

Particle Acidity and Seed Aerosol Drive the Spatiotemporal Dynamics of Isoprene-Epoxydiol-Derived Secondary Organic Aerosols in Eastern China

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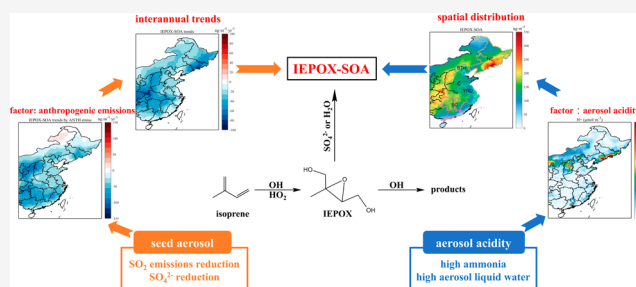
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ABSTRACT: Isoprene, a major global precursor to secondary organic aerosol (SOA), affects air quality and radiative forcing. A key SOA formation pathway is the reactive uptake of isoprene epoxydiol (IEPOX), a process influenced by multiple environmental factors. Here, we simulate the spatial distribution and interannual trend of IEPOX-SOA over Eastern China from 2014 to 2019 using CMAQ and quantify the contributions of different factors. Our results indicate that ambient IEPOX-SOA concentrations are elevated in central and northeast China, averaging $135 \text{ ng}\cdot\text{m}^{-3}$ and with a recent declining trend between -19.1 and $-34.8 \text{ ng}\cdot\text{m}^{-3}\cdot\text{yr}^{-1}$. Long-term trends of IEPOX-SOA are primarily driven by changes in sulfate ($-50.5 \text{ ng}\cdot\text{m}^{-3}\cdot\text{yr}^{-1}$), which serve as seed aerosols, while a decrease in organic carbon reduces the coating effects and partially offsets ($+16.1 \text{ ng}\cdot\text{m}^{-3}\cdot\text{yr}^{-1}$) the decline. Aerosol acidity plays a key role in governing its spatial distribution by affecting reactive rates. In Eastern China, high ammonia levels effectively neutralize acidity, thereby suppressing abundant IEPOX-SOA formation, resulting in lower concentrations compared to other regions, such as the United States. Sensitivity tests indicate that substantial future NH_3 reductions in China could increase the IEPOX-SOA by up to 100%. This study clarifies the key chemical mechanisms governing IEPOX-SOA production and supports regional air pollution control strategies.

KEYWORDS: isoprene epoxides, secondary organic aerosols, aerosol acidity, anthropogenic emissions



1. INTRODUCTION

Secondary organic aerosol (SOA), a major constituent of fine particulate matter ($\text{PM}_{2.5}$), significantly impacts air quality, climate radiative forcing, and human health.^{1–3} As one of the most important biogenic precursors of SOA,^{4,5} isoprene has been estimated to contribute up to 70% of the global SOA burden.^{6–8} This highly reactive compound is rapidly oxidized by atmospheric oxidants such as OH and HO_2 ,^{9–11} leading to the formation of isoprene epoxide (IEPOX). IEPOX is subsequently taken up by acidic sulfate aerosols, producing various highly oxidized particle-phase SOAs such as organic sulfates, 2-methyltetrols, 2-methyl sulfate, C_5 olefin triols, and oligomers.^{12–14} IEPOX-derived SOA (IEPOX-SOA) tracers account for 12–19% of the total SOA in certain regions,¹⁵ with methyltetrols alone contributing 5.2–8.9% of the organic aerosol (OA) in the southeastern United States. These findings underscore the importance of IEPOX-SOA, particularly in heavily polluted environments.^{16–18}

IEPOX-SOA formation is significantly modulated by isoprene concentrations, ambient pollution levels, and aerosol acidity. For instance, the presence of nitrogen oxides (NO_x) can inhibit IEPOX production by accelerating the conversion of isoprene to methacrylic acid epoxide (MAE) or hydroxymethyl methyl- α -lactone (HMML).^{14,19–22} In addition,

IEPOX-SOA formation is highly dependent on sulfate (SO_4^{2-}), which acts as seed aerosols, providing reaction sites for SOA generation.²³ Consistent with this, Xu et al.²⁴ observed concurrent peaks of isoprene-derived SOA in SO_4^{2-} -rich plumes over Centerville. Several modeling studies have also attributed long-term trends in IEPOX-SOA to changes in SO_4^{2-} levels.^{25,26} Additionally, numerous chamber experiments have demonstrated that acidity is a critical parameter for IEPOX-SOA formation as it enhances the rate of ring-opening reactions.²⁷ For example, Surratt et al.¹⁴ reported markedly higher SOA yields from acidified ammonium sulfate seed aerosols compared to their neutral counterparts. Nevertheless, substantial uncertainties remain in quantitatively linking aerosol acidity to IEPOX-SOA formation in both U.S. and Chinese field studies.^{23,28} Further

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investigation is therefore essential to elucidate the precise role of aerosol acidity in ambient IEPOX-SOA production.

Organic coatings also play a significant role in suppressing the uptake of IEPOX onto acidic sulfate seed aerosols. In ambient conditions, oligomeric organic matter can form surface coatings on particles, significantly reducing IEPOX uptake by SO_4^{2-} aerosols.^{29–32} Zheng et al.³³ notably improved the simulation of long-term OA trends in the southeastern United States by incorporating such coating effects into the GEOS-Chem model, thereby reducing the model's overestimation of IEPOX-SOA dependence on SO_4^{2-} . However, the contribution of the coating effects to IEPOX-SOA in China remains unquantified, and severe OA pollution in China may significantly impact IEPOX uptake rates. Therefore, a critical challenge remains in precisely understanding the mechanisms by which anthropogenic emissions modulate IEPOX-SOA formation via these processes.

