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Improved representation of isoprene-derived secondary organic aerosol in CAM6-Chem reveals regional contrasts in its long-term changes over China

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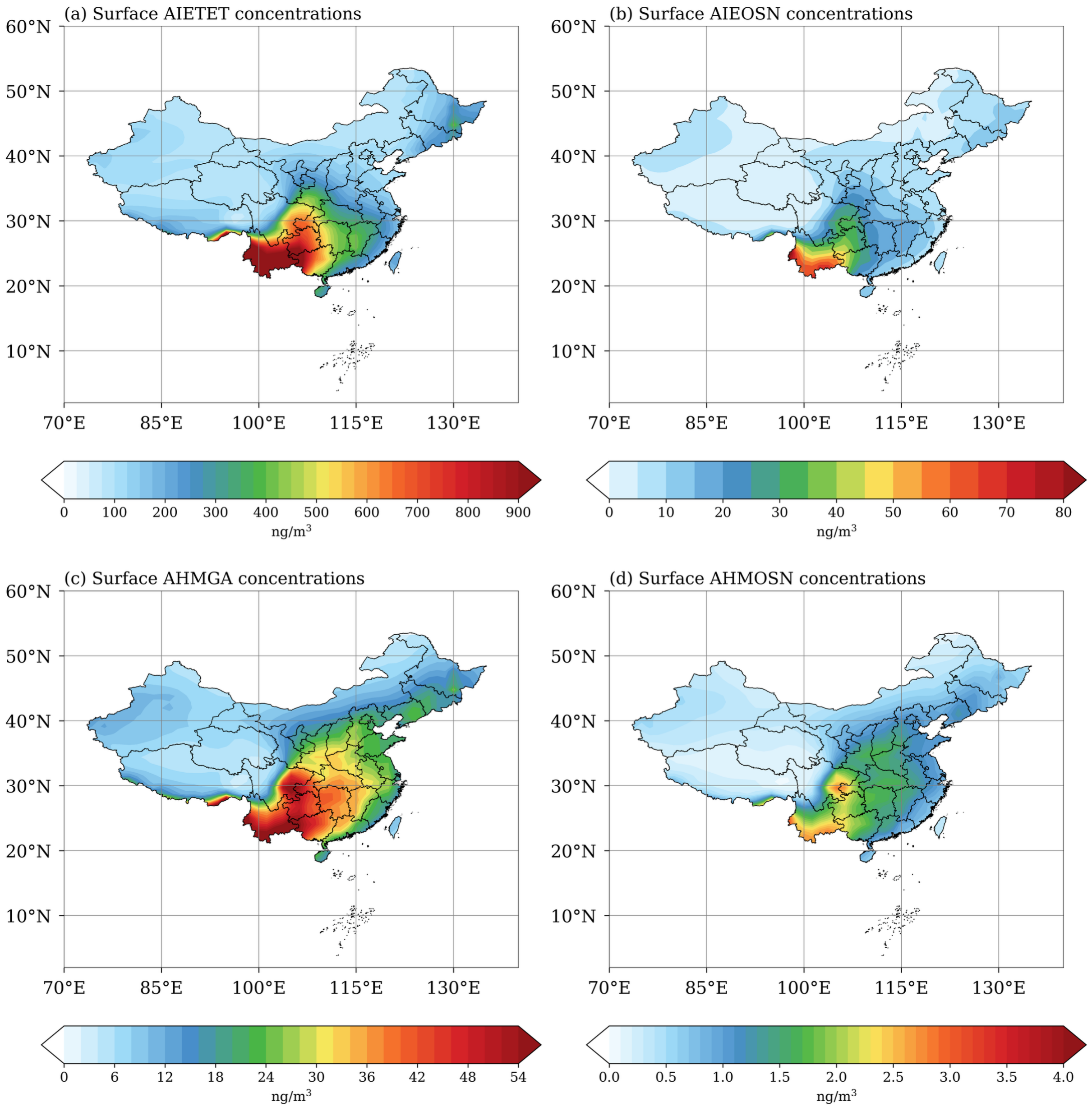
S1. Multiple regression supplement. The standardized regression analysis was based on regional-mean monthly time series derived by spatially averaging the original monthly gridded data for each variable over Southwest China (SWC) and the Shaanxi–Gansu–Ningxia region (SGN). The mean seasonal cycle was then removed from each time series to obtain monthly anomalies, followed by z-score standardization so that all variables had zero mean and unit variance and could be compared on a common scale. Multiple linear regression was subsequently applied to the standardized anomalies, and the resulting standardized regression coefficients (β) were used to compare the relative statistical importance of individual predictors. To further compare their regression-based importance, we calculated the normalized importance of each factor as $|\beta|/\Sigma|\beta|$. As in the main text, this analysis should be interpreted as a diagnostic of statistical associations rather than as a strict causal attribution. Because this analysis is based on deseasonalized monthly anomalies, the standardized β values primarily reflect the leading statistical predictors of regional month-to-month isoprene-derived secondary organic aerosol (ISOA) variability (Table S1). The regression results show that biogenic isoprene emissions and sulfate are the two leading statistical indicators of monthly ISOA variability, but their relative importance differs between SWC and SGN. In SWC, isoprene emissions have the largest standardized coefficient ($\beta = 0.383$, $p = 0.001$) and the highest normalized regression-based importance (43.39%; Table S1), indicating that isoprene precursor supply is most strongly associated with ISOA variability in this region. Sulfate emerges as the second most important statistical indicator, with a normalized importance of 31.29% and a positive standardized coefficient ($\beta = 0.276$), although its regression coefficient is not statistically significant at the 0.05 level ($p = 0.154$). Aerosol liquid water shows a smaller but non-negligible regression-based importance (15.03%), whereas anthropogenic NOx emissions and $\log_{10}(H^+)$ contribute less to the statistical explanation of monthly ISOA variability in SWC (Table S1). In SGN, sulfate shows the highest normalized regression-based importance (42.94%; Table S1) and the largest positive standardized coefficient ($\beta = 0.560$, $p = 0.049$), suggesting that sulfate-related heterogeneous processing is strongly associated with monthly ISOA variability in this region. Isoprene emissions show the second-highest regression-based importance (18.91%) and a statistically significant positive coefficient ($\beta = 0.247$, $p = 0.042$), indicating that precursor supply also contributes to ISOA variability in SGN. Aerosol liquid water shows moderate regression-based importance (16.73%), although its standardized coefficient is not statistically significant ($\beta = -0.218$, $p = 0.544$). Anthropogenic NOx emissions and $\log_{10}(H^+)$ show smaller regression-based importance and non-significant standardized coefficients in SGN (Table S1). Overall, the regression analysis indicates that month-to-month ISOA variability in SWC is most strongly associated with biogenic isoprene emissions, suggesting that precursor supply is the leading statistical indicator in this region. In contrast, ISOA variability in SGN is more strongly associated with sulfate-related heterogeneous processing, while isoprene precursor supply remains a secondary but statistically significant contributor. These results suggest that regional differences in ISOA variability reflect different balances between biogenic precursor supply and the aerosol reaction environment.

