Effects of Anthropogenic Pollutants on Biogenic Secondary Organic Aerosol Formation in the Atmosphere of Mt. Hua, China

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Text S1 Estimation the IEPOX reactive uptake on particles at MS site

To quantitatively assess the effects of aerosol water on isoprene-derived SOA formation, the pseudo-first-order heterogeneous reaction rate constant for IEPOX uptake to particle (k_{het}, 1/s) is calculated using the method of Gaston et al. (2014), in which the gas phase diffusion is not considered due to its minor effects on k_{het} (eq. (1)). And the possibility of IEPOX reactive uptake (i.e., uptake coefficient, γ_{IEPOX}) was also calculated using eqs 2-3.

$$k_{het} \approx \frac{\gamma_{IEPOX} S_a \omega}{4} \qquad \text{Eq. (1)}$$

$$\frac{1}{\gamma_{IEPOX}} = \frac{R_p \omega}{4D_g} + \frac{1}{\alpha} + \frac{1}{\Gamma_{aq}} \qquad \text{Eq. (2)}$$

$$\Gamma_{aq} = \frac{4VRTH_{aq}k_{aq}}{S_a \omega} \qquad \text{Eq. (3)}$$

$$k_{aq} = \left(k_{H^+}[H^+]\right) + \left(k_{nuc}[nuc]\alpha_{H^+}\right) + k_{ga}[ga] \qquad \text{Eq. (4)}$$

Where S_a represents the total surface area concentration of particles (cm^2/cm^3); The S_a, particle radium (R_p, m) and total particle volume (V, cm^3/cm^3) were measured using a scanning mobility particle sizer (SMPS) here, more details can be found elsewhere (Cao, 2018). In equations 2-3, ω is the mean molecular speed of an epoxide molecule (231 m/s, at 298 K), D_g the gas-phase diffusion coefficient (0.1 cm^2/s); α is the mass accommodation coefficient, with a mean value of 0.1. R is the universal gas constant (L atm/mol K), T represent the temperature (K). The Henry's law coefficient in the aqueous phase, H_{aq}, is estimated to be 1.7×10^8 (M/atm). The pseudo-first-order aqueous-phase rate constant, k_{aq} (1/s), is based on an acid-catalyzed, epoxide ring-open mechanism. k_{H^+} is the reaction rate taken to be 0.036 (M/s); [H^+] and α_{H^+} are the concentration (mol/L) and activity of proton, respectively. k_{nue} is the reaction rate due to the presence of specific nucleophiles (e.g., sulfate, nitrate), which is estimated to be 2.0×10^4 (M/s); [nue] is the nucleophiles concentration (mol/L). [ga] represent the concentration of general acids (e.g., bisulfate, mol/L), of which reaction rate is taken to 2.0×10^4 (M/s). All the key parameters applied here are consistent with Gaston et al. (2014).

Table S1 RF model performance for testing dataset.

	R^2	MSE	RMSE	MAE
Training dataset	0.91	0.012	0.11	0.07
Testing dataset	0.80	0.008	0.09	0.07

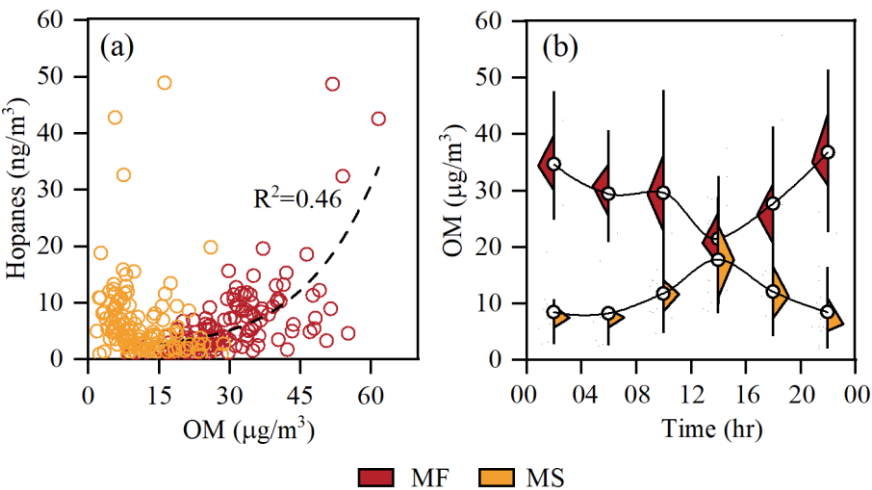Note: MSE: mean square error; RMSE: root-mean-square error; MAE: mean absolute error.