Eastern China features abundant anthropogenic and biogenic emissions, creating an environment conducive to IEPOX-SOA formation through synergistic anthropogenic–biogenic interactions.^{34,35} Nevertheless, available field measurements indicate that IEPOX-SOA concentrations in China remain relatively low, typically ranging from 36.5 to 330 $\text{ng}\cdot\text{m}^{-3}$.^{36–38} Reports indicate that China emissions of NO_x and sulfur dioxide (SO_2) are 2–4 times higher than those in the United States.³⁹ IEPOX-SOA levels in Eastern China are significantly lower than those in the southeastern United States.^{23,39} The underlying causes of this discrepancy remain poorly understood and warrant further investigation. In recent years, the atmospheric environment in Eastern China has undergone substantial changes, with notable reductions in emissions of SO_2 , NO_x , and primary organic carbon (POC).^{40,41} Recent studies suggest that declining SO_4^{2-} concentrations are a primary driver of decreasing IEPOX-SOA over Eastern China.^{25,42} However, the roles of other factors—such as aerosol acidity and organic coating effects—remain insufficiently quantified and are not yet fully understood in this context. A better understanding of these processes is essential for evaluating the effectiveness of current air-quality policies and guiding future mitigation strategies.

This study aims to advance our understanding of key factors influencing the spatiotemporal distribution of IEPOX-SOA over Eastern China. We employed the Community Multiscale Air Quality Modeling System version 5.4 (CMAQ version 5.4) and added the organic coating effect mechanism, improving the representation of IEPOX uptake kinetics. We simulated the distribution and interannual trends of IEPOX-SOA during the summer months from 2014 to 2019 and evaluated model results against observed tracer compounds. Furthermore, we conducted systematic sensitivity analyses to quantify the impacts of various environmental drivers on the IEPOX-SOA trend and discussed the potential significance of IEPOX-SOA under future emission control scenarios.

2. MATERIALS AND METHODS

2.1. Model Configuration

Summertime IEPOX-SOA over Eastern China was simulated using the `saprc07_aero7i_aq` mechanism within the Community Multiscale Air Quality Model (CMAQ) version 5.4. This mechanism includes explicit treatment of isoprene chemistry and parametrization of IEPOX-SOA based on uptake coefficients.^{43,44} The coating effects on IEPOX uptake were incorporated into the model; a detailed description of this implementation is provided in Section 2.2.

The simulation domain encompasses mainland China and surrounding regions in East and Southeast Asia, with a horizontal resolution of 36×36 km. Anthropogenic emissions in China are derived from the Multiresolution Emission Inventory of China (MEIC) version 1.4, with a resolution of $0.25^\circ \times 0.25^\circ$. Biogenic emissions were generated using the Model for Emissions of Gases and Aerosols from Nature (MEGAN) v2.1,⁴⁵ based on annual specific leaf area index data from the 8-day moderate resolution imaging spectroradiometer (MODIS) LAI product (MOD15A2). The Fire Inventory from the National Center for Atmospheric Research (FINN)⁴⁶ was used for open-air biomass burning emissions.

Meteorological fields for driving both MEGAN and CMAQ were generated using the Weather Research and Forecasting (WRF) model, version 4.2. The WRF configuration incorporates physical parametrizations for subgrid-scale processes including radiation, planetary boundary layer turbulence, advection, diffusion, and dry/wet deposition. Initial and boundary conditions for the WRF simulations were derived from the NCEP Global Final Analysis (FNL) data, with a temporal resolution of 6 h and a spatial resolution of $1^\circ \times 1^\circ$. A summary of the physical parametrization schemes and experimental configuration is provided in Tables S1, S2 and Text S1.

2.2. IEPOX-SOA Formation

The default IEPOX-SOA generation mechanism in CMAQ is parametrized using an uptake coefficient γ , derived from SO_4^{2-} and aerosol liquid water (ALW). γ is calculated as follows:

$$\frac{1}{\gamma} = \frac{1}{\alpha} + \frac{\nu}{4HRT\sqrt{D_a k_{\text{particle}}}} \frac{1}{f(q)}$$

$$f(q) = \coth(q) - \frac{1}{q}$$

$$q = r_p \sqrt{\frac{k_{\text{particle}}}{D_a}}$$

$$k_{\text{particle}} = \sum_{i=1}^N \sum_{j=1}^M k_{i,j} [\text{nuc}_i] [\text{acid}_j]$$

where α is the mass accommodation (0.02^{20}), ν is the average molecular speed, H is Henry's law coefficient ($3.0 \times 10^7 \text{ M}\cdot\text{atm}^{-1}$), R is the gas constant, T is the temperature, D_a is the diffusion coefficient in the particle phase, k_{particle} is the pseudo-first-order particle-phase rate constant, q is the diffusion reaction parameter, and r_p is the effective particle radius. k_{particle} is calculated with N as the nucleophiles and M as the acids. The third-order rate constants ($k_{i,j}$) for the particle-phase reactions are derived from the work of Eddingsaas et al.⁴⁷ Acids include H^+ and HSO_4^- . The concentration of H^+ is calculated by ISORROPIA II based on the equilibrium Aitken and Accumulation modes. In CMAQ, ISORROPIA II defaults to the metastable assumption, assuming that inorganic aerosols are always in a liquid state. Metastable states better reflect the observed reality of fine particles in the atmosphere and are more numerically stable. Metal cations (Na^+ , K^+ , Ca^{2+} , Mg^{2+}) are considered nonvolatile components, preferentially participating in charge neutralization, not undergoing gas-particle phase transformation, and significantly affecting the nitrate, ammonium salt, and aerosol water contents by altering the acid–base balance. The H^+ and charge balances predicted by ISORROPIA II are used to separate the SO_4^{2-} (nucleophile) and HSO_4^- (acid) for epoxide uptake. The parametrization produces three SOA species from IEPOX reactive absorption: dimethyl tetraol, organic sulfate, and oligomers. The details of this parametrization are described by Pye et al.⁴³

