



Divergent impacts of summertime extreme heat on O₃ and PM_{2.5} levels in the Beijing-Tianjin-Hebei and Yangtze River Delta regions: Driving chemical and physical processes

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ABSTRACT

As global warming increases the frequency of summertime extreme heat events in China, understanding their impact on secondary pollutants is essential for air quality management. This study investigates the influence of extreme heat (defined as a daily maximum temperature exceeding 35 °C) on surface ozone (O₃) and fine particulate matter (PM_{2.5}) in the Beijing-Tianjin-Hebei (BTH) and Yangtze River Delta (YRD) regions. We analyze observational data from 2013 to 2022 and perform GEOS-Chem model simulations for 2013–2020. During extreme heat, enhanced chemical production at 850–950 hPa strongly promotes O₃ formation. For each 1 °C rise in the daily maximum temperature, the maximum daily 8-h average (MDA8) O₃ concentration increases by 11.79 µg m⁻³ in BTH and by 5.08 µg m⁻³ in YRD. In contrast, the PM_{2.5} response to extreme heat diverges notably between the regions. In BTH, observed PM_{2.5} decreases by 2.48 µg m⁻³ °C⁻¹ under the typical dry extreme heat (mean RH = 50.13%), which favors the thermal dissociation of ammonium and nitrate. Conversely, in YRD, PM_{2.5} increases by 0.98 µg m⁻³ °C⁻¹. Influenced by the Western Pacific Subtropical High, the YRD experiences higher humidity (mean RH = 69.71%) under extreme heat, facilitating secondary inorganic aerosol formation. Analysis reveals relative humidity thresholds of approximately 58% in BTH and 60% in YRD, above which the negative chemical contributions to nitrate and ammonium decline linearly and eventually turn positive. These findings clarify the chemical mechanisms driving air pollutant behavior during extreme heat and highlight important implications for the health risks posed by compounded heat and pollution events.

1. Introduction

Under the background of global warming, the surface air temperature in China has been increasing, with large increases in the observed frequency of extreme heat events in summer (Zhang et al., 2024). For example, in June–August 2022, new records were established for daily maximum temperatures (Tmax) > 42 °C in urban areas along the Yangtze River, and the widespread heatwaves (Tmax > 35 °C) lasted for over 40 days in the regions of Yangtze River Delta, Sichuan-Chongqing, and Wuhan (Yuan et al., 2023). The occurrence of extreme heat can have significant impacts on the formation of secondary pollutants in the atmosphere. Recent studies indicated that the increases in frequency and intensity of heatwaves in China have significantly exacerbated urban ozone pollution (Li et al., 2024; Qin et al., 2025). Even under strict

emission controls, the co-occurrence of extreme heat, ozone, and PM_{2.5} events was projected to intensify in the future (Gao et al., 2024).

Monthly or seasonally mean surface O₃ concentrations in polluted regions usually increase with temperature (Szopa et al., 2021). However, O₃ concentrations during extreme heat events have complex relationship with temperature; O₃ levels can increase with temperature, remain stable as temperature increases, or even decrease with temperature. Steiner et al. (2010) analyzed relationship between O₃ levels and temperature by using observations from 1980 to 2005 in four air basins of California, United States. They found that the daily 1-h maximum O₃ concentrations ([O₃]_{max}) increased approximately linearly with temperature with a slope of 2–8 ppb K⁻¹ as temperatures were in the range of 295–312 K. However, as temperatures exceeded 312 K, [O₃]_{max} levels exhibited stability or a slight decrease in some air basins. Their

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simulations with a photochemical box model showed that the stability was predominantly caused by peroxyacetyl nitrate (PAN) chemistry. The formation of PAN serves as sinks for both NO_x and HO_x at low temperatures, while the thermal decomposition of PAN becomes rapid as temperature increases, causing increases in O_3 concentrations at warmer temperatures. However, at extreme heat (for example, above 312 K), the lifetime of PAN decreases with a greater e-folding rate, which leads to a reduced effect of PAN on O_3 chemistry and hence a plateau in O_3 concentration (Jacob et al., 1993; Cardelino and Chameides, 1995). Steiner et al. (2010) also reported that the observed isoprene levels increase with temperatures within the 290–312 K range, followed by a decline with further temperature increases, a pattern of temperature dependence comparable to observed O_3 . Shen et al. (2016) examined the O_3 -temperature slopes using the observed daily maximum 8 h average O_3 (MDA8 O_3) and daily maximum temperature for May–September of 2003–2012 across the United States, and found that 20% of the U.S. sites exhibited significant decreases in O_3 -temperature slopes at very high temperatures (above the 95th percentile). Their analysis showed that high temperatures enhance the atmosphere's capacity for transport and removal of O_3 by intensifying vertical turbulent mixing and horizontal advection (Pu et al., 2017). Ma et al. (2019) reported that a linear correlation of $4.21 \text{ ppbv } ^\circ\text{C}^{-1}$ was observed between summer MDA8 O_3 and daily maximum temperature in summer of 2017 in the North China Plain (NCP). They suggested that under heat wave conditions, biogenic emissions may be further enhanced through the effect of vapor pressure deficit (VPD). Li et al. (2025) examined the characteristics of O_3 changes under high temperature conditions in eastern China for 2016–2020 by using observations. Their results show that, while O_3 concentrations in the Beijing-Tianjin-Hebei (BTH) region generally increased with temperature, O_3 levels were mostly reduced under high-temperature conditions in the regions of Yangtze River Delta (YRD) and Pearl River Delta (PRD), with the cutoff temperature ranging between 28.0 and 34.5 $^\circ\text{C}$. Statistical analysis and machine learning model calculation revealed that relative humidity (RH) was the primary driver of the regional differences in O_3 -temperature relationship. High humidity in central and southern China enhances O_3 uptake by plant leaves (Kavassalis and Murphy, 2017). Therefore, the variations of O_3 under extreme high temperatures exhibit diverse patterns across different regions, contingent upon environmental disparities.

Numerous studies have analyzed the linear relationship between $\text{PM}_{2.5}$ and temperature in different regions using observations. Tai et al. (2010) utilized long-term observations (1998–2008) to calculate the linear correlation coefficients between $\text{PM}_{2.5}$ and temperature for different locations in the United States. Throughout the United States, $\text{PM}_{2.5}$ and temperature generally exhibited positive correlations. In terms of chemical components of $\text{PM}_{2.5}$, sulfate, organic carbon (OC), and elemental carbon (EC) had positive correlations with temperature, in which the positive correlation between sulfate and temperature were the highest. However, in most regions, particularly in the southern United States, nitrate showed strong negative correlations with temperature. By using observations from 14 monitoring stations in Nagasaki, Japan, Wang and Ogawa (2015) also reported positive correlations between observed $\text{PM}_{2.5}$ concentrations and temperature during the summer months (June–August) of 2013. Wang et al. (2023) reported positive correlation coefficients between $\text{PM}_{2.5}$ concentrations and temperature in the three developed regions (NCP, YRD, PRD) in eastern China in summers of 2015–2019.

The mechanisms of temperature impacts on $\text{PM}_{2.5}$ components can be classified through the roles of biogenic volatile organic compounds (BVOCs) emissions, gas-aerosol partitioning, gas-phase reaction rates, and atmospheric dynamics. As temperature rises, the emission of BVOCs increases. On one hand, this leads to an increase in biogenic secondary organic aerosol (SOA) concentration, with biogenic SOA concentration accounting for nearly 90% of the increase in organic aerosol (OA) (Megaritis et al., 2014). On the other hand, the increase in BVOCs results in a reduction hydroxyl radicals (OH) in some regions (Zhang et al.,

2008), which slows down the gas-phase formation of sulfate (through SO_2 oxidation) and also leads to a decrease in ammonium nitrate (Tagaris et al., 2014). From the aspect of gas-aerosol partitioning, the increase in temperature shifts the partitioning of volatile and semi-volatile compounds between gas and condensed phases (Seinfeld and Pandis, 2006). This primarily enhances ammonium nitrate volatilization, reducing nitrate and ammonium concentrations. Conversely, as the nitrate levels decrease, cloud pH increases, accelerating the formation of aqueous-phase sulfate (Dawson et al., 2007). Additionally, at higher temperatures, gas-phase reactions accelerate (Jacob and Winner, 2009; Day and Pandis, 2011; Im et al., 2011). This mainly results in an increase in nitrate levels, followed by OA (mainly attributed to secondary OA) and sulfate increases (Megaritis et al., 2014). In addition to influencing chemical reaction rates, temperature fluctuations also affect the transport and dispersion of pollutants. Tai et al. (2012) carried out a temperature sensitivity experiment on sulfate and nitrate in the United States using the GEOS-Chem model. Their analysis revealed that most of the correlations of $\text{PM}_{2.5}$ with temperature do not arise from direct dependence on temperature but from covariation with synoptic transport. The occurrence of extreme heat days is often associated with an anomalous high-pressure system featuring strong descending airflows (Tai et al., 2010; Sun et al., 2023). Characterized by reduced precipitation, lower wind speeds, and diminished cloud cover, such weather pattern increases solar radiation reaching the ground, creating favorable conditions for pollutant formation and accumulation (Zhu et al., 2020). Rising temperatures can directly or indirectly influence the concentrations and chemical composition of $\text{PM}_{2.5}$. However, studies on the changes of $\text{PM}_{2.5}$ components during summer, particularly under extreme heat, remain insufficient. In China, due to significantly higher $\text{PM}_{2.5}$ concentrations in winter compared to summer, the variations of $\text{PM}_{2.5}$ in summer have often been overlooked.

Previous studies on O_3 or $\text{PM}_{2.5}$ under extreme high temperatures were mostly single-site or case-based, limiting the general and systematic understanding of their changes under extreme heat. This study used long-term, multi-station observations to systematically examine the effects of daily maximum temperature on O_3 and $\text{PM}_{2.5}$ in polluted regions of BTH and YRD, which are representative of dry-heat and humid-heat meteorological conditions, respectively. We analyzed firstly the variations of O_3 , $\text{PM}_{2.5}$ and secondary inorganic particulate matter (sulfate, nitrate, ammonium) with different daily maximum temperatures in BTH and YRD in China based on observations in summers of 2013–2022, with special attention to the changes in concentrations under extreme heat conditions. We then carried out process analyses to understand the key chemical and physical processes for O_3 and secondary $\text{PM}_{2.5}$ components during extreme heat days by using the global chemical transport model GEOS-Chem. The specific content regarding observational data, GEOS-Chem model, process analysis and sample selection methods is presented in Section 2. Section 3 consists of the results of this study. Section 3.1 shows the observed variations of O_3 , $\text{PM}_{2.5}$ and secondary inorganic particulate matter (sulfate, nitrate, ammonium) with different daily maximum temperatures. Section 3.2 presents the model simulation results. Section 3.3 identifies the key chemical and physical processes for O_3 and secondary $\text{PM}_{2.5}$ components during extreme heat. The meteorological fields under extreme heat and their roles in the formation of secondary air pollutants are presented in Section 3.4. The conclusions are summarized in Section 4.