Driver	Southwest China (SWC)					Shaanxi–Gansu–Ningxia region (SGN)				
	r	p_r	β	p_β	Importance (%)	r	p_r	β	p_β	Importance (%)
ISOP emis	0.419	0.001	0.383	0.001	**43.39**	0.245	0.059	0.247	0.042	18.91
SO_4^{2-}	0.441	<0.001	0.276	0.154	31.29	0.412	0.001	0.560	0.049	**42.94**
Anthro NOx emis	0.353	0.006	0.072	0.625	8.107	-0.100	0.447	-0.161	0.275	12.31
AeroWater	0.397	0.002	0.133	0.582	15.03	0.279	0.031	-0.218	0.544	16.73
$\log_{10}(H^+)$	0.329	0.010	-0.019	0.916	2.170	0.266	0.040	0.119	0.616	9.116

Table S1: Standardized multiple linear regression results for monthly isoprene-derived secondary organic aerosol (ISOA) variability in Southwest China (SWC) and the Shaanxi–Gansu–Ningxia region (SGN). The regression is based on deseasonalized monthly anomalies that were subsequently z-score standardized, using data from the five simulation years (2000, 2006, 2012, 2016, and 2019). For each driver, the table lists the Pearson correlation coefficient (r), significance level (p_r), standardized regression coefficient (β), significance level (p_β), and normalized relative importance (|β|/Σ|β|; %). Bold values indicate the largest normalized relative importance in each region.