2.3. Coating Effects

In the real atmosphere, the presence of organic coatings may reduce the uptake efficiency. We adopted the methodology of Zheng et al.³³ in GEOS-CHEM to incorporate a linear coating effect into CMAQ. The parameter γ , accounting for the coating effects, was determined

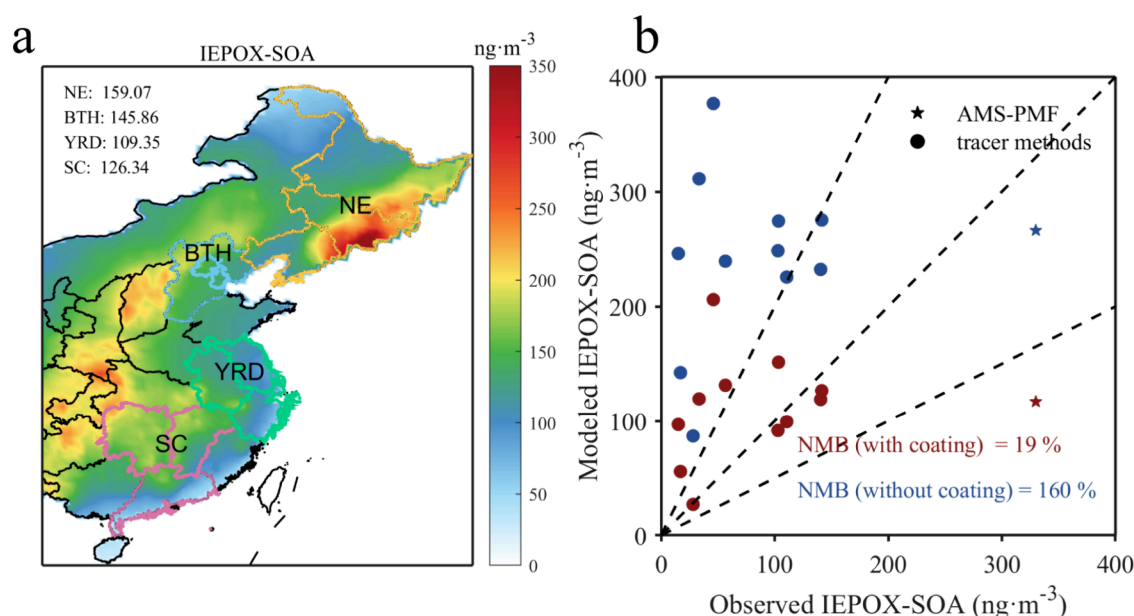


Figure 1. Simulated spatial distribution of IEPOX-SOA in the summer from 2014 to 2019 (a) and scatter plot of simulated versus observed surface IEPOX-SOA concentrations (b). The black dashed lines represent ratios of 2:1, 1:1, and 1:2. The blue dots represent IEPOX-SOA simulations without coating effects. The red dots represent IEPOX-SOA simulations that included coating effects. The results of PMF-AMS are marked with pentagrams, while the tracer method is represented by circles.

based on the laboratory findings of Gaston et al.²⁹ The specific calculation method is as follows:

$$\gamma_{\text{coating}} = \gamma \cdot (1 - 1.3 \cdot x_{\text{org}})$$

x_{org} represents the mass fraction of OA in mixed particles, including inorganic aerosol and OA. When x_{org} exceeds 0.7, IEPOX uptake ceases, resulting in $\gamma_{\text{coating}} = 0$. In calculating the IEPOX reactive uptake, we assume that all OA coats the inorganic aerosol core. However, this simplified linear function does not account for the diminished coating effect under high relative humidity (RH) conditions⁴⁸ and limits the further increase of IEPOX-SOA when x_{org} exceeds 0.7. These uncertainties necessitate further studies on the coating effects.^{49,50}

3. RESULTS AND DISCUSSION

3.1. Model Validation

Accurate meteorological simulation is essential for reliably capturing key processes in atmospheric chemical transport including reaction rates, advection, and diffusion. The meteorological parameters simulated by the WRF model were initially evaluated against observations from 136 meteorological stations across four study regions: Northeast China (NE), Beijing–Tianjin–Hebei (BTH), the Yangtze River Delta (YRD), and Southern China (SC) (Figure S1).

The model captures the magnitude of the temperature and wind speed effectively. Figures S2 and S3 show the comparison of time series between the observations and simulations. The simulated summer mean temperature (25.85 °C) and wind speed (2.50 m·s^{−1}) agree closely with the observed values (25.97 °C and 2.54 m·s^{−1}). The normalized mean bias (NMB) for temperature ranges from −2 to 1%, while that for wind speed varies between −11 and 8%. Furthermore, the model reproduces the interannual variations in temperature and wind speed observed in recent years. Correlation coefficients for temperature and wind speed reach 0.81–0.98 and 0.56–0.86, respectively. The index of agreement (IOA) values ranged

from 0.8 to 0.94 for temperature and from 0.41 to 0.62 for wind speed.

