The Role of Naphthalene and Its Derivatives in the Formation of Secondary Organic Aerosols in the Yangtze River Delta Region, China

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Abstract. Naphthalene (Nap) and its derivatives, including 1-methylnaphthalene (1-MN) and 2-methylnaphthalene (2-MN), serve as prominent intermediate volatile organic compounds (IVOCs) contributing to the formation of secondary organic ~~carbon (SOC~~aerosol (SOA). In this study, the Community ~~Multi-Scale~~Multiscale Air Quality (CMAQ) model coupled with detailed emissions and reactions of these compounds was utilized to examine their roles in the formation of ~~SOC~~SOA and other secondary pollutants in the Yangtze River Delta (YRD) region during summer. ~~Remarkably, significant~~Significant underestimations of Nap and MN concentrations (by 79% and 85%) were observed at the Taizhou site~~. To better capture the temporal variations~~ based on the model results using the default emissions. Constrained by the observations, anthropogenic emissions of Nap and MN~~, their emissions~~ in the ~~YRD~~entire region were ~~scaled up~~multiplied by ~~a factor of~~ 5 and 7, respectively, ~~with constraints based on field measurements. After adjusting their emissions,~~ to better capture the evolution of pollutants. The average concentration of Nap ~~concentrations~~ reached ~~27~~25 ppt in the YRD, ~~accounting for~~ with Nap contributing 4.1% and ~~9~~8.1% (up to ~~13.7~~12.6%) of total ~~aromatics~~aromatic emissions and aromatic-derived secondary organic carbon (SOC~~,~~), respectively. The concentrations of 1-MN and 2-MN were relatively low, ~~with an average of 3 and 6~~averaging at 2 ppt ~~in the YRD,~~ and ~~contributed 3.1~~5 ppt. Together, they accounted for only 2.4% of the aromatic-derived SOC. The ~~influences~~impacts of Nap and MN oxidation on ozone and radicals ~~might be trivial on a~~were insignificant at regional ~~scale~~scales but were not negligible when considering daily fluctuations~~, particularly~~ in ~~Shanghai~~locations with high emissions of Nap and ~~Suzhou~~MN. This study ~~emphasizes the high SOC~~highlights the significant roles of Nap and MN in the formation ~~potentials~~ of ~~Nap and MN~~SOA, which may pose environmental risks and adverse health effects.

1 Introduction

Secondary organic aerosols (SOA) are formed from the condensation and multiphase evolution of less volatile organic compounds (VOCs), which can be directly emitted or produced from the oxidation of higher volatile organics in the atmosphere. SOA not only affects visibility and human health but also ~~has impacts~~exerts direct effects on the climate ~~directly~~ by absorbing and reflecting solar radiation ~~and indirectly~~, as well as indirect effects by ~~affecting~~influencing cloud formation ~~(Chen et al., 2016; Zhang and Ying, 2012)~~(Chen et al., 2016; Zhang and Ying, 2012). Semi-volatile and intermediate-volatile organic compounds (S/IVOCs) have been identified as the key precursors of SOA (Robinson et al., 2007; Hu et al., 2022). IVOCs are categorized by small polycyclic aromatic hydrocarbons (PAHs), intermediate-length alkanes (e.g. ~~n-hexadecane), and phenols(Pye and Seinfeld, 2010)~~n-hexadecane), and phenols(Pye and Seinfeld, 2010). PAHs are organic compounds containing multiple aromatic rings. In 2004, China ~~was responsible for~~ exhibited the highest annual PAH emissions ~~at~~ (114 Gg ~~with a portion of~~) globally, accounting for 22% of ~~global~~the total ~~PAH~~ emissions ~~in 2004(Zhang and Tao, 2009).~~worldwide (Zhang and Tao, 2009). Naphthalene (Nap) and methylnaphthalene (MN), such as 1-methylnaphthalene (1-MN) and 2-methylnaphthalene (2-MN), are the most abundant airborne PAHs (Chen et al., 2016; Fang et al., 2021), ~~which are mainly~~primarily emitted from ~~the~~ combustion of fossil fuels, biomass burning, and industrial sectors ~~(Fang et al., 2021)~~(Fang et al., 2021).

~~Chamber studies have identified the gas- and particle-phase products from Nap reacting with hydroxyl radical (OH·) (Huang et al., 2019). Ring-retaining products (e.g., 1,4-naphthoquinone) with lower volatilities are dominant under low nitrogen oxide (NO_x) conditions, and ring-opening products (e.g., 2-formylcinnamaldehyde) with higher volatilities are dominant in the presence of high NO_x. Chan et al. (2009) evaluated the SOA yields of Nap, 1-MN, 2-MN, and 1,2-dimethyl naphthalene in chambers and applied these yields to estimate SOA formation from primary~~

~~emissions of diesel engines and wood burning. The SOA yields were 55–75% under low-NO_x conditions at a total organic aerosol loading of 15 μg m^{-3}, which was more efficient than high-NO_x conditions (25–45%). In the photo-oxidation period of less than 12 h, these PAHs produced 3–5 times more SOA than light aromatic compounds and were responsible for up to 54% of total SOA from the oxidation of diesel emissions. Huang et al. (2019) applied a tracer method and discovered that 14.9% of SOA was owing to the oxidation of Nap and MN in the afternoon during the wintertime haze in Beijing. Shakya and Griffin (2010) also reported 36–162 kg day^{-1} of SOA production from the mobile source emitted PAHs (including Nap, 1-MN, and 2-MN) in Houston based on the yields from their study and that of Chan et al. (2009). Based on the yield from Shakya and Griffin (2010), Liu et al. (2015) showed that Nap contributed 8–52% of the total SOA originating from benzene, toluene, C2-benzene, C3-benzene, C4-benzene, and Nap in light-duty gasoline vehicle exhausts. All these experimental findings demonstrate the significant role of Nap and MN in SOA formation in the environment with anthropogenic influences dominated. However, these results might not accurately reflect the actual atmospheric conditions due to the simplicity of reaction conditions and the limited precursors involved in chamber studies~~ Chamber studies have identified the gas- and particle-phase products from Nap reacting with hydroxyl radicals (OH·) (Huang et al., 2019). Ring-retaining products (such as 1,4-naphthoquinone) with lower volatilities dominate under conditions of low nitrogen oxides (NO_x), and ring-opening products (such as 2-formyl cinnamaldehyde) with higher volatilities dominate in the presence of high NO_x. Chan et al. (2009) evaluated the SOA yields of Nap, 1-MN, 2-MN, and 1,2-dimethyl naphthalene in chambers to estimate SOA formation from primary emissions of diesel engines and wood burning. It was found that SOA is more efficiently produced under low-NO_x conditions than high-NO_x conditions, with yields of 55–75% and 25–45%, respectively, at a total organic aerosol loading of 15 μg m^{-3}.

During photo-oxidation of less than 12 h, these PAHs produced 3–5 times more SOA than light aromatic compounds, accounting for up to 54% of the total SOA from the oxidation of diesel emissions. Huang et al. (2019) applied a tracer method to determine that 14.9% of SOA was attributed to the oxidation of Nap and MN in the afternoon during wintertime haze in Beijing. Shakya and Griffin (2010) also reported 37–162 kg day^{-1} of SOA production from the mobile source emitted PAHs (including Nap, 1-MN, and 2-MN) in Houston, based on the yields from their study and that of Chan et al. (2009). By adopting the SOA yields from Shakya and Griffin (2010), Liu et al. (2015) showed that Nap accounted for 8–52% of the total SOA derived from benzene, toluene, C2-benzene, C3-benzene, C4-benzene, and Nap in exhaust emissions from light-duty gasoline vehicles. All these experimental findings demonstrate the significant role of Nap and MN in SOA formation in environments dominated by anthropogenic influences. However, these results might not accurately reflect the actual atmospheric conditions due to the simplicity of reaction conditions and the limited precursors involved in chamber studies (Ling et al., 2022).

Numerical models have been developed and utilized to assess the contribution of S/IVOCs to SOA (Hayes et al., 2015; Pye and Seinfeld, 2010; An et al., 2023). ~~Zhang and Ying (2011) showed that PAHs emitted from anthropogenic sources could produce SOA mass as much as 10% of that from the traditional light aromatics or around 4% of total anthropogenic SOA by using the Community Multiscale Air Quality (CMAQ) model. However, the products from several explicit PAH species (Nap, MN, dimethyl naphthalene, ethyl naphthalene, acenaphthylene, acenaphthene, fluorene, phenanthrene, fluoranthene) were lumped rather than separated for their contributions to SOA due to limited experimental data. Pye and Pouliot (2012) utilized the CMAQ model and tracked 10% of peroxy radicals produced from the ARO2 (lumped aromatics in CMAQ) and OH· reaction as for that of Nap without considering the emissions and the accurate OH· reactivity of~~

~~Nap. According to Cohan et al. (2013), the modeled SOA increased by roughly 1–10% when Nap emissions from on-road gasoline and diesel vehicles were considered. Their simulations showed a lower bound in the SOA production from Nap due to underestimations in the emission inventory in the South Coast Air Basin of California. Majdi et al. (2019) found that Nap and MN contributed 2.4% to the total organic aerosol (OA) originating from wildfires over the Euro-Mediterranean region during the summer of 2007 by using a 3D chemistry transport model (CTM). The contributions of Nap and MN to SOA over a regional scale in China had not been quantified.~~

. Zhang and Ying (2011) showed that PAHs emitted from anthropogenic sources could produce SOA mass as much as 10% of that from the traditional light aromatics or approximately 4% of the total anthropogenic SOA by using the Community Multiscale Air Quality (CMAQ) model. However, the SOA products of several PAH species such as Nap and MN were lumped together due to limited experimental data for explicit parameterization. Pye and Pouliot (2012) assumed that 10% of ARO2 (lumped aromatic species) reacted with OH· to represent SOA formation from PAHs in the CMAQ model, using Nap as a surrogate for parameterization, without considering individual PAH's emissions and OH· reactivity. According to Cohan et al. (2013), the modeled SOA increased by roughly 1–10% when Nap emissions from on-road gasoline and diesel vehicles were considered. Their simulations showed a lower limit in the SOA production from Nap due to underestimations in the emission inventory in the South Coast Air Basin of California. Majdi et al. (2019) found that Nap and MN contributed 2.4% of the total organic aerosol (OA) originating from wildfires over the Euro-Mediterranean region during the summer of 2007 by using a 3D chemical transport model (CTM). The contributions of Nap and MN to SOA at regional scales in China had not been quantified.

