes,  
184 and how to add AH fluxes into the urban canopy can refer to Xie et al. (2016a, b). Figure 3 gives  
185 the spatial distribution of AH fluxes in the innermost domain. In the urban areas, the AH fluxes  
186 usually exceed  $20 \text{ W m}^{-2}$ . Some big cities, like Shanghai, can have a value of AH flux as high as  
187  $200 \text{ W m}^{-2}$ . Except for the urban areas, the AH fluxes are generally less than  $5 \text{ W m}^{-2}$  in most parts  
188 of the YRD region. In particular, in those places where there is no human activity, the AH flux is 0.  
189



190

191 **Figure 3.** Spatial distribution of anthropogenic heat fluxes in the innermost domain.

192

#### 193 **2.4 Model set-up and experimental designs**

194 The WRF-Chem model is a fully coupled online numerical weather prediction model with  
195 chemistry component (Grell et al., 2005), in which air quality and the meteorological component  
196 use the same coordinates, transport schemes and physics schemes in space and time. In this study,  
197 the WRF-Chem version 3.9.1 is applied. The initial and boundary conditions of meteorological  
198 fields are from the National Centers for Environmental Prediction (NCEP) global final analysis  
199 fields every 6 h with a spatial resolution of  $1^\circ \times 1^\circ$ . There are 32 vertical levels extending from the  
200 surface to 100 hPa with 12 levels located below 2 km to resolve the boundary layer processes.  
201 Furthermore, the domain and options for physical and chemical parameterization schemes are  
202 summarized in Table 1. The anthropogenic emissions are provided by the Multiresolution Emission  
203 Inventory for China (MEIC) in 2017 with a resolution of  $0.25^\circ$  (<http://meicmodel.org/>), which  
204 includes 10 air pollutants and  $\text{CO}_2$  from power, industry, residential, transportation and agriculture  
205 sectors. The biogenic emissions are estimated online by the Model of Emissions of Gases and  
206 Aerosols from Nature (MEGAN) in WRF-Chem (Guenther et al., 2006).

207

208 **Table 1.** The domains and major options for WRF-Chem

Items	Contents
Dimensions (x, y)	(101, 96), (146, 121), (236, 206)
Grid spacing (km)	25, 5, 1



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Time step (s)	75
Microphysics	Purdue Lin microphysics scheme (Chen and Sun, 2002)
Longwave radiation	RRTM scheme (Mlawer et al., 1997)
Shortwave radiation	Goddard scheme (Kim and Wang, 2011)
Surface layer	Revised MM5 Monin-Obukhov scheme
Land-surface layer	Noah land-surface model (Chen and Dudhia, 2001)
Planetary boundary layer	YSU scheme (Hong et al., 2006)
Cumulus parameterization	Grell 3D ensemble scheme (Grell and Devenyi, 2002)
Gas-phase chemistry	RADM2 (Stockwell et al., 1990)
Photolysis scheme	Fast-J photolysis (Fast et al., 2006)
Aerosol module	MADE/SORGAM (Schell et al., 2001)

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209

210 As shown in Table 2, three numerical experiments are performed to study the effects of land-  
211 surface forcing and AH on meteorology and O<sub>3</sub> in the YRD. The MODIS\_noAH experiment is a  
212 control simulation with commonly used settings. Compared with MODIS\_noAH, USGS\_noAH  
213 selects the USGS data at run-time through the geogrid program. Thus, the difference between the  
214 modeling results of MODIS\_noAH and USGS\_noAH can illustrate the changes caused by land  
215 cover. As for the impact of AH, it can be identified by comparing the modeling results of  
216 MODIS\_withAH and MODIS\_noAH. All three simulations run from 00:00 on 21 May to 00:00 on  
217 4 June in 2017 with the first 88 h as spin-up time, using the same physical and chemical  
218 parameterization schemes (Table 1).

219

220 **Table 2.** The three numerical experiments.

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Cases	Land use categories	Whether to add AH
MODIS_noAH	MODIS-based	No
USGS_noAH	USGS	No
MODIS_withAH	MODIS-based	Yes

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221

222 **2.5 Model evaluation**



223 The simulation results in the innermost domain, including  $O_3$  concentration, 2-m air  
224 temperature ( $T_2$ ), relative humidity (RH), 10-m wind speed ( $WS_{10}$ ) and 10-m wind direction ( $WD_{10}$ )  
225 are examined against the surface observations described in Sect. 2.1. The statistical metrics,  
226 including the mean bias (MB), root mean square error (RMSE) and correlation coefficient (COR),  
227 are used to evaluate the model performance. They are defined as follows:

$$228 \quad MB = \frac{1}{N} \sum_{i=1}^N (S_i - O_i), \quad (1)$$

$$229 \quad RMSE = \sqrt{\frac{1}{N} \sum_{i=1}^N (S_i - O_i)^2}, \quad (2)$$

$$230 \quad COR = \frac{\sum_{i=1}^N (S_i - \bar{S})(O_i - \bar{O})}{\sqrt{\sum_{i=1}^N (S_i - \bar{S})^2} \sqrt{\sum_{i=1}^N (O_i - \bar{O})^2}}, \quad (3)$$

231 where  $S_i$  and  $O_i$  are the simulations and observations, respectively.  $N$  is the total amount of valid  
232 data, and  $\bar{S}$  and  $\bar{O}$  represent the average of simulations and observations, respectively. Generally,  
233 the model performance is acceptable if the values of MB and RMSE are close to 0, and that of COR  
234 is close to 1 (Xie et al., 2016a, b; Zhan et al., 2020).

235

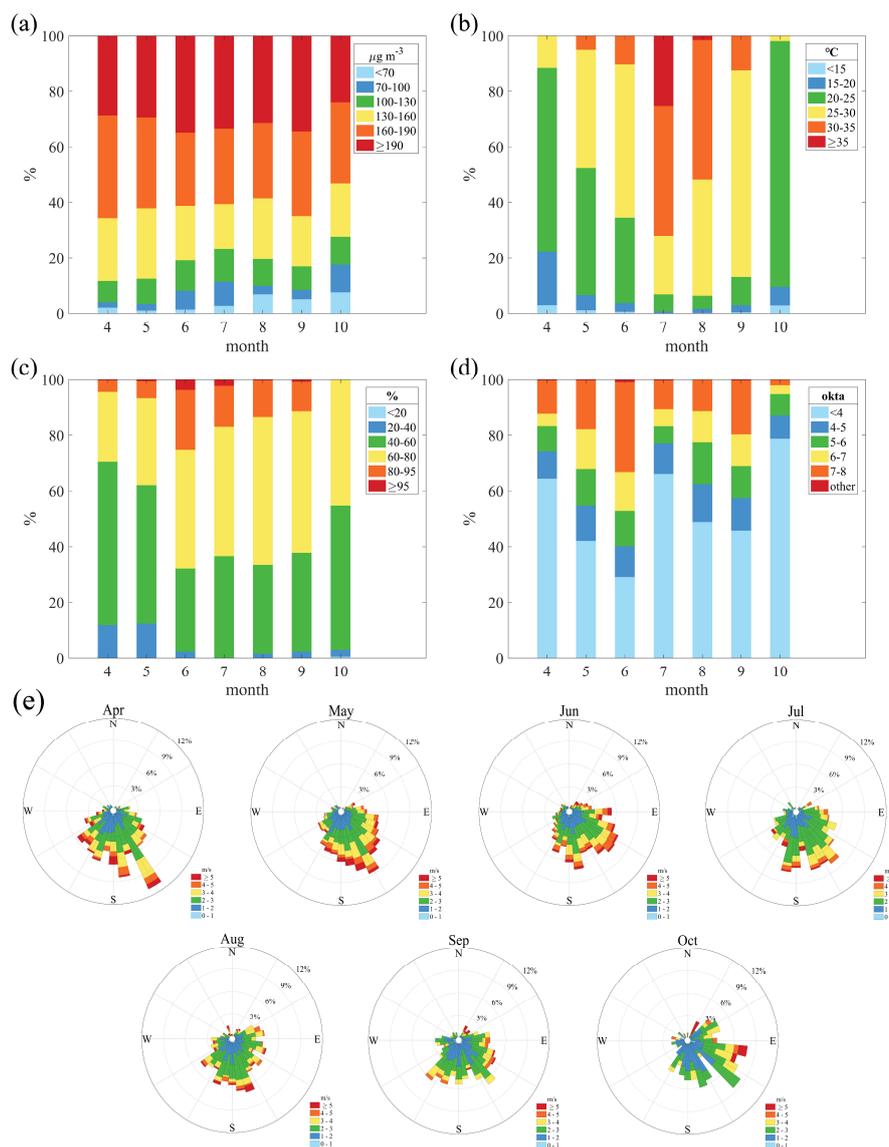
### 236 **3 Results and discussions**

#### 237 **3.1 Regional $O_3$ pollution episodes in the YRD**

238 Under adverse weather conditions,  $O_3$  pollution episodes occur frequently in the YRD (Gao et  
239 al., 2020; Zhan et al., 2021). Sometimes,  $O_3$  pollution can spread throughout the YRD and cause  
240 regional  $O_3$  pollution, affecting an area of up to 3.5 million square kilometers and harming more  
241 than 200 million people. Based on the surface  $O_3$  observations, we define the regional  $O_3$  pollution  
242 in the YRD as when more than half of the 26 typical cities in the YRD fail to meet the national  $O_3$   
243 standard (In China, the national ambient air quality standard for MDA8  $O_3$  is  $160 \mu\text{g m}^{-3}$ ), and then  
244 sort out all regional  $O_3$  pollution episodes and the corresponding weather patterns from 2015 to  
245 2019 (Table S1). There were 20, 19, 34, 28 and 30 regional  $O_3$  pollution cases in the YRD from  
246 2015 to 2019, respectively. These cases mainly occurred in April to October of each year, and were  
247 usually related to high pressure, uniform pressure field and typhoon activity.



248           Figure 4 further displays the monthly distribution of meteorological factors during the day  
249 (from 8:00 to 20:00 local time) when regional O<sub>3</sub> pollution occurs in the YRD. All the variables  
250 show significant monthly variations. The highest (lowest) temperature is found in July (April), and  
251 the relative humidity is highest in June. This may be related to the Meiyu in June, and the hot weather  
252 in July as the YRD is usually dominated by the western Pacific subtropical high after Meiyu. As for  
253 the cloud cover, the sky is covered with fewer clouds in October than other months. In addition,  
254 southeast wind prevails in the YRD from April to October under the influence of monsoon climate.  
255 As shown in Figure 4, O<sub>3</sub> pollution episodes are likely to occur in the YRD on days when the  
256 temperature exceeds 20 °C (Figure 4b), the relative humidity is less than 80% (Figure 4c), the cloud  
257 cover is less than 5 (Figure 4d), and the wind speed is less than 3 m s<sup>-1</sup> (Figure 4e). Interestingly,  
258 the local circulations induced by thermal differentiation is clearest when in absence of clouds,  
259 radiative heating is strongest and wind is weakest. Thus, both O<sub>3</sub> pollution and local circulations  
260 tend to appear in calm conditions characterized by high temperature, cloudless sky and weak wind,  
261 and the local circulation will inevitably have an impact on the distribution of O<sub>3</sub> in this case.  
262





270 For simplicity but without loss of generality, the longest-lasting regional O<sub>3</sub> pollution case in  
271 Table S1 is selected to investigate the impacts of land-surface forcing and AH on meteorology and  
272 O<sub>3</sub> pollution in the YRD. This 10-day regional O<sub>3</sub> pollution episode occurred from 25 May to 3 June  
273 in 2017. During this period, an average of 18 out of the 26 cities experienced O<sub>3</sub> pollution every day,  
274 and the MDA8 O<sub>3</sub> concentrations ranged from 168.1 to 205.1 μg m<sup>-3</sup>. Moreover, the daily maximum  
275 air temperature ranged from 28.5 to 33.9 °C over the central YRD (the innermost domain) under  
276 high pressure/uniform pressure field (Figure S1). This case meets the requirements of calm weather  
277 and high O<sub>3</sub> concentration. And the relatively long duration also provide a representative result.