Subsequently, model simulations of IEPOX-SOA and SO₄^{2−}, the key aerosol species examined in this study, were evaluated against the observational data. For IEPOX-SOA, observational data compiled from 12 regions across multiple periods based on previous studies were used for model evaluation.^{20,23,51} Discrepancies in measurement techniques (e.g., aerosol mass spectrometry with PMF vs SOA tracer methods) may introduce uncertainties in reported IEPOX-SOA concentrations. In general, PMF-AMS measurements tend to yield higher IEPOX-SOA values than the tracer method in China. Considering that the collected observational data do not completely correspond to the simulated time period, we used observations from the year closest to it for verification. For example, we use observations from the summer of 2013 to verify the simulation for 2014. The original parametrization scheme of the model did not explicitly consider the inhibitory influence of organic coatings, which consequently resulted in a systematic overestimation of IEPOX-SOA concentrations (NMB = 160%). With the incorporation of the coating effects, the revised model demonstrates substantially improved agreement with observational data, as reflected by a reduction in the NMB to 19% (Figure 1b). However, the underestimation of wind speed in some areas may reduce the diffusion efficiency of IEPOX-SOA. The uncertainties in the isoprene emissions calculated by MEGAN and the contribution of the coating effects may lead to an overestimation of IEPOX-SOA. Further details regarding observational data sets and model evaluation procedures are provided in the Supporting Information (Texts S2, S3, Table S3, and Figure S1).

In addition, two typical megacities, Beijing and Shanghai, were selected for SO₄^{2−} evaluation.^{52,53} The CMAQ model effectively captured both the magnitude (NMB ranging from −13 to 2%) and interannual variability ($r = 0.67$ – 0.92) of SO₄^{2−} (Figure S4). A clear decreasing trend in SO₄^{2−} was

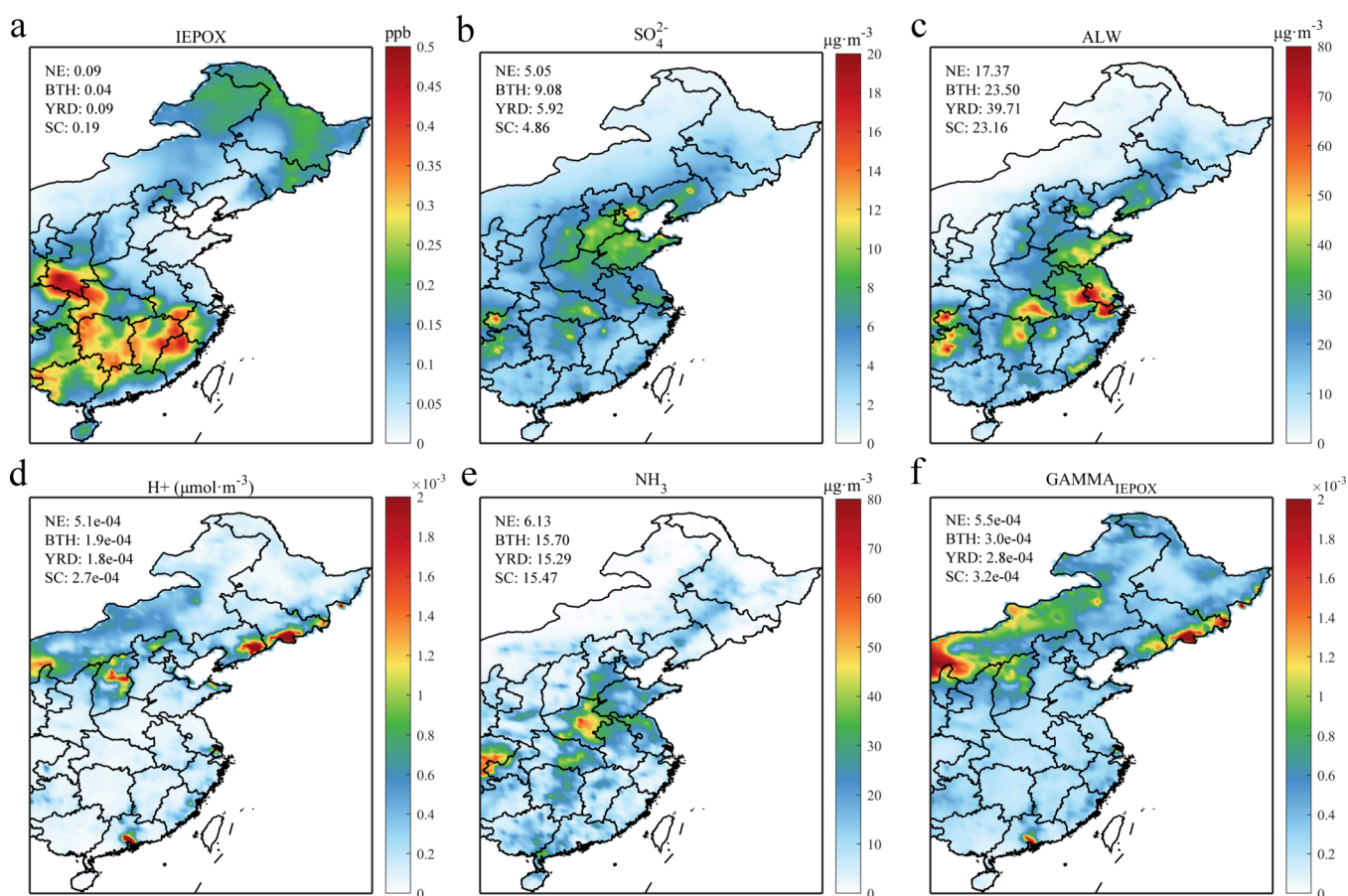


Figure 2. Spatial distribution of the simulated various impact factors including IEPOX (a), sulfate (b), ALW (c), H^+ (equilibrium particle hydronium ion concentration per volume air) (d), NH_3 (e), and γ_{IEPOX} (f).

identified in both cities, consistent with the stringent SO_2 emissions control implemented in China in recent years. Since 2014, SO_2 emissions have decreased by 62% (Figure S5), largely owing to energy structure transitions and advances in emission control technologies.