In this study, SOA formation from Nap, 1-MN, and 2-MN in the Yangtze River Delta (YRD) region during the EXPLORE-YRD ~~-~~(EXPeriment on the eLucidation of the atmospheric Oxidation capacity and aerosol foRmation~~,~~ and their Effects in the Yangtze River Delta) campaign period (May 20 − June 18, 2018) was investigated ~~with~~by using an updated CMAQ model that incorporated explicit SOA schemes for these PAHs. Emission inventories of Nap, 1-MN, and 2-MN were estimated based on different sources and methods and validated against observations. After that, the influences of Nap and MN on secondary organic carbon (SOC), ozone (O_3), and radical concentrations were examined in ~~the~~ locations with high ~~concentrations~~levels of Nap and MN as well as at the regional scale~~ were examined separately~~. The newly added SOA parameterizations for 1-MN and 2-MN were fitted by both two-product and one-product methods to compare the differences. We ~~find~~found that Nap and its derivatives, although accounting for a small fraction of emitted aromatics (5.1%), contributed ~~12.1~~10.4% of aromatic-derived SOC in the YRD.

2 Methods

2.1 Modified SOA formation pathways of MN

The CMAQ model version 5.2, coupled with the SAPRC07tic atmospheric chemical mechanism and the AERO6i aerosol module, was updated to include the oxidation of 1-MN and 2-MN by OH· and the corresponding SOA formation pathways. In the original CMAQ model, Nap reacts with OH· to form SOA under ~~low~~high- and ~~high~~low-NO_x conditions, ~~which are~~ represented by two different counter species PAHNRXN and PAHHRXN~~ and PAHNRXN~~, respectively (Fig. ~~S1~~1a). Similar to Nap, 1-MN, and 2-MN were ~~treated~~ explicitly treated as reacting with OH· and forming SOA counter species under high NO_x (aMPAHNRXN and bMPAHNRXN) and low NO_x (aMPAHHRXN and bMPAHHRXN), along with other products following ~~Zhang and Ying~~

~~(2012).~~Zhang and Ying (2012). These counter species were used to calculate the production of SOA through gas-particle partitioning based on yields (α_i) and partitioning coefficients ($K_{\mathrm{om},i}$, $\mathrm{m^3\ \mu g^{-1}}$) of condensable organic products derived from chamber experiment data. ~~The detailed descriptions~~Details of gas-particle partitioning ~~to fit~~for fitting SOA ~~yield through~~formation using one-product and two-product methods are ~~depicted~~described in the Supplement.

~~In gas-particle partitioning of~~In the original CMAQ model, a two-product method (SV_PAH1 and SV_PAH2) was used to represent the SOA formation from Nap under high-NO_x conditions, ~~which are~~ denoted as APAH1J and APAH2J, respectively (Fig. ~~S1a~~1a). Under low-NO_x conditions, a one-product method was used to represent the SOA formation from Nap, denoted as APAH3J. It was assumed that APAH3J (with a yield of α_3) was non-volatile and resided in the particle phase. Similar to Nap, a two-product method for the ~~oxidation products of~~SOA formation from 1-MN ~~was added~~ under high-NO_x conditions was added as shown in Fig. ~~S1b~~1b, with the SOA species denoted as AaMPAH1J and AaMPAH2J. ~~A~~Additionally, a one-product method ~~to characterize~~characterizing the ~~oxidation products of~~SOA formation from 1-MN under high-NO_x conditions was ~~also~~ applied to compare ~~the difference~~differences caused by ~~the~~different fitting ~~approach~~approaches. As shown in Fig. ~~S1c~~1c, the semi-volatile organic product SV_aMPAH1' undergoes equilibrium partitioning to form SOA (AaMPAH1J'). Under low-NO_x conditions, a non-volatile SOA product AaMPAH3J is formed ~~by the~~through oxidation of 1-MN. The SOA ~~pathways~~scheme of 2-MN ~~follow~~ followed that of 1-MN~~,~~ with ~~the~~ corresponding ~~SOA~~ products ~~of~~ AbMPAH1J~~,~~ and AbMPAH2J~~,~~ (or AbMPAH1J') under high-NO_x conditions and AbMPAH3J under low-NO_x conditions, respectively. ~~In addition~~Moreover, all semi-volatile SOA products originating from MN undergo condensed-phase oligomerization reactions at the same rate ~~of~~as APAH1J and APAH2J ~~and produce~~, generating anthropogenic non-volatile oligomers (AOLGAJ~~)~~

~~that belong to the anthropogenic source.~~). Other processes and parameters involved in the newly added SOA pathways for 1-MN and 2-MN, such as the dry and wet deposition and the molecular weight of the oxidation products, were set to be the same as Nap due to limited experimental data. Details of all the parameters, i.e., α_i, $K_{\mathrm{om},i}$, and $\Delta H_{\mathrm{vap},i}$ are summarized in Table S1.

2.2 Model application

The simulation domain, which covers Jiangsu, Zhejiang, Anhui, Shanghai, and neighboring provinces, has a horizontal resolution of 4 km × 4 km (238 × 268 grids) and a vertical structure of 18 layers as shown in Fig. ~~S2~~S1. Details of the domain setup can be found in previous studies (Li et al., ~~2021~~2022; Li et al., ~~2022~~2021). The meteorological field was predicted by the Weather Research and Forecasting (WRF) model version 4.0 with the ECMWF Reanalysis v5.0 (ERA5) reanalysis data as ~~the~~ inputs. More details about the WRF configuration ~~were~~have been summarized by ~~Wang et al. (2021)~~Wang et al. (2021). A spin-up of two days was used to minimize the influence of initial conditions.

Biogenic emissions were generated from the Model for Emissions of Gases and Aerosols from Nature (MEGAN) version 2.1 ~~(Guenther et al., 2012).~~(Guenther et al., 2012). Open biomass burning emissions were based on the Fire INventory from the National Center for Atmospheric Research (FINN) ~~(Wiedinmyer et al., 2011)~~(Wiedinmyer et al., 2011). Anthropogenic emissions were generated from the updated 2017 emission inventory for the YRD ~~(Cheng et al., 2021)~~(Cheng et al., 2021) and the Multi-resolution Emission Inventory for China (MEIC, http://www.meicmodel.org, last access: 1 June 2023) for the rest of the domain. Currently, there is ~~no available data to use in more~~ a lack of localized ~~sources~~ source profiles in China~~. The detailed emissions of 1-MN~~, particularly regarding Nap and ~~2-~~MN ~~of different sources~~. These data were ~~calculated~~obtained from the ~~US EPA (~~U.S. Environmental Protection Agency's (EPA's)

repository of organic gas and particulate matter (PM) speciation profiles of air pollution sources (SPECIATEv5.2) ~~and~~along with the source information reported by ~~An et al. (2021)~~An et al. (2021) and Li et al. (2014). ~~See the~~ Relevant details of emission calculations can be found in the Supplement ~~for more details about the calculating process.~~. There ~~were~~are two sets of emission data consisting of different Nap and MN emissions ~~in the YRD~~. The emis-orig used the original Nap emissions from the 2017 YRD inventory ~~and~~as well as the calculated Nap emissions in the rest of the domain and MN emissions~~.~~ in the entire domain. We show later that Nap and MN were underestimated ~~in emis-orig~~ and required an adjustment in their emissions to capture the observed concentrations. ~~Therefore, the~~Considering their predominantly anthropogenic origin, their anthropogenic emissions ~~of Nap and MN~~ in the ~~YRD~~entire region from emis-orig were multiplied by 5 and 7~~,~~ respectively~~, and unchanged in other regions~~ in the emis-adjust case. All the emission ratios applied in this study are shown in Table S2. According to Fig. ~~S3~~S2, Nap and MN emissions were mainly located in Shanghai, southern Jiangsu, and parts of Zhejiang ~~in the YRD region.~~. After adjustments, the total ~~Nap and MN~~ emission rate ~~over~~of Nap and MN in the YRD region in emis-adjust (~~3.9 kg~~85.0 tons day^{-1}) was approximately ~~fourfold~~4 times higher than that in emis-orig (~~0.9 kg~~18.2 tons day^{-1}). The total MN emission rate ~~over~~in the YRD region in emis-adjust was ~~0.9 kg~~20.3 tons day^{-1} ~~and was~~, lower than that of Nap. For emis-adjust, the dominant source of MN was residential-related (47.0%), followed by industry process (25.8%) and on-road ~~transport~~transportation (20.8%). ~~On~~Among all sources, on-road ~~transport~~transportation contributed the most to Nap emissions in both emis-orig (78.2%) and emis-adjust (87.5%). It should be noted that uncertainties associated with the emission inventory and source profiles, which are based on sector-specific mass ratios presented in Table S2, may potentially affect both

the distribution and source contributions of Nap and MN ~~may be influenced by the uncertainties in the source profiles~~.

Table ~~S3~~1 lists the scenarios conducted in this study. In case-1product-orig, the anthropogenic emissions ~~in the YRD used~~were based on emis-orig, along with ~~default Nap and added MN emissions, and~~ the SOA parameterization for MN ~~was~~ fitted by ~~the~~a one-product method~~.~~ in Fig. 1c and that of Nap fitted by a two-product method in Fig. 1a under high-NO_x conditions. To assess the impacts of different SOA parameterizations, ~~the~~ case-2products-orig ~~shared~~adopted the same setting ~~with~~as case-1product-orig except ~~that a two-product method~~ for ~~MN generated~~utilizing a two-product method for MN-derived SOA ~~was employed. Both~~under high-NO_x conditions (Fig. 1b). For accurate representations of the fate of Nap and MN in the atmosphere, both case-1product and case-2products ~~used~~ employed adjusted emissions (emis-adjust ~~as the emission inventory but~~) along with different SOA parameterizations for MN. ~~In~~SOA formation from Nap and MN under low-NO_x conditions in the above cases were all characterized by a fixed yield as shown in Table S1. Overall, the contributions of Nap, 1-MN, and 2-MN to the aromatic SOC were estimated based on different emission inventories and ~~two~~ SOA ~~parameterization~~ schemes. To evaluate the effects of Nap, 1-MN, and 2-MN on O_3, SOC, and radical concentrations, their emissions in case-1product were set to zero and named ~~base1.~~ base_zeroNapMN. A case named base_zeroMN was conducted to quantify the individual effects of Nap and MN by setting the emissions of 1-MN and 2-MN to zero.