2. Data and methods

2.1. Observations

The datasets of daily maximum temperatures were obtained from the website of tianqihoubao (<http://www.tianqihoubao.com>), which archives meteorological observations from official China Meteorological Administration (CMA) weather stations. We collected daily maximum temperature data for each city included in this study to ensure

consistency with the spatial scale of city-level air pollutant observations. Quality control procedures were applied to remove missing values and abnormal records and to ensure temporal continuity.

The hourly observations of PM_{2.5} and O₃ for summers of 2013–2022 were taken from the website of the Chinese Ministry of Ecology and Environment (MEE) (<https://www.mee.gov.cn>). Prior to September 2018, MEE reported O₃ and PM_{2.5} concentrations in $\mu\text{g m}^{-3}$ under the standard conditions of 273 K and 1013 hPa. From September 2018 onward, observed values adopted the reference state of 298 K and 1013 hPa. To ensure consistency in long-term trend analysis, we converted the post-August 2018 O₃ and PM_{2.5} data to the former standard state. To guarantee the quality of data, the daily averaged PM_{2.5} concentration was computed only when valid data were available for over 20 h on that day. Similarly, the MDA8 O₃ concentration was calculated under the condition of having valid data for a minimum of 6 h within every 8-h period. In the BTH and YRD regions, the observed concentrations of O₃ and PM_{2.5} cover the summers (June to August) of 2013–2022. The BTH region includes 13 cities, while the YRD comprises 36 cities. These two regions are indicated by black rectangles in the first panel of Fig. 1.

We also analyzed the daily observations of the secondary inorganic components (sulfate, nitrate, ammonium) of PM_{2.5} in Beijing and Nanjing. The observation stations were located, respectively, at Peking University in Beijing (Tan et al., 2018; Zhang et al., 2022) and on the rooftop of Nanjing Environmental Protection Building in Nanjing (118.75°E, 32.06°N) (Yu et al., 2020; Xie et al., 2022). The observed concentrations of secondary inorganic aerosols in Beijing were available for June–August of 2013–2016, 2018, and 2019, while those in Nanjing were available for June–August of 2017–2022.

2.2. ERA5 reanalysis data

This study also utilized hourly wind speed, wind direction, sea level pressure, and geopotential height data from ERA5 reanalysis data with a resolution of 0.25° latitude by 0.25° longitude. ERA5 is the fifth-generation global high-resolution atmospheric reanalysis dataset developed and maintained by the European Centre for Medium-Range Weather Forecasts (ECMWF). It offers a continuous, consistent, and high-quality datasets of various meteorological variables.

2.3. Extreme heat days

The World Meteorological Organization's definition of extreme weather events, as released in 2016, does not provide specific numerical standards for extreme heat. Instead, it defines it as an abnormal condition where temperatures surpass the normal range for a particular region. In this study, extreme heat days are defined as days with daily maximum temperature exceeding 35 °C (Pu et al., 2017; Sun et al., 2018; Coppola et al., 2021).

2.4. GEOS-chem model

For simulations of O₃ and PM_{2.5}, we utilized the 3-D Goddard Earth Observing System chemical transport model (GEOS-Chem) which includes fully coupled HO_x-NO_x-VOC-O₃-aerosol chemistry with more than 80 species and 300 reactions and online calculations of aerosols including sulfate (Park et al., 2004), nitrate (Pye et al., 2009), ammonium, BC and organic carbon (OC) (Park et al., 2003), mineral dust

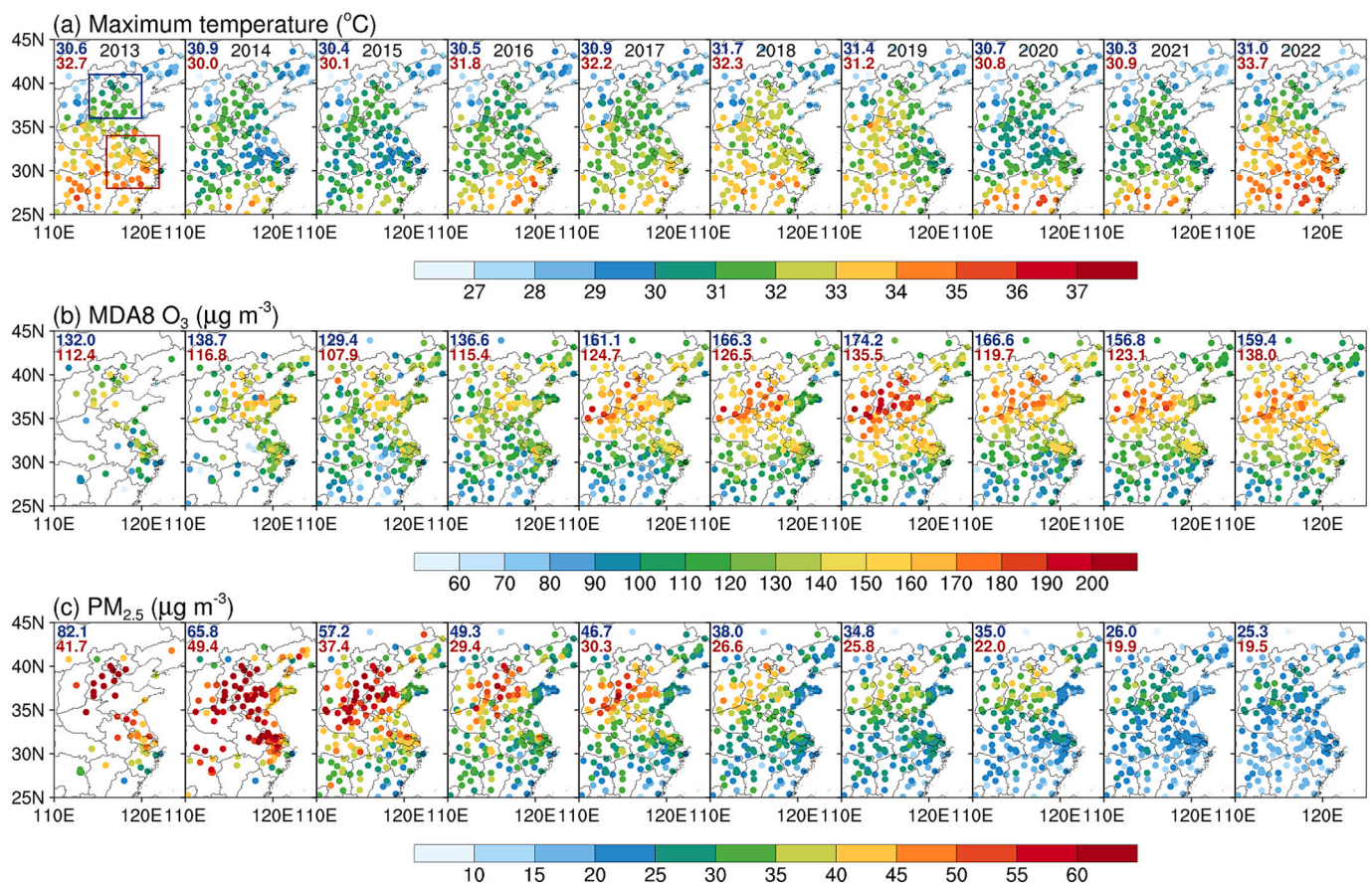


Fig. 1. The observed year-by-year variations of seasonal mean (June–August) (a) daily maximum temperature (°C), (b) MDA8 O₃ concentration ($\mu\text{g m}^{-3}$), and (c) PM_{2.5} concentration ($\mu\text{g m}^{-3}$) in eastern China from 2013 to 2022. The solid rectangles in the top left panel indicate the BTH (blue) and YRD (red) regions. The numbers displayed in each panel represent the mean values in BTH (blue) and YRD (red). (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

maximum temperatures. Since 2013, due to the implementation of Clean Air Actions, PM_{2.5} concentrations in China have decreased significantly. The seasonal mean PM_{2.5} concentrations in BTH and YRD showed downward trends of -5.8 and $-3.0 \mu\text{g m}^{-3} \text{y}^{-1}$, respectively, over 2013–2022.

Fig. 2 shows the distributions and mean values of observed MDA8 O₃ and PM_{2.5} concentrations in BTH and YRD at different daily maximum temperatures considering all observations in summers of 2013–2022. In BTH, considering all the data samples, the MDA8 O₃ concentrations gradually expanded to higher values as the daily maximum temperature increased (Fig. 2a). As averaged over all the samples at specific daily maximum temperature, the concentration of MDA8 O₃ had a positive correlation with daily maximum temperature, with a linear trend of $11.79 \mu\text{g m}^{-3} \text{°C}^{-1}$ under extreme heat conditions ($T_{\text{max}} > 35 \text{°C}$, Fig. 2c). For PM_{2.5}, its concentration distribution exhibited a conical pattern, with the highest number of samples occurring when the daily maximum temperature was 32°C (Fig. 2b). The mean concentrations of PM_{2.5} had a trend of increase as the daily maximum temperature was below 34°C . During extreme heat events ($T_{\text{max}} > 35 \text{°C}$), PM_{2.5} concentrations showed a decreasing trend of $2.48 \mu\text{g m}^{-3} \text{°C}^{-1}$ with increasing daily maximum temperature (Fig. 2c). Furthermore, city-specific trends of MDA8 O₃ and PM_{2.5} during extreme heat were calculated for both regions. In BTH, 12 of 13 cities (92.31%) exhibited trends consistent with the regional mean concentrations, with MDA8 O₃ showing increasing trends and PM_{2.5} showing decreasing trends during extreme heat events (Supplementary Materials Tables S1–2 and Fig. S1).