3.2. IEPOX-SOA and Its Impact Factors

3.2.1. Spatial Distributions. Figure 1a presents the simulated summer average IEPOX-SOA concentrations from 2014 to 2019. Across the four study regions, mean IEPOX-SOA concentrations ranged from 110 to 160 $ng\cdot m^{-3}$. The spatial distribution of IEPOX-SOA showed prominent hotspots over the North China region, the Qinling Mountains, and Shanxi Province. These spatial patterns are consistent with the simulated results in the summer of 2012 given by Qin et al.³⁹

IEPOX-SOA formation is strongly influenced by its major precursor isoprene and IEPOX, as well as reactive factors, such as organic coatings, seed aerosol, ALW content, and aerosol acidity. Figures 2a and S6 show the spatial distributions of IEPOX and isoprene, both of which differ noticeably from that of IEPOX-SOA. High isoprene emissions and concentrations are concentrated in Southeast China, the Qinling Mountains, and Northeast China, which is primarily driven by temperature.⁴⁵ The distribution of gaseous IEPOX broadly mirrors that of isoprene with similarly high concentrations occurring in these regions. In terms of magnitude, IEPOX in Eastern China (~ 0.1 ppb) is only 20% of that in the southeastern United States (~ 0.5 ppb), which can be largely attributed to the

suppression by substantial anthropogenic emissions.¹⁹ In Eastern China, elevated NO_x levels accelerate the conversion of isoprene into MAE and HMML, thereby inhibiting the formation of IEPOX.

To elucidate the discrepancy between IEPOX and IEPOX-SOA, we further investigated the influence of key reactive factors on the spatial pattern of IEPOX-SOA. Aerosol acidity (H^+) is likely the dominant factor driving the spatial disparities between IEPOX and IEPOX-SOA, as evidenced by the similar distribution patterns of γ_{IEPOX} and H^+ . In heavily polluted regions such as BTH and YRD, elevated levels of ammonia (NH_3) (BTH: 15.70 ppb, YRD: 15.29 ppb) and ALW (BTH: 23.50 $\mu g\cdot m^{-3}$, YRD: 39.71 $\mu g\cdot m^{-3}$) lead to reduced aerosol acidity and consequently higher aerosol pH compared to those in the United States and Europe.⁵⁴ Under these conditions, excess NH_3 largely suppresses the formation of IEPOX-SOA across most parts of China. In contrast, regions with higher γ_{IEPOX} , such as the southeast corner of the NE region, are characterized by lower NH_3 and ALW, facilitating greater IEPOX-SOA production.

To quantitatively evaluate the sensitivity of IEPOX-SOA to aerosol acidity, we conducted a simulation by reducing the pH by 1 unit (a 10-fold amplification of H^+ ; only modifying the module for calculating γ_{IEPOX} , while other inorganic aerosol components remained unchanged). The results demonstrate that a 1-unit decrease in pH leads to a 2–5-fold increase in IEPOX-SOA concentration (Figure S7). Experimental studies by Surratt et al.¹⁴ found that changes in aerosol acidity can increase IEPOX-SOA concentrations from 0.1 $\mu g\cdot m^{-3}$ under

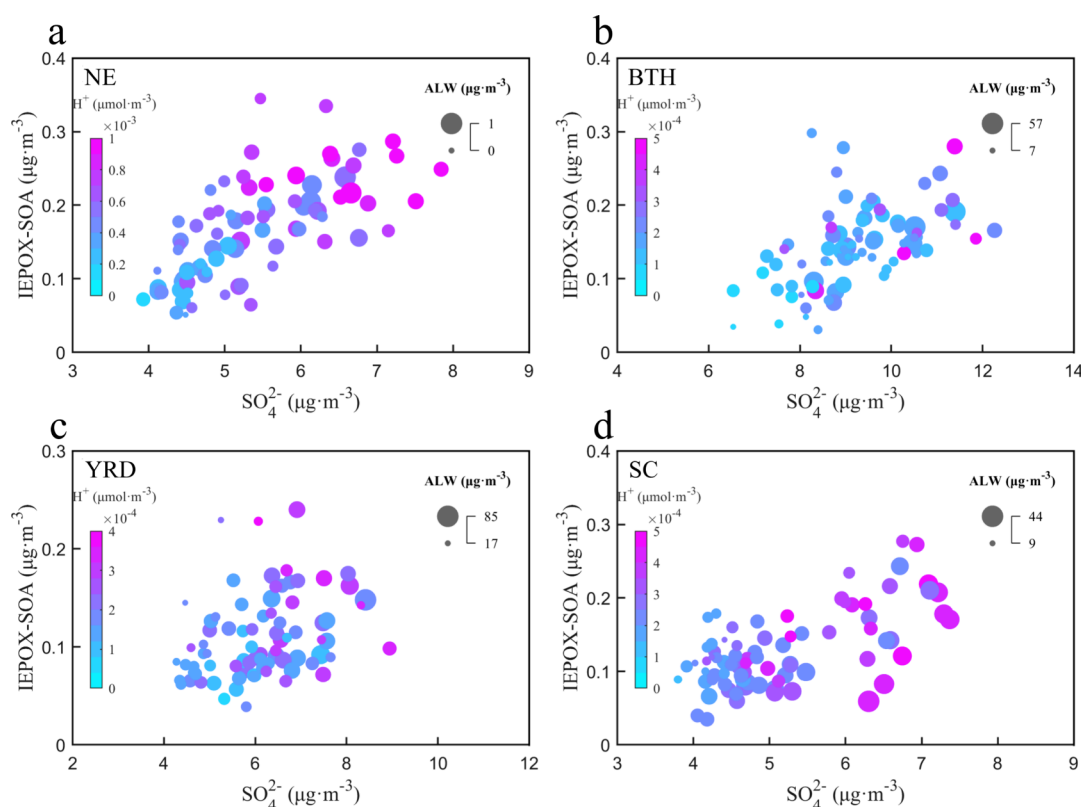


Figure 3. Correlation between IEPOX-SOA and various influencing factors. The data points are color-coded by H^+ concentrations, and the marker sizes indicate the values of the ALW. (a–d) Represent the four regions of NE, BTH, YRD, and SC, respectively.

neutral conditions to $5.1 \mu\text{g}\cdot\text{m}^{-3}$ under highly acidic conditions.