2.3 Observation data for model validation

In May-June 2018, the EXPLORE-YRD field campaign was launched at a rural site in Taizhou (32.558°N, 119.994°E) and simultaneously monitored VOCs (including Nap and MN), O_3, NO_x, ~~SOC,~~ organic carbon (OC), OH~~,~~·, hydroperoxy radical (HO_2·), and other various

pollutants, which provides a good opportunity for model validation and understanding the evolution of air pollution in the YRD (Wang et al., ~~2020~~2020a; Huang et al., 2020; Yu et al., 2021; Gao et al., 2022). Details of the measurement method and accuracy for each species refer to these references. The simulated ~~MDA8~~daily maximum 8-hour average (MDA8) O_3, fine particulate matter ($PM_{2.5}$), sulfur dioxide (SO_2), nitrogen dioxide (NO_2), and carbon monoxide (CO) were also compared with the observations from the National Real-Time Urban Air Quality Release Platform of the China Environmental Monitoring Center (http://106.37.208.233:20035/, last access on May 17, 2023) in Suzhou, Nanjing, Hangzhou, Hefei, and Shanghai cities as shown in Fig. ~~S2. The statistical metrics including NMB, NME, and r were calculated for several air pollution species. The model performance benchmarks followed the recommendations by Emery et al. (2017) and are listed in Table S4.~~S1. The statistical metrics including normalized mean bias (NMB), normalized mean error (NME), and correlation coefficient (r) were calculated for several air pollution species. The benchmarks for model performance followed the recommendations by Emery et al. (2017) and are listed in Table S3. The meteorological parameters predicted by WRF have been examined to be robust during the same episode by ~~Wang et al. (2021)~~Wang et al. (2021).

3 Results

3.1 Model validation

~~Fig. 1~~Figure 2 and Fig. ~~S4~~S3 show the comparison of observed and simulated hourly variations of Nap, MN, O_3, ~~organic carbon (~~OC~~),~~, and $PM_{2.5}$ at the Taizhou site during the study period. ~~As shown in Fig. 1, in the original settings, the~~The concentrations of Nap in case-1product-orig and case-2products-orig were ~~largely~~significantly underestimated ~~in emis-orig~~ by 79% compared ~~with~~to the observations~~, with the value of NMB being -0.79~~. In contrast, emis-adjust better represented the temporal variations of Nap (NMB=0.01, r=0.68) than emis-orig, with the

averagedaverage concentration increasedincreasing by 375%a factor of 4 and more comparable toagreeing well with the observations. The concentrationsmodeled concentration of MN simulated by emis-adjust (1.40E-2 ppb) were14.0 ppt) was also comparable to the observations (1.50E-2 ppbobserved value (15.0 ppt) and showed a good correlation withbetween the observationstwo (r=0.59). For other species, the concentrations of OC and $PM_{2.5}$ were also improved slightly increased in emis-adjust compared to that of emis-orig, although they were underestimated in both scenarios. The NMB and NME of $PM_{2.5}$ satisfied the benchmarkbenchmarks recommended by Emery et al. (2017)Emery et al. (2017), while the NMB of the maximum daily 8-hour average (MDA8) O_3 exceeded the benchmarkcriteria. Table S5S4 shows that the concentrations of NO_2 and nitric oxide (NO) were underestimated at the Taizhou site suggested by the negative NMB values.. The simulated OH radicals comparedagreed well with the observationobservations while the concentrations of HO_2· were underestimated at the Taizhou site (Fig. S5).S4). It should be noted that the influences of different SOA schemes for MN on the aforementioned species are negligible. The predicted concentrations of MDA8 O_3, $PM_{2.5}$, SO_2, NO_2, and CO in other cities were also examined as shown in Table S4.. Overall, the model agreed well with observations in most of the cities except for a significant underestimation of MAD8 O_3 in Shanghai. We chose the (Table S3). The results fromof case-1product and case-2products using emis-adjust as the emission data were superior compared to the cases using emis-orig. These findings will be further discussed in the subsequent analysis.

3.2 Influences of Nap and MN on SOC in Taizhou

Figure 23 depicts the diurnal variations of emissions and concentrations of Nap, 1-MN, and 2-MN, as well as the corresponding SOC products SOC-Nap, SOC-1MN, and SOC-2MN at the Taizhou site in both case-1product and case-2products. The emissions of Nap, 1-MN, and 2-MN

exhibited a bimodal pattern. For Nap, the bimodal characteristics were the most pronounced, accompanied by two peaks that occurred between 8:00~9:00 and 16:00~17:00, respectively. This ~~was~~is likely attributed to the dominant source of Nap from ~~transport~~transportation as described in Sect. 2.2. Nap and MN concentrations were relatively low during the daytime and peaked in the morning and at night~~, which was~~. This is caused by the fast photochemical removal and increased dilution during the daytime, along with the facilitated accumulation due to low mixing heights at night (~~Cohan et al., 2013;~~ Huang et al., 2019; Cohan et al., 2013)~~.~~. The simulated diurnal variation of Nap agreed well with observations, but the daytime MN concentration was underpredicted as shown in Fig. S5. The concentrations of SOC generated by Nap, 1-MN, and 2-MN were high during the daytime, especially from 10:00 to 15:00. This ~~was~~is attributed to the removal of Nap and MN by OH radicals to form SOC. The potential removal by ~~nighttime~~ nitrate radicals (NO_3) was negligible in this study, leading to a ~~certain degree of declining trend for~~decline in SOC formation at night. Nap-derived SOC was the most abundant, followed by SOC from 2-MN ~~(SOC-2MN)~~ and 1-MN ~~(SOC-1MN).~~. This is attributed to the combined effects of the OH· reactivity, SOA yields, as well as abundances of the three compounds (Li et al., 2017; Yu et al., 2021). ~~Apart from the highest emissions of Nap, Nap is also more reactive with OH· and has the highest SOA yield in case-2products compared to the other two species. In case-1product, although the SOA yields of MN are the highest, the OH· reaction rate with Nap is faster than MN.~~Apart from having the highest emissions, Nap also exhibits greater reactivity with OH·. Although its SOA yield under high-NO_x conditions is lower than that of MN fitted by the one-product scheme (Fig. S6), its SOA yield under low-NO_x conditions is the highest among the three PAHs (Table S1). Overall, Nap contributed the most to SOC. 2-MN demonstrates higher SOA yields than 1-MN under high-NO_x conditions in both cases, but a lower SOA yield under low-NO_x conditions. Considering the impact

of a higher emission rate (Fig. 3a and 3c), 2-MN contributed two times more SOC compared to 1-MN. The SOC generated by MN in case-2products was lower than that in case-1product due to the lower SOA yield ~~of MN~~ applied in case-2products ~~as shown in Table S1.~~(Fig. S6).

Figure ~~3~~4 shows the contributions of major aromatic species, i.e., Nap, 1-MN, 2-MN, 1,2,4-trimethyl benzene (B124), xylene (MPO), benzene (BENZ), toluene (TOLU), aromatics with k_{OH} (reaction rate constant with OH•) < 2×10^4 ppm^{-1} min^{-1} (ARO1) and ARO2MN' (ARO2 excluding Nap and MN) to the total emissions of aromatics and the aromatic-derived SOC in both case-1product and case-2products at the Taizhou site. Among all the species, ARO2MN', MPO, and B124 showed the largest fraction ~~of~~in emissions, accounting for 58.6%, followed by ARO1 and TOLU (31.8%), and BENZ (6.3%). Nap and MN contributed the least to the total aromatic emissions, with Nap ~~to be~~being the most abundant species. The daily average concentrations of SOC produced from all the aromatics ~~was~~were quite similar in case-1product and case-2products, ~~which were 102.0~~with the values of 101.3 and 100.~~7~~2 ng m^{-3}, respectively (Fig. ~~S6~~S7). The contribution of ARO2MN', MPO, and B124 to the total aromatic-derived SOC was the most significant, ~~which was~~ranging from 45.6% to 46.2~~–45.8~~%. Nap ~~showed~~indicated a remarkable contribution to SOC, accounting for 8.~~7–8.8%, although it~~2–8.3%, despite constituting only ~~made up~~ 2.6% of the total emitted aromatics. 2-MN was also an important SOC precursor, contributing ~~to~~ 1.~~3–2~~.2–2.0% of the aromatic-derived SOC. 1-MN ~~was~~showed the ~~least emitted aromatic compound~~lowest emissions, accounting for 0.2% of the total aromatic emissions and less than 1.0% of the aromatic-derived SOC. ~~All of~~Overall, Nap, 1-MN, and 2-MN ~~had~~exhibited the same trait of contributing ~~much~~significantly more to SOC than to ~~SOC~~ precursor emissions, especially for Nap. The total contributions of MN and Nap to SOC were higher than that of BENZ, even though their emissions were significantly lower than BENZ. Similar results were also found in field campaigns

conducted in Guangzhou ~~(Fang et al., 2021)~~(Fang et al., 2021) and Beijing ~~(Huang et al., 2019)~~(Huang et al., 2019) where Nap and MN showed higher contributions. Compared to ~~BENZ~~benzene and other ~~single-ring~~monocyclic aromatics, the oxidation products of Nap and MN ~~belong to IVOCs with lower saturation vapor pressure, which is~~are much less volatile and are more ~~likely to generate SOA through coagulation and absorption~~efficient at aerosol growth (~~Gao~~Wang et al., ~~2021; Zhao et al., 2014~~2020b). Thus, their considerably higher SOA yields and reactivity with OH· lead to an important contribution to SOA formation. ~~In general, we~~We found that 3.3% of aromatic emissions from Nap and derivatives ~~could contribute~~contributed up to ~~11.7%~~10.9% of SOC generated from aromatics at the Taizhou site.