Figure S1 The fit regressions for OM with hopanes **(a)** and diurnal cycle of OM **(b)** at both sampling sites.
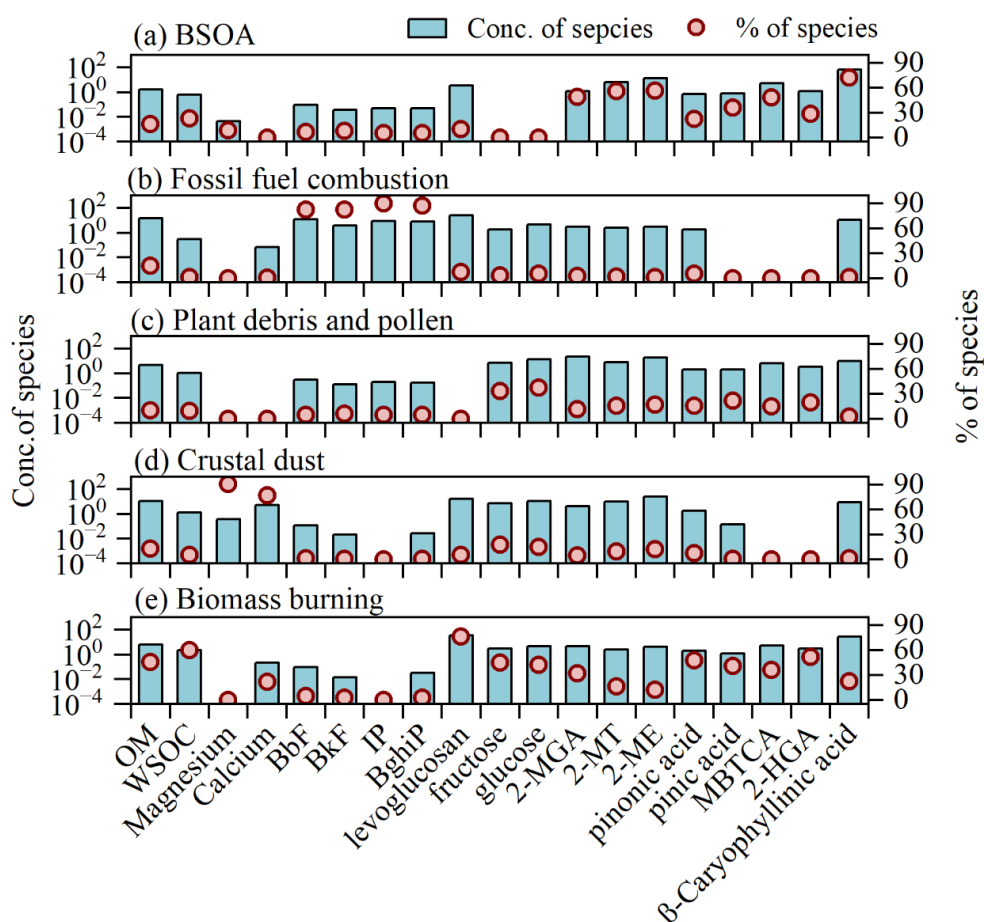
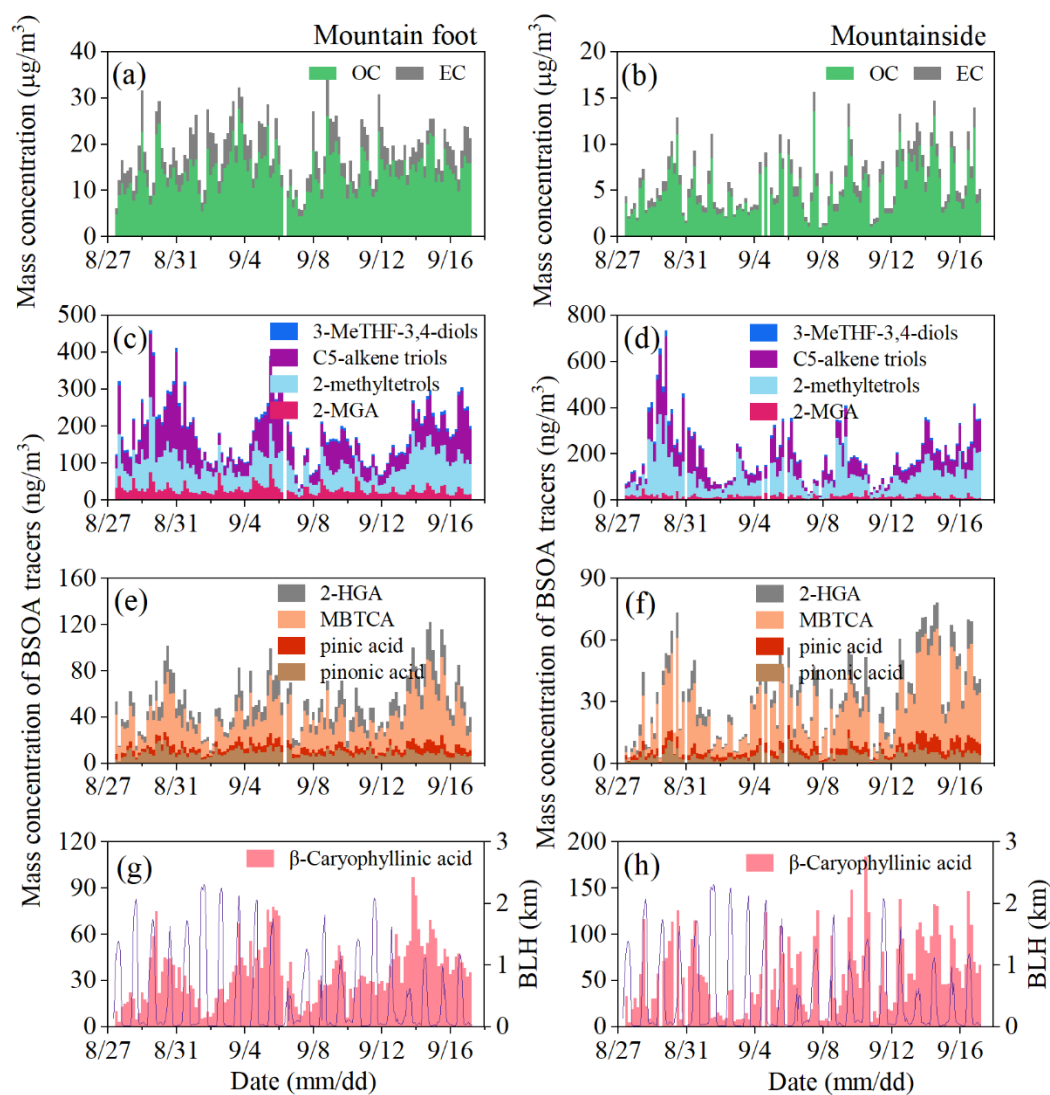**Figure S2** Factor profiles resolved by PMF mode for OM source apportionment.