45 **Figure S1: Annual mean surface concentrations of four isoprene-derived secondary organic aerosol (ISOA) subspecies (AIETET, AIEOSN, AHMGA, and AHMOSN) over China, averaged over the five simulation years (2000, 2006, 2012, 2016, and 2019) (unit: ng m^{-3}).**

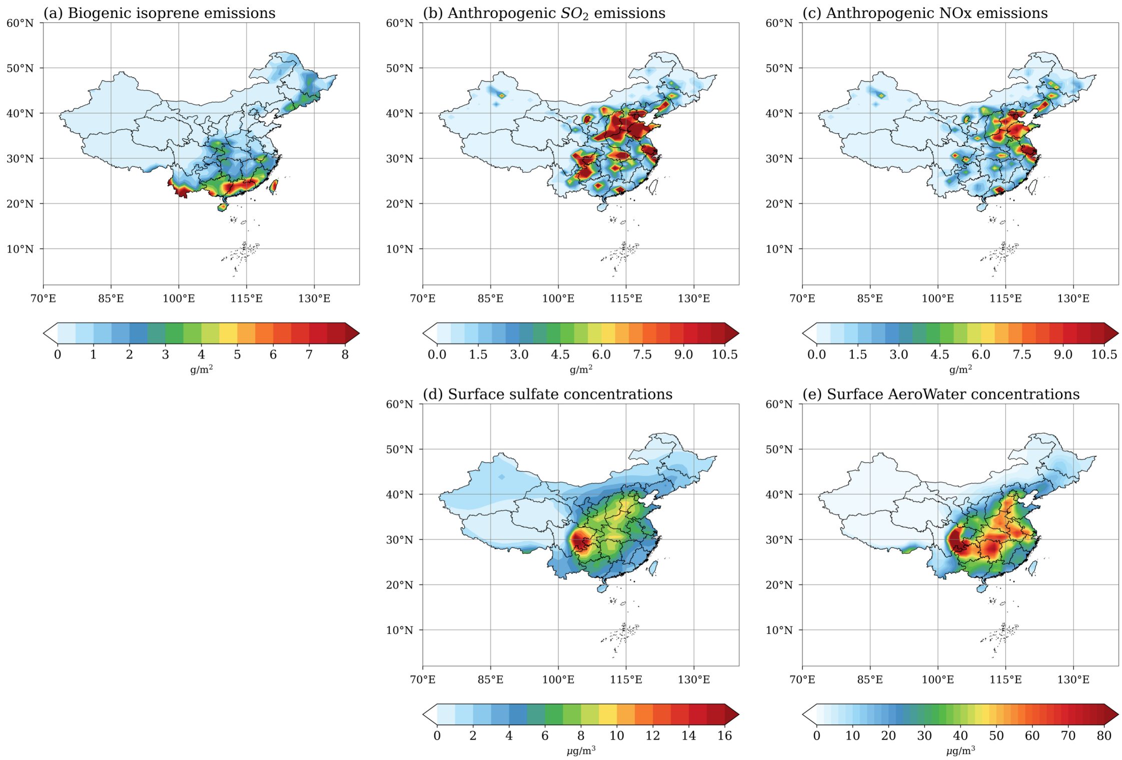


Figure S2: Annual mean biogenic isoprene emissions (a; unit: g m^{-2}), anthropogenic sulfur dioxide (SO_2) emissions (b; unit: g m^{-2}), anthropogenic nitrogen oxides (NOx) emissions (c; unit: g m^{-2}), surface sulfate concentrations (d; µg m^{-3}), and surface aerosol liquid water (AeroWater) concentrations (e; µg m^{-3}) over China, averaged over the five simulation years (2000, 2006, 2012, 2016, and 2019).