3.3 Regional distributions of Nap and MN and the influences on secondary pollutants

In the YRD, ~~the average contribution of~~ Nap ~~to aromatic emissions was 4.1% (Fig. S7), while the Nap-derived SOC~~ accounted for ~~9~~4.1% of aromatic emissions and contributed 8.0% and ~~9~~8.1% of the total SOC generated by aromatics in case-1product and case-2products, respectively~~.~~ (Fig. S8). We found extremely high contributions of Nap-derived SOC in areas with high Nap emissions ~~(Fig. S8),~~, reaching up to ~~13.7~~12.6% in case-2products. 2-MN ~~constituted~~contributed 0.6% of the total aromatic emissions and ~~contributed~~ up to ~~3.8~~2.5% of the aromatic-derived SOC in case-1product. Among the three PAHs, 1-MN showed the lowest emissions (about 0.4% of the aromatic emissions) and contributed minimally to the ~~smallest~~ regional average ~~contribution to~~ SOC (0.~~6~~4–0.~~9~~7%). The SOC derived from MN in case-2products was approximately 38% lower than that in case-1product across the entire YRD region (Fig. ~~S8~~S9), while minor differences were observed in O_3 and the total SOC ~~showed minor differences in~~between the two cases with different SOA parameterization of MN (Fig. ~~S9~~S10). In general, the concentrations of SOC produced by the three PAHs in case-1product were higher than ~~those in case-2products, which may minimize the~~

~~discrepancy between the simulated and observed OC given the existing underestimation of OC at least in Taizhou, as shown in Fig. 1 and Fig. S6. Therefore, we opted for~~that in case-2products, exhibiting similar spatial distribution patterns in both cases. We will focus on the results from case-1product in the subsequent analysis.

~~The accurate reproduction and quantitative constraints~~Accurate representation of Nap and MN ~~are~~sources and sinks in model simulations is crucial for ~~understanding~~comprehending the atmospheric oxidation capacity~~ in model simulations.~~. The relative differences between ~~base1~~base_zeroNapMN and case-1product were calculated to evaluate the effects of Nap, 1-MN, and 2-MN on O_3, SOC, and radical concentrations. As shown in Fig. ~~4a~~5a, the SOC concentrations ~~over~~in the YRD ~~region~~ increased by approximately ~~1.~~0.9% on average, with the most significant ~~increase~~change observed in areas with high emissions of Nap and MN, such as Shanghai and southern Jiangsu Province, reaching up to 1.7%. The impact on O_3 was relatively limited, with a maximum increase of 0.3~~%.~~%, primarily attributed to Nap rather than MN (Fig. S11). Similar to SOC, the spatial distribution of O_3 variations was consistent with that of Nap and MN emissions. ~~When~~By considering the oxidation of Nap and MN ~~oxidation was considered~~ in the model, HO_2· concentration was enhanced across the domain by up to 1.6% (in Shanghai), likely due to the production of HO_2· through the reaction of Nap and MN with OH·. However, the variations in OH· concentration exhibited regional heterogeneity, with a maximum increase of 0.~~8% (~~7% in Shanghai~~)~~ and a maximum decrease of 0.3% ~~(~~in Wenzhou~~).~~. The areas with elevated OH· coincided with the locations experiencing notable increases in O_3. As an OH· source in the troposphere, the photolysis of O_3 produces electronically excited O(^{1}D) atoms that react with water molecules to form fresh OH· (Qin et al., 2022; Tan et al., 2019~~; Qin et al., 2022~~). Moreover, the areas with elevated OH· also exhibited a significant increase in HO_2·. HO_2· can react with O_3 ~~to~~

~~produce OH·, thereby offsetting the OH· consumption by Nap and MN oxidations (Zhu et al., 2020).~~or NO to produce OH·, thereby offsetting the OH· consumption by Nap and MN oxidation (Zhu et al., 2020). In the areas with decreased OH·, the ~~increase~~increases of O_3 and HO_2· ~~was not significant~~were insignificant, resulting in ~~fewer newly generated~~a reduced generation of OH· to compensate for the OH· consumption by Nap and MN. Similar to O_3, variations in OH· and HO_2· were primarily influenced by Nap rather than MN (Fig. S11).

To ~~minimize the potential obfuscation of~~avoid obscuring the true magnitude by averaging over the entire episode~~ average variation, the hourly~~, daily relative differences of SOC, O_3, and radicals at the Shanghai and Suzhou sites, which exhibit significant variations, are ~~depicted~~shown in Fig. ~~4b~~5b and ~~Fig. 4c, respectively~~5c. Overall, the influences of Nap and MN varied daily. At the Shanghai site, the most pronounced effects ~~of~~on OH· and HO_2· were observed, with increases of up to 1.~~7~~9% and 3.~~7~~8%, respectively. At the Suzhou site, the maximum daily variations of OH· and HO_2· (1.5% and 2.9%) were ~~marginally~~slightly lower than those in Shanghai~~; whereas~~. However, the ~~maximum~~ daily ~~variations of~~ SOC and O_3 were elevated by up to 3.0% and 1.1% ~~at the~~in Suzhou ~~site~~, respectively. It was found that both OH· and HO_2· displayed bimodal variations at the two sites, with the most pronounced changes of 0.7–1.0% and 1.6–2.2% occurring in the morning, respectively (Fig. S12). The concentrations of SOC and O_3 were elevated in the daytime, reaching peak increments of 2.1–2.3% and 0.4–0.5% at noon. Consequently, the influences of Nap and MN on SOC, O_3, and the atmospheric oxidation capacity were substantial at the daily scale in those regions.

4 Discussion

Our results revealed that the contributions of Nap and MN to the total aromatic emissions were minimal, which were 5.1% in the YRD and 3.3% at the Taizhou site. However, the SOC

produced by Nap and MN ~~constituted 12.1~~accounted for 10.4% of the total aromatic-derived SOC in this region and ~~11.7~~10.9% at the Taizhou site. Given the overestimation of other aromatic species in the current model (Table ~~S5~~S4), the contributions of Nap and MN to aromatic SOC ~~might~~may be underestimated. ~~Yu et al. (2021)~~Yu et al. (2021) demonstrated an augmented fraction of SOC derived from a yield method to that using the EC tracer method after the inclusion of Nap and MN oxidation (from 25.3% to 39.5%) during the same episode at the Taizhou site. That is to say, Nap and MN ~~contributed~~contribute 35.9% of the total SOC estimated by using the SOA yield multiplied by the consumption of VOCs, which ~~was~~is higher than the value (~~11.7~~10.9%) in this study. Other field studies have also found significant SOA formation from Nap and MN among aromatics in the Pearl River Delta region (12.4%) ~~(Fang et al., 2021)~~(Fang et al., 2021) and in Beijing during haze days (10.2±1.3%) ~~(Huang et al., 2019)~~(Huang et al., 2019), with relatively smaller contributions to emissions of aromatics by less than 2% and 7%, respectively. This study highlights the ~~crucial~~important roles of Nap and MN, which exhibit high SOA ~~production~~formation potentials with trace amounts emitted into the atmosphere. In addition, the average concentrations of Nap and MN in this study were ~~27~~25 and ~~9~~7 ppt during summer over the YRD region (Fig. ~~S8~~S9), respectively. Previous studies have confirmed that the concentrations of Nap and MN exhibited a seasonal variation, with maxima in winter and minima in summer, attributed to the increased heating and cooking activities in households during the cold season (~~Tang et al., 2020;~~ Huang et al., 2019; Fang et al., 2021; Tang et al., 2020). Consequently, the ambient concentration of Nap and MN, along with the potential SOA production may be more severe in winter. Cleaner fuel types and household cleaning products are recommended for vehicular and domestic usage.

The ~~urgent demand for enhancing the~~improvement in simulation and assessment of Nap and MN chemistry is ~~necessitated~~crucial. Firstly, the characterization of Nap and MN from local sources and additional field observations are indispensable to reduce the disparities between the modeled and observed Nap and MN concentrations. Secondly, the SOA parameterizations of Nap and MN, including the enthalpy of vaporization and SOA yields, are derived from limited chamber experiments and require further validation. Previous studies have reported that the SOA yields obtained from chamber studies were contingent on OH· exposure, NO_x levels, relative humidity, and seed particles, which may not represent the actual atmospheric conditions (Yu et al., 2021; Ling et al., 2022). Thirdly, chlorine radicals (Cl), NO_3 radicals, and O_3 also play an important role in the atmospheric reactions of Nap and MN (Wang et al., 2005; Cohan et al., 2013; ~~Matthieu et al., 2014;~~ Riva et al., 2015~~; Wang et al., 2005;~~ , 2014; Aleman, 2006), which were missing in the current study due to the lack of parameterization.~~–~~ The formation of gas- and particle-phase products through reactions between Cl atoms and Nap has been confirmed. For instance, chloronaphthalene and chloroacenaphthenone have been identified as potential SOA markers for the Cl-initiated oxidation of Nap in the ambient atmosphere ~~(Riva et al., 2015).~~(Riva et al., 2015). As important sources of Cl atoms, abundant nitryl chloride ($ClNO_2$) and molecular chlorine (Cl_2) ~~were~~are attributed to sea salt, coal combustion, biomass burning (Le Breton et al., 2018), and urban-originated ~~transports~~transport (Li et al., 2021; Tham et al., ~~2013~~2014). Consequently, the Cl-initiated SOA formation process may be pronounced in specific regions, such as the marine boundary layer and industrial areas. Using the rate constant of Cl with Nap ($(4.22\pm0.46)\times10^{-12}$) ~~(Matthieu et al., 2014)~~ (Riva et al., 2014) and corresponding SOA yields (0.91±0.05) ~~(Riva et al., 2015), which is approximately~~(Riva et al., 2015), which is up to three times higher than those determined from OH-initiated oxidation (Chan et al., 2009; Shakya and Griffin, 2010), we