Figure S3 Time series of the mass concentration of BSOA tracers and boundary layer height (BLH) at both sampling sites.
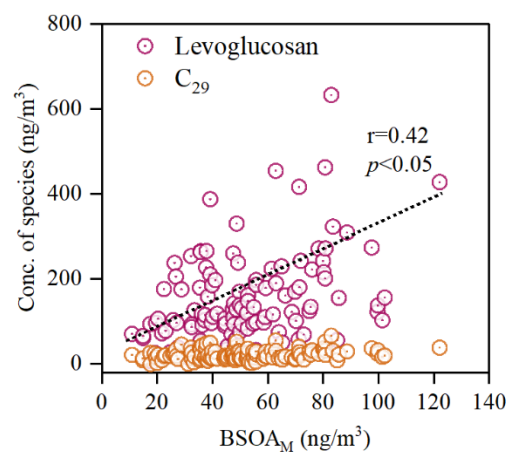
Figure S4 Correlation of $BSOA_M$ with levoglucosan and C_{29}-alkane at MF site.
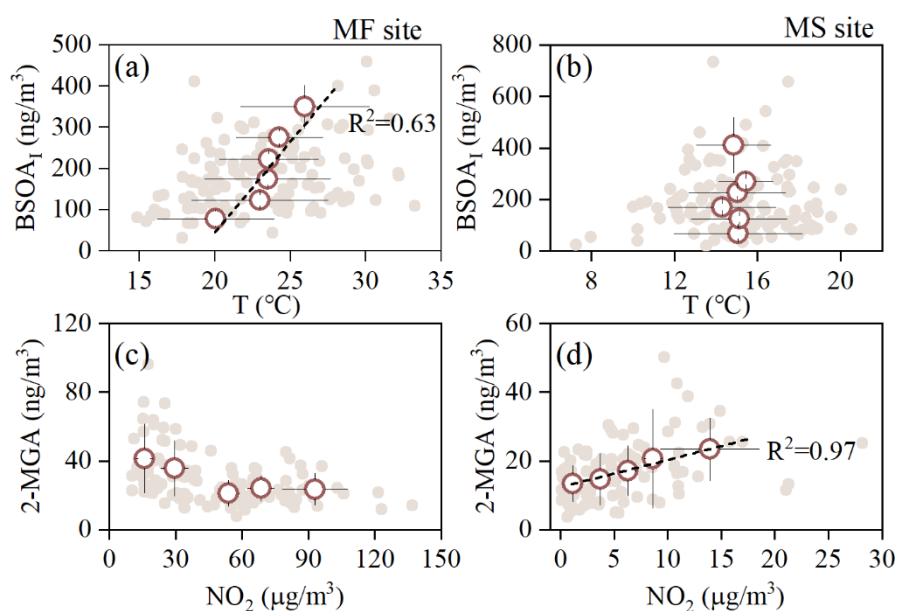