### 278 3.2.2 Evaluation of model performance

279 In this study, three numerical experiments are conducted using WRF-Chem (Sect. 2.4) during  
280 the period of the previously mentioned O<sub>3</sub> episode. The simulation results are validated in the  
281 innermost domain by comparing with the observational data. Table 5 presents the statistical metrics  
282 in meteorological variables that includes 2-m air temperature (T<sub>2</sub>), relative humidity (RH), 10-m  
283 wind speed (WS<sub>10</sub>) and direction (WD<sub>10</sub>). Figure 5 further illustrates time series comparisons  
284 between these meteorological factors and their modeling results. T<sub>2</sub> is reasonably well simulated as  
285 the mean CORs (the mean of all the sites) are 0.875, 0.865 and 0.863 in MODIS\_noAH,  
286 USGS\_noAH and MODIS\_AH, respectively. The small negative MBs at all sites suggest that our  
287 simulations underestimate T<sub>2</sub> to some extent, though this light underestimation is acceptable because  
288 of the small mean RMSE (2.3, 3.1 and 2.3 °C). The mean MBs for T<sub>2</sub> in USGS\_noAH,  
289 MODIS\_noAH and MODIS\_AH are -2.4, -1.0, and -0.8 °C, indicting an improvement in  
290 temperature when new land use and AH are taken into account. These results can be confirmed by  
291 Figure 5a. With respect to RH, the mean CORs are 0.823, 0.753 and 0.825 for the three numerical  
292 experiments, respectively. All three simulations can well capture the diurnal variation of RH, but  
293 have different performance on different sites (Figure 5b). In USGS\_noAH, RH is overestimated at  
294 all sites, especially Pudong site, and the mean MB is 11.2%. While RH is only overestimated at the  
295 two coastal sites (Pudong and Shanghai) but underestimated at other two sites (Hongqiao and  
296 Xiaoshan) in MODIS\_noAH and MODIS\_AH. Moreover, USGS\_noAH has the highest mean  
297 RMSE of RH (16.3%), followed by MODIS\_AH (12.4%) and MODIS\_noAH (12.1%). As for WS<sub>10</sub>,  
298 the modeling values are slightly overestimated at all sites in all three simulations. The  
299 overestimation of WS<sub>10</sub> may partly be attributed to the unresolved terrain features by the default



300 surface drag parameterization causing an overestimation of wind speed in particular at low values  
301 (Jimenez and Dudhia, 2012). Specially,  $WS_{10}$  in USGS\_noAH is the most overestimated, followed  
302 by MODIS\_AH and MODIS\_noAH, with the mean MBs are 1.2, 1.0 and  $0.8 \text{ m s}^{-1}$ , respectively.  
303 Additionally, a high mean MB is found to correspond to a high mean RMSE (1.9, 1.8 and  $1.7 \text{ m s}^{-1}$ )  
304 in our simulations. In terms of  $WD_{10}$ , the model captures well the shift in wind direction during  
305 the study period (Figure 5d). Thus, our modeling results of wind speed and direction basically reflect  
306 the characteristics of wind fields. In summary, both the statistical metrics in Table 3 and time series  
307 in Figure 5 illustrate that all the numerical experiments can reflect the major characteristics of  
308 meteorological conditions during this  $O_3$  pollution episode. Nevertheless, using new land-use data  
309 and adding AH can reduce the underestimation of  $T_2$  and the overestimation of RH and  $WS_{10}$  to  
310 some extent.



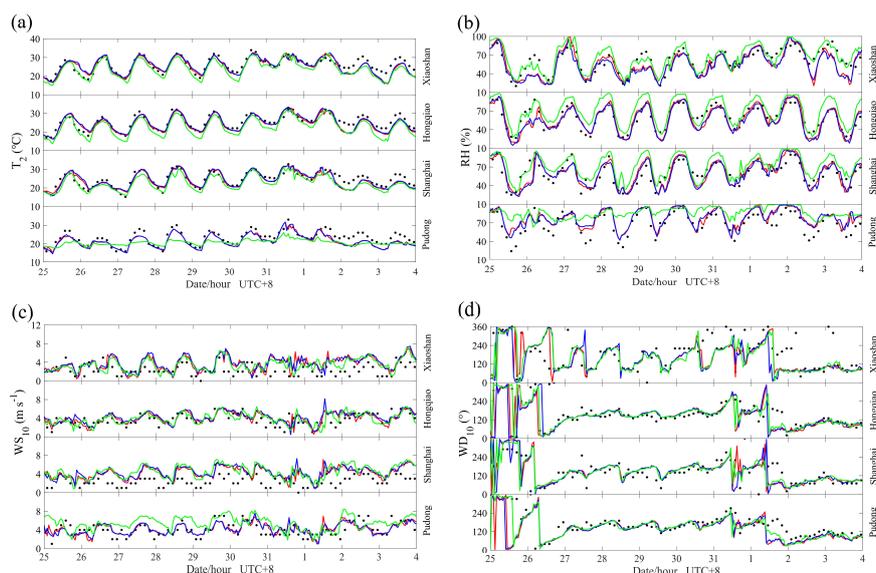
311 **Table 3.** Statistical metrics in meteorological variables between observations and simulations.

Variables	Site	MODIS <sub>noAH</sub>				USGS <sub>noAH</sub>				MODIS <sub>AH</sub>				
		$\bar{O}^a$	$\bar{S}^b$	MB <sup>c</sup>	RMSE <sup>d</sup>	COR <sup>e</sup>	$\bar{S}$	MB	RMSE	COR	$\bar{S}$	MB	RMSE	COR
T <sub>2</sub> (°C)	Pd	23.2	21.5	-1.7	2.4	0.89	20.7	-2.5	3.8	0.70	21.5	-1.7	2.4	0.89
	Sh	24.6	23.9	-0.7	2.2	0.87	22.5	-2.1	2.7	0.90	24.2	-0.5	2.3	0.84
	Hq	25.3	24.4	-0.9	2.0	0.89	22.7	-2.6	3.0	0.95	24.8	-0.5	1.9	0.89
	Xs	25.9	25.1	-0.8	2.4	0.85	23.8	-2.2	2.8	0.91	25.5	-0.4	2.4	0.83
RH (%)	Pd	69.1	77.7	8.6	13.5	0.81	86.2	17.2	23.4	0.45	77.7	8.7	13.3	0.83
	Sh	59.3	60.6	1.3	11.7	0.81	71.1	11.8	16.1	0.81	59.4	0.1	12.4	0.78
	Hq	59.5	57.7	-1.8	9.8	0.88	70.6	11.1	14.5	0.89	56.2	-3.3	9.8	0.89
	Xs	60.6	55.4	-5.2	13.5	0.79	65.3	4.8	11.3	0.86	53.5	-7.1	14.1	0.80
WS <sub>10</sub> (m s <sup>-1</sup> )	Pd	4.1	4.1	0.0	1.4	0.47	5.5	1.3	2.1	0.35	4.2	0.1	1.3	0.51
	Sh	2.5	4.2	1.7	2.2	0.36	4.5	2.0	2.4	0.54	4.3	1.9	2.3	0.35
	Hq	3.7	3.9	0.2	1.2	0.54	3.9	0.2	1.2	0.53	4.2	0.5	1.3	0.50
	Xs	2.3	3.6	1.3	2.0	0.26	3.4	1.1	1.8	0.30	3.8	1.5	2.1	0.24
WD <sub>10</sub> (°)	Pd	160.4	136.1	-26.2	78.7	0.42	148.1	-14.3	55.1	0.72	137.3	-24.7	77.5	0.42
	Sh	141.6	146.4	4.8	66.4	0.60	141.7	0.1	63.9	0.59	142.6	1.0	69.9	0.56
	Hq	159.7	140.2	-23.4	80.2	0.46	153.1	-10.6	74.9	0.52	142.8	-20.4	91.8	0.29
	Xs	188.6	160.2	-28.4	99.5	0.48	161.4	-27.3	109.6	0.35	152.0	-36.6	109.9	0.38

312 <sup>a</sup>  $\bar{O}$  and <sup>b</sup>  $\bar{S}$  indicate the average of observations and simulations, respectively. <sup>c</sup> MB indicates the mean bias, <sup>d</sup> RMSE indicates the root mean square error and <sup>e</sup> COR  
 313 indicate the correlation coefficient, with statistically significant at 99% confident level.



314



315

316 Figure 5. Time series of  $T_2$ , RH,  $WS_{10}$  and  $WD_{10}$  for observations and simulations at different  
 317 meteorological stations. The black dots are the surface observations. The simulation results of  
 318 MODIS\_noAH, USGS\_noAH and MODIS\_withAH are shown in red, green and blue, respectively.

319

320 Table 4 lists the statistical metrics in  $O_3$ , and Figure 6 gives the hourly variations of  $O_3$  for  
 321 observations and simulations at different sites. With high CORs (the mean CORs are 0.80, 0.81 and  
 322 0.80 in MODIS\_noAH, USGS\_noAH and MODIS\_AH, respectively), all the simulations can  
 323 reproduce the diurnal variation of  $O_3$ , which shows that  $O_3$  concentration reaches its maximum in  
 324 the afternoon and gradually decreases to its minimum in the morning. The magnitude of  $O_3$   
 325 modeling results is reasonable (Figure 6), but the peak and valley values of  $O_3$  simulations are  
 326 sometimes differ greatly from the observations, especially the peak value, like Huzhou. This may  
 327 be related to the resolution of the emission inventory and the distribution of  $O_3$  precursors.  
 328 Considering the relatively low mean MB (6.9, -1.6 and  $9.0 \mu\text{g m}^{-3}$ ) and mean RMSE (49.3, 46.2 and  
 329  $49.0 \mu\text{g m}^{-3}$ ), the modeling results of  $O_3$  are generally reasonable and acceptable.

330

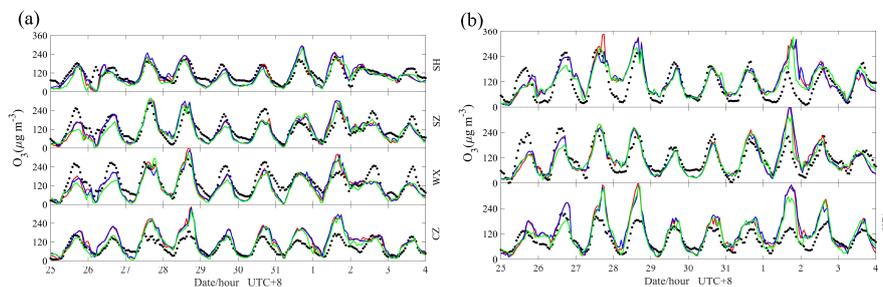
331 **Table 4.** Statistical metrics in  $O_3$  between observations and simulations.

