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The effect of particle acidity on secondary organic aerosol formation from α -pinene photooxidation under atmospherically relevant conditions

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S1 High-NO_x regime assessment

The Master Chemical Mechanism (MCM v3.3.1, <http://mcm.leeds.ac.uk/MCMv3.3.1/home.htm>) was incorporated into a box model to assess the NO_x regime for the gas-phase reactions of α -pinene photooxidation under high-NO_x conditions. The box model was constrained with the initial experimental conditions including temperature, pressure, and the concentrations of α -pinene, NO, water vapor, and H₂O₂ for the individual chamber experiments in this study. The photooxidation reaction of α -pinene was simulated for 6 hours with the box model. The output of the box model was the time series of the concentrations of α -pinene, NO, O₃, HO₂, and organic peroxy radicals (RO₂) (molecule cm⁻³) from each time step with a 1-min resolution. The fraction of RO₂ radicals reacted with NO compared to the total reacted RO₂ radicals (with NO, HO₂, and RO₂) was calculated by

$$\frac{k_{\text{NO}}[\text{NO}]}{k_{\text{NO}}[\text{NO}] + k_{\text{HO}_2}[\text{HO}_2] + k_{\text{RO}_2}[\text{RO}_2]}$$

where k_{NO} , k_{HO_2} , and k_{RO_2} are the reaction rates of RO₂ + NO, RO₂ + HO₂ and RO₂ + RO₂, respectively and [NO], [HO₂], and [RO₂] are the concentration of NO, HO₂, and RO₂, respectively. The results from the box model are presented in Figure S1. At the start of the simulations, more than 99% of the RO₂ radicals were reacting with NO; while by the end of the experiments (after 6 hours), at least 62% of the RO₂ radicals continued to react with NO (Figure S1a). The time series for α -pinene, NO, and O₃ from the measurements were reasonably well captured by the box model (Figure S1b, c, and d).

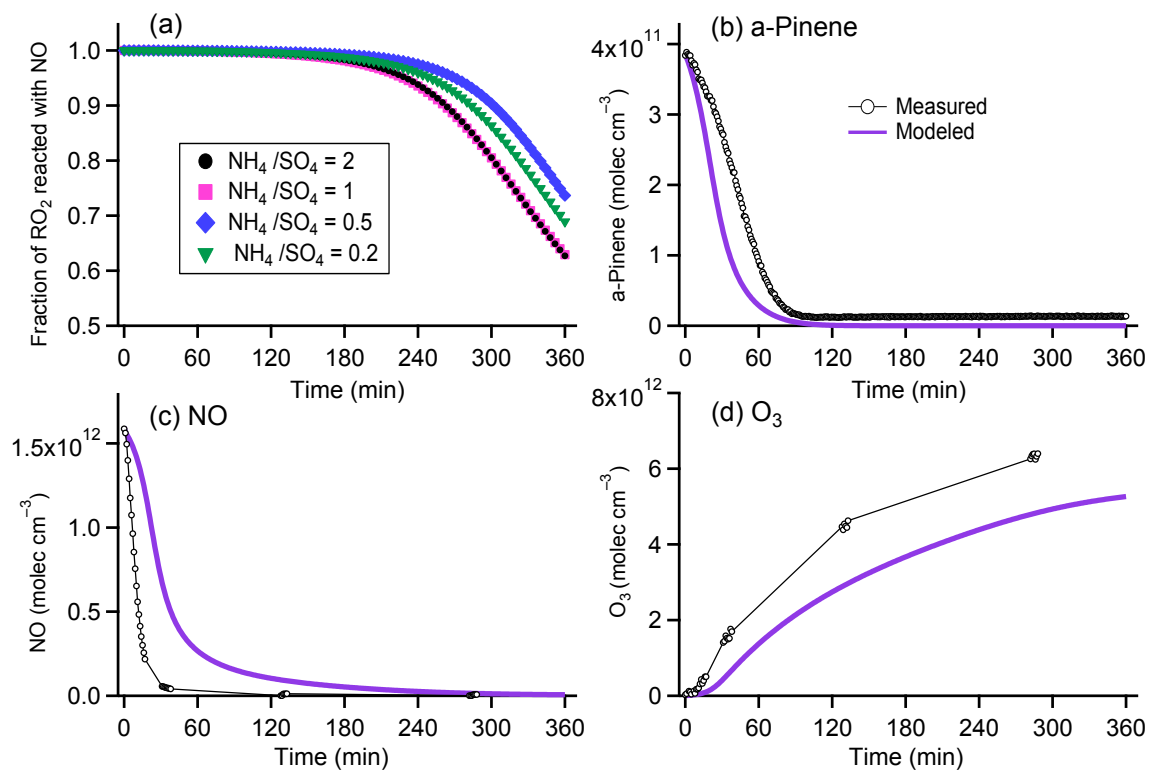


Figure S1. (a) Fraction of RO₂ reacted with NO compared to the total reacted RO₂ radicals for high-NO_x experiments with ammonium sulfate and acidic seed particles. The measured and the modeled time series of the concentrations of (b) *α*-pinene, (c) NO, and (d) O₃ for the high-NO_x experiment with ammonium sulfate particles (NH₄/SO₄ = 2). The variations in time for each species in all experiments with acidic particles under high-NO_x conditions are similar to (b), (c), and (d).