estimated the potential SOA formation from the reaction of Nap and Cl atoms via a yield method (Huang et al., 2019; Yu et al., 2021). ~~Assuming a global average Cl concentration of 1×10^4 molecules cm^{-3} and a tropospheric lifetime of 275 days as determined by Matthieu et al. (2014), SOA generated from Nap initiated by Cl atoms is three times higher than that from the oxidation by OH· with a 12-h average daytime concentration of 2×10^6 molecules cm^{-3} and a tropospheric lifetime of 6 hours.~~Assuming a 12-h average daytime OH· concentration of 2×10^6 molecules cm^{-3} and a photooxidation age of 6 h, the SOA generated from Nap oxidation by Cl atoms can reach up to 56% of that from the Nap + OH pathway in highly polluted regions with a Cl/ OH ratio greater than 0.8 (Choi et al., 2020). This suggests that the omission of Cl-initiated chemistry in this study might lead to an underestimation of Nap-derived SOA by approximately ~~75~~36%. Given the underestimation of anthropogenic chlorine emissions in China (~~Li et al., 2021;~~ Choi et al., 2020; Li et al., 2021), further studies are recommended to estimate chlorine emissions with finer spatial resolution and the impacts on Nap SOA under atmospherically realistic conditions. Lastly, a precise depiction of Nap and MN chemistry is crucial for gaining a deeper understanding of the health implications of these noxious compounds. The health risks associated with inhalation exposure to outdoor Nap and other PAHs have been assessed by calculating the incremental lifetime cancer risk (ILCR) values in China and the United States (Han et al., 2020; Zhang et al., 2016). Nonetheless, there has been no systematic evaluation of the health risks resulting from exposure to PAH-derived SOA and by-products, despite previous studies verifying the toxicological impacts (e.g. oxidation potential, OP) of Nap-derived SOA (~~Lima de Albuquerque et al., 2021;~~ Wang et al., 2018; Tuet et al., 2017a; Tuet et al., 2017b; Lima de Albuquerque et al., 2021). More precise measurements of the OP of ~~the~~ different ~~individual~~ SOA components are needed ~~in order~~ to evaluate the overall oxidative potentials of ambient SOA ~~using individual~~

~~intrinsic OP of different types of SOA in conjunction with SOA loadings in models~~. Future studies are needed to develop rational parameterization schemes for assessing the health risks associated with Nap- and MN-derived SOA.

5 Conclusions

In this study, we investigated the impacts of Nap, 1-MN, and 2-MN oxidation on the formation of SOC, O_3, and radicals from May 20 to June 18, 2018, in the YRD using a revised CMAQ model and explicit emission inventories. The ~~simulating~~ results of case-1product, using the adjusted emissions (emis-adjust) and a one-product method ~~to fit~~for fitting MN ~~yields~~SOA, best ~~reproduced~~captured the observed evolution of Nap (NMB=0.01) and MN (NMB=-0.07) when compared ~~with~~to the default case (NMB=-0.79 for Nap, NMB=-0.85 for MN). The primary sources of Nap and MN were transportation and residential-related ~~and thus led to~~ sectors, resulting in a bimodal emission pattern ~~for their emissions. Whereas the Nap and MN~~ . The concentrations of Nap and MN were ~~relatively low~~lowest during the daytime ~~and peaked~~, peaking in the morning~~,~~ ~~the generated~~ and at night. Their SOC ~~peaked in~~concentrations reached the maximum value during the daytime ~~affected by~~due to the ~~photochemistry~~photooxidation of Nap and MN and ~~the evolution of the~~ boundary layer~~. All of~~ evolution. Nap, 1-MN, and 2-MN ~~had~~exhibited the same trait of contributing ~~much~~ more to aromatic-derived SOC than to ~~SOC precursor~~ emissions of aromatic hydrocarbons, especially for Nap. ~~In general, we found that 3.3% of aromatic emissions from Nap and derivatives could contribute up to 11.7% SOC generated from aromatics at the Taizhou site.~~ The average concentration of Nap ~~concentrations reached 27~~was 25 ppt in the YRD, accounting for 4.1% and ~~9~~8.1% (up to ~~13.7~~12.6%) of total ~~aromatics~~aromatic emissions and aromatic-derived SOC, respectively. The concentrations of 1-MN and 2-MN were relatively low, with ~~an~~ average values of ~~3 and 6~~2 ppt ~~in the YRD, and~~and 5 ppt, respectively, Together, they contributed ~~3.1~~only

2.4% of the aromatic-derived SOC. At the regional scale, the impacts of Nap and MN oxidation on O_3 and radical concentrations were limited. However, substantial increases still occurred in areas with high Nap and MN emissions ~~and~~, which cannot be ~~disregarded~~ignored. The high SOA formation ~~potential~~potentials of Nap and MN and ~~its impact~~their impacts on secondary pollutants ~~proved in this study implied~~highlight the ~~significance~~importance of ~~such~~considering these IVOCs ~~except for~~alongside traditional VOCs when implementing air pollution control policies, energy use strategies, and health risks evaluation.

Code and data availability

The codes used for all the analyses are available on reasonable request to the corresponding author. All data used in this research are freely available and may be downloaded from the links and cited references given in the methods section.

Author contributions

F.Y., J.L., and J.H. designed the research and conducted the simulations~~,~~. Y.G., H.W., S.G., and K.L. collected the ~~observed~~observation data. J.A. and C.H. provided emission data. F.Y~~.,~~, led data analysis and drafted the main text. J.L., J.H., and M.Q. analyzed the data~~, all~~. All authors ~~discussed~~contributed to interpreting the results~~. F.Y. prepared the manuscript and all authors helped improve~~ and editing the manuscript.

Competing interests

The authors declare no competing interests.

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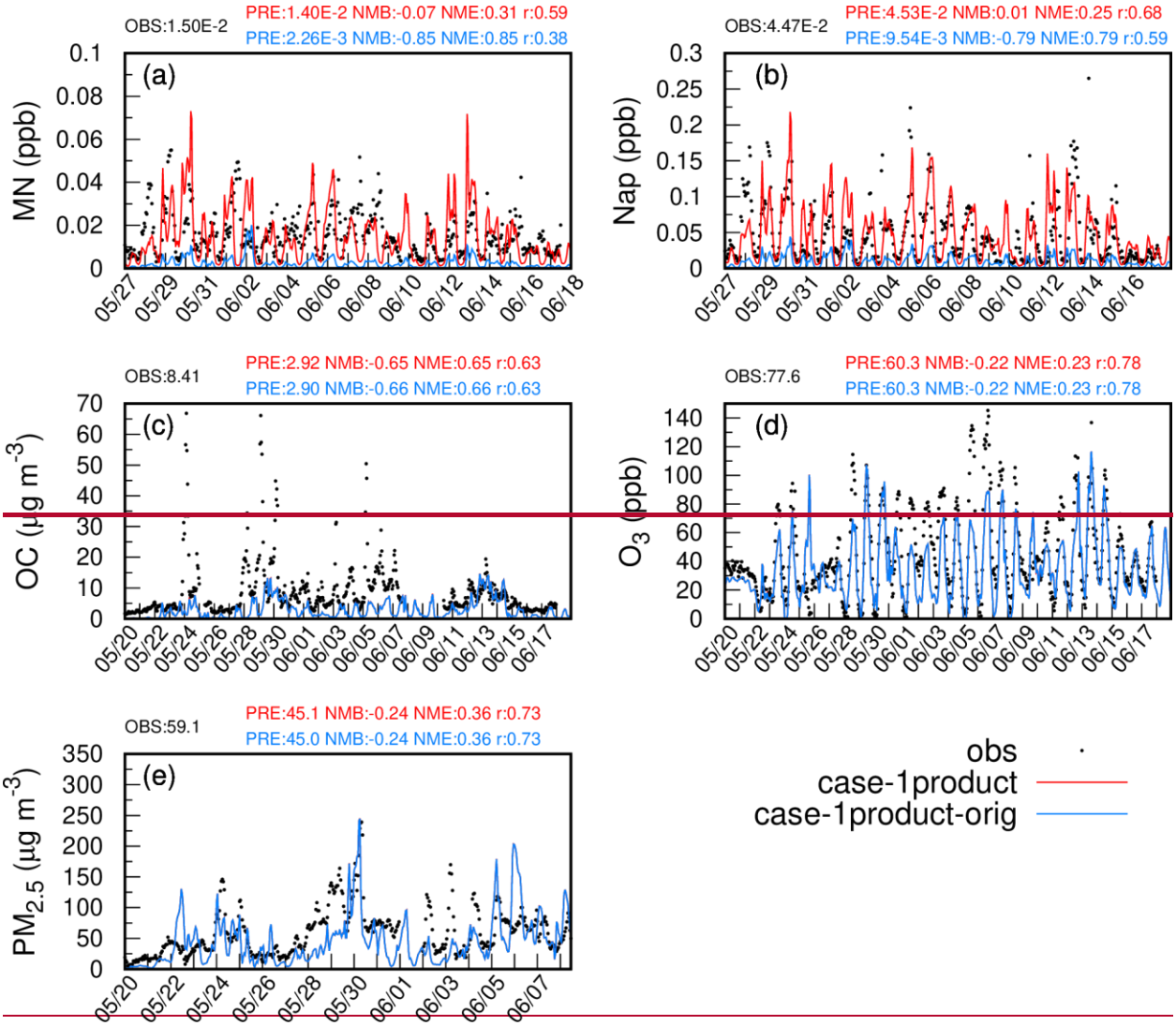

OBS:1.50E-2
PRE:1.40E-2 NMB:-0.07 NME:0.31 r:0.59
PRE:2.26E-3 NMB:-0.85 NME:0.85 r:0.38
(a)
MN (ppb)
OBS:4.47E-2
PRE:4.53E-2 NMB:0.01 NME:0.25 r:0.68
PRE:9.54E-3 NMB:-0.79 NME:0.79 r:0.59
(b)
Nap (ppb)
OBS:8.41
PRE:2.92 NMB:-0.65 NME:0.65 r:0.63
PRE:2.90 NMB:-0.66 NME:0.66 r:0.63
(c)
OC (μg m-3)
OBS:77.6
PRE:60.3 NMB:-0.22 NME:0.23 r:0.78
PRE:60.3 NMB:-0.22 NME:0.23 r:0.78
(d)
O3 (ppb)
OBS:59.1
PRE:45.1 NMB:-0.24 NME:0.36 r:0.73
PRE:45.0 NMB:-0.24 NME:0.36 r:0.73
(e)
PM2.5 (μg m-3)
obs
case-1product
case-1product-orig

~~Figure 1.~~

Table 1. Settings of the scenarios.