Case	Index	Site
------	-------	------



		CZ	WX	SZ	SH	HZ1	JX	HZ
	$\bar{O}$	89.7	141.8	121.7	112.8	95.8	113.2	104.8
MODIS_noAH	$\bar{S}$	123.2	117.6	116.2	103.4	128.1	112.5	127.5
	MB	33.3	-24.2	-5.6	-9.1	32.1	-0.6	22.7
	RMSE	53.8	49.1	42.8	36.4	59.9	44.4	58.6
	COR	0.85	0.83	0.82	0.80	0.83	0.78	0.71
USGS_noAH	$\bar{S}$	108.1	106.8	107.1	93.8	118.6	111.0	122.5
	MB	18.5	-35.0	-14.7	-18.9	23.0	-2.0	18.0
	RMSE	43.5	56.0	44.7	37.7	50.1	41.1	50.0
	COR	0.83	0.81	0.80	0.81	0.82	0.80	0.77
MODIS_AH	$\bar{S}$	124.5	119.8	119.1	108.0	130.3	113.7	127.8
	MB	34.7	-21.9	-2.7	-4.6	34.3	0.6	23.0
	RMSE	53.5	47.3	42.4	37.4	59.4	44.7	58.2
	COR	0.84	0.83	0.81	0.80	0.82	0.78	0.71

332



333

334 Figure 6. Same as Figure 5, but for O<sub>3</sub>.

335

336 Above all, the WRF-Chem model using our configuration has a good capability in simulating  
 337 the meteorology and O<sub>3</sub> air quality over the studied region in this study. It is still noteworthy that  
 338 the object of inter-comparison between the three numerical experiments is not to determine which  
 339 setting is most skillful in reproducing the observations. Rather, it is to diagnose and understand the  
 340 differences induced by land-surface forcing and AH, and then to provide valuable insight into the  
 341 formation of the O<sub>3</sub> pollution episodes.

342

### 343 3.3 Overall behaviors of O<sub>3</sub> and local circulations

344 Based on the results of the control simulation (MODIS\_noAH), we first give an overall  
 345 behavior of O<sub>3</sub> and local circulations during the study period. And then the differences induced by  
 346 land-surface forcing and AH are discussed via intercomparisons between the numerical experiments.

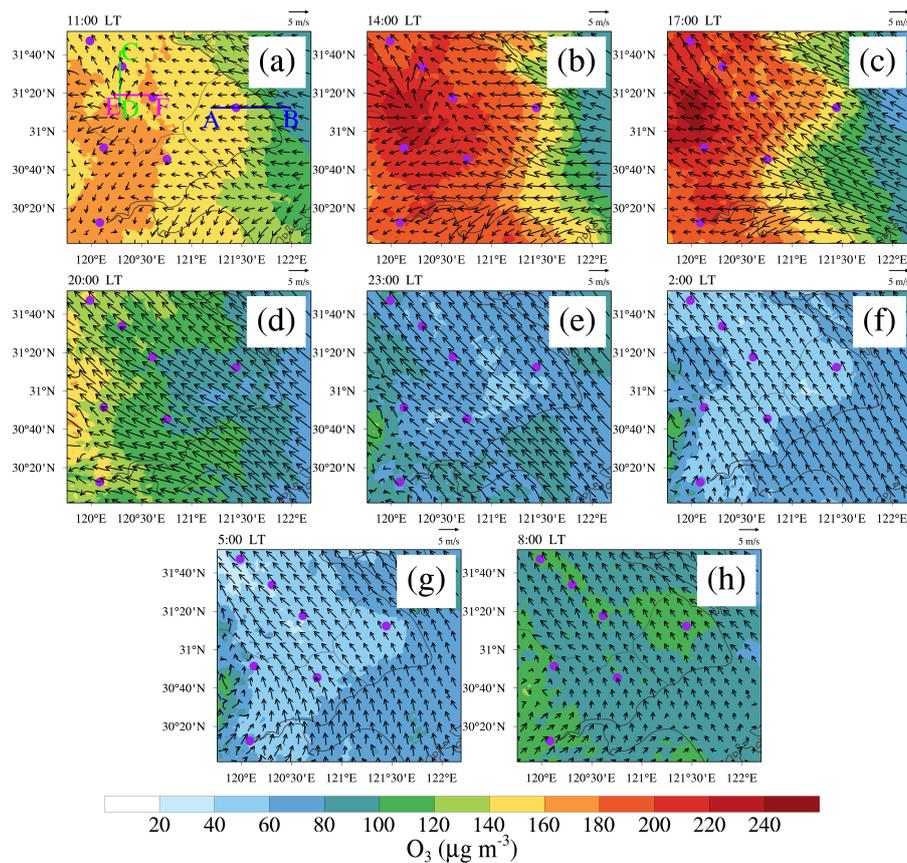


347 Thereby, only difference plots between USGS\_noAH/MODIS\_withAH and MODIS\_noAH are  
348 shown in this paper, but the corresponding original plots for USGS\_noAH and MODIS\_withAH  
349 can be found in supplementary materials (Figure S2-5).

### 350 **3.3.1 Spatiotemporal variations of O<sub>3</sub>**

351 As show in Figure 7, O<sub>3</sub> concentration began to rise around 8:00 local time (LT = UTC + 8 h)  
352 after sunrise, and became noticeable after only 3 hours (Figure 7a and h). During this stage, the  
353 nocturnal residual layer vanished due to the development of the convective boundary layer (Figure  
354 8). The O<sub>3</sub>-rich air mass in the residual layer was mixed with the O<sub>3</sub>-poor air mass on the ground,  
355 which enhanced the surface O<sub>3</sub> in the morning (Hu et al., 2018). Around 11:00 LT, the convective  
356 boundary layer was established, and high O<sub>3</sub> produced by photochemical reactions appeared over  
357 the central YRD and persisted until 18:00 LT (Figure 7b, 7c and 8). The maximum O<sub>3</sub> production  
358 was in the middle of the boundary layer (~800 m) instead of at the surface (Figure 8). After sunset,  
359 surface O<sub>3</sub> concentrations decreased sharply due to nitrogen oxide (NO) titration. The loss of O<sub>3</sub>  
360 caused by NO titration almost ceased around 2:00 LT when O<sub>3</sub> was at its lowest level of the day  
361 (Figure 7f and g). In general, O<sub>3</sub> has a typical diurnal variation with high concentration in the  
362 daytime and low concentration at night. This is consistent with the results in Figure 6, and this rule  
363 of O<sub>3</sub> can be applied to most parts of the world. Therefore, the situation during the daytime (We  
364 select 11:00, 14:00, 17:00 and 20:00 LT in this study) should be paid attention to when it comes to  
365 O<sub>3</sub> pollution.

366



367

368 **Figure 7.** Horizontal distributions of  $O_3$  and wind at the lowest model level in MODIS\_noAH. (a),

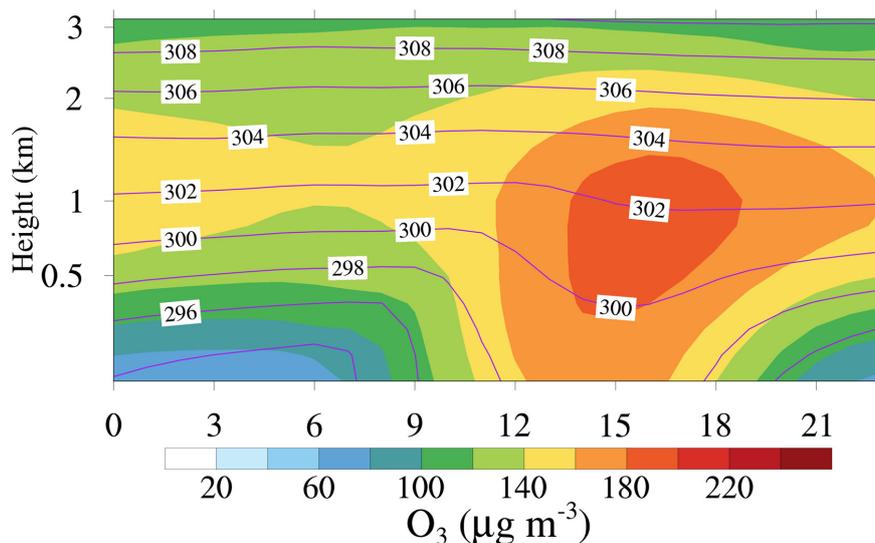
369 (b), (c) and (d) are the results at 11:00, 14:00, 17:00 and 20:00 LT, referring to the daytime. (e), (f),

370 (g) and (h) are the results at 23:00, 2:00, 5:00 and 8:00 LT, referring to the night. The purple dots

371 represent the locations of cities (red dots in Figure 1b) in the innermost domain. To obtain general

372 feature, all results are the average of the study period, and the same for the subsequent results.

373



374  
375 **Figure 8.** Temporal-vertical distribution of O<sub>3</sub> and potential temperature over the innermost domain  
376 in MODIS\_noAH.

377

### 378 3.3.2 Sea and lake breezes

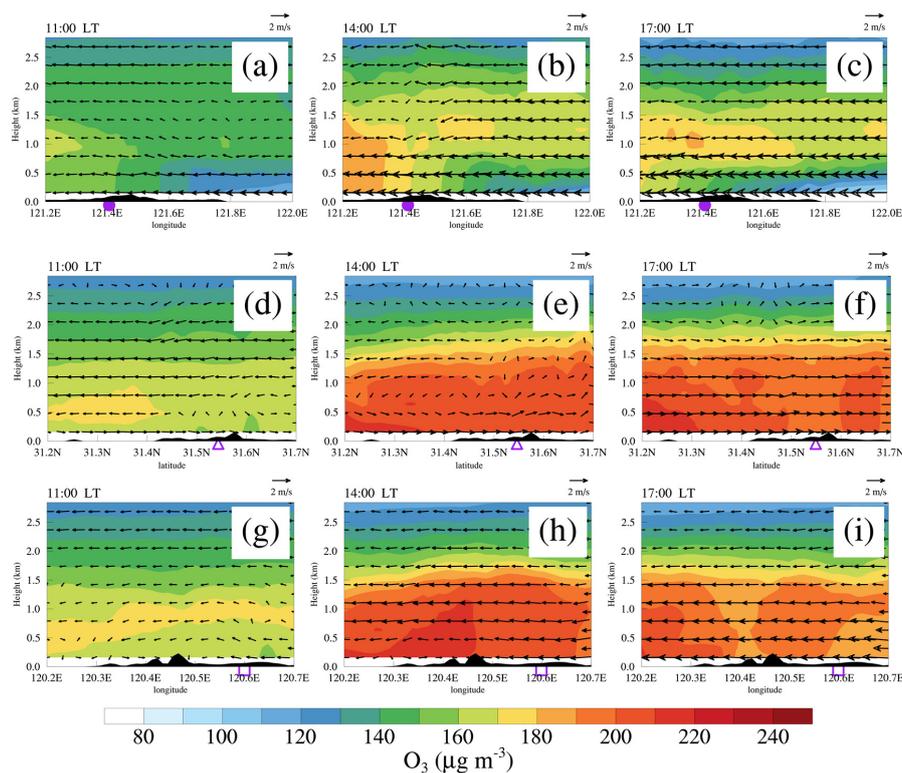
379 As shown in Figure 7a and b, in the areas where the local circulations meet the background  
380 dominant winds (the southeast wind), the converging airflows make O<sub>3</sub> concentrations higher than  
381 those in the surrounding areas. Furthermore, the typical local circulations in the central YRD are the  
382 sea and the lake breezes around the Tai Lake. In this study, the sea-breeze usually affected a wide  
383 area and lasted a long time, which may be related to the local background field since they are mostly  
384 in same direction, and it is difficult to separate the sea-breeze from the southeast wind. The sea-  
385 breeze was obvious around 14:00 LT and matured around 17:00 LT, and continuously transported  
386 high O<sub>3</sub> from coastal to the inland areas during this period (Figure 7b-d). Compared with the sea-  
387 breeze, the lake-breeze had a much smaller influencing area and a shorter duration. Around 11:00  
388 LT, the lake-breeze was established. It reached its maximum intensity around 14:00 LT, and then  
389 disappeared sharply due to the predominant sea-breeze (Figure 7c). Both the sea and the lake breezes  
390 played important roles in the horizontal distributions of O<sub>3</sub> in the central YRD.