The spatial abundance of IEPOX-SOA is not dependent on nucleophile concentrations such as SO_4^{2-} and ALW. As shown in Figure 2b,c, neither BTH with high SO_4^{2-} concentrations nor YRD with high ALW concentrations shows corresponding high IEPOX-SOA values. The coating effects inhibit IEPOX-SOA generation, as organic matter coating the aerosol surface reduces IEPOX uptake capacity. As shown in Figures S8c and S9, the coating effects are particularly significant in regions with high OA concentrations, such as the SC region ($-194.83 \text{ ng}\cdot\text{m}^{-3}$). Compared to the simulation accounting for the coating effects, the scenario neglecting this process produced higher average IEPOX-SOA concentrations in the SC region (Figure S8a). However, the overall spatial pattern remained relatively consistent between the two simulations. Furthermore, no significant correlation was observed between X_{org} and IEPOX-SOA (Figure S9), suggesting that the coating effect is not the dominant driver governing the spatial distribution of IEPOX-SOA over Eastern China.

Particle morphology represents an important source of uncertainty in quantifying the coating effects on IEPOX-SOA formation.^{55–57} Mixed particles are represented as an idealized inorganic-core/organic-shell. However, the actual phase state of ambient particles is highly sensitive to the RH. Under high-RH conditions, increased water uptake by the inorganic phase and the high hydrophilicity of IEPOX-SOA may suppress liquid–liquid phase separation, resulting in a more internally mixed or even a single-phase particle. In such cases, the formation of a continuous organic shell may be limited or transient. Consequently, the coating effects estimated in this study should be interpreted as an upper-bound estimate under

the conditions of sustained phase separation. If particles remain internally mixed at elevated RH, the suppression of reactive uptake due to coating would be less pronounced than predicted by the core–shell model.^{31,48} Overall, real atmospheric behavior is expected to lie between the limiting cases of fully phase-separated and fully internally mixed particles, and the conclusions presented here likely represent the maximum possible impact of the coating effects.

3.2.2. Correlation Analysis. To investigate the relationship between daily variations in IEPOX-SOA and key factors, including SO_4^{2-} , ALW, and aerosol acidity, a correlation analysis was conducted. Figure 3 compares the characteristics of IEPOX-SOA across the four study regions under different influencing conditions.

IEPOX-SOA exhibited a strong positive correlation with SO_4^{2-} across all regions, with correlations ranging from 0.33 to 0.68, aligning with previous studies.^{24,28,39,58} In contrast, the correlation between ALW (as a nucleophile) and IEPOX-SOA is weak, with correlation coefficients (r) ranging from 0.10 to 0.18 (Table S4). Although ALW can directly provide reaction sites for IEPOX uptake, an increased level of ALW may also dilute the concentrations of SO_4^{2-} and H^+ , thereby inhibiting IEPOX-SOA formation. Furthermore, the reactions of IEPOX with multiple nucleophiles are competitive. Zhang et al.³⁷ reported that nucleophilic addition with SO_4^{2-} dominates IEPOX formation in Beijing, whereas ALW plays a more critical role in Kunming and Hefei—a regional discrepancy not fully captured in our simulations.

H^+ exhibited significant positive correlations in the YRD, SC, and NE regions ($r = 0.40$ – 0.64), and a comparatively weak correlation ($r = 0.28$) was observed in the BTH region. This result contrasts with the findings reported by Xu et al.²⁸ in

the United States. The discrepancy may be attributed to the consistently high aerosol acidity typical of U.S. regions. For instance, at the Centreville monitoring site, the average pH is as low as 0.94,⁵⁹ indicating that IEPOX-SOA formation there is less sensitive to H^+ . Conversely, field measurements in China have demonstrated a strong correlation between IEPOX-SOA and H^+ , highlighting the important role of acid-catalyzed mechanisms under these conditions.³⁶ The results confirmed that differences in aerosol acidity are the most likely explanation for the divergent patterns of IEPOX-SOA formation observed in China versus in the United States.

3.3. Long-Term Trends and Drivers

In recent years, China has implemented strict emission control measures. Against this backdrop, we conducted a detailed investigation of the interannual trends of IEPOX-SOA and their driving factors. IEPOX-SOA levels changed at the rate of -19.14 to -34.77 $ng\cdot m^{-3}\cdot yr^{-1}$ in Eastern China. IEPOX-SOA concentrations exhibit an inverse relationship with their precursor IEPOX (Figure S10), underscoring the critical role of anthropogenic influences. As shown in Figure S10, the interannual variations in IEPOX-SOA closely follow those of SO_4^{2-} , rather than other examined factors. Over Eastern China, ALW decreased in tandem with overall pollution levels; however, its weak correlation with IEPOX-SOA (Table S4 and Figure S10) suggests it is not the primary driver behind the decline in IEPOX-SOA. Meanwhile, H^+ showed no significant trend in most regions except for NE. This may be attributed to differential reduction rates between acidic gases (e.g., NO_x , SO_2) and alkaline gas (NH_3) under current emission policies, which collectively modulate pH.