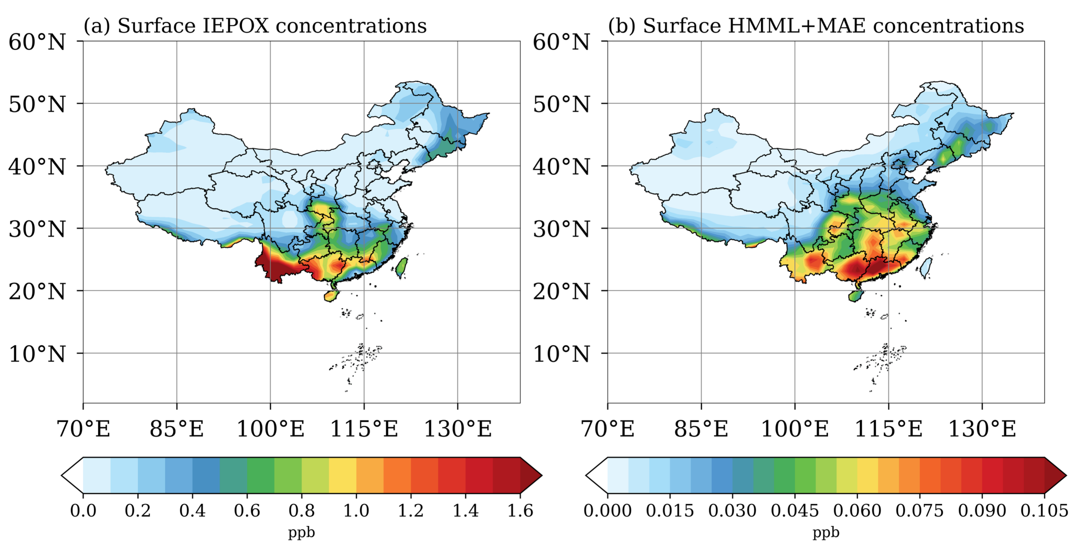


Figure S3: Annual mean surface isoprene epoxydiols (IEPOX) concentrations (a; unit: ppb) and surface hydroxymethyl-methyl-α-lactone plus methacrylic acid epoxide (HMML + MAE) concentrations (b; unit: ppb) over China, averaged over the five simulation years (2000, 2006, 2012, 2016, and 2019).

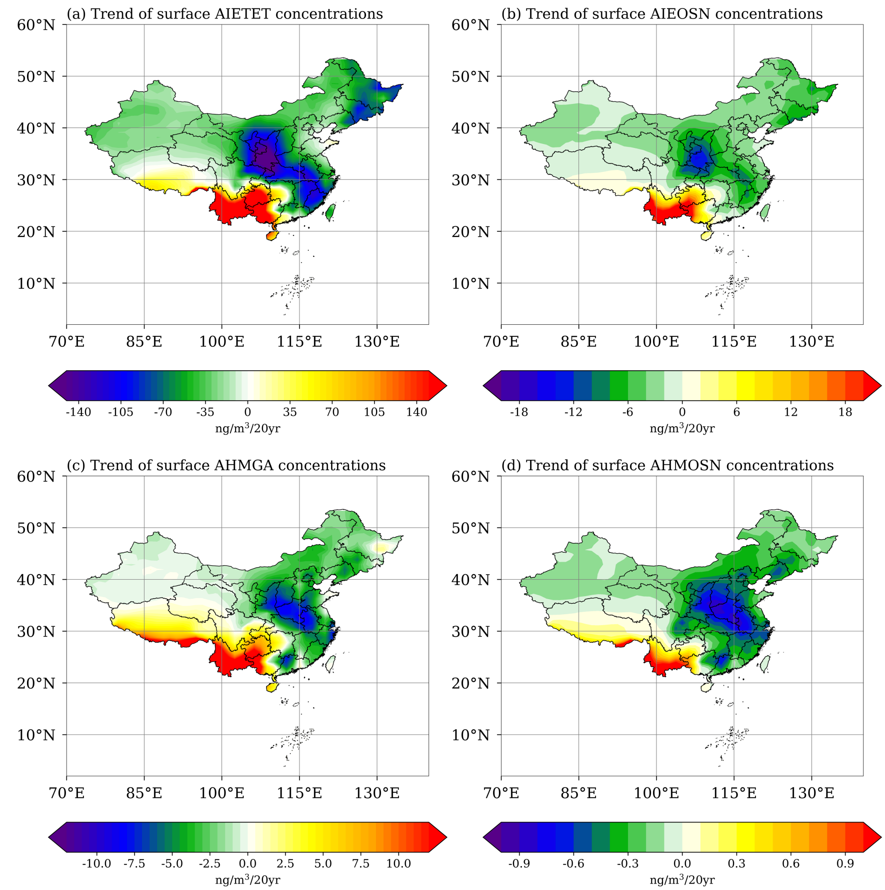


Figure S4: Long-term trends in annual mean surface concentrations of four isoprene-derived secondary organic aerosol (ISOA) subspecies (AIETET, AIEOSN, AHMGA, and AHMOSN) surface concentrations (ng m^{-3} per 20 years), in China from 2000 to 2019.