391 As the coastline is generally north-south (Figure 1b), the cross sections along line AB depicted  
392 in Figure 7a are illustrated to show representative example of the vertical structure of the sea breezes



393 (Figure 9a-c). The sea-breeze below 500m had already developed by 11:00 LT. A sea-breeze front  
394 was found in front of Shanghai (~121.6°E), with a height of 1.5 km. The speed of sea-breeze  
395 increased around 14:00 LT, which can exceed  $5 \text{ m s}^{-1}$ . The intensified sea-breeze penetrated inland  
396 for a distance of 20-30 km, and the sea-breeze front (~121.4°E) lifted the boundary layer top over  
397 Shanghai up to ~2 km (Figure 9b). Strong sea-breeze swept across the central YRD around 17:00  
398 LT, reducing the  $\text{O}_3$  concentration near the surface in coastal areas. But the  $\text{O}_3$  in the mixed layer  
399 still maintained a high level, which can result in an  $\text{O}_3$ -rich reservoir forming in the nocturnal  
400 residual layer (Figure 9c and 8). The penetration of sea-breeze front and its effect on surface  $\text{O}_3$  can  
401 be also observed in other regions, such as the Pearl River Delta Region (You et al., 2019), Taiwan  
402 (Lin et al., 2007), the Athens basin (Mavrakou et al., 2012) and Paulo (Freitas et al., 2007).

403 As for the lake breezes, the cross sections along line CD (Figure 9d-f) and EF (Figure 9g-i) are  
404 given since the lake is usually inside the land so that the lake breezes can have different directions.  
405 The lake-breeze was established when the surface wind was weak by 11:00 LT (Figure 9d and g)  
406 though it was shallow at that time. Around 14:00 LT, the lake-breeze strengthened. The extension  
407 of the lake-breeze circulation zone can even reach up to 2 km in the vertical dimension. The offshore  
408 flow ( $\sim 2 \text{ m s}^{-1}$ ) of the lake-breeze circulation transported high  $\text{O}_3$  concentration from urban areas  
409 to the lake, while the onshore flow blew the  $\text{O}_3$  back to urban areas (Figure 9e and h). Thus, the net  
410 effect is that the lake-breeze “accelerated” the vertical mixing in the boundary layer, resulting in  
411 high concentration of  $\text{O}_3$  in the lakeside cities. The high surface  $\text{O}_3$  concentration caused by the lake  
412 breezes has also been confirmed near other lakes, such as the Lake Michigan (Lennartson and  
413 Schwartz, 2002), the Great Lakes (Sills et al., 2011) and the Great Salt Lake (Blaylock et al., 2017).  
414 Finally, the lake-breeze was destroyed by the prevailing southwest wind by 17:00 LT.  
415



416  
417 **Figure 9.** Vertical cross sections of  $O_3$  and wind for sea-breeze at (a) 11:00, (b) 14:00 and (c) 17:00  
418 LT along the line AB in Figure 7a. (d), (e) and (f) are the same as (a), (b) and (c), respectively, but  
419 for lake-breeze along the line CD in Figure 7a. (g), (h) and (i) are also the same as (a), (b) and (c),  
420 respectively, but for lake-breeze along the line EF in Figure 7a. The purple dots, triangles and  
421 rectangle represent the locations of Shanghai, Wuxi and Suzhou, respectively. The black shaded  
422 areas represent the terrain, and the terrain has been multiplied by a factor of 10 when plotting.

423

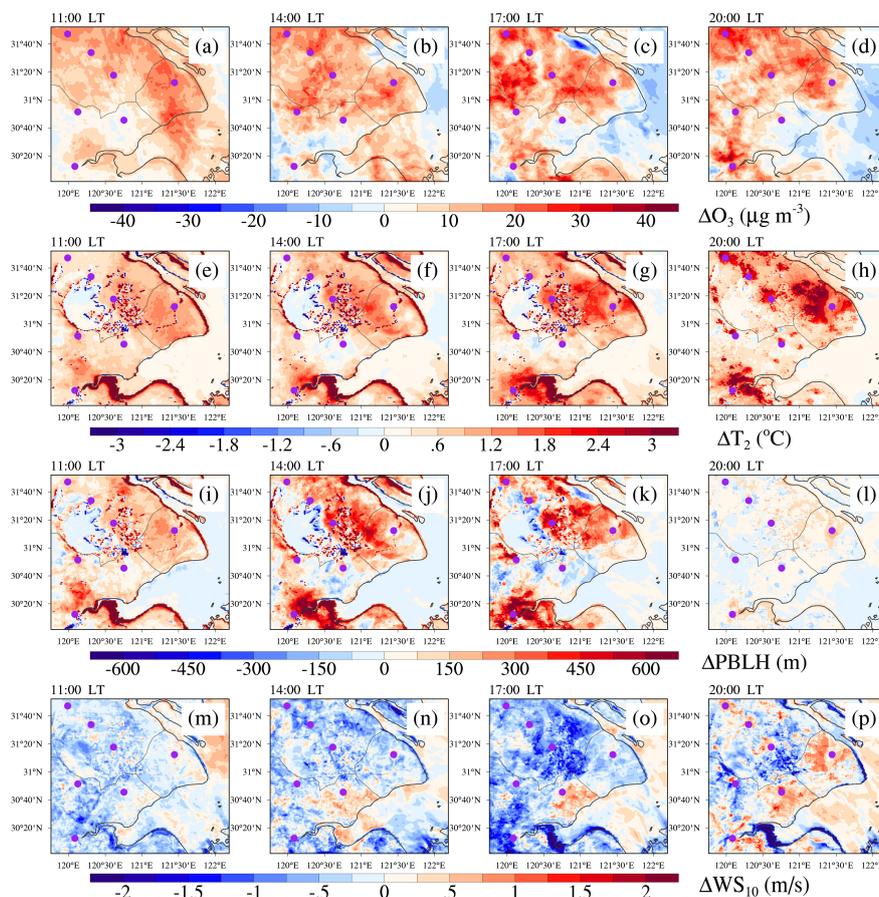
### 424 3.4 Impacts of land-surface forcing on meteorology and $O_3$

#### 425 3.4.1 The changes in horizontal direction

426 Figure 10 presents the spatial differences of the main factors, including  $O_3$ ,  $T_2$ , PBLH and  $WS_{10}$ ,  
427 between MODIS\_noAH and USGS\_noAH. Obviously, higher  $O_3$  was produced in the  
428 MODIS\_noAH, indicating that urban expansion will increase surface  $O_3$  concentrations. The largest  
429 increment of  $O_3$  occurred in the afternoon, with a value of  $20 \mu\text{g m}^{-3}$  around 17:00 LT in Changzhou.  
430  $T_2$  is directly affected by the land-atmosphere heat fluxes resulting from land-surface forcing. The



431 spatial pattern of remarkable warming effect for  $T_2$  was consistent with the urban-fraction change  
432 (Figure 2a and b), which is that the positive temperature anomaly often appeared in large cities and  
433 their surrounding areas. This positive forcing for  $T_2$  is associated with the enhanced surface heating  
434 through upward sensible heat fluxes during the day. In megacities like Shanghai,  $T_2$  can increase by  
435 3 °C. It should be noted that there was a confusing “false” warming at the junction of land and  
436 sea/lake, which was mainly caused by the different treatment of the MODIS-based and USGS land  
437 use classifications at the boundary conditions of land versus water (Figure 2a and b). The change in  
438 PBLH was similar to that in  $T_2$ , but it was less obvious after sunset around 20:00 LT. This is because  
439 that the warming up of  $T_2$  can enhance the vertical air movement in the boundary layer and thereby  
440 increase the PBLH. The maximum positive change of PBLH reached up to 500 m in the urban areas  
441 at noon but downed to 100 m after sunset. The roughness of cities and forest is greater than that of  
442 cropland, so there was a decrease in  $WS_{10}$  in the MODIS\_noAH (Figure 9m-p), with a maximum  
443 decrease up to 1.5 m  $s^{-1}$  in Hangzhou around 17:00 LT.  
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### 3.4.2 The changes in vertical direction

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**Figure 10.** Horizontal distributions of the (a-d)  $O_3$ , (e-h)  $T_2$ , (i-l) PBLH and (m-p)  $WS_{10}$  differences between MODIS\_noAH and USGS\_noAH (MODIS\_noAH – USGS\_noAH) at different times (11:00, 14:00, 17:00 and 20:00 LT) of the day. The purple dots represent the locations of cities (red dots in Figure 1b) in the innermost domain.