In YRD, the highest MDA8 O₃ concentrations remained plateau as the daily maximum temperature was higher than 31°C (Fig. 2d). As averaged over all the samples at specific daily maximum temperature, the concentration of MDA8 O₃ increased with temperature over $22\text{--}30 \text{°C}$, remained flat over $31\text{--}34 \text{°C}$, and increased sharply over $35\text{--}40 \text{°C}$, and then decreases with temperature over $40\text{--}42 \text{°C}$. Such decline has been reported to be driven by changes in NO_x-VOC chemical sensitivity that reduce net O₃ production (Lu et al., 2023) and by enhanced vertical mixing and boundary layer turbulence that dilute near-surface O₃ (Pu et al., 2017). The overall linear trend for $T_{\text{max}} > 35 \text{°C}$ remains positive,

with a slope of $5.08 \mu\text{g m}^{-3} \text{°C}^{-1}$ (Fig. 2f). Such changes in MDA8 O₃ in YRD are more complex than the changes in BTH. A high density of PM_{2.5} samples (54%) in the YRD region was concentrated in the $30\text{--}35 \text{°C}$ temperature window (Fig. 2e). As shown in Fig. 2f, PM_{2.5} peaked at 30°C , and increased with temperature during extreme heat episodes ($35 \text{°C} < T_{\text{max}} < 42 \text{°C}$), at a rate of $0.98 \mu\text{g m}^{-3} \text{°C}^{-1}$. A city-scale analysis for the YRD region indicated that, during extreme heat events, PM_{2.5} concentrations in 80.56% of the 36 cities increased, and MDA8 O₃ concentrations in 41.67% of the cities displayed a turning point around 40°C followed by a decline (a behavior consistent with the regional mean) (Supplementary Materials Tables S1–2 and Fig. S2). In summary, extreme heat not only exacerbates O₃ pollution but is also associated with elevated PM_{2.5} pollution in the YRD.

Fig. 3 presents the averages of observed concentrations of MDA8 O₃, PM_{2.5}, sulfate, nitrate, and ammonium concentrations at different daily maximum temperatures in Beijing (considering all observations in summers of 2013–2016, 2018, 2019) and Nanjing (considering all observations in summers of 2017–2022). In Beijing, the mean MDA8 O₃ concentration increased linearly with daily maximum temperature (Fig. 3a), with a linear trend of $10.38 \mu\text{g m}^{-3} \text{°C}^{-1}$. Unlike the distinct unimodal pattern shown in Fig. 2c, PM_{2.5} concentrations in Beijing exhibited two peaks at temperatures of 29°C and 34°C and kept decreasing over $34\text{--}38 \text{°C}$. For sulfate, nitrate, and ammonium, their variations below 35°C were consistent with those of PM_{2.5}, indicating their significant roles in driving PM_{2.5} concentration variations on non-extreme heat days. When the daily maximum temperature exceeded 30°C , nitrate concentrations exhibited a decreasing trend while sulfate and nitrate remained relatively stable.

In Nanjing, MDA8 O₃ concentrations showed an increase over $25\text{--}30 \text{°C}$, a subsequent stagnation over $31\text{--}34 \text{°C}$, and a resurgence under extreme heat conditions. These characteristics of fluctuating changes corresponded well to the regional variations shown in Fig. 2f, except for that MDA8 O₃ concentrations in Nanjing did not show a turning point at about 40°C . PM_{2.5} exhibited only modest variability with daily maximum temperature and persisted at high levels during extreme heat events (Fig. 3 g). PM_{2.5} concentrations in Nanjing did not

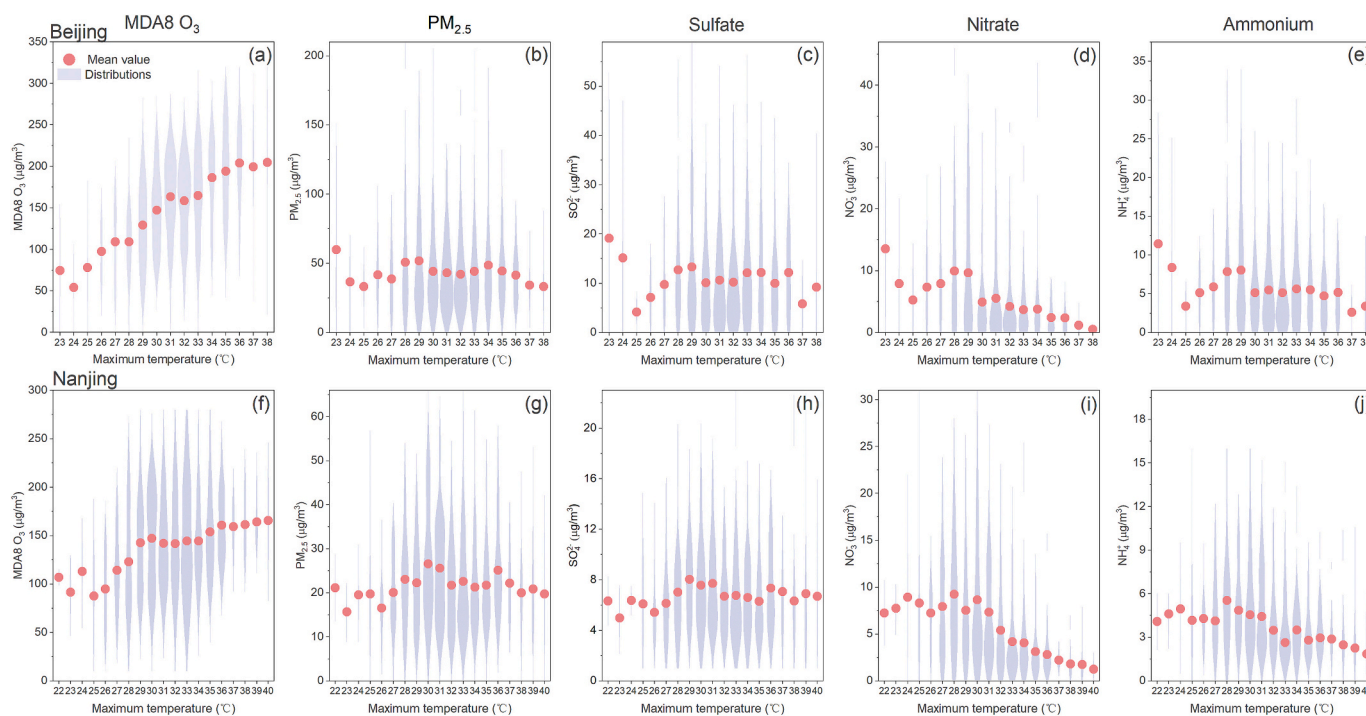


Fig. 3. (a)–(e) The averages of observed concentrations ($\mu\text{g m}^{-3}$) of MDA8 O₃, PM_{2.5}, sulfate, nitrate, and ammonium at different daily maximum temperatures in Beijing considering all observations in summers of 2013–2016, 2018, and 2019. (f)–(j) are similar to (a)–(e) but for Nanjing considering all observations in summers of 2017–2022.

increase during extreme heat, which is not consistent with the regional trend of increasing with temperature in YRD as shown in Fig. 2f. Secondary inorganic species constituted more than half of the $PM_{2.5}$ mass in Nanjing, in which sulfate was the dominant component (Supplementary Materials Fig. S3). This fraction of sulfate in $PM_{2.5}$ was further enhanced during extreme heat days because of the decreases in nitrate and ammonium concentrations (Fig. 3 h).

3.2. The simulated vs. observed variations of O_3 and secondary $PM_{2.5}$ components with daily maximum temperature

To identify the key chemical and physical processes for O_3 and secondary $PM_{2.5}$ components during extreme heat, processes analyses will be conducted using the global 3-D model of atmospheric chemistry driven by meteorological input from the Goddard Earth Observing System (GEOS-Chem). Summertime concentrations of O_3 and $PM_{2.5}$ from 2013 to 2020 were simulated and the roles of processes (chemical production, transport (including both horizontal and vertical advection), turbulent mixing, and dry deposition) were quantified. Fig. 4 shows the comparisons of the simulated and observed daily mean surface-layer MDA8 O_3 and $PM_{2.5}$ concentrations in BTH and YRD during the summers of 2013–2020. The model captures fairly well the daily variations (peaks and troughs), with high correlation coefficients of 0.62–0.78. Simulated daily concentrations of MDA8 O_3 and $PM_{2.5}$ have normalized mean biases (NMB), respectively, of 2.7% and 5.5% in BTH and 20.5% and 5.7% in YRD. The NMB of MDA8 O_3 of 20.5% in YRD may result from complex photochemical and meteorological processes under humid and hot conditions (Ye et al., 2022; Yang and Zhao, 2023). Nevertheless, our study is focused on the responses of O_3 and $PM_{2.5}$ to daily maximum temperature, which have been captured by the model as shown in Fig. 6. Therefore, we would not expect that the model biases influence the trends, process analyses, and mechanistic insights of our study.

We also carried out brief validation for secondary inorganic aerosols. In Beijing, the correlation coefficient between observed and simulated sulfate is the highest (0.62), followed by ammonium (0.56) and nitrate (0.43). In Nanjing, ammonium exhibits the highest correlation (0.60), followed by sulfate (0.58) and nitrate (0.55). We further analyzed the averages of simulated concentrations of sulfate, nitrate, and ammonium concentrations at different daily maximum temperatures in Beijing and Nanjing (Supplementary Materials Fig. S4). The simulated changes of these components across daily maximum temperature are similar to observations (Fig. 3), confirming that GEOS-Chem captures fairly well

the temperature-pollutant relationship.

As described in Section 2, samples for process analyses for each grid cell in the studied regions were selected as the days with absolute difference between MERRA-2 daily maximum temperature and observed daily maximum temperature less than 1 °C. As a result, over summers of 2013–2020, there were 2968 selected samples (31% of total) from 13 BTH cities (in which 298 (10.0%) were extreme heat days) and 8641 selected samples (33% of total) from 36 YRD cities (in which 898 (10.4%) were extreme heat days). A comparison of the observed and simulated values of MDA8 O_3 and $PM_{2.5}$ concentrations for the selected samples is presented in Fig. 5. The results indicate fairly well agreement between observations and simulations. Correlation coefficients for MDA8 O_3 are 0.53 (BTH) and 0.66 (YRD), and for $PM_{2.5}$ 0.62 (BTH) and 0.55 (YRD). To assess whether the <1 °C temperature matching criterion introduces biases in selecting samples, we compared the results of the full dataset (without any temperature matching filter) during 2013–2020 with those of the filtered subset. The two datasets yielded essentially identical trends and mechanistic conclusions (Supplementary Materials Fig. S5–7).