Sensitivity experiments isolating the influences of meteorology, anthropogenic emissions, and biogenic emissions further support the dominant role of SO_4^{2-} reductions in driving IEPOX-SOA trends. As shown in Figure 4, variations in

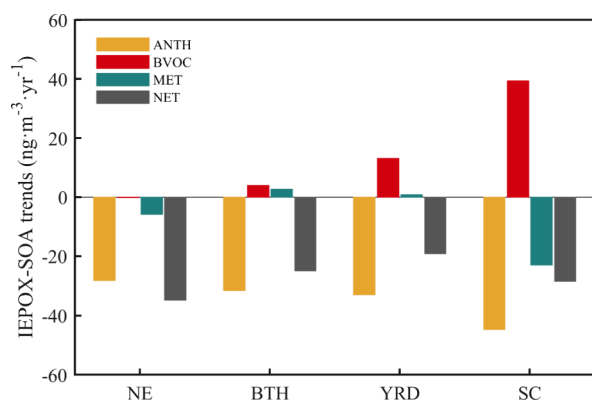


Figure 4. Driving factors of interannual variation of IEPOX-SOA. Contributions of anthropogenic emissions (ANTH), biological emissions (BVOC), and meteorological factors (MET) changes to the trends in IEPOX-SOA. NET represents the sum of contributions from BVOC, MET, and ANTH.

anthropogenic emissions resulted in substantial decreases in IEPOX-SOA concentrations, with trends ranging from -28.18 to -44.67 $ng\cdot m^{-3}\cdot yr^{-1}$. These reductions are attributed to combined effects from declining SO_4^{2-} and changes in coating effects. In recent years, coating effects have weakened synchronously with the overall decrease in OA concentrations. Sensitivity experiments revealed that the attenuation of coating effects caused a slight increase in IEPOX-SOA (Figure S8d),

ranging from $+8.8$ to $+20.65$ $ng\cdot m^{-3}\cdot yr^{-1}$. Although this partially offsets the overall decline, anthropogenic emission reductions remained the primary driver of the decrease. The reduced SO_4^{2-} availability limits the reactive uptake of IEPOX, thereby suppressing IEPOX-SOA formation.

Changes in BVOC emissions also play a notable role in certain regions. For instance, in the SC region, increased BVOC emissions contributed to an upward trend in IEPOX-SOA concentrations at the rate of $+39.41$ $ng\cdot m^{-3}\cdot yr^{-1}$, nearly offsetting the anthropogenic-induced decrease (-44.67 $ng\cdot m^{-3}\cdot yr^{-1}$). Elevated isoprene emissions enhance atmospheric IEPOX production, thus promoting IEPOX-SOA formation. Meteorological factors moderately influence reaction rates, diffusion, and deposition processes, though their contributions remain relatively minor, ranging from -23.05 to $+2.69$ $ng\cdot m^{-3}\cdot yr^{-1}$.

3.4. Uncertainty in IEPOX-SOA Simulations

It is worth noting that many uncertainties in the model simulations can significantly influence the assessment results such as the selection of IEPOX kinetic parameters, emission uncertainties, and potential missing chemical mechanisms. To evaluate the robustness of our findings, additional sensitivity experiments were conducted to quantify uncertainties associated with different kinetic parametrizations and emission inputs.

Reported kinetic parameters for the reactive uptake of IEPOX vary across the literature. Here, we performed baseline simulations for July 2014 and July 2019 and compared them with simulations using two alternative, representative sets of kinetic parameters (Table S5).^{60,61} The results show that varying these parameters leads to changes in IEPOX-SOA concentrations in the range of approximately -14 to -19% (Figure S11a–c). However, the spatial distribution pattern of IEPOX-SOA remains consistent across all simulations: elevated concentrations persistently occur over the NE regions and the Qinling Mountains. Moreover, irrespective of the specific third-order rate constant adopted for the particle-phase reaction, the simulated temporal trend of IEPOX-SOA is uniformly characterized by a nationwide decrease (Figure S11d,e), with the most pronounced reductions occurring precisely in those high-concentration regions (NE and the Qinling Mountains). In summary, although the selected kinetic parameters can moderately affect the predicted absolute levels of IEPOX-SOA, they do not alter the simulated spatial distributions or the overall downward trend. This consistency strengthens confidence in the robustness of the key conclusions drawn from this study.

Furthermore, the MEIC 2.0 emission inventory was employed to evaluate uncertainties associated with the emission inputs. Relative to the prior version, changes in SO_2 , NO_x , and NH_3 were modest (each below 9%), whereas OC emissions increased by 27% (Figure S5). July 2014 and July 2019 were selected as representative periods to examine the influence of these updated emissions. Spatially, the simulated pattern of IEPOX-SOA remained consistent with the baseline simulation (Figure S12), confirming that aerosol acidity continues to dominate its geographical distribution in eastern China. The correlation between SO_4^{2-} and IEPOX-SOA remained statistically significant, with coefficients ranging from approximately 0.45 to 0.8 (Figure S13). However, elevated OC emissions enhanced the suppressing effect of organic coatings on IEPOX uptake. In summary, although

emission uncertainties can influence the quantitative estimation of IEPOX-SOA, the key drivers identified in this analysis remain robust.

3.5. Responses of IEPOX-SOA to Future Emission Reductions

Given that reductions in different anthropogenic emissions may lead to contrasting effects on IEPOX-SOA formation, we conducted a series of sensitivity experiments to evaluate the possible response of IEPOX-SOA to future changes in specific emission species. Using July 2019 as the baseline case, we quantified changes in IEPOX-SOA concentrations and related factors under 30% individual and synergistic reductions in SO_2 , NH_3 , NO_x and POC emissions (Figures 5 and S14–S16).