Case	Emission setting	SOA parameterization for MN
case-1product-orig	Nap emissions in the YRD were based on the 2017 YRD inventory; Nap emissions in the rest of the domain and MN emissions in the entire domain were calculated using sector-specific mass ratios and total emissions of non-methane volatile organic compounds (emis-orig)	one-product method
case-2products-orig		two-product method
case-1product	The anthropogenic emissions of Nap and MN in the entire domain from emis-orig were multiplied by 5 and 7, respectively (emis-adjust)	one-product method
case-2products		two-product method
base_zeroNapMN	Emissions of Nap and MN were set to zero based on emis-adjust	one-product method
base_zeroMN	Emissions of MN were set to zero based on emis-adjust	one-product method

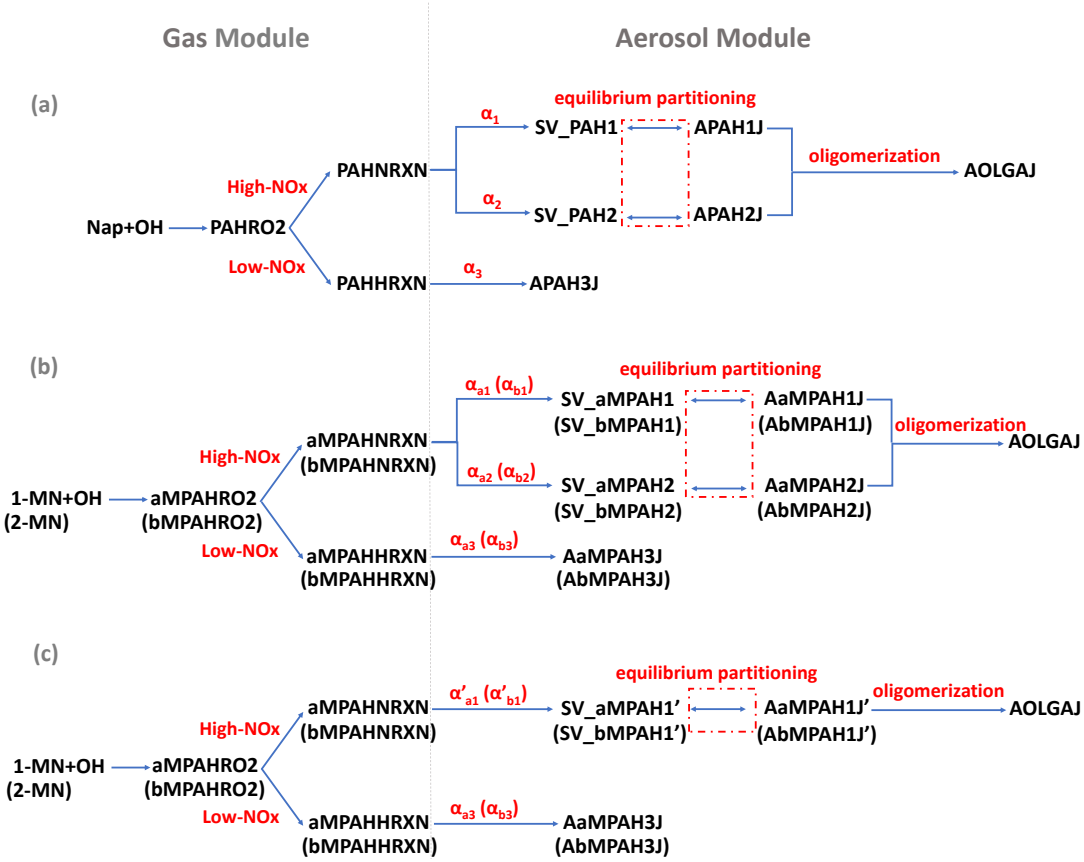


Figure 1. SOA schemes for naphthalene (Nap), 1-methylnaphthalene (1-MN), and 2-methylnaphthalene (2-MN) in the updated CMAQ model. (a) pre-existing Nap-derived SOA formation pathways fitted by two products under high NO_x; (b) newly added SOA formation pathways for 1-MN and 2-MN fitted by two products under high NO_x; (c) newly added SOA formation pathways for 1-MN and 2-MN fitted by one product under high NO_x. SOA formation from Nap and MN oxidation by OH radicals under low-NO_x conditions is represented by a fixed yield. Parameters for 2-MN are indicated in brackets in (b) and (c). The values of α refer to Table S1.

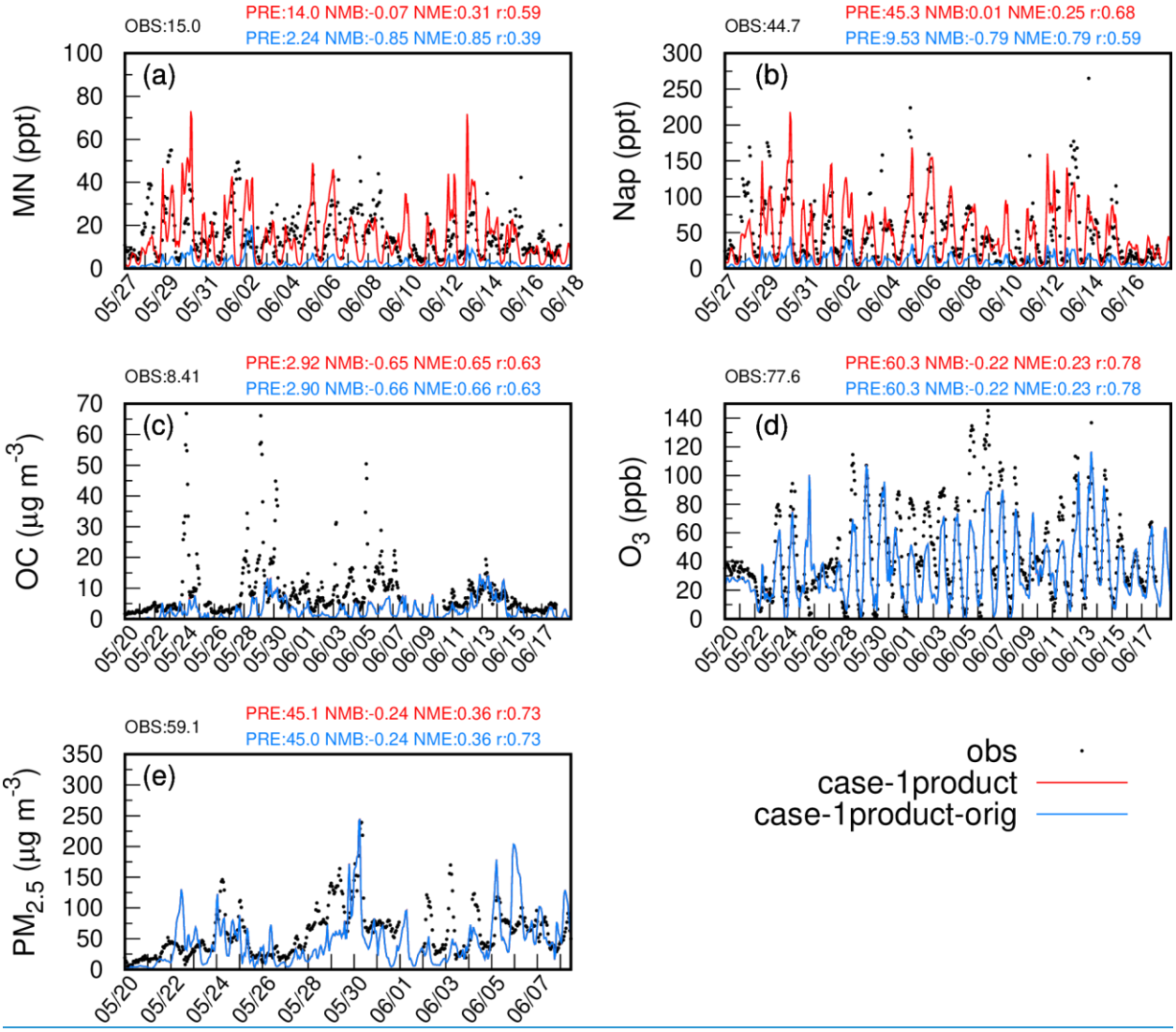
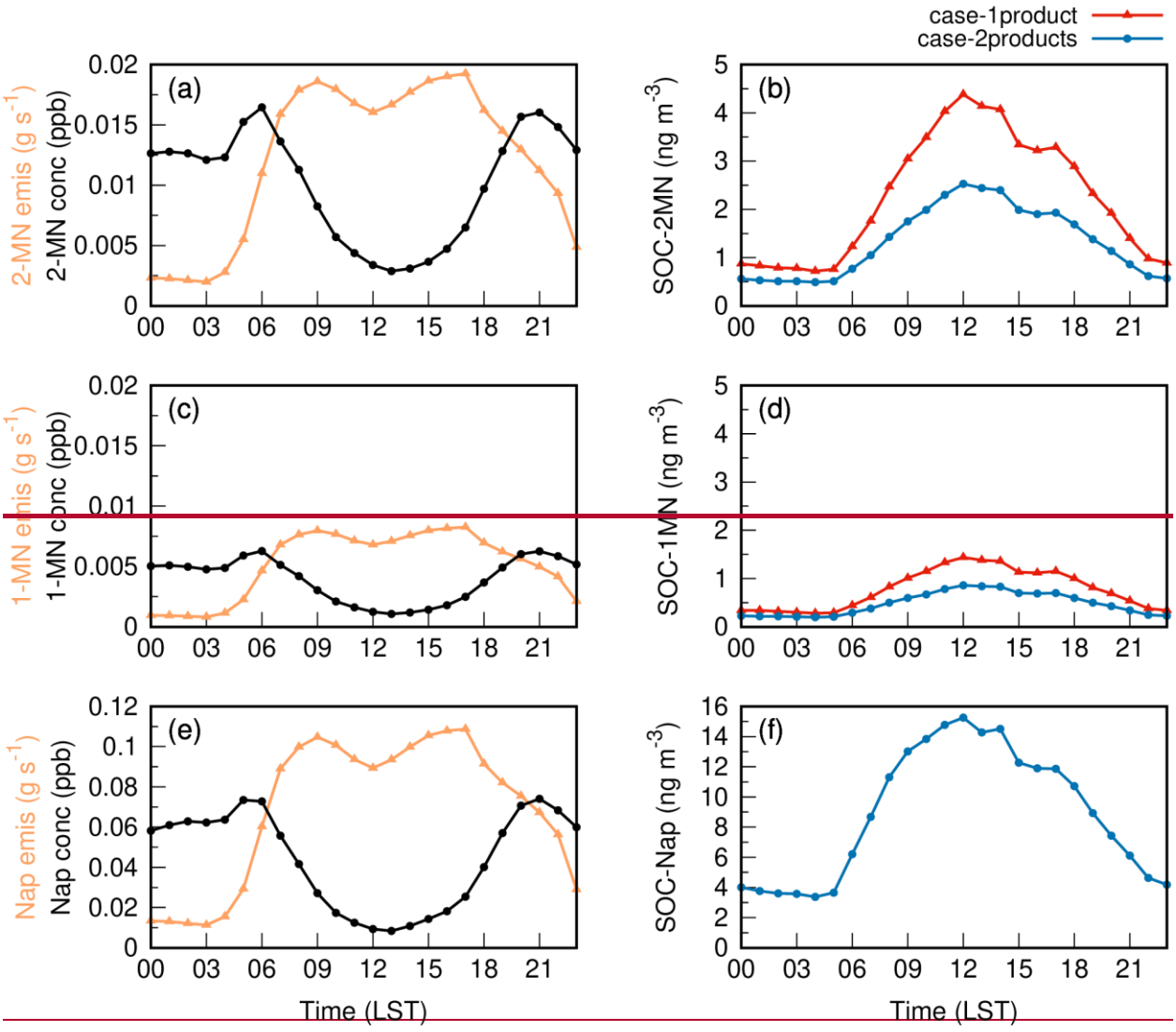