Figs. 6a and 6b show the variations of observed daily concentrations of MDA8 O_3 and $PM_{2.5}$ with daily maximum temperature for BTH and YRD as we consider only the above selected samples. The variations of MDA8 O_3 and $PM_{2.5}$ with temperature in Figs. 6a and 6b are quite similar to those shown in Fig. 2c and f, confirming that the selected observation samples can well represent the observed variations of pollutants' concentrations with daily maximum temperature in summers of 2013–2022. It should be noted that no samples can meet the selection criteria as maximum temperature exceeded 40 °C in both BTH and YRD.

Fig. 6c shows the variations of simulated O_3 and $PM_{2.5}$ concentrations with daily maximum temperature considering only the days of selected samples in BTH. The simulated MDA8 O_3 concentrations increased with daily maximum temperature over 23–39 °C, consistent with the observed trend (Fig. 6a), although the slope of increases was weaker from simulation than from observations. For $PM_{2.5}$, the increasing trend of both observed and simulated $PM_{2.5}$ concentrations changed around 33–34 °C, shifting to a general decline trend when daily maximum temperatures exceeded this threshold.

Fig. 6d shows the relationship between simulated O_3 and $PM_{2.5}$ concentrations and daily maximum temperature considering the selected samples in YRD. The simulated trend in MDA8 O_3 concentration with daily maximum temperature was $4.30 \mu g m^{-3} ^\circ C^{-1}$, which agreed closely with the observed trend of $5.08 \mu g m^{-3} ^\circ C^{-1}$ (Fig. 6b). For $PM_{2.5}$, the observed and simulated concentrations peaked around 30 °C,

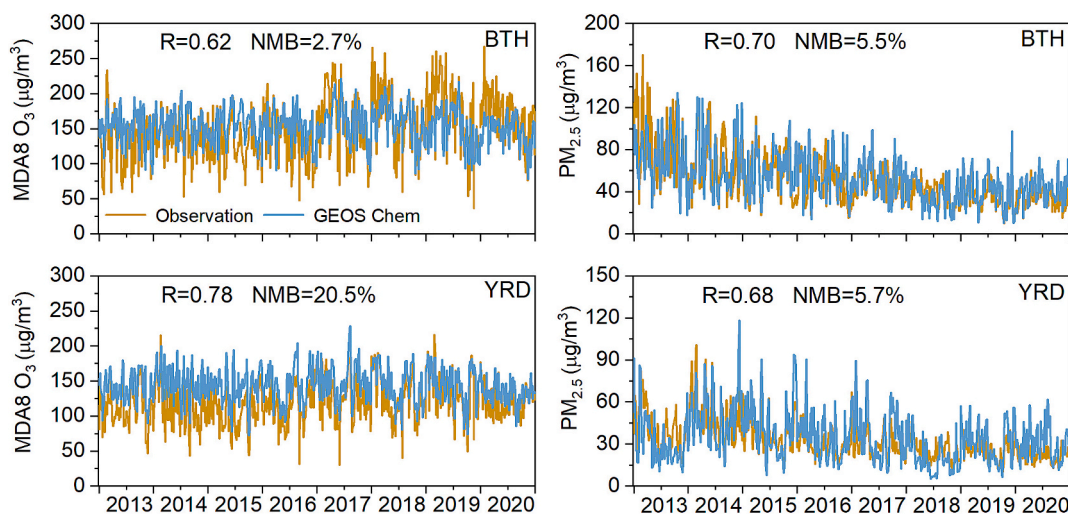


Fig. 4. Comparisons of the simulated and observed daily mean surface-layer MDA8 O_3 and $PM_{2.5}$ concentrations ($\mu g m^{-3}$) in BTH and YRD during the summers of 2013–2020. The correlation coefficient (R) and normalized mean bias (NMB) values are also shown. $NMB = (\sum_{i=1}^N (M_i - O_i) / \sum_{i=1}^N O_i) \times 100\%$, where O_i and M_i are the observed and simulated concentrations, respectively, i denotes the i^{th} day, and N is the total number of days.

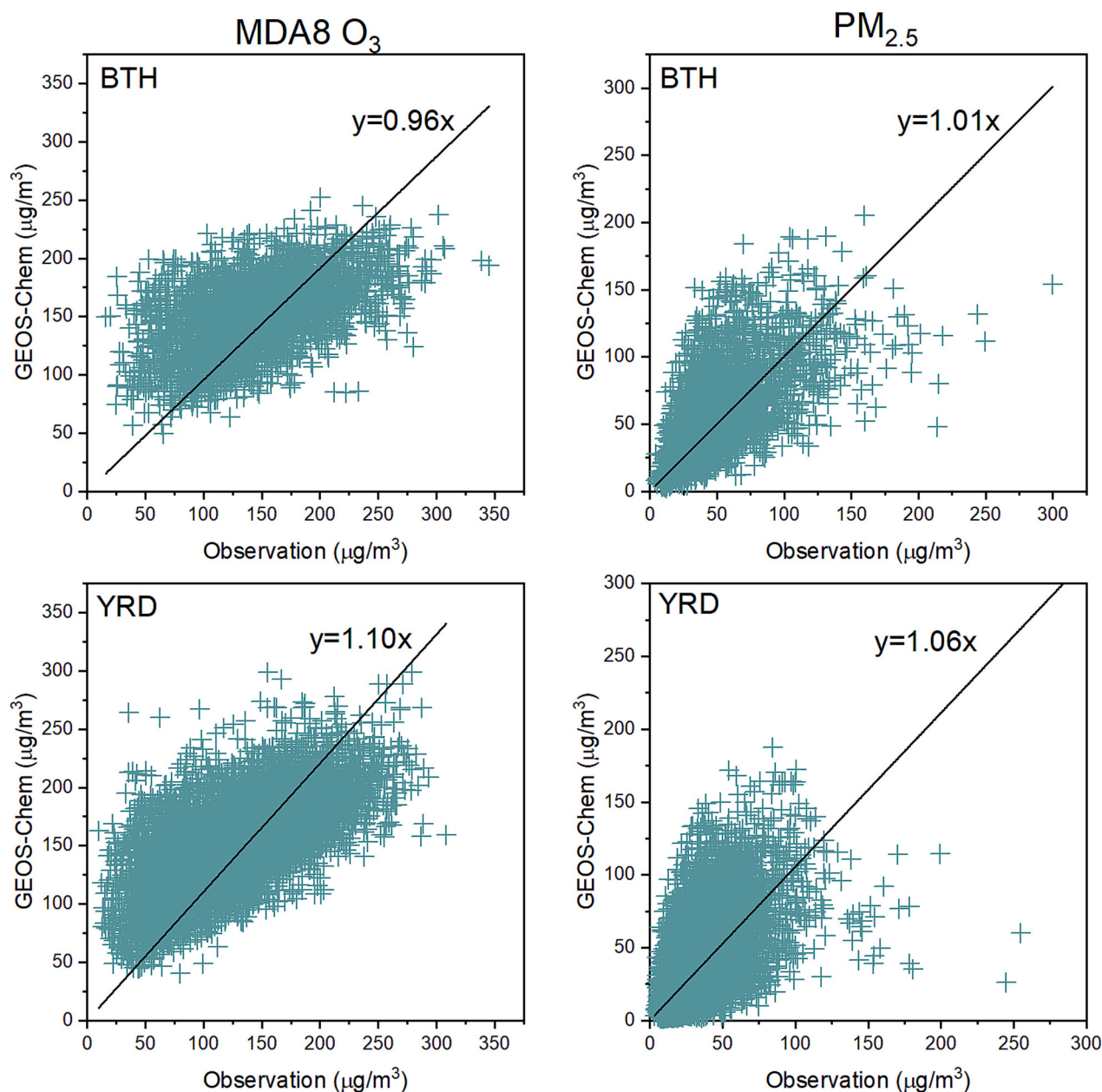


Fig. 5. The scatter plots of observed vs. simulated MDA8 O₃ and PM_{2.5} concentrations of selected samples (with absolute difference between MERRA-2 daily maximum temperature and observed daily maximum temperature less than 1 °C) in the BTH and YRD regions during summer in 2013–2020. It also provides the fitted line between observed and simulated values with the intercept forced through the origin.

decreased over 30–35 °C, and then had an increasing trend under extreme heat (> 35 °C). Such increases in PM_{2.5} under extreme heat in YRD was quite different from the decreases at highest temperatures in BTH.

3.3. Changes in chemical and physical processes with daily maximum temperature for O₃ and secondary PM_{2.5} components

3.3.1. Process analyses for BTH

Fig. 7a presents the daily net changes in mass concentrations of various pollutants at different vertical levels below 850 hPa under different daily maximum temperature in the BTH region. The selected samples over all the grid cells within BTH were grouped according to daily maximum temperature. For each temperature bin, all process contributions were summed and averaged over all samples. For O₃, chemical production above the surface layer was positive, with this

effect intensifying as temperatures increased. The maximum chemical production of O₃ was located at 850–950 hPa altitudes when daily maximum temperature was around 30–39 °C. At the surface, the titration of O₃ by high concentrations of NO_x led to a negative chemical production (Gong and Liao, 2019; Andreev et al., 2023). Transport contributed positively to O₃ mass at the surface because of the strong inflow of pollutants at the southern boundary. Above the surface layer, the contribution of transport changed from positive to negative as daily maximum temperature increased. Under extreme heat, this negative contribution became more pronounced at higher altitudes. The strong westerlies at upper levels during extreme heat (Supplementary Materials Fig. S8) over BTH facilitated the outflow of pollutants through the eastern boundary. Meanwhile, diffusion (atmospheric turbulence) exhibited a positive effect on O₃ mass at the surface, while contributing negatively above ground level. The dry deposition process, which represents the total deposition flux across the entire vertical column, was