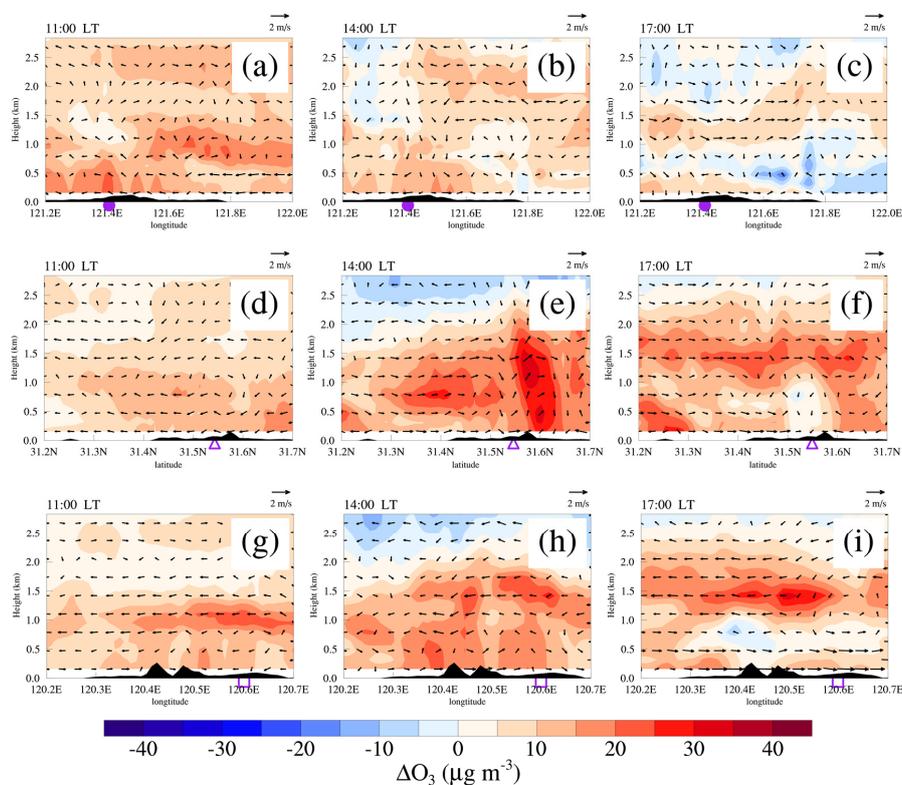
As shown in Figure 11a-c, the sea-breeze below 500 m increased by 1-2 m s<sup>-1</sup> due to the existence of the cities which enhanced the temperature contrast between the land and the sea. Strong turbulent mixing and updraft induced by the sea-breeze front promote the development of the urban boundary layer, contributing to elevated  $O_3$  levels at surface in the city during the advance of the sea-breeze front inland (Figure 11a and b). When the sea-breeze matured around 17:00 LT, its transport effect reduced the surface  $O_3$  concentration of the coastal cities (Figure 9c). However, this



458 “removal” was weakened because the sea-breeze near the surface was slowed due to the rough urban  
459 surface. Finally, surface  $O_3$  of about  $10 \mu\text{g m}^{-3}$  was left compared to the scenario without cities  
460 (Figure 11c).

461 As for the lake-breeze, it was also enhanced by  $1\text{--}2 \text{ m s}^{-1}$  after the establishment because of the  
462 larger temperature contrast resulting from the cities, just like the sea-breeze (Figure 11e and h). And  
463 the life of the lake-breeze was extended to 17:00 LT (Figure 11f and i) when the city exists. Because  
464 the lake-breeze was conducive to the vertical mixing of the boundary layer and its onshore flow can  
465 blow high concentration of  $O_3$  from the lake to the city (Sect. 3.3.2), the urban  $O_3$  concentration will  
466 eventually increase, with a maximum of  $30 \mu\text{g m}^{-3}$  in Wuxi at 14:00 LT.

467



468

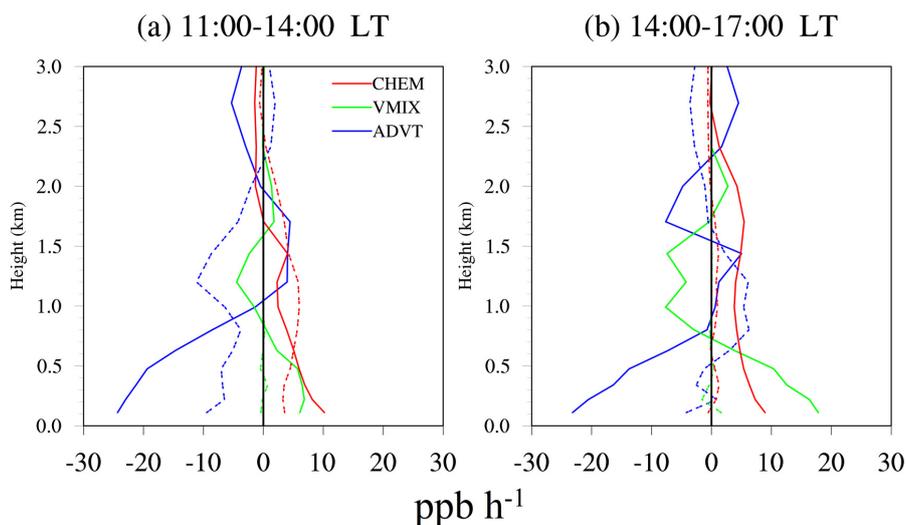
469 **Figure 11.** Same as Figure 9, but for the differences between MODIS\_noAH and USGS\_noAH  
470 (MODIS\_noAH – USGS\_noAH).

471

472 **3.4.3 The mechanism of land-surface forcing modulating  $O_3$**



473 Land-surface forcing plays an important role in the evolution of O<sub>3</sub> by changing the local  
474 meteorology (meteorological factors and local circulations). Changing land-surface forcing from  
475 USGS to MODIS leads to an increase in T<sub>2</sub> by maximum 3 °C, an increase in PBLH by maximum  
476 500 m and a decrease in WS<sub>10</sub> by maximum 1.5 m s<sup>-1</sup> in the YRD, which is comparable to those in  
477 the BTH region (Yu et al., 2012), the PRD region (Li et al., 2014) and the National Capital Region  
478 of India (Sati and Mohan, 2017). And these changes are particularly evident in and around cities.  
479 The elevated air temperature is conducive to the photochemical production of O<sub>3</sub>, and the well-  
480 developed boundary layer favors the vertical mixing of O<sub>3</sub> (Figure 12), which increases the O<sub>3</sub>  
481 concentration near the surface by maximum 20 µg m<sup>-3</sup>. This change magnitude in O<sub>3</sub> is consistent  
482 with the findings reported in Seoul (Ryu et al., 2013b) and Southern California (Li et al., 2019).  
483 Local circulations (the sea and the lake breezes) are also influenced by the land-surface forcing,  
484 chiefly from the urban expansion as the most significant land-surface forcing in the YRD comes  
485 from urban expansion over the past few decades. For the coastal cities, like Shanghai, the larger  
486 temperature contrast induced by cities enhances the sea-breeze below 500 m. As the sea-breeze front  
487 moves inland, it can induce stronger upward air flow that deepens the boundary layer. Thus, high  
488 O<sub>3</sub> concentration in the middle of boundary layer can be more easily transported to the surface.  
489 However, the movement of the sea-breeze is slowed due to the rough urban surface after the sea-  
490 breeze matures. The removal of the sea-breeze is then weakened and the surface O<sub>3</sub> increases by 10  
491 µg m<sup>-3</sup>. The similar response of the sea breezes to urban expansion as well as its impact on O<sub>3</sub> has  
492 been also reported in the PRD region (You et al., 2019) and Paulo (Freitas et al., 2007). For the  
493 lakeside cities, like Wuxi and Suzhou, the lifetime of the lake breezes is extended to the afternoon  
494 due to the existence of the city. The offshore flow of the lake-breeze transports high O<sub>3</sub> concentration  
495 in the middle of the boundary layer from the land to the lake, while the onshore flow brings the O<sub>3</sub>  
496 back to the land, which accelerates the vertical mixing of O<sub>3</sub> and can increase the surface O<sub>3</sub> by even  
497 30 µg m<sup>-3</sup>. High surface O<sub>3</sub> appears when the lake breezes have been established can also be  
498 observed in the Greater Toronto Area (Wentworth et al., 2015) and the Lake Michigan (Abdi-  
499 Oskouei et al., 2020).  
500



501

502 **Figure 12.** Vertical profiles of the changes in individual processes between MODIS\_noAH and  
503 USGS\_noAH (MODIS\_noAH – USGS\_noAH) at (a) 11:00-14:00 LT and (b) 14:00-17:00 LT over  
504 Shanghai (solid lines) and Wuxi (dashed lines). CHEM (in red), VMIX (in green) and ADVT (in  
505 blue) represent gas-phase chemical reactions, turbulent mixing and advection transport, respectively.

506

### 507 3.5 Impacts of anthropogenic heat on meteorology and O<sub>3</sub>

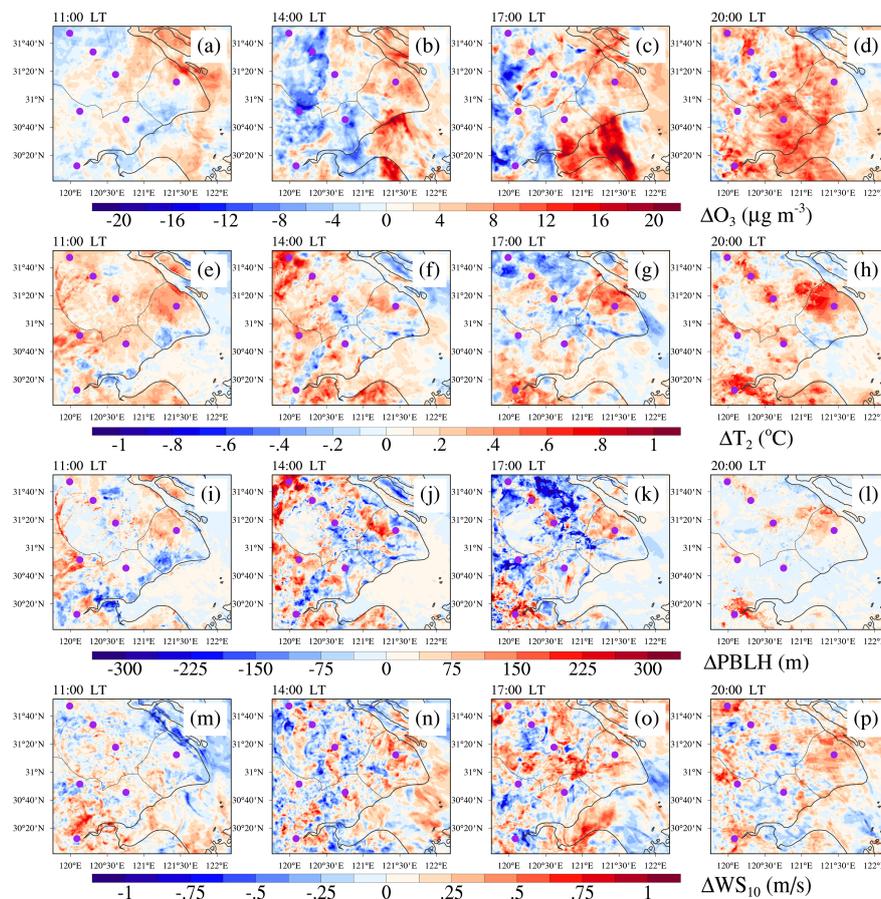
#### 508 3.5.1 Horizontal changes

509 Compared with land-surface forcing, the changes caused by AH are much smaller (Figure 13).  
510 Furthermore, these changes in meteorology and O<sub>3</sub> mainly occur in and around cities as there are  
511 more AH emissions in these areas (Figure 3). Surface O<sub>3</sub> concentration increased in the urban areas  
512 by about 4 μg m<sup>-3</sup> in the simulation with adding AH, and this phenomenon was clearer after sunset  
513 (Figure 13d). By adding more surface sensible heat into the atmosphere, the AH fluxes can lead to  
514 an increase in T<sub>2</sub> of 0.2 °C during the day, with the typical value of 0.42 °C in Shanghai. Vertical air  
515 movement in the boundary layer can be enhanced by the warming up of the surface air temperature,  
516 thereby the PBLH will increase as well. According to the simulations, the PBLH increased by about  
517 75 m in the urban areas. With regards to WS<sub>10</sub>, it increased by about 0.3 m s<sup>-1</sup> in the urban areas,  
518 which is contrary to the decrease in WS<sub>10</sub> caused by land-surface forcing (Sect. 3.4.1). This is  
519 ascribed to the strengthened urban-breeze circulations induced by the AH fluxes, which is



520 mentioned in previous studies (Ryu et al., 2013a, b; Xie et al., 2016a, b).