Figure 2. Observed and simulated hourly concentrations of MN, Nap, OC, $PM_{2.5}$, and O_3 based on emis-adjust (red) and emis-orig (blue) at the Taizhou site. Model performances ~~of~~for daily MN, Nap, OC, $PM_{2.5}$, and MDA8 O_3 are shown in blue for case-1product-orig and in red for case-1product. OBS and PRE represent ~~averaged concentrations~~the average of observations and predictions, respectively. Note that the red and blue lines overlap in (c)-(e).


case-1product
case-2products
(a)
(b)
(c)
(d)
(e)
(f)
2-MN emis (g s-1)
2-MN conc (ppb)
SOC-2MN (ng m-3)
1-MN emis (g s-1)
1-MN conc (ppb)
SOC-1MN (ng m-3)
Nap emis (g s-1)
Nap conc (ppb)
SOC-Nap (ng m-3)
Time (LST)
Time (LST)

754

755

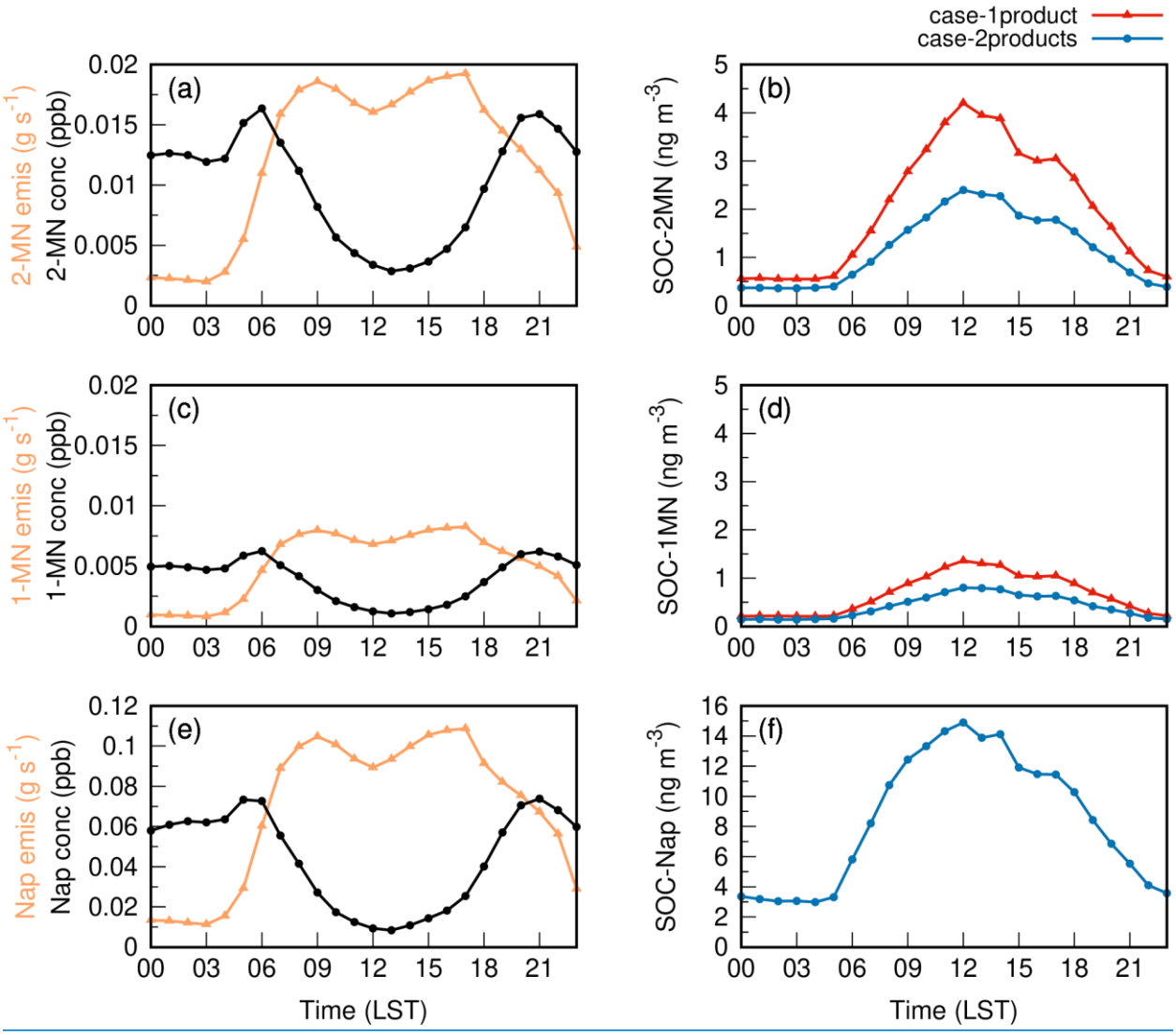


Figure ~~2~~3. Diurnal variations of emissions (yellow line) and predicted concentrations (black line) for 2-MN (a), 1-MN (c), and Nap (e), as well as the corresponding SOC concentrations (b, d, f) at the Taizhou site. Note that the red and blue lines overlap in (f).