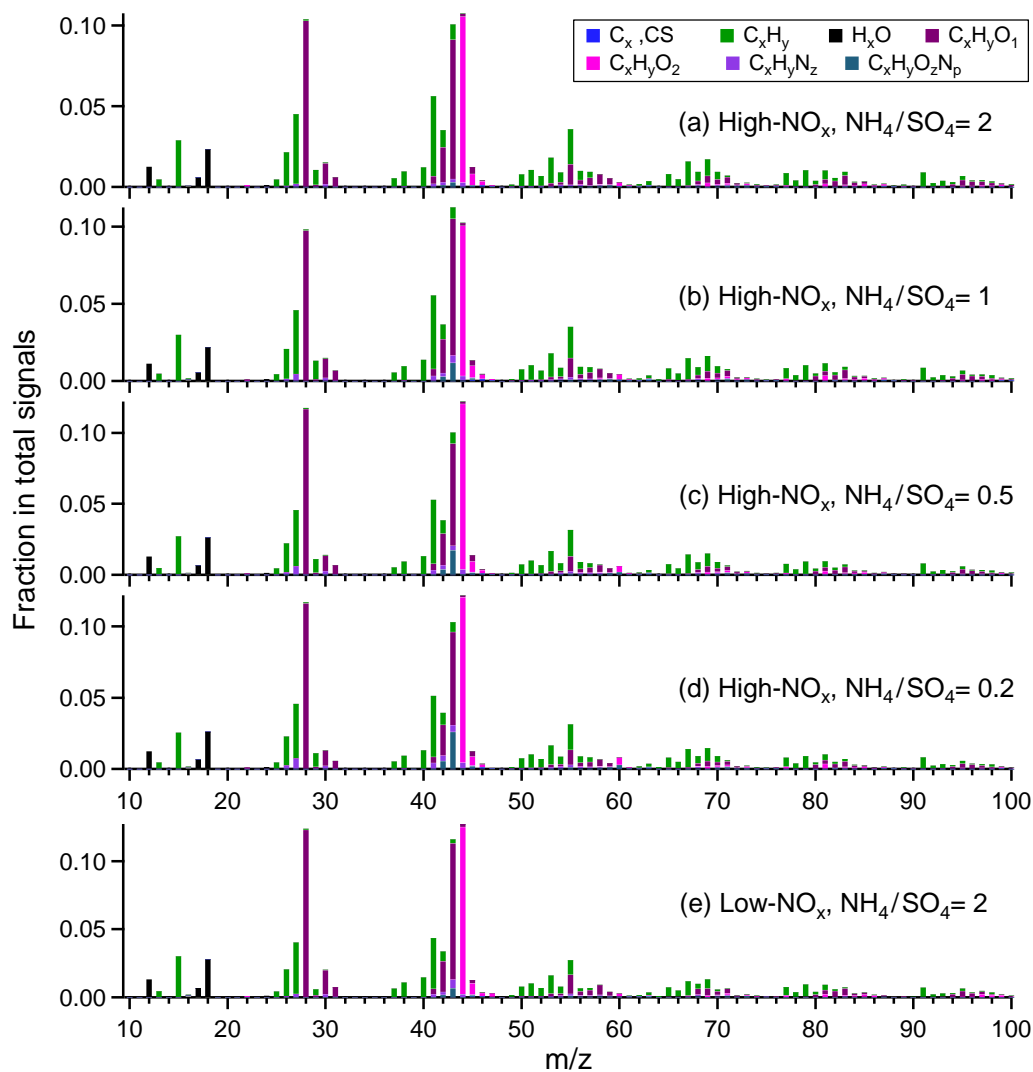


Figure S2. High-resolution mass spectra of α -pinene SOA under (a–d) high- and (e) low- NO_x conditions. The mass spectra were averaged on the irradiation times of 1–5 h and 2–12 h under high- and low- NO conditions, respectively. The mass spectra of α -pinene SOA under low- NO_x conditions for acidic particles, which are not presented here, resemble that of ammonium sulfate particles in (e).