Figure S5 Linear correlations of $BSOA_I$ with temperature (**a** and **b**), and 2-MGA with NO_2 (**c** and **d**) at both sampling sites.
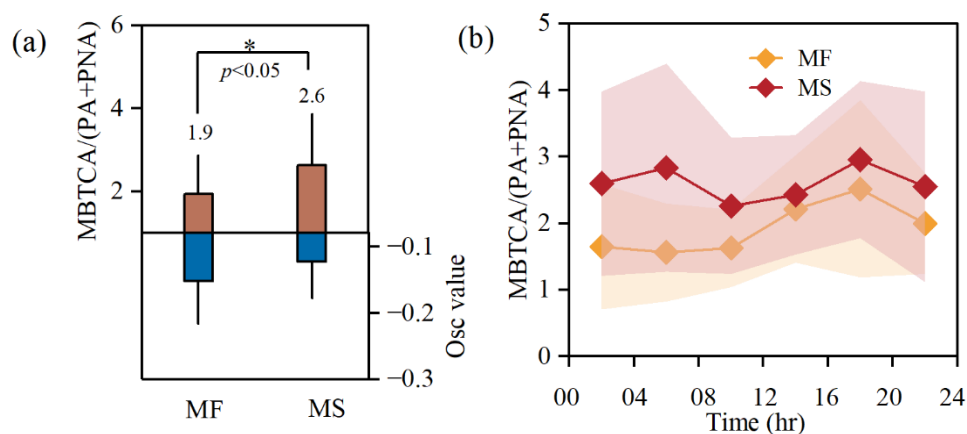
Figure S6 A comparison of BSOA$_M$ tracer among two sampling sites; (a) aging state, (b) diurnal variation of MBTCA/(PA+PNA) ratio. (Error bar of Osc value has been reduced by half)

References

Cao, C.: Vertical distribution of physical and chemical characteristics of PM2.5 at Mt. Hua and the new particle formation, 2018.

Gaston, C. J., Riedel, T. P., Zhang, Z., Gold, A., Surratt, J. D., and Thornton, J. A.: Reactive Uptake of an Isoprene-Derived Epoxydiol to Submicron Aerosol Particles, Environmental Science & Technology, 48, 11178-11186, 10.1021/es5034266, 2014.