521



522

523 **Figure 13.** Same as Figure 10, but for the differences between MODIS\_withAH and MODIS\_noAH  
524 (MODIS\_withAH – MODIS\_noAH).

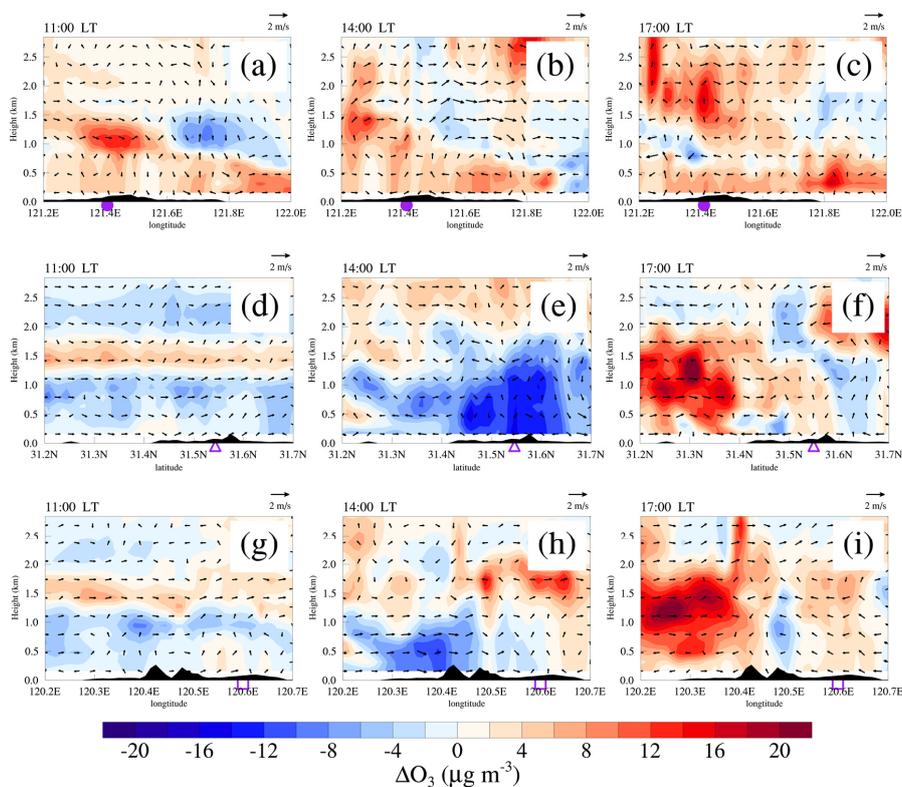
525

### 526 3.5.2 Vertical changes

527 The phenomenon that cities are almost always warmer than their surroundings is known as the  
528 urban heat island (UHI), and the difference between the urban and the rural surface energy balance  
529 can further initiate the UHI circulation. It is clearly seen that an enhanced UHI circulation driven  
530 by AH appeared in the megacity Shanghai around 14:00 LT (Figure 14b). This circulation extended  
531 horizontally 20-30 km from the city center to the urban edge, and vertically to nearly 2 km from the  
532 ground to the top of the urban boundary layer. Under this condition, there was a small increase (4–6



533  $\mu\text{g m}^{-3}$ ) in  $\text{O}_3$  concentrations in the low boundary layer. However, for the lakeside cities, the  
534 enhanced UHI circulation was not visibly noticed, and the  $\text{O}_3$  concentration in urban areas was  
535 reduced on average, with a maximum of  $16 \mu\text{g m}^{-3}$  in Wuxi around 14:00 LT (Figure 14e). The  
536 lower  $\text{O}_3$  concentration may be affected by the increased wind on the lake (Figure 13), which was  
537 beneficial to the diffusion and dilution processes. Furthermore, it seems that AH has a limited effect  
538 on local circulations, regardless of the sea or lake breeze, though it play an important role in the  
539 urban-breeze circulations. In our simulation cases, AH does not continuously and significantly affect  
540 any branch of the local circulations like the land-surface forcing.  
541



542  
543 **Figure 14.** Same as Figure 8, but for the differences between MODIS\_withAH and MODIS\_noAH  
544 (MODIS\_withAH – MODIS\_noAH).

545  
546 **3.5.3 The mechanism of anthropogenic heat modulating  $\text{O}_3$**



547 AH and land-surface forcing play different roles in meteorology and O<sub>3</sub>. AH allows the  
548 atmosphere to reserve more energy via the additional sensible heat fluxes, which increases T<sub>2</sub> by  
549 about 0.2 °C. Higher temperature is conducive to the development of the convective boundary layer  
550 and can induce stronger upward air movement, which rises the PBLH by about 75 m. In the  
551 convective boundary layer, the atmosphere is associated with turbulent motions, and is unstable.  
552 Together with the urban-breeze circulations enhanced by AH, WS<sub>10</sub> can increase by 0.3 m s<sup>-1</sup>. These  
553 findings are comparable to the values estimated in other cities all around the world, such as  
554 Philadelphia in the United States (Fan and Sailor, 2005), Winnipeg in Canada (Ferguson and  
555 Woodbury, 2007), Berlin in German (Menberg et al., 2013) and Tokyo in Japan (Dhakal and Hanaki,  
556 2002). It is noteworthy that the abovementioned changes mainly appear in large cities and their  
557 surrounding areas, where AH emission centers are located. And these changes eventually caused an  
558 increase in surface O<sub>3</sub> concentration by about 4 μg m<sup>-3</sup>. Additionally, though AH can play an  
559 important role in urban-breeze circulations, it may not be powerful enough to affect the local  
560 circulations such as the sea and the lake breezes.

561

#### 562 **4 Summary and conclusions**

563 Land-surface forcing related to the urban expansion and AH release from human activities can  
564 change the meteorology (meteorological factors and local circulations) and thereby affect O<sub>3</sub> air  
565 quality in and around cities. In this study, the YRD region, a highly urbanized place with sever O<sub>3</sub>  
566 pollution and complex geography, is selected to discuss this issue. Firstly, we briefly describe the  
567 general characteristics of O<sub>3</sub> pollution in the YRD based on the surface observations. Secondly, we  
568 simulate a representative case using WRF-chem and evaluate the model performance by comparing  
569 with the observational data. Finally, the response of meteorology as well as O<sub>3</sub> to land-surface  
570 forcing and AH are investigated from the model results. The main findings are listed as below:

571 (1) Regional O<sub>3</sub> pollution occurs frequently in the YRD (~ 26 times per year). Like other  
572 regions, these O<sub>3</sub> pollution episodes mainly occur in warm season (April to October) under calm  
573 conditions characterized by high temperature (over 20 °C), low relative humidity (less than 80%),  
574 light wind (less than 3 m s<sup>-1</sup>) and shallow cloud cover (less than 5). In this case, the local circulations  
575 induced by thermal differentiation tend to develop and will have an important impact on the  
576 distribution of O<sub>3</sub>.



577 (2) By updating the land-use data from USGS to MODIS, we find an increase in  $T_2$  by  
578 maximum 3 °C, an increase in PBLH by maximum 500 m and a decrease in  $WS_{10}$  by maximum 1.5  
579  $m s^{-1}$  in the YRD, which is comparable to those in the BTH region (Yu et al., 2012), the PRD region  
580 (Li et al., 2014) and the National Capital Region of India (Sati and Mohan, 2017). The higher  
581 temperature and PBLH elevate the  $O_3$  level by maximum  $20 \mu g m^{-3}$  via the photochemical and the  
582 vertical mixing processes, respectively. For changes in local circulations, the sea-breeze below 500  
583 m is enhanced due to larger temperature contrast induced by the urban expansion. During the  
584 advance of the sea-breeze front inland, the upward air flow in front of the front is conducive to the  
585 vertical mixing of  $O_3$ . When the sea-breeze is well formed in the late afternoon, further progression  
586 inland is stalled on account of the rough urban surface. The transport of high  $O_3$  from coastal to the  
587 inland areas is weakened and thereby  $O_3$  can be  $10 \mu g m^{-3}$  higher in the case with cities than without.  
588 The similar results have been also reported in the Paulo (Freitas et al., 2007) and the PRD region  
589 (You et al., 2019). With respect to the lake breezes, its lifetime will be extended from the noon to  
590 the afternoon because of the urban expansion. Since the net effect of the lake-breeze is to accelerate  
591 the vertical mixing in the boundary layer, the surface  $O_3$  can increase as much as  $30 \mu g m^{-3}$   
592 influenced by the lake-breeze. Similar phenomenon also be observed in the Greater Toronto Area  
593 (Wentworth et al., 2015) and the Lake Michigan (Abdi-Oskouei et al., 2020).

594 (3) The changes caused by AH are different from land-surface forcing. These changes are  
595 relatively small and mainly appear around the cities where there are large AH emissions. Through  
596 regulating the land-atmosphere heat fluxes,  $O_3$ ,  $T_2$ , PBLH and  $WS_{10}$  increases by about  $4 \mu g m^{-3}$ ,  
597 0.2 °C, 75 m and  $0.3 m s^{-1}$  under the effect of the additional sensible heat fluxes induced by AH.  
598 The magnitudes of these changes are consistent with the values estimated in other cities all around  
599 the world, including Philadelphia in the United States (Fan and Sailor, 2005), Winnipeg in Canada  
600 (Ferguson and Woodbury, 2007), Tokyo in Japan (Dhakal and Hanaki, 2002) and Berlin in German  
601 (Menberg et al., 2013). Additionally, our results show that AH may have a quite limited impact on  
602 local circulations, such as the sea and the lake breezes. But the urban-breeze circulations in and  
603 around big cities are sensitive to AH inputs, which can further affect the urban air pollutants.

604 Estimating the impacts of land-surface forcing and AH on urban climate and air quality is a  
605 complex but necessary issue as these two are important manifestations of urbanization. Although  
606 our study only focuses on the YRD region, most of the results can be supported by previous studies



607 that conducted in other region around the world. Thus, our work may provide valuable insight into  
608 the formation of O<sub>3</sub> pollution in those rapidly developing regions with unique geographical features.  
609

610 ***Data Availability Statement.***

611 Air quality monitoring data were acquired from a mirror of data from the official NEMC real-time  
612 publishing platform (<https://quotsoft.net/air/>). Meteorological data were issued by the NCDC  
613 (<ftp://ftp.ncdc.noaa.gov/pub/data/noaa/isd-lite/>). The FNL meteorological data were acquired from  
614 NCEP (<https://doi.org/10.5065/D6M043C6/>). These data can be downloaded for free as long as you  
615 agree to the official instructions.

616

617 ***Author contributions.***

618 CZ and MX had the original ideas, designed the research, collected the data and prepared the original  
619 draft. CZ did the numerical simulations and carried out the data analysis. MX acquired financial  
620 support for the project leading to this publication.