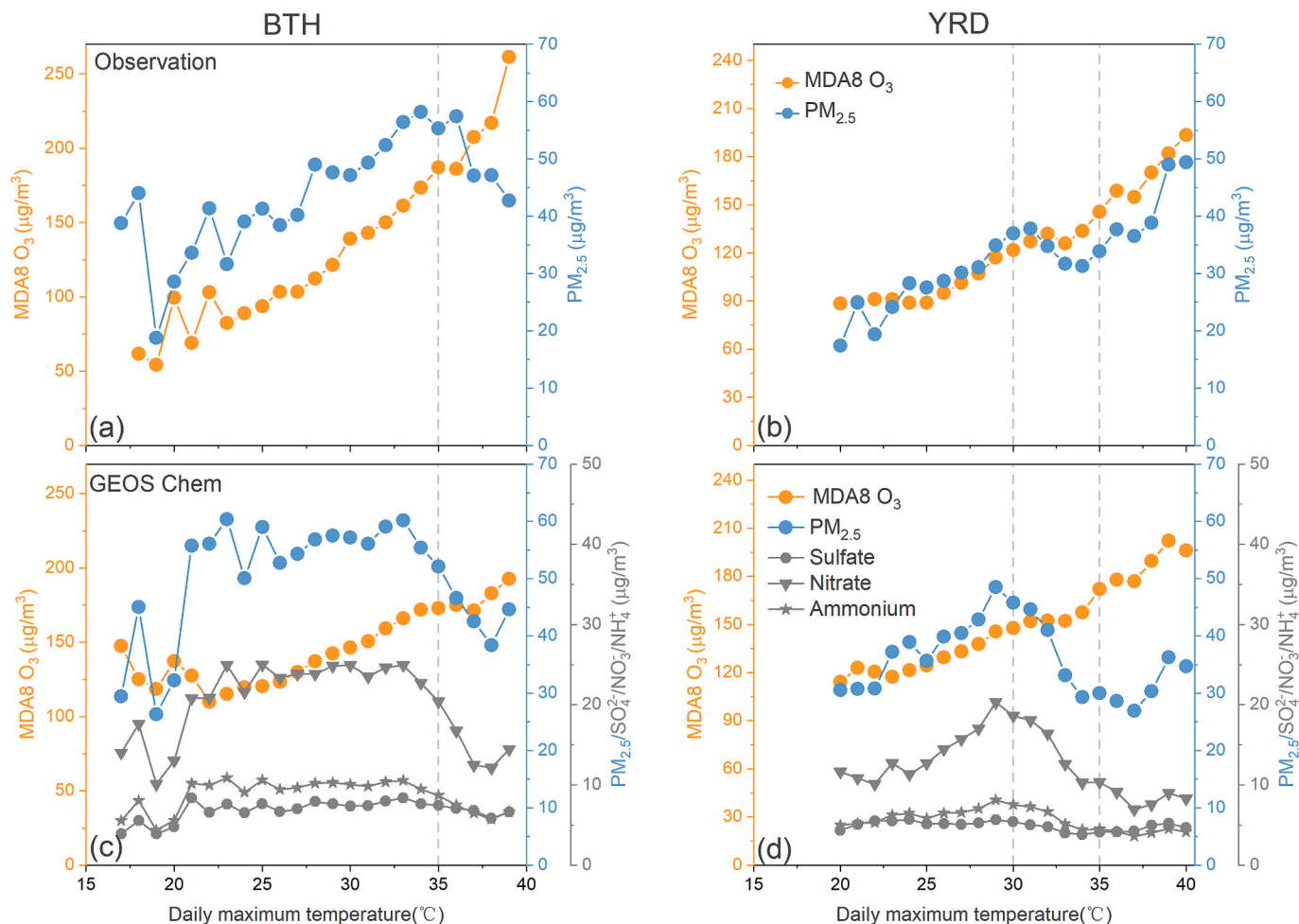


Fig. 6. (a)–(b) The mean concentrations of observed MDA8 O₃ and PM_{2.5} across different daily maximum temperatures considering only the selected samples during the summer of 2013–2020. (c)–(d) The averages of simulated concentrations of MDA8 O₃, PM_{2.5}, sulfate, nitrate, and ammonium at different daily maximum temperatures in the BTH and YRD regions considering only the selected samples during summer 2013–2020.

included in the calculation of the net mass change at the surface (1005 hPa) from all processes. Above 975 hPa, as daily maximum temperatures reached 28–37 °C, the positive chemical production effectively offset the negative contributions from atmospheric transport and turbulent processes, leading to a pronounced net positive mass change of O₃.

For sulfate, the vertical distribution of chemical production above the surface was similar to that of O₃, since SO₂ was converted to sulfate by atmospheric oxidants. The large positive contribution to sulfate mass occurred within 850–950 hPa when daily maximum temperatures reached 30–39 °C. Below 850 hPa, atmospheric transport exerted a negative influence on sulfate mass, which intensified when daily maximum temperatures exceeded 28 °C due to the higher sulfate concentrations under these conditions (Fig. 7b). Under extreme heat, diffusion provided a slight positive contribution to sulfate mass at the surface but a minor negative contribution above the ground level. Sulfate exhibited a high dry deposition, and showed an increasing trend under extreme heat (Supplementary Materials Fig. S11), which resulted in a decline in sulfate concentration at the surface. Chemical processes played a dominant role, resulting in a generally positive net change from all processes above the surface.

PM_{2.5}, nitrate, and ammonium exhibited similar patterns across different processes, and chemical production dominated the net changes. Chemical processes contributed negatively to mass change near the surface but positively above about 930 hPa. The high volatility of ammonium nitrate led to conversion of it to gaseous substances at elevated temperatures (Seinfeld and Pandis, 2006). Furthermore,

intense summer solar radiation heated the surface and generated up-drafts (Supplementary Materials Fig. S10), which transported gaseous precursors such as NO_x and NH₃ from the surface and the lower boundary layer to the higher altitudes, enhancing the chemical formation of secondary pollutants. Extreme heat amplified the negative changes near the surface and the positive changes aloft. In the lower atmosphere, diffusion contributed positively to PM_{2.5}, nitrate, and ammonium mass, and this effect intensified under extreme heat. As expected, dry deposition reduced the mass of PM_{2.5}, nitrate, and ammonium, with the dry deposition flux of PM_{2.5} increasing during extreme heat (Supplementary Materials Fig. S11).

The daily net changes from all processes (Fig. 7a) corresponded well with the concentrations shown in Fig. 7b. O₃ daily mean concentrations increased with daily maximum temperatures, with pronounced enhancement above 950 hPa, especially during extreme heat events. Surface-layer PM_{2.5} concentrations peaked at 33 °C (Figs. 6a and 7b) and then started to decrease with temperature. The peak was determined by the peak of chemical production and the highest concentration of sulfate, and the decreases in PM_{2.5} above 33 °C were caused by the decreases in nitrate and ammonium.

3.3.2. Process analyses for YRD

Fig. 8a presents the daily net contributions of individual processes to pollutant mass at different vertical levels below 850 hPa in the YRD under different daily maximum temperatures. The chemical production of O₃ averaged over all temperatures and all vertical layers below 850

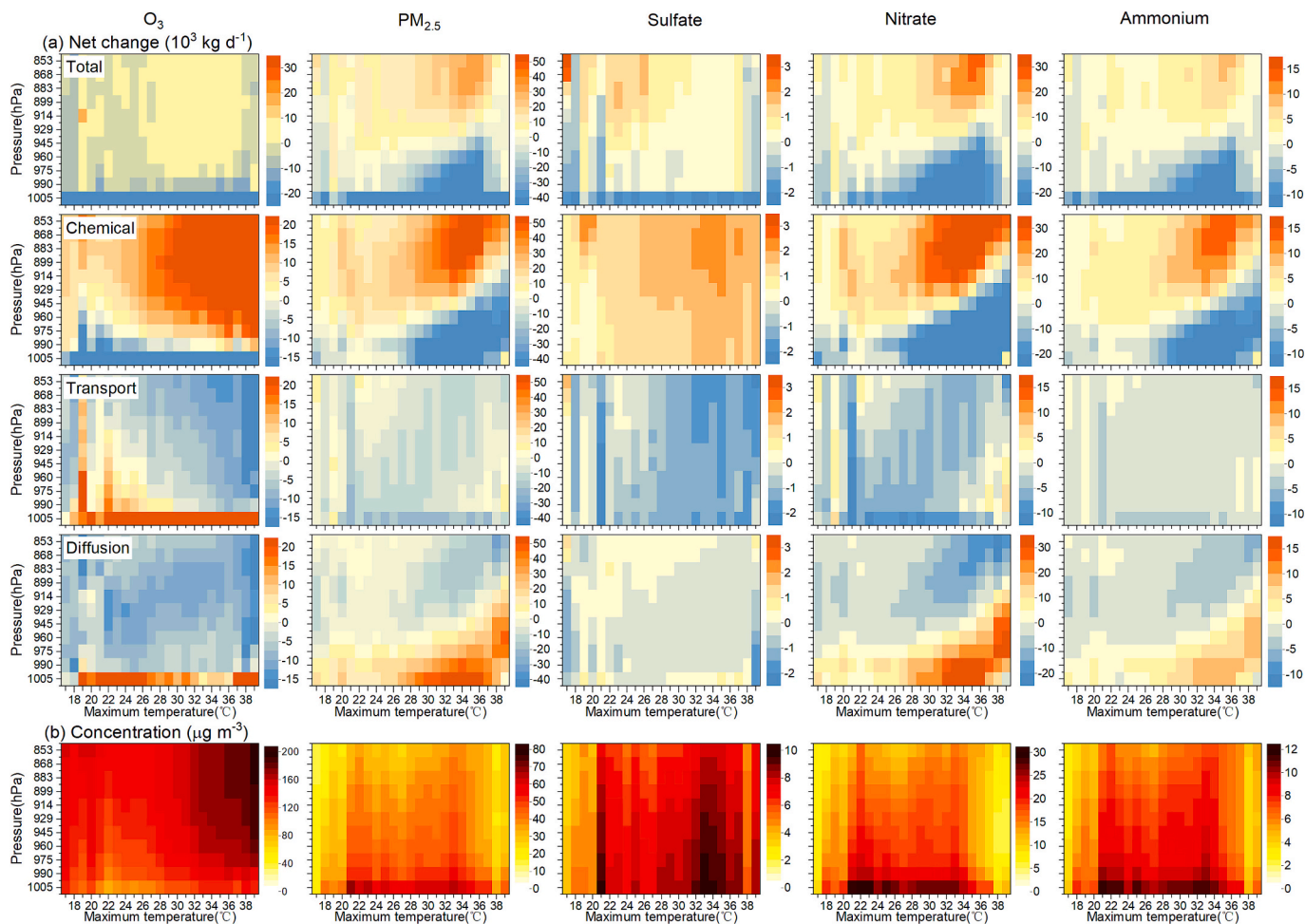


Fig. 7. (a) Daily integrated mass net changes (10^3 kg d^{-1}) of O_3 , $\text{PM}_{2.5}$, sulfate, nitrate, and ammonium caused by individual processes, as well as the total contribution of all processes, at different vertical layers below 850 hPa in BTH under different daily maximum temperatures. (b) Simulated daily mean concentrations of O_3 , $\text{PM}_{2.5}$, sulfate, nitrate, and ammonium at different vertical layers below 850 hPa in BTH under different daily maximum temperatures. The values shown represent the averaged process contributions over all samples within specific bins of daily maximum temperature.

hPa was higher in YRD than in BTH (the value in YRD was three times that in BTH). The reason for this was that the daily mean temperature was generally higher in YRD than in BTH even under identical daily maximum temperatures, which promoted more O_3 chemical production in the YRD. With this higher concentration of atmospheric oxidants as well as the larger humidity (Fig. 9), chemical production of sulfate was also stronger in YRD than in BTH. Transport generally contributed negatively to pollutant mass because of the strong outflows in the northern boundary and minimal fluxes at the southern boundary of YRD (Supplementary Materials Fig. S9).