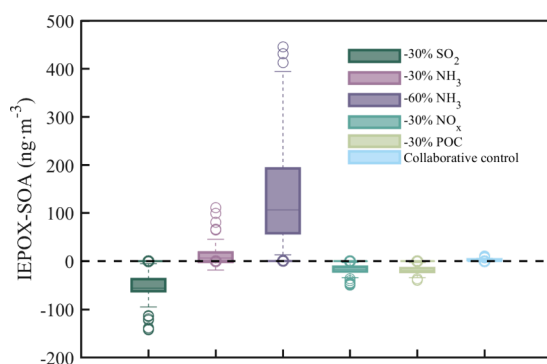


Figure 5. Change in IEPOX-SOA for July 2019 for the sensitivity simulations relative to the base case. The distribution is shown as median (line), 25th and 75th percentiles (bottom and top of box), and 10th and 90th percentiles (bottom and top whiskers).

All emission control scenarios resulted in decreases in IEPOX-SOA concentrations with the exception of NH_3 reduction and collaborative control. As anticipated, reducing SO_2 emissions led to a decrease in the level of SO_4^{2-} , which subsequently reduced the level of IEPOX-SOA formation. NO_x reduction, on the one hand, promotes the conversion of isoprene to IEPOX, while on the other hand, it reduces ALW, overall slightly suppressing IEPOX-SOA production. POC reduction can diminish the organic coating effect. The response of IEPOX-SOA to POC reductions was similar to that of NO_x controls: a concurrent decrease in ALW largely offsets the potential enhancement from a weaker coating effect.

In contrast, a 30% reduction in NH_3 emissions resulted in an increase in IEPOX-SOA concentrations ranging from +5.32 to +35.26 $\text{ng}\cdot\text{m}^{-3}$, consistent with our earlier conclusion that NH_3 suppresses IEPOX-SOA formation. This finding is consistent with the research by Du et al.,⁶² who reported that the presence of NH_3 can neutralize particle acidity generated from SO_2 oxidation, thereby diminishing the catalytic capacity of acidic seed particles—such as sulfuric acid—in promoting SOA formation. Recent studies further indicate that NH_3 emissions in China could potentially be reduced by up to 60%.⁶³ Under such a scenario, IEPOX-SOA concentrations would increase by 57.64–245.40 $\text{ng}\cdot\text{m}^{-3}$, underscoring the critical role of ammonia in modulating SOA formation. The reduction in NH_3 perturbs the aerosol acid–base balance, leading to elevated H^+ levels and thereby enhancing acid-catalyzed formation of IEPOX-SOA. Although some studies have proposed that the presence of NH_3 may promote SOA formation via the production of particulate ammonium nitrate,^{64–66} our results provide an alternative perspective

regarding the potential impacts of future NH_3 emission controls. Specifically, we suggest that reducing NH_3 emissions may unexpectedly enhance IEPOX-SOA formation due to increased aerosol acidity. Collaborative control leads to mutual constraints among various factors, resulting in a slight enhancement of IEPOX-SOA (1.87–5.15 $\text{ng}\cdot\text{m}^{-3}$). Overall, these sensitivity experiments underscore the critical roles of sulfate and aerosol acidity in governing IEPOX-SOA concentrations.

4. ATMOSPHERIC IMPLICATIONS

This study employed the CMAQ model to investigate the spatial distribution and interannual trends of IEPOX-SOA across Eastern China during the summer. The results demonstrate that IEPOX-SOA formation is substantially modulated by organic coating effects, SO_4^{2-} availability, and aerosol acidity. Organic coatings significantly suppress the reactive uptake of IEPOX, and although recent reductions in OA have slightly weakened this effect, its inhibitory role remains substantial. Daily variability and long-term trends in IEPOX-SOA are primarily influenced by sulfate concentrations.

In contrast, aerosol acidity is a key factor governing the spatial distribution of IEPOX-SOA across China. High NH_3 levels prevalent in most Chinese regions effectively neutralize particle-phase acidity, thereby suppressing IEPOX-SOA formation. Recent studies indicated that aerosol pH in China is generally 1–2 units higher—equivalent to 10–100 times lower H^+ concentration—than that in the United States, which can be attributed to higher aerosol loadings and a larger fraction of total ammonia partitioning into the aerosol phase.^{67,68} Our sensitivity experiments confirmed that a one-unit decrease in pH resulted in a 2–5-fold increase in IEPOX-SOA yields. Taken together, these findings collectively indicate that differences in aerosol pH are likely the major reason for the considerably lower IEPOX-SOA concentrations observed in China relative to those in the United States.

With effective control of acid gas emission, NH_3 plays an increasingly important role in air pollution⁶⁹ and has attracted growing attention in China's emission mitigation planning, with several policies already proposed to reduce NH_3 emissions.⁶³ If future policies lead to stringent NH_3 reduction, increased aerosol acidity could subsequently enhance IEPOX-SOA yields—particularly under conditions of low aerosol mass, low ALW, low total ammonia, and elevated acidity. Consequently, IEPOX-SOA may become a more substantial component of OA. It is therefore imperative to strengthen the monitoring of aerosol acidity and related particulate matter components to support the formulation of effective emission control strategies.

■ ASSOCIATED CONTENT

Supporting Information

The Supporting Information is available free of charge at <https://pubs.acs.org/doi/10.1021/acs.est.5c14957>.

Additional text, including sensitivity experiment setup, observation data sources, and introduction to simulation validation methods; figures, including research area, model validation results, emission changes, and sensitivity experiment results; and tables, including model parametrization settings, model sensitivity experimental settings, observation data, and correlation

coefficients between IEPOX-SOA and each factor (PDF)

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Notes

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