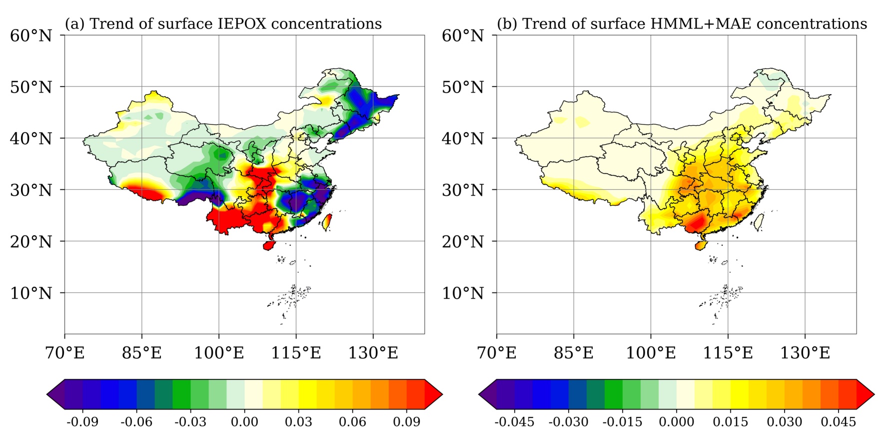


Figure S5: Long-term trends in annual mean surface concentrations of (a) surface isoprene epoxydiols (IEPOX) concentrations and (b) surface hydroxymethyl-methyl-α-lactone plus methacrylic acid epoxide (HMML + MAE) concentrations (ppb per 20 years), in China from 2000 to 2019.

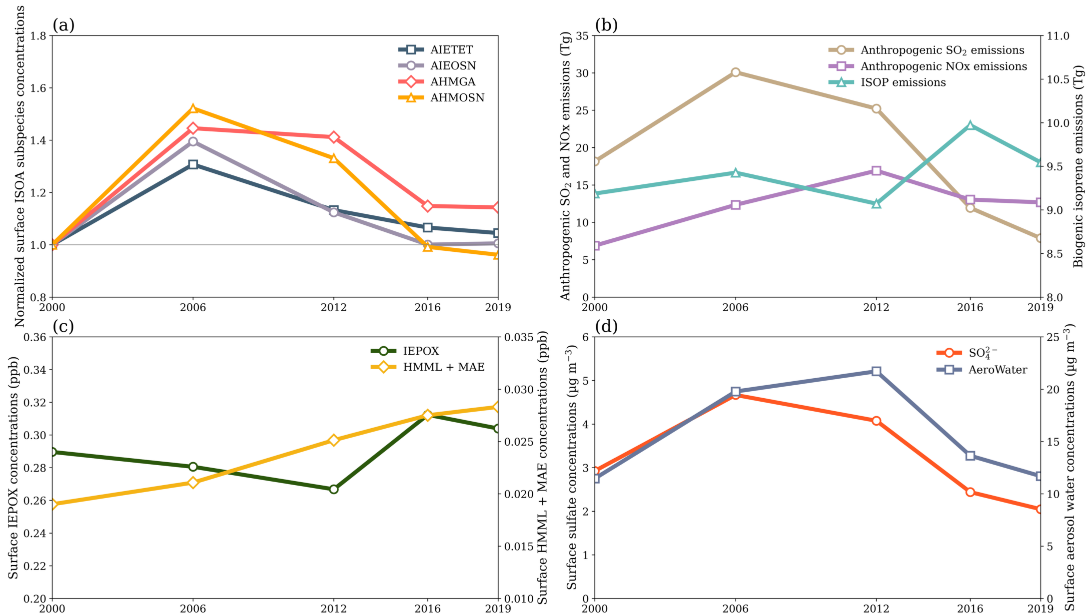


Figure S6: Time series for China, showing (a) normalized surface isoprene-derived secondary organic aerosol (ISOA) subspecies concentrations, including AIETET (dark blue), AIEOSN (gray-purple), AHMGA (rose red), and AHMOSN (earthy yellow). The normalized values are calculated as the ratio of the value in each year to that in 2000; (b) anthropogenic sulfur dioxide (SO_2) emissions (tan; left y axis; unit: Tg) and anthropogenic nitrogen oxides (NOx) emissions (purple; left y axis; unit: Tg), and biogenic isoprene emissions (blue; right y axis; unit: Tg); (c) surface isoprene epoxydiols (IEPOX) concentrations (dark green; left y axis; unit: ppb) and surface hydroxymethyl-methyl-α-lactone plus methacrylic acid epoxide (HMML + MAE) concentrations (yellow; right y axis; unit: ppb); and (d) surface sulfate (SO_4^{2-}) concentrations (red-orange; left y axis; unit: μg m^{-3}) and surface aerosol liquid water (AeroWater) concentrations (blue-gray; right y axis; unit: μg m^{-3}).