As mentioned above, the observed and simulated $\text{PM}_{2.5}$ concentrations peaked around 30 °C, decreased over 30–35 °C, and then had an increasing trend under extreme heat (> 35 °C). Chemical production of sulfate, nitrate, and ammonium were overall positive at the surface as daily maximum temperatures remained below 28 °C. Above 30 °C, chemical formation of nitrate and ammonium was positive above about 900 hPa but was negative below this level. The maximum negative contribution of chemical process occurred at the surface over 30–35 °C. Interestingly, and chemical formation of nitrate and ammonium at the surface was positive under extreme heat, because of the high humidity and high O_3 concentration (Yan et al., 2023; Sun et al., 2025). The diffusion process had a significant positive contribution to the mass of $\text{PM}_{2.5}$ and its components (sulfate, nitrate, and ammonium) near the surface under extreme heat (daily maximum temperature > 35 °C) because of the diffusion from high altitude (high chemical production)

to the surface. Consequently, at the surface during extreme heat, the positive contribution from diffusion effectively offset the negative contributions from transport and dry deposition, thereby suppressing the decrease in concentrations of $\text{PM}_{2.5}$, nitrates, and ammonium.

Fig. 8b shows the distributions of O_3 and $\text{PM}_{2.5}$ daily mean concentrations below 850 hPa. Driven predominantly by chemical production, the region maintained high O_3 concentrations. During extreme heat, O_3 levels increased significantly throughout the vertical column examined. $\text{PM}_{2.5}$ concentrations peaked at 29 °C, decreased around 30–35 °C because of larger chemical loss of nitrate and ammonium, and rebounded under extreme heat as results of positive contributions from diffusion and enhanced chemical production of ammonium and nitrate under high humidity and high O_3 concentration.

3.4. Roles of weather patterns in net chemical productions of O_3 and $\text{PM}_{2.5}$ under extreme heat

To examine weather patterns under different temperature ranges, summer days from 2013 to 2022 in the BTH and YRD regions were categorized into three ranges: below 30 °C, 30–35 °C, and above 35 °C when more than half of the cities in either BTH or YRD recorded daily maximum temperatures within these intervals.

Fig. 9 shows the vertical profiles of the daily mean temperature and RH below 850 hPa in BTH and YRD that were averaged over the days that fall within the three temperature ranges mentioned above. For both

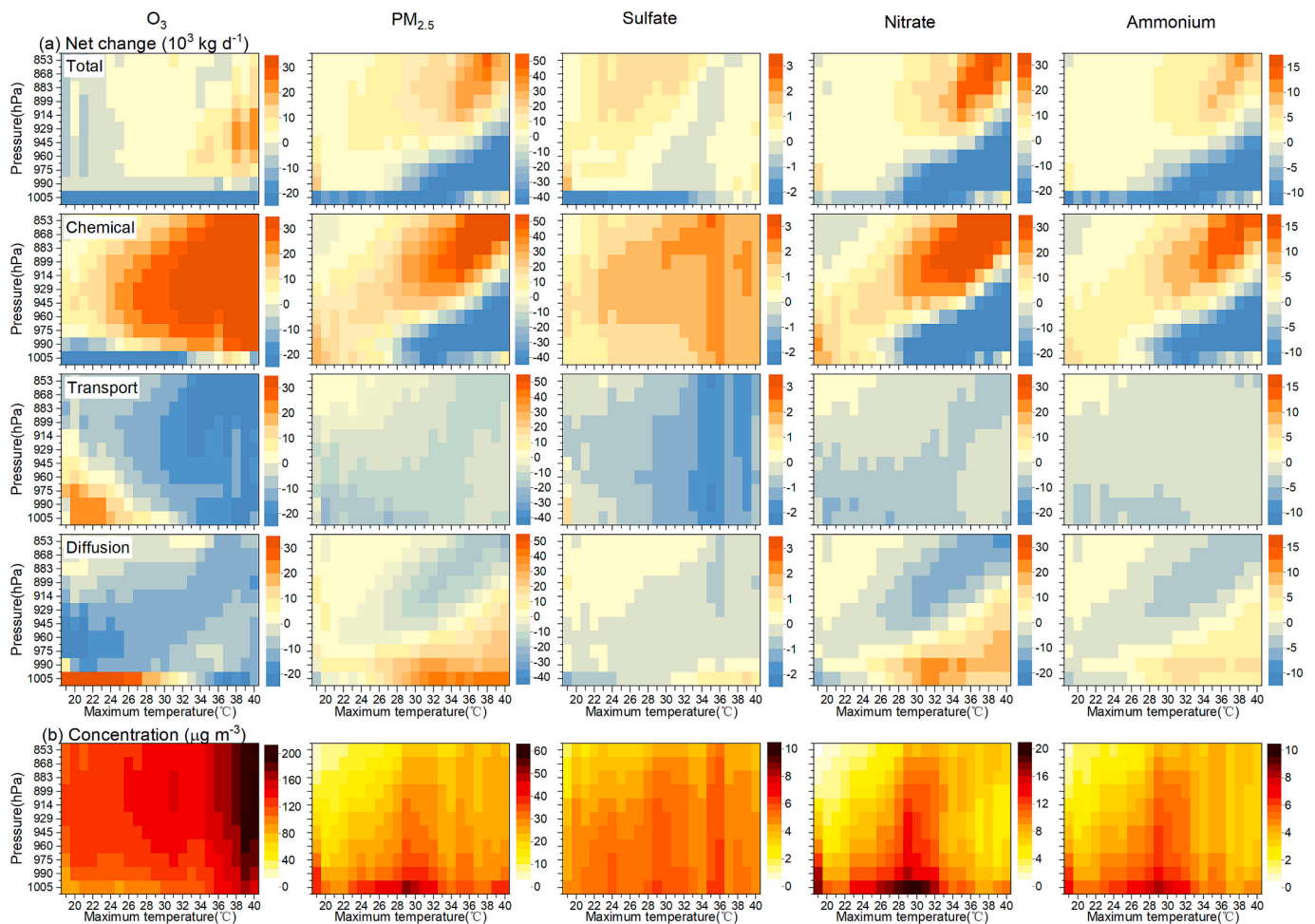


Fig. 8. Same as Fig. 7 but for the YRD region.

regions, the daily mean temperature increased while RH decreased with rising daily maximum temperature. During extreme heat, the regional mean surface daily mean temperature and relative humidity were, respectively, 28.91 °C and 50.13% in BTH and 30.03 °C and 69.71% in YRD. YRD experienced both higher temperature and higher relative humidity under extreme heat, promoting secondary inorganic aerosol formation and leading to higher PM_{2.5} levels (shown in Fig. 12). High temperatures coincided with high O₃ levels, leading to a sharp increase in the sulfur oxidation ratio (Fang et al., 2019). In the meantime, elevated O₃ promoted the formation of N₂O₅, which subsequently hydrolyzed to generate nitrate (Yan et al., 2023). Sun et al. (2025) showed a monotonic increase of the nitrogen oxidation ratio with RH by using observations and reported that RH dominated nitrate formation and the partitioning of HNO₃ to aerosol phase throughout the year. Therefore, the notably higher RH in YRD than in BTH under extreme heat corresponded to the positive chemical production of PM_{2.5}, nitrate, and ammonium at the surface in YRD (Fig. 8a).

Figs. 10 and 11 present the composited weather patterns for the BTH and YRD regions for summer-mean (June–July–August) and regional extreme heat ($\geq 50\%$ of cities affected) conditions during 2013–2022. Additionally, the anomalies in sea level pressure, geopotential height, and wind during extreme heat days relative to the seasonal mean were quantified. In BTH, under extreme heat, an anomalous high-pressure system at 500 hPa resulted in high daily maximum temperatures and low RH. These conditions promoted substantial chemical production of O₃ within the 850–950 hPa layer but induced thermal decomposition of nitrate and ammonium near the surface (Fig. 7a). In BTH, during extreme heat, strong southerlies prevailed at the surface and

southwesterlies entered the region and transitioned into strong westerly winds. These wind patterns agreed with the O₃ and PM_{2.5} horizontal transport pathways identified in the process analysis (Supplementary Materials Fig. S4).

Under extreme heat conditions, YRD was under the influence of the western Pacific subtropical high, which was accompanied by a marked rise in geopotential heights at 850 and 500 hPa. Under the hot conditions brought by the subtropical high, the chemical productions of both O₃ and sulfate were significantly enhanced, which increased atmospheric oxidant (O_x) levels and further increased the formation of nitrate and ammonium at the surface (Fig. 8a). At the surface, moist south-easterlies from the ocean transported humid air into the region, creating favorable conditions for secondary pollutant formation and increased PM_{2.5} concentrations (Fig. 8a).