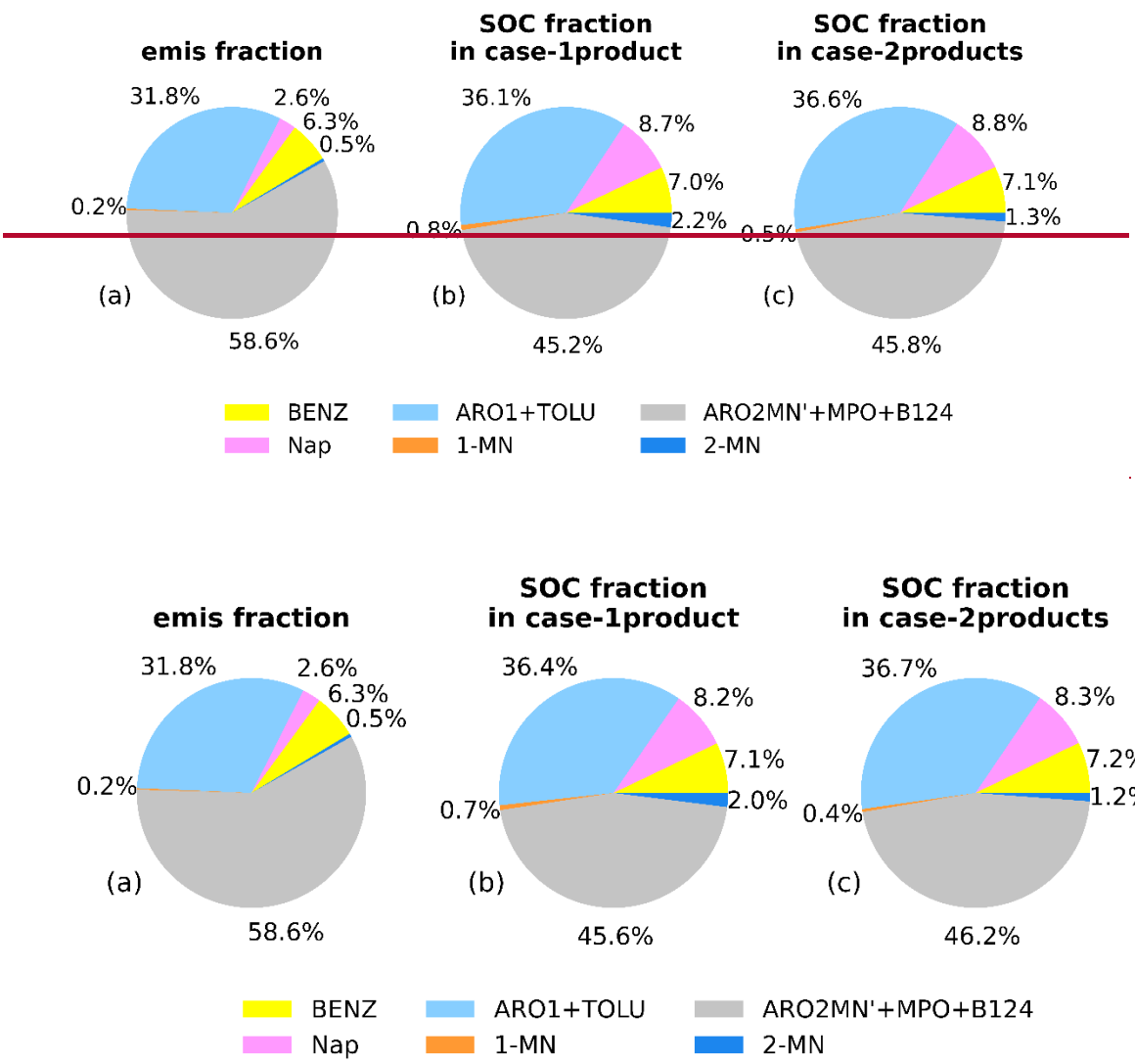
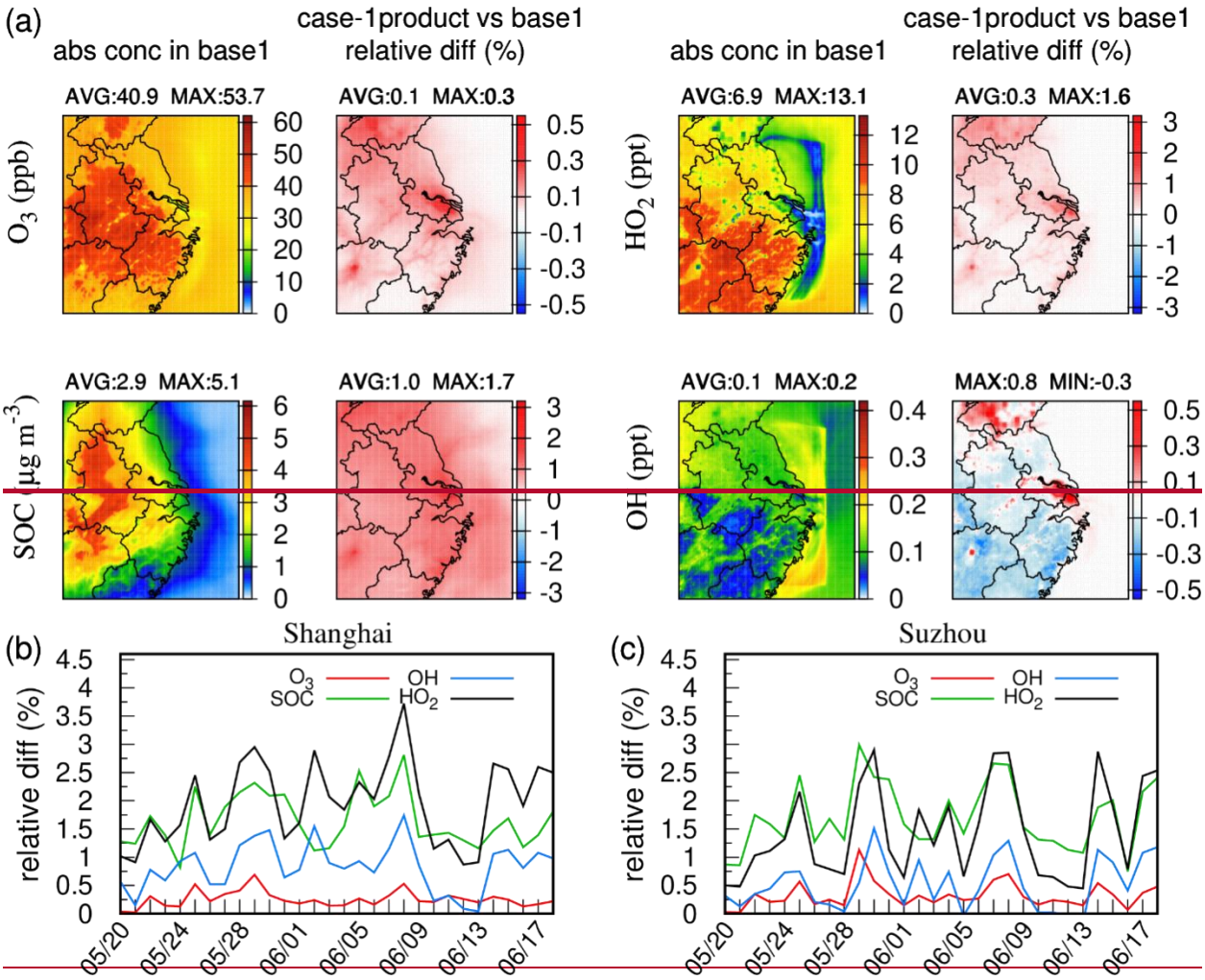


Figure ~~3~~4. Contributions of the major aromatic species to (a) the total emissions of aromatics (weight fraction) and the aromatic-derived SOC in (b) case-1product and (c) case-2products at the Taizhou site. ~~These~~The aromatic species ~~are~~include Nap, 1-MN, 2-MN, BENZ, the sum of toluene and aromatics with k_{OH} < 2x10^4 ppm^{-1} min^{-1} (ARO1+TOLU), and the sum of xylenes, 1,2,4-trimethyl benzene and aromatics with k_{OH} > 2x10^4 ppm^{-1} min^{-1} excluding Nap and MN (ARO2MN'+MPO+B124).


(a)
abs conc in base1
case-1product vs base1
relative diff (%)
AVG:40.9 MAX:53.7
AVG:0.1 MAX:0.3
AVG:6.9 MAX:13.1
AVG:0.3 MAX:1.6
O3 (ppb)
HO2 (ppt)
AVG:2.9 MAX:5.1
AVG:1.0 MAX:1.7
AVG:0.1 MAX:0.2
MAX:0.8 MIN:-0.3
SOC (μg m-3)
OH (ppt)
(b)
Shanghai
(c)
Suzhou
relative diff (%)
O3
OH
SOC
HO2
05/20
05/24
05/28
06/01
06/05
06/09
06/13
06/17

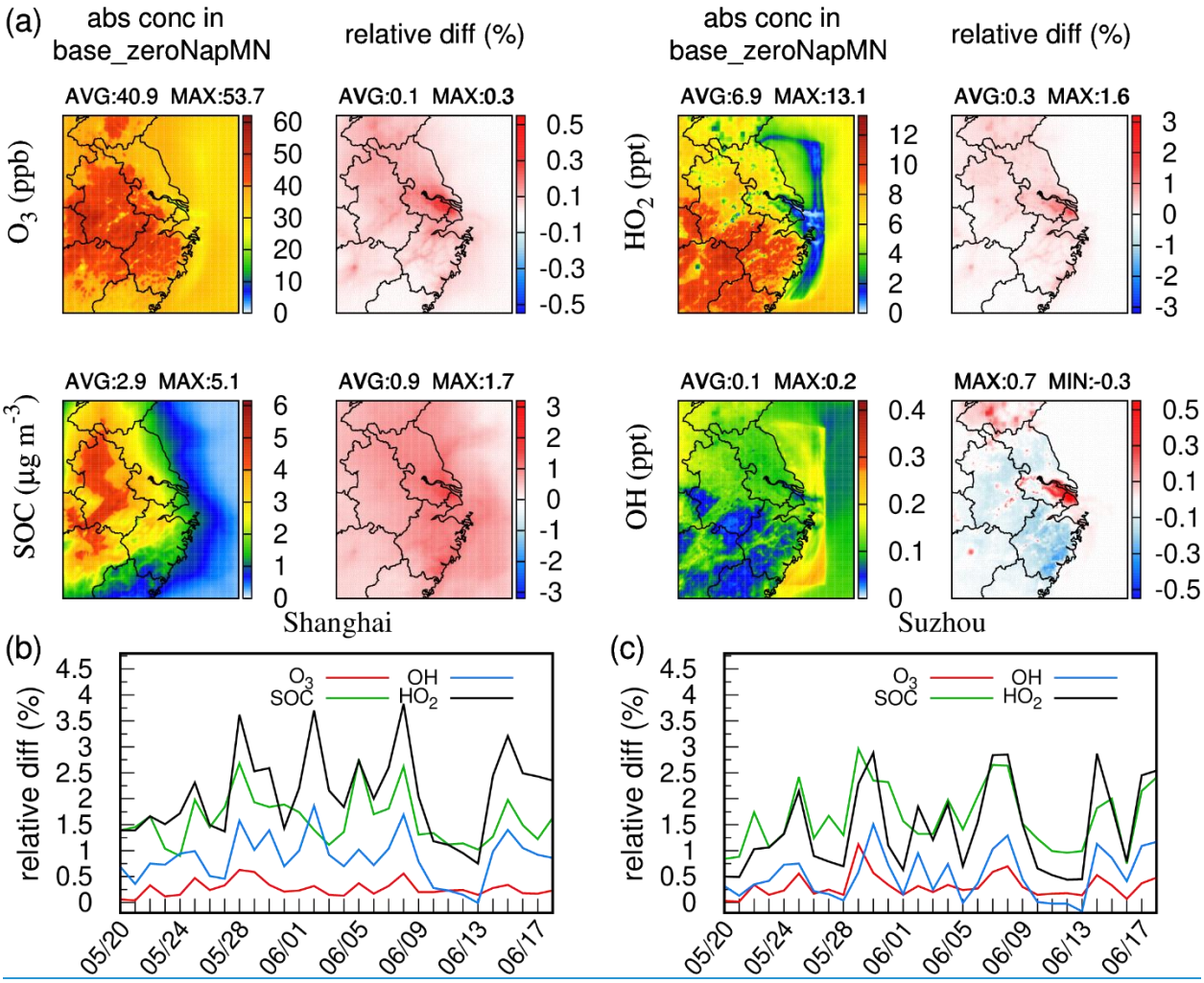


Figure 45. (a) ~~Absolute~~Average concentrations of SOC, O_3, OH~~,~~, and HO_2 in ~~base1,~~base_zeroNapMN and changes in case-1product relative to ~~base1, respectively.~~base_zeroNapMN. Daily relative changes in case-1product compared to ~~base1 at~~base_zeroNapMN in (b) Shanghai and (c) Suzhou.