621

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630

631 **References**

632 Abdi-Oskouei, M., Carmichael, G., Christiansen, M., Ferrada, G., Roozitalab, B., Sobhani, N., Wade,  
633 K., Czarnetzki, A., Pierce, R. B., Wagner, T., and Stanier, C.: Sensitivity of Meteorological  
634 Skill to Selection of WRF-Chem Physical Parameterizations and Impact on Ozone Prediction  
635 During the Lake Michigan Ozone Study (LMOS), *J Geophys Res-Atmos*, 125, 2020.  
636 Blaylock, B. K., Horel, J. D., and Crosman, E. T.: Impact of Lake Breezes on Summer Ozone



- 637 Concentrations in the Salt Lake Valley, *Journal of Applied Meteorology and Climatology*, 56,  
638 353-370, 2017.
- 639 Buchholz, S., Junk, J., Krein, A., Heinemann, G., and Hoffmann, L.: Air pollution characteristics  
640 associated with mesoscale atmospheric patterns in northwest continental Europe, *Atmospheric*  
641 *Environment*, 44, 5183-5190, 10.1016/j.atmosenv.2010.08.053, 2010.
- 642 Chameides, W., and Walker, J. C. G.: A photochemical theory of tropospheric ozone, *Journal of*  
643 *Geophysical Research*, 78, 8751-8760, 10.1029/JC078i036p08751, 1973.
- 644 Chen, F., and Dudhia, J.: Coupling an advanced land surface-hydrology model with the Penn State-  
645 NCAR MM5 modeling system. Part II: Preliminary model validation, *Monthly Weather*  
646 *Review*, 129, 587-604, 2001.
- 647 Chen, S. H., and Sun, W. Y.: A one-dimensional time dependent cloud model, *J Meteorol Soc Jpn*,  
648 80, 99-118, 2002.
- 649 Crosman, E. T., and Horel, J. D.: Sea and Lake Breezes: A Review of Numerical Studies, *Boundary-*  
650 *Layer Meteorology*, 137, 1-29, 10.1007/s10546-010-9517-9, 2010.
- 651 Dhakal, S., and Hanaki, K.: Improvement of urban thermal environment by managing heat discharge  
652 sources and surface modification in Tokyo, *Energ Buildings*, 34, 13-23, 2002.
- 653 Ding, A., Wang, T., Zhao, M., Wang, T., and Li, Z.: Simulation of sea-land breezes and a discussion  
654 of their implications on the transport of air pollution during a multi-day ozone episode in the  
655 Pearl River Delta of China, *Atmospheric Environment*, 38, 6737-6750,  
656 10.1016/j.atmosenv.2004.09.017, 2004.
- 657 Ding, A. J., Fu, C. B., Yang, X. Q., Sun, J. N., Zheng, L. F., Xie, Y. N., Herrmann, E., Nie, W., Petäjä,  
658 T., Kerminen, V. M., and Kulmala, M.: Ozone and fine particle in the western Yangtze River  
659 Delta: an overview of 1 yr data at the SORPES station, *Atmospheric Chemistry and Physics*,  
660 13, 5813-5830, 10.5194/acp-13-5813-2013, 2013.
- 661 Fan, H. L., and Sailor, D. J.: Modeling the impacts of anthropogenic heating on the urban climate  
662 of Philadelphia: a comparison of implementations in two PBL schemes, *Atmospheric*  
663 *Environment*, 39, 73-84, 2005.
- 664 Fast, J. D., Gustafson, W. I., Easter, R. C., Zaveri, R. A., Barnard, J. C., Chapman, E. G., Grell, G.  
665 A., and Peckham, S. E.: Evolution of ozone, particulates, and aerosol direct radiative forcing  
666 in the vicinity of Houston using a fully coupled meteorology-chemistry-aerosol model, *J*



- 667 Geophys Res-Atmos, 111, 2006.
- 668 Ferguson, G., and Woodbury, A. D.: Urban heat island in the subsurface, Geophysical Research  
669 Letters, 34, 2007.
- 670 Flanner, M. G.: Integrating anthropogenic heat flux with global climate models, Geophysical  
671 Research Letters, 36, n/a-n/a, 10.1029/2008gl036465, 2009.
- 672 Freitas, E. D., Rozoff, C. M., Cotton, W. R., and Dias, P. L. S.: Interactions of an urban heat island  
673 and sea-breeze circulations during winter over the metropolitan area of Sao Paulo, Brazil,  
674 Boundary-Layer Meteorology, 122, 43-65, 2007.
- 675 Friedl, M. A., Sulla-Menashe, D., Tan, B., Schneider, A., Ramankutty, N., Sibley, A., and Huang,  
676 X.: MODIS Collection 5 global land cover: Algorithm refinements and characterization of new  
677 datasets, Remote Sensing of Environment, 114, 168-182, 10.1016/j.rse.2009.08.016, 2010.
- 678 Gao, D., Xie, M., Chen, X., Wang, T. J., Liu, J., Xu, Q., Mu, X. Y., Chen, F., Li, S., Zhuang, B. L.,  
679 Li, M. M., Zhao, M., and Ren, J. Y.: Systematic classification of circulation patterns and  
680 integrated analysis of their effects on different ozone pollution levels in the Yangtze River Delta  
681 Region, China, Atmospheric Environment, 242, 2020.
- 682 Gong, P., Liu, H., Zhang, M., Li, C., Wang, J., Huang, H., Clinton, N., Ji, L., Li, W., Bai, Y., Chen,  
683 B., Xu, B., Zhu, Z., Yuan, C., Ping Suen, H., Guo, J., Xu, N., Li, W., Zhao, Y., Yang, J., Yu, C.,  
684 Wang, X., Fu, H., Yu, L., Dronova, I., Hui, F., Cheng, X., Shi, X., Xiao, F., Liu, Q., and Song,  
685 L.: Stable classification with limited sample: transferring a 30-m resolution sample set  
686 collected in 2015 to mapping 10-m resolution global land cover in 2017, Science Bulletin, 64,  
687 370-373, 10.1016/j.scib.2019.03.002, 2019.
- 688 Grell, G. A., and Dévényi, D.: A generalized approach to parameterizing convection combining  
689 ensemble and data assimilation techniques, Geophysical Research Letters, 29, 38-31-38-34,  
690 10.1029/2002gl015311, 2002.
- 691 Grell, G. A., Peckham, S. E., Schmitz, R., McKeen, S. A., Frost, G., Skamarock, W. C., and Eder,  
692 B.: Fully coupled “online” chemistry within the WRF model, Atmospheric Environment, 39,  
693 6957-6975, 10.1016/j.atmosenv.2005.04.027, 2005.
- 694 Guenther, A., Karl, T., Harley, P., Wiedinmyer, C., Palmer, P. I., and Geron, C.: Estimates of global  
695 terrestrial isoprene emissions using MEGAN (Model of Emissions of Gases and Aerosols from  
696 Nature), Atmospheric Chemistry and Physics, 6, 3181-3210, 2006.



- 697 Hong, S. Y., Noh, Y., and Dudhia, J.: A new vertical diffusion package with an explicit treatment of  
698 entrainment processes, *Monthly Weather Review*, 134, 2318-2341, 2006.
- 699 Hu, J., Li, Y., Zhao, T., Liu, J., Hu, X.-M., Liu, D., Jiang, Y., Xu, J., and Chang, L.: An important  
700 mechanism of regional O<sub>3</sub> transport for summer smog over the  
701 Yangtze River Delta in eastern China, *Atmospheric Chemistry and Physics*, 18, 16239-16251,  
702 10.5194/acp-18-16239-2018, 2018.
- 703 Jacob, D. J., and Winner, D. A.: Effect of climate change on air quality, *Atmospheric Environment*,  
704 43, 51-63, 10.1016/j.atmosenv.2008.09.051, 2009.
- 705 Jerrett, M., Burnett, R. T., Pope, C. A., Ito, K., Thurston, G., Krewski, D., Shi, Y. L., Calle, E., and  
706 Thun, M.: Long-Term Ozone Exposure and Mortality., *New Engl J Med*, 360, 1085-1095, 2009.
- 707 Jimenez, P. A., and Dudhia, J.: Improving the Representation of Resolved and Unresolved  
708 Topographic Effects on Surface Wind in the WRF Model, *Journal of Applied Meteorology and  
709 Climatology*, 51, 300-316, 2012.
- 710 Kim, H.-J., and Wang, B.: Sensitivity of the WRF model simulation of the East Asian summer  
711 monsoon in 1993 to shortwave radiation schemes and ozone absorption, *Asia-Pacific Journal  
712 of Atmospheric Sciences*, 47, 167-180, 10.1007/s13143-011-0006-y, 2011.
- 713 Lennartson, G. J., and Schwartz, M. D.: The lake breeze-ground-level ozone connection in eastern  
714 Wisconsin: A climatological perspective, *International Journal of Climatology*, 22, 1347-1364,  
715 2002.
- 716 Li, M., Song, Y., Huang, X., Li, J., Mao, Y., Zhu, T., Cai, X., and Liu, B.: Improving mesoscale  
717 modeling using satellite-derived land surface parameters in the Pearl River Delta region, China,  
718 *Journal of Geophysical Research: Atmospheres*, 119, 6325-6346, 10.1002/2014jd021871,  
719 2014.
- 720 Li, Y., Zhang, J., Sailor, D. J., and Ban-Weiss, G. A.: Effects of urbanization on regional meteorology  
721 and air quality in Southern California, *Atmospheric Chemistry and Physics*, 19, 4439-4457,  
722 10.5194/acp-19-4439-2019, 2019.
- 723 Li, K., Jacob, D. J., Shen, L., Lu, X., De Smedt, I., and Liao, H.: Increases in surface ozone pollution  
724 in China from 2013 to 2019: anthropogenic and meteorological influences, *Atmospheric  
725 Chemistry and Physics*, 20, 11423-11433, 10.5194/acp-20-11423-2020, 2020.
- 726 Liao, Z., Gao, M., Sun, J., and Fan, S.: The impact of synoptic circulation on air quality and