Since chemical productions of sulfate, nitrate, and ammonium gradually shifts from negative to positive at the surface during extreme heat in the YRD (Figs. 8a), the relationships between the net chemical production of PM_{2.5} and its inorganic components at the surface and RH and daily maximum temperature were examined. The sensitivity of net chemical production to T_{max} (defined as $S_{T_{max}} = \Delta \text{chemical production} / \Delta T_{max}$) and RH (defined as $S_{RH} = \Delta \text{chemical production} / \Delta RH$) regressed using all the data points are shown in Fig. 12. In both BTH and YRD, linear regression analyses show that while higher T_{max} promoted sulfate formation but suppressed the net chemical productions of total PM_{2.5}, nitrate, and ammonium, higher RH promoted the chemical production of PM_{2.5} and secondary inorganic components. The chemical production of PM_{2.5}, nitrate, and ammonium showed a stronger negative sensitivity to T_{max} in BTH than in YRD. $S_{T_{max}}$ values of PM_{2.5}, nitrate,

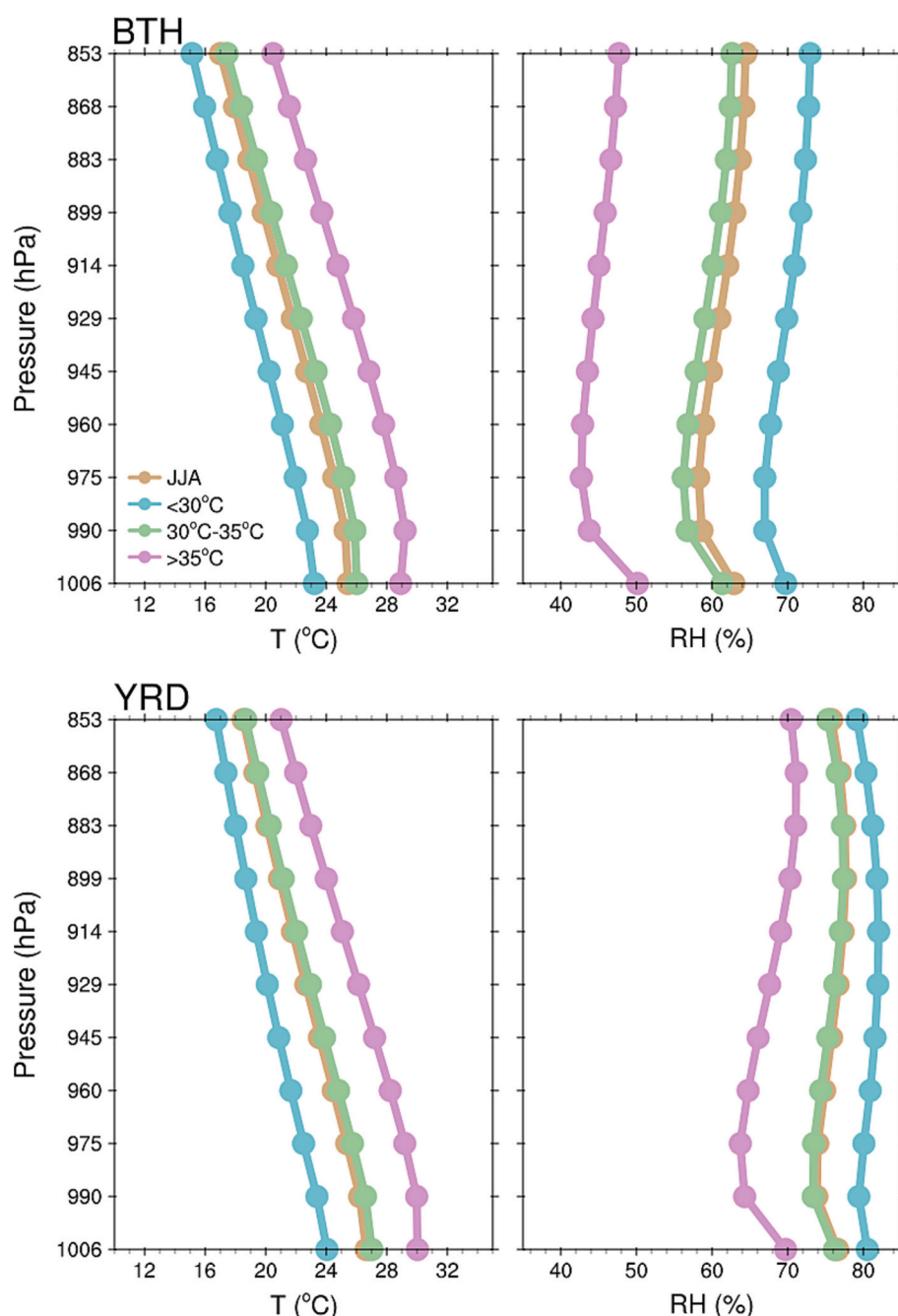


Fig. 9. The vertical profiles of daily mean temperature (T) and relative humidity (RH) below 850 hPa across temperature bins (below 30 °C, 30–35 °C, and above 35 °C) in the BTH and YRD regions during summers of 2013–2022. The values shown are spatial averages for the region.

and ammonium were, respectively, -6.60 , -5.16 , and -1.48 in BTH and -3.73 , -2.95 , and -0.85 in YRD. The net chemical production of nitrate had the largest negative sensitivity among all the secondary components (Fig. 12).

YRD exhibited a much stronger positive sensitivity of $\text{PM}_{2.5}$, nitrate, and ammonium chemical production to RH compared to BTH. S_{RH} values of $\text{PM}_{2.5}$, nitrate, and ammonium were, respectively, 0.52 , 0.38 , and 0.12 in BTH and 1.67 , 1.29 , and 0.38 in YRD. As shown in Fig. 12, positive net chemical production of $\text{PM}_{2.5}$, nitrate, and ammonium occurred primarily when the RH exceeded 60%. We performed a bin analysis of RH from 30% to 90% in 2% intervals to examine the net chemical production of $\text{PM}_{2.5}$, sulfate, nitrate, and ammonium in BTH and YRD. A transition was observed at $\text{RH} = 58\%$ in BTH and 60% in YRD, above which negative chemical contributions became smaller and

eventually positive, highlighting the key role of humidity in secondary aerosol formation (Supplementary Materials Fig. S12). Beyond this threshold, S_{RH} values of $\text{PM}_{2.5}$, nitrate, and ammonium increased to be, respectively, 3.59 , 2.75 , and 0.82 in BTH and 2.99 , 2.33 , and 0.68 in YRD. Overall, under extreme heat in the YRD ($\text{RH} = 69.71\%$), the atmosphere is simultaneously humid and highly oxidative (Supplementary Materials Fig. S13), which enhances both gas-phase and aqueous-phase reactions and thereby promotes the formation of secondary inorganic aerosols.

4. Conclusion

This study carried out the composited analyses of the changes in summertime daily concentrations of O_3 and $\text{PM}_{2.5}$ with daily maximum

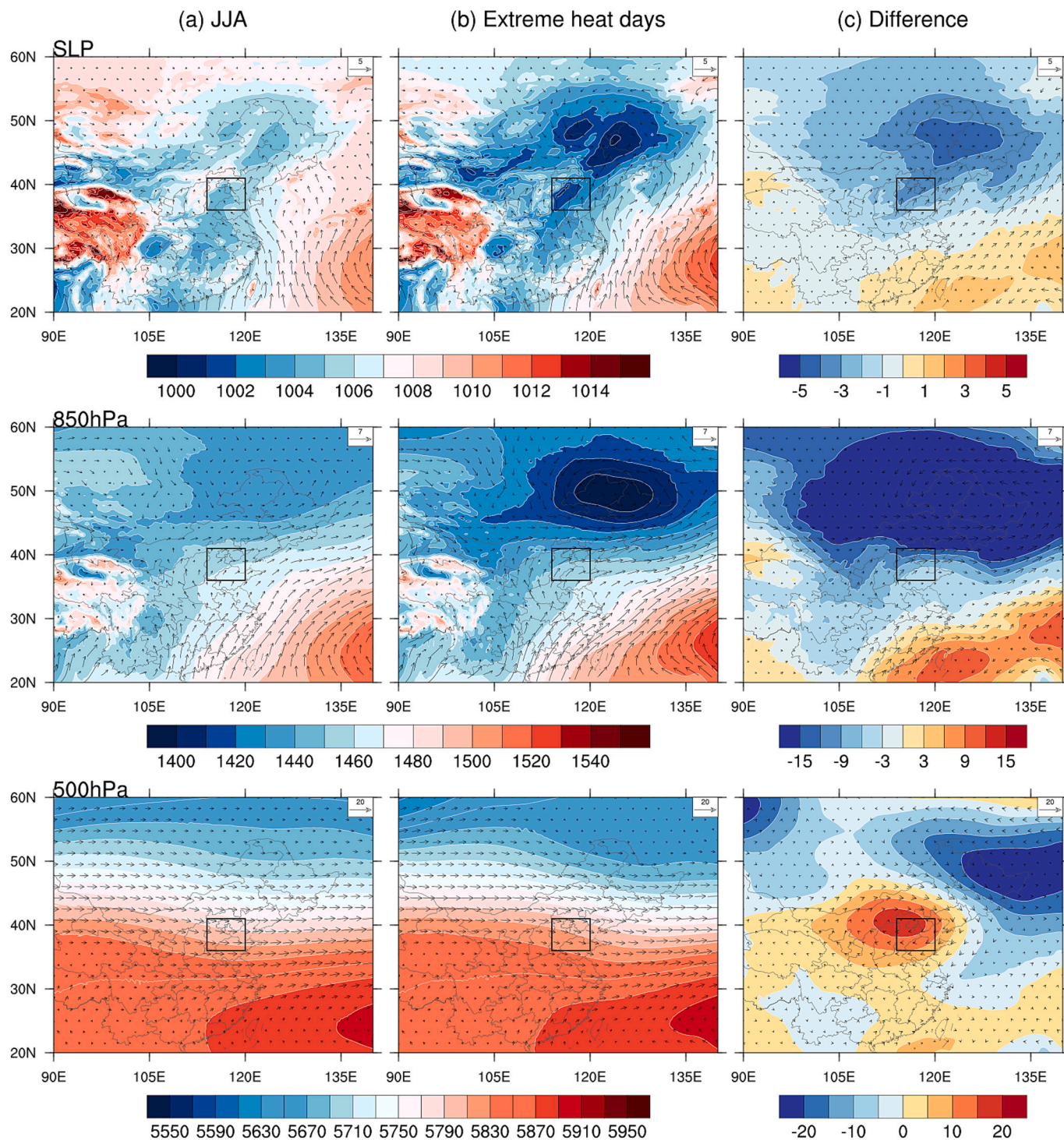


Fig. 10. Composed weather patterns (winds (m s^{-1}), SLP (sea level pressure), and geopotential height at 850 and 500 hPa) for the BTH region for (a) summer-mean (June–July–August) of 2013–2022 and (b) regional extreme heat ($\geq 50\%$ of cities with daily maximum temperature $> 35^\circ\text{C}$) conditions during 2013–2022. (c) The difference ((b) minus (a)). The data were taken from the ERA5 datasets. The solid black rectangle indicates BTH region.

temperature for BTH and YRD based on observed data from 2013 to 2022 and the GEOS-Chem model simulations from 2013 to 2020. We pay special attention to understand the changes in O_3 and $\text{PM}_{2.5}$ under extreme heat through process analyses to quantify the roles of chemical and physical production.