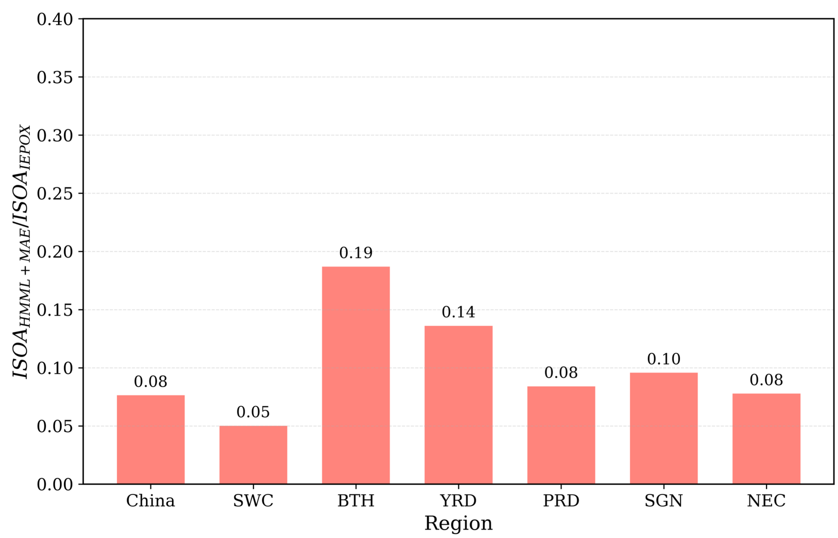


Figure S7: Ratios of multi-year mean surface concentrations of ISOA derived from HMML and MAE ($ISOA_{HMML+MAE}$) to those derived from IEPOX ($ISOA_{IEPOX}$) in China and selected subregions from 2000 to 2019, including Southwest China (SWC), the Beijing–Tianjin–Hebei region (BTH), the Yangtze River Delta (YRD), the Pearl River Delta (PRD), the Shaanxi–Gansu–Ningxia region (SGN), and Northeast China (NEC).

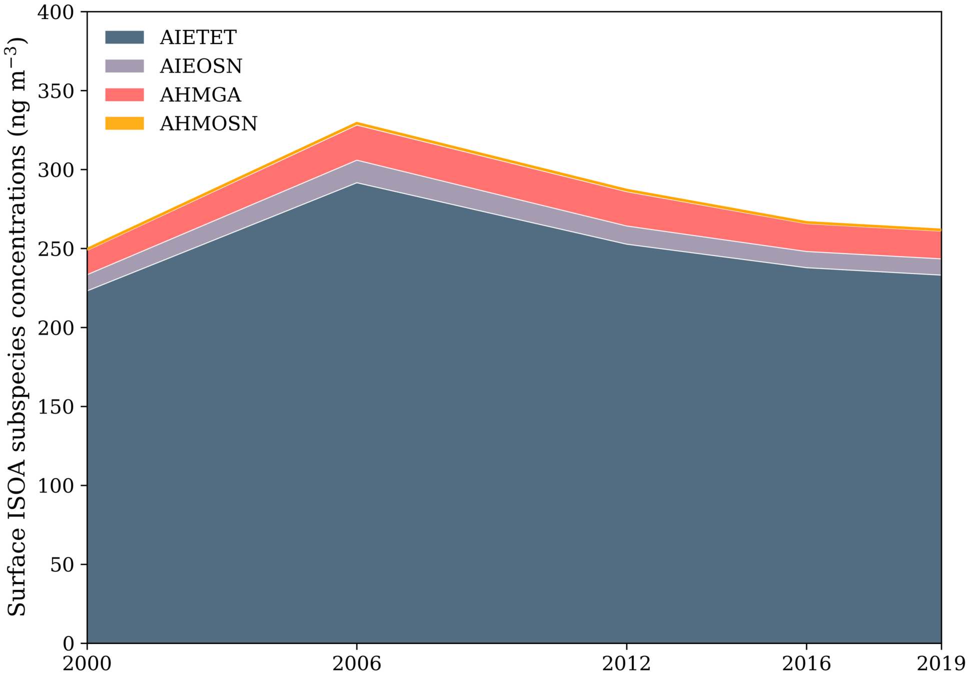


Figure S8: Interannual variations of average surface isoprene-derived secondary organic aerosol (ISOA) subspecies concentrations from 2000 to 2019 (unit: ng m^{-3}).