- 727 pollution-related human health in the Yangtze River Delta region, *Sci Total Environ*, 607-608,  
728 838-846, 10.1016/j.scitotenv.2017.07.031, 2017.
- 729 Lin, C. H., Lai, C. H., Wu, Y. L., Lin, P. H., and Lai, H. C.: Impact of sea breeze air masses laden  
730 with ozone on inland surface ozone concentrations: A case study of the northern coast of  
731 Taiwan, *J Geophys Res-Atmos*, 112, 2007.
- 732 Liu, M., and Tian, H.: China's land cover and land use change from 1700 to 2005: Estimations from  
733 high-resolution satellite data and historical archives, *Global Biogeochemical Cycles*, 24, n/a-  
734 n/a, 10.1029/2009gb003687, 2010.
- 735 Loveland, T. R., Reed, B. C., Brown, J. F., Ohlen, D. O., Zhu, Z., Yang, L., and Merchant, J. W.:  
736 Development of a global land cover characteristics database and IGBP DISCover from 1 km  
737 AVHRR data, *International Journal of Remote Sensing*, 21, 1303-1330,  
738 10.1080/014311600210191, 2000.
- 739 Lu, X., Hong, J., Zhang, L., Cooper, O. R., Schultz, M. G., Xu, X., Wang, T., Gao, M., Zhao, Y., and  
740 Zhang, Y.: Severe Surface Ozone Pollution in China: A Global Perspective, *Environmental*  
741 *Science & Technology Letters*, 5, 487-494, 10.1021/acs.estlett.8b00366, 2018.
- 742 Mavrakou, T., Philippopoulos, K., and Deligiorgi, D.: The impact of sea breeze under different  
743 synoptic patterns on air pollution within Athens basin, *Science of the Total Environment*, 433,  
744 31-43, 2012.
- 745 Menberg, K., Bayer, P., Zosseder, K., Rumohr, S., and Blum, P.: Subsurface urban heat islands in  
746 German cities, *Sci Total Environ*, 442, 123-133, 10.1016/j.scitotenv.2012.10.043, 2013.
- 747 Miao, Y., Hu, X.-M., Liu, S., Qian, T., Xue, M., Zheng, Y., and Wang, S.: Seasonal variation of local  
748 atmospheric circulations and boundary layer structure in the Beijing-Tianjin-Hebei region and  
749 implications for air quality, *Journal of Advances in Modeling Earth Systems*, 7, 1602-1626,  
750 10.1002/2015ms000522, 2015.
- 751 Mlawer, E. J., Taubman, S. J., Brown, P. D., Iacono, M. J., and Clough, S. A.: Radiative transfer for  
752 inhomogeneous atmospheres: RRTM, a validated correlated-k model for the longwave, *Journal*  
753 *of Geophysical Research: Atmospheres*, 102, 16663-16682, 10.1029/97jd00237, 1997.
- 754 Oke, T. R.; Mills, G.; Christen, A.; Voegt, J. A. *Urban Climates*; Cambridge University Press:  
755 Cambridge, 2017.
- 756 Ryu, Y. H., Baik, J. J., Kwak, K. H., Kim, S., and Moon, N.: Impacts of urban land-surface forcing



- 757 on ozone air quality in the Seoul metropolitan area, *Atmospheric Chemistry and Physics*, 13,  
758 2177-2194, 10.5194/acp-13-2177-2013, 2013b.
- 759 Ryu, Y.-H., Baik, J.-J., and Lee, S.-H.: Effects of anthropogenic heat on ozone air quality in a  
760 megacity, *Atmospheric Environment*, 80, 20-30, 10.1016/j.atmosenv.2013.07.053, 2013a.
- 761 Sailor, D. J.: A review of methods for estimating anthropogenic heat and moisture emissions in the  
762 urban environment, *International Journal of Climatology*, 31, 189-199, 10.1002/joc.2106, 2011.
- 763 Sati, A. P., and Mohan, M.: The impact of urbanization during half a century on surface meteorology  
764 based on WRF model simulations over National Capital Region, India, *Theoretical and Applied  
765 Climatology*, 134, 309-323, 2017.
- 766 Schell, B., Ackermann, I. J., Hass, H., Binkowski, F. S., and Ebel, A.: Modeling the formation of  
767 secondary organic aerosol within a comprehensive air quality model system, *J Geophys Res-  
768 Atmos*, 106, 28275-28293, 2001.
- 769 Shao, M., Tang, X. Y., Zhang, Y. H., and Li, W. J.: City clusters in China: air and surface water  
770 pollution, *Front Ecol Environ*, 4, 353-361, 2006.
- 771 Sills, D. M. L., Brook, J. R., Levy, I., Makar, P. A., Zhang, J., and Taylor, P. A.: Lake breezes in the  
772 southern Great Lakes region and their influence during BAQS-Met 2007, *Atmospheric  
773 Chemistry and Physics*, 11, 7955-7973, 10.5194/acp-11-7955-2011, 2011.
- 774 Stockwell, W. R., Middleton, P., Chang, J. S., and Tang, X. Y.: The 2nd Generation Regional Acid  
775 Deposition Model Chemical Mechanism for Regional Air-Quality Modeling, *J Geophys Res-  
776 Atmos*, 95, 16343-16367, 1990.
- 777 Van Dingenen, R., Dentener, F. J., Raes, F., Krol, M. C., Emberson, L., and Cofala, J.: The global  
778 impact of ozone on agricultural crop yields under current and future air quality legislation,  
779 *Atmospheric Environment*, 43, 604-618, 10.1016/j.atmosenv.2008.10.033, 2009.
- 780 Wang, T., Xue, L., Brimblecombe, P., Lam, Y. F., Li, L., and Zhang, L.: Ozone pollution in China:  
781 A review of concentrations, meteorological influences, chemical precursors, and effects, *Sci  
782 Total Environ*, 575, 1582-1596, 10.1016/j.scitotenv.2016.10.081, 2017.
- 783 Wang, Y., Gao, W., Wang, S., Song, T., Gong, Z., Ji, D., Wang, L., Liu, Z., Tang, G., Huo, Y., Tian,  
784 S., Li, J., Li, M., Yang, Y., Chu, B., Petäjä, T., Kerminen, V.-M., He, H., Hao, J., Kulmala, M.,  
785 Wang, Y., and Zhang, Y.: Contrasting trends of PM<sub>2.5</sub> and surface-ozone concentrations in  
786 China from 2013 to 2017, *National Science Review*, 7, 1331-1339, 10.1093/nsr/nwaa032, 2020.



- 787 Wentworth, G. R., Murphy, J. G., and Sills, D. M. L.: Impact of lake breezes on ozone and nitrogen  
788 oxides in the Greater Toronto Area, *Atmospheric Environment*, 109, 52-60,  
789 10.1016/j.atmosenv.2015.03.002, 2015.
- 790 Worden, H. M., Bowman, K. W., Worden, J. R., Eldering, A., and Beer, R.: Satellite measurements  
791 of the clear-sky greenhouse effect from tropospheric ozone, *Nature Geoscience*, 1, 305-308,  
792 2008.
- 793 Xie, M., Zhu, K., Wang, T., Yang, H., Zhuang, B., Li, S., Li, M., Zhu, X., and Ouyang, Y.:  
794 Application of photochemical indicators to evaluate ozone nonlinear chemistry and pollution  
795 control countermeasure in China, *Atmospheric Environment*, 99, 466-473,  
796 10.1016/j.atmosenv.2014.10.013, 2014.
- 797 Xie, M., Liao, J., Wang, T., Zhu, K., Zhuang, B., Han, Y., Li, M., and Li, S.: Modeling of the  
798 anthropogenic heat flux and its effect on regional meteorology and air quality over the Yangtze  
799 River Delta region, China, *Atmospheric Chemistry and Physics*, 16, 6071-6089, 10.5194/acp-  
800 16-6071-2016, 2016a.
- 801 Xie, M., Zhu, K., Wang, T., Feng, W., Gao, D., Li, M., Li, S., Zhuang, B., Han, Y., Chen, P., and  
802 Liao, J.: Changes in regional meteorology induced by anthropogenic heat and their impacts on  
803 air quality in South China, *Atmospheric Chemistry and Physics*, 16, 15011-15031,  
804 10.5194/acp-16-15011-2016, 2016b.
- 805 Xie, M., Shu, L., Wang, T.-j., Liu, Q., Gao, D., Li, S., Zhuang, B.-l., Han, Y., Li, M.-m., and Chen,  
806 P.-l.: Natural emissions under future climate condition and their effects on surface ozone in the  
807 Yangtze River Delta region, China, *Atmospheric Environment*, 150, 162-180,  
808 10.1016/j.atmosenv.2016.11.053, 2017.
- 809 You, C., Fung, J. C. H., and Tse, W. P.: Response of the Sea Breeze to Urbanization in the Pearl  
810 River Delta Region, *Journal of Applied Meteorology and Climatology*, 58, 1449-1463, 2019.
- 811 Young, P. J., Archibald, A. T., Bowman, K. W., Lamarque, J. F., Naik, V., Stevenson, D. S., Tilmes,  
812 S., Voulgarakis, A., Wild, O., Bergmann, D., Cameron-Smith, P., Cionni, I., Collins, W. J.,  
813 Dalsøren, S. B., Doherty, R. M., Eyring, V., Faluvegi, G., Horowitz, L. W., Josse, B., Lee, Y.  
814 H., MacKenzie, I. A., Nagashima, T., Plummer, D. A., Righi, M., Rumbold, S. T., Skeie, R. B.,  
815 Shindell, D. T., Strode, S. A., Sudo, K., Szopa, S., and Zeng, G.: Pre-industrial to end 21st  
816 century projections of tropospheric ozone from the Atmospheric Chemistry and Climate Model



817 Intercomparison Project (ACCMIP), *Atmospheric Chemistry and Physics*, 13, 2063-2090,  
818 10.5194/acp-13-2063-2013, 2013.

819 Yu, M., Carmichael, G. R., Zhu, T., and Cheng, Y.: Sensitivity of predicted pollutant levels to  
820 urbanization in China, *Atmospheric Environment*, 60, 544-554,  
821 10.1016/j.atmosenv.2012.06.075, 2012.

822 Zhan, C.-c., Xie, M., Fang, D.-x., Wang, T.-j., Wu, Z., Lu, H., Li, M.-m., Chen, P.-l., Zhuang, B.-l.,  
823 Li, S., Zhang, Z.-q., Gao, D., Ren, J.-y., and Zhao, M.: Synoptic weather patterns and their  
824 impacts on regional particle pollution in the city cluster of the Sichuan Basin, China,  
825 *Atmospheric Environment*, 208, 34-47, 10.1016/j.atmosenv.2019.03.033, 2019.

826 Zhan, C., Xie, M., Huang, C., Liu, J., Wang, T., Xu, M., Ma, C., Yu, J., Jiao, Y., Li, M., Li, S.,  
827 Zhuang, B., Zhao, M., and Nie, D.: Ozone affected by a succession of four landfall typhoons  
828 in the Yangtze River Delta, China: major processes and health impacts, *Atmospheric Chemistry  
829 and Physics*, 20, 13781-13799, 10.5194/acp-20-13781-2020, 2020.

830 Zhan, C., Xie, M., Liu, J., Wang, T., Xu, M., Chen, B., Li, S., Zhuang, B., and Li, M.: Surface Ozone  
831 in the Yangtze River Delta, China: A Synthesis of Basic Features, Meteorological Driving  
832 Factors, and Health Impacts, *Journal of Geophysical Research: Atmospheres*, 126,  
833 10.1029/2020jd033600, 2021.

834 Zhang, N., Zhu, L., and Zhu, Y.: Urban heat island and boundary layer structures under hot weather  
835 synoptic conditions: A case study of Suzhou City, China, *Advances in Atmospheric Sciences*,  
836 28, 855-865, 10.1007/s00376-010-0040-1, 2011.

837 Zhang, H., Wang, Y., Hu, J., Ying, Q., and Hu, X. M.: Relationships between meteorological  
838 parameters and criteria air pollutants in three megacities in China, *Environ Res*, 140, 242-254,  
839 10.1016/j.envres.2015.04.004, 2015.

840 Zhu, B., Kang, H., Zhu, T., Su, J., Hou, X., and Gao, J.: Impact of Shanghai urban land surface  
841 forcing on downstream city ozone chemistry, *Journal of Geophysical Research: Atmospheres*,  
842 120, 4340-4351, 10.1002/2014jd022859, 2015.

843