MDA8 O_3 concentrations showed an overall positive relationship with daily maximum temperature in both BTH and YRD, except in YRD where concentrations declined when temperatures exceeded 40°C . Under extreme heat, observed MDA8 O_3 in BTH exhibited a strong linear

increase of $11.79 \mu\text{g m}^{-3} ^\circ\text{C}^{-1}$, which was driven by enhanced chemical production, particularly between 850 and 950 hPa, offsetting the losses from transport and diffusion. In YRD, the MDA8 O_3 response to daily maximum temperature was $5.08 \mu\text{g m}^{-3} ^\circ\text{C}^{-1}$ under extreme heat. The YRD experiences significantly higher overall chemical production than BTH due to generally warmer daily mean temperatures.

The changes in $\text{PM}_{2.5}$ concentrations under extreme heat differed in BTH and YRD due to the differences in prevailing meteorological conditions. During extreme heat, the observed $\text{PM}_{2.5}$ levels in BTH actually

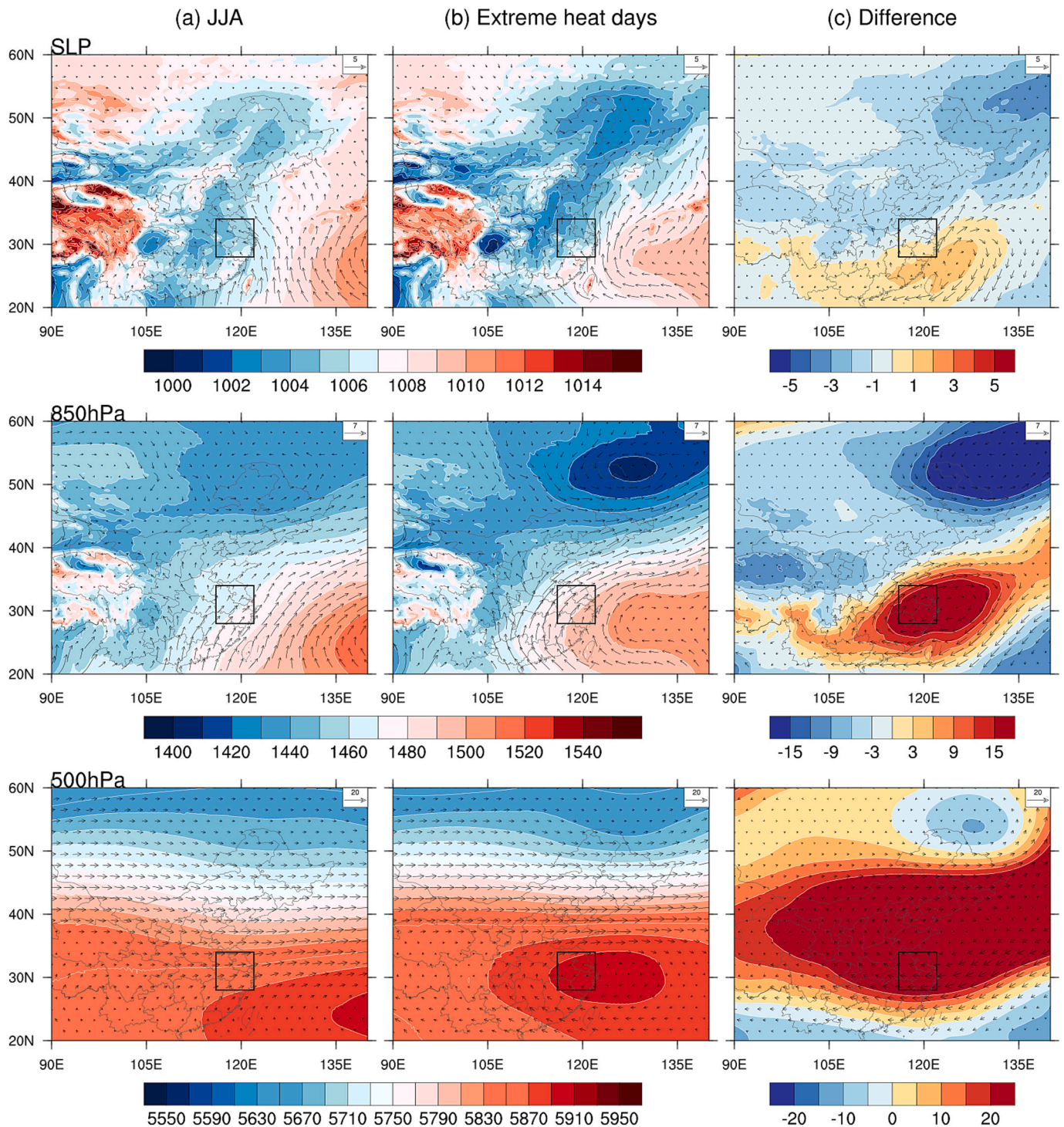


Fig. 11. Same as Fig. 10 but for the YRD region.

decreased at a rate of $2.48 \mu\text{g m}^{-3} \text{ } ^\circ\text{C}^{-1}$. This decline was primarily attributed to the hot and dry conditions that promoted the thermal dissociation of nitrate and ammonium. Conversely, in the YRD, observed $\text{PM}_{2.5}$ concentration increased during extreme heat at a rate of $0.98 \mu\text{g m}^{-3} \text{ } ^\circ\text{C}^{-1}$. Influenced by the Western Pacific Subtropical High, YRD experiences high temperatures coupled with high RH. Process analyses showed that such humid conditions enhanced the formation of secondary inorganic aerosols.

In both BTH and YRD, linear regression analyses showed that while higher T_{max} promoted sulfate formation but suppressed the net

chemical productions of total $\text{PM}_{2.5}$, nitrate, and ammonium, higher RH promoted the chemical production of $\text{PM}_{2.5}$ and secondary inorganic components. Relative humidity thresholds of about 58% in BTH and 60% in YRD are identified, beyond which the negative chemical contributions to nitrate and ammonium decrease linearly and ultimately become positive.

This study, based on long-term multi-station observations and model simulations, systematically reveals region-specific responses and mechanisms of O_3 and $\text{PM}_{2.5}$ under extreme heat for BTH and YRD with different meteorological features. Note that uncertainties may arise from

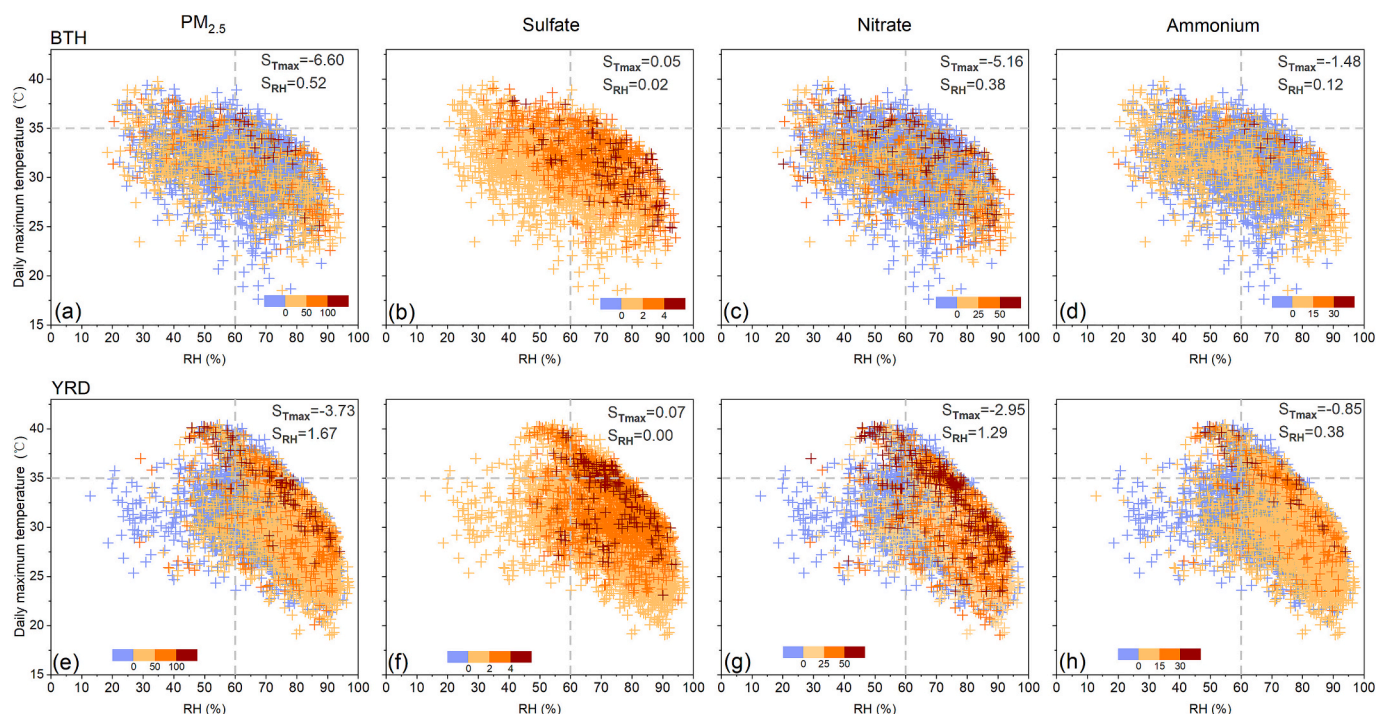


Fig. 12. The distributions of surface net chemical production (10^3 kg d^{-1}) of PM_{2.5} and its secondary inorganic components with relative humidity and daily maximum temperature in BTH (a-d) and YRD (e-h). The sensitivity of net chemical production to Tmax (S_{Tmax} , Δ chemical production/ Δ Tmax) or RH (S_{RH} , Δ chemical production/ Δ RH) is also shown, which was derived from linear regression using all the selected simulated samples in summers of 2013–2020. Different colors indicate the magnitude of net mass change.

emission changes, single-model limitations, site representativeness of component observations and sample screening. The findings of this study enhance our understanding of chemical characteristics of air pollutants under extreme heat and have important implications for understanding health impacts of compounded extreme heat and air pollution.

CRediT authorship contribution statement

Peifu Xie: Writing – original draft, Visualization, Validation, Methodology, Investigation, Formal analysis, Data curation. **Hong Liao:** Writing – review & editing, Supervision, Resources, Project administration, Methodology, Investigation, Funding acquisition, Formal analysis, Conceptualization. **Huibin Dai:** Writing – review & editing, Data curation.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Appendix A. Supplementary data

Supplementary data to this article can be found online at <https://doi.org/10.1016/j.atmosres.2026.109094>.

Data availability

Data will be made available on request.

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