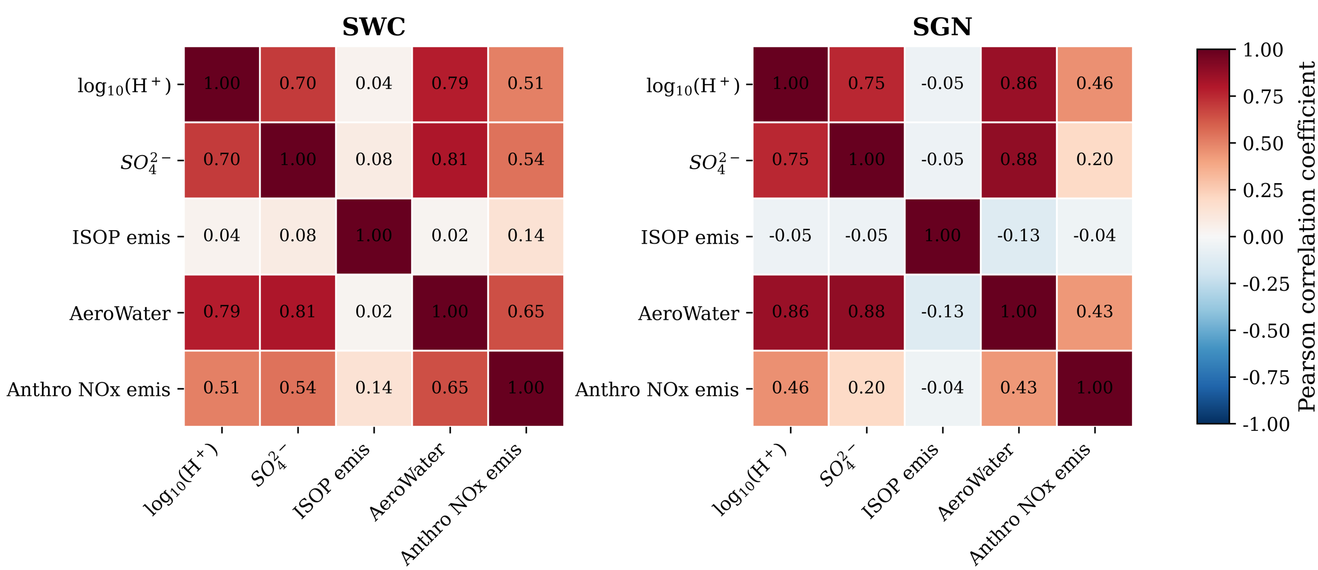


Figure S9: Pairwise Pearson correlation coefficients among predictors used in the multiple linear regression analysis for Southwest China (SWC) and the Shaanxi–Gansu–Ningxia region (SGN). The predictors include aerosol acidity represented by $\log_{10}(H^+)$, sulfate (SO_4^{2-}), biogenic isoprene emissions (ISOP emis), aerosol liquid water (AeroWater), and anthropogenic NOx emissions (Anthro NOx emis). Warm colors indicate positive correlations, whereas cool colors indicate negative correlations.

Equation	Rate coefficient/parameters
MACR + NO_2 -> MPAN	9.7e-29, 5.6, 9.3e-12, 1.5, 0.6
MPAN + OH -> 0.75*HMML + 0.02*MAE + 0.23*HYAC + 0.23*CO + NO_3	3.00e-11

Table S2: Newly added gas-phase reactions for the updated high-NOx isoprene chemistry and their rate constants in this study. For the first reaction, the listed five parameters follow the standard CESM/MOZART falloff formulation and represent the low-pressure-limit pre-exponential factor, its temperature exponent, the high-pressure-limit pre-exponential factor, its temperature exponent, and the broadening factor, respectively. For the second reaction, the listed value is the temperature-independent Arrhenius rate constant.