Supplement of

Explicit simulation of chemical composition, size distribution and cloud condensation nuclei of secondary organic aerosol from α-pinene ozonolysis

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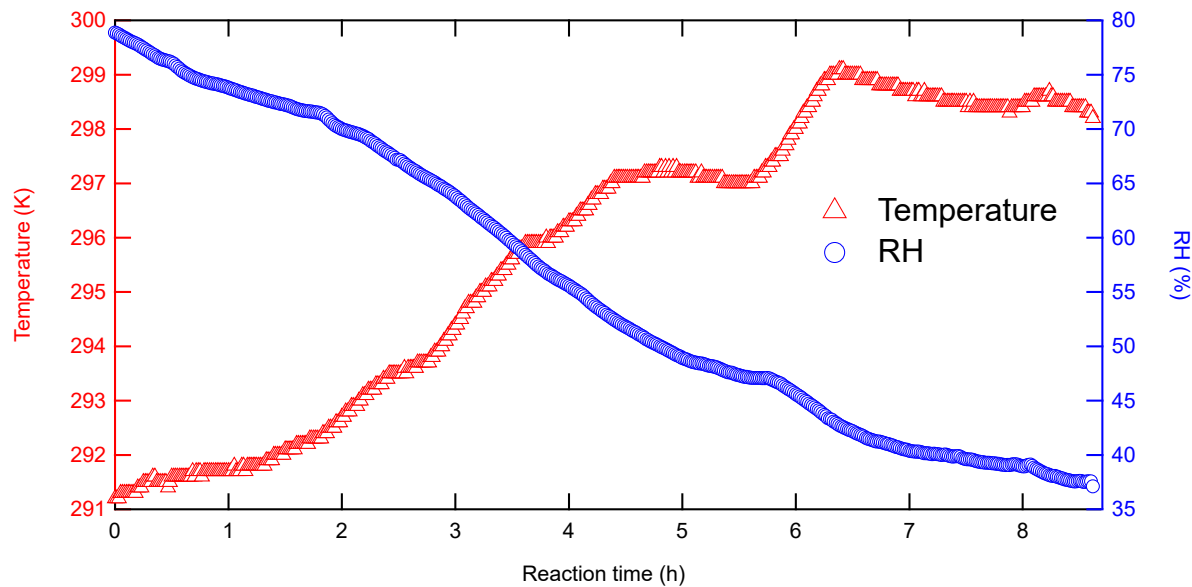
Table S1: The simulated hygroscopicity parameter (κ) of SOA calculated by different chemical composition and corresponding particle size (nm).

Particle size (nm)	κ
50.6	0.179
63.0	0.178
84.8	0.177

25 **Figure S1: The time evolution of measured temperature (Unit: K) and relative humidity (RH; %) during the experiment of α-pinene ozonolysis in the dark.**

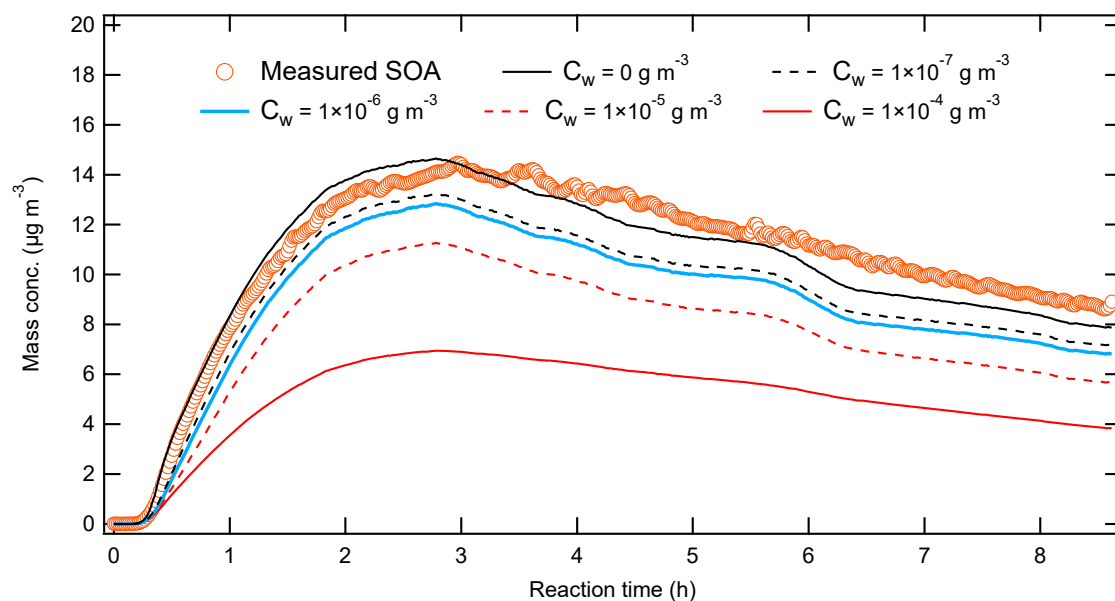



Figure S2: The sensitivity of SOA mass concentration to parameter C_w which represents effective absorbing wall mass concentration (g m^{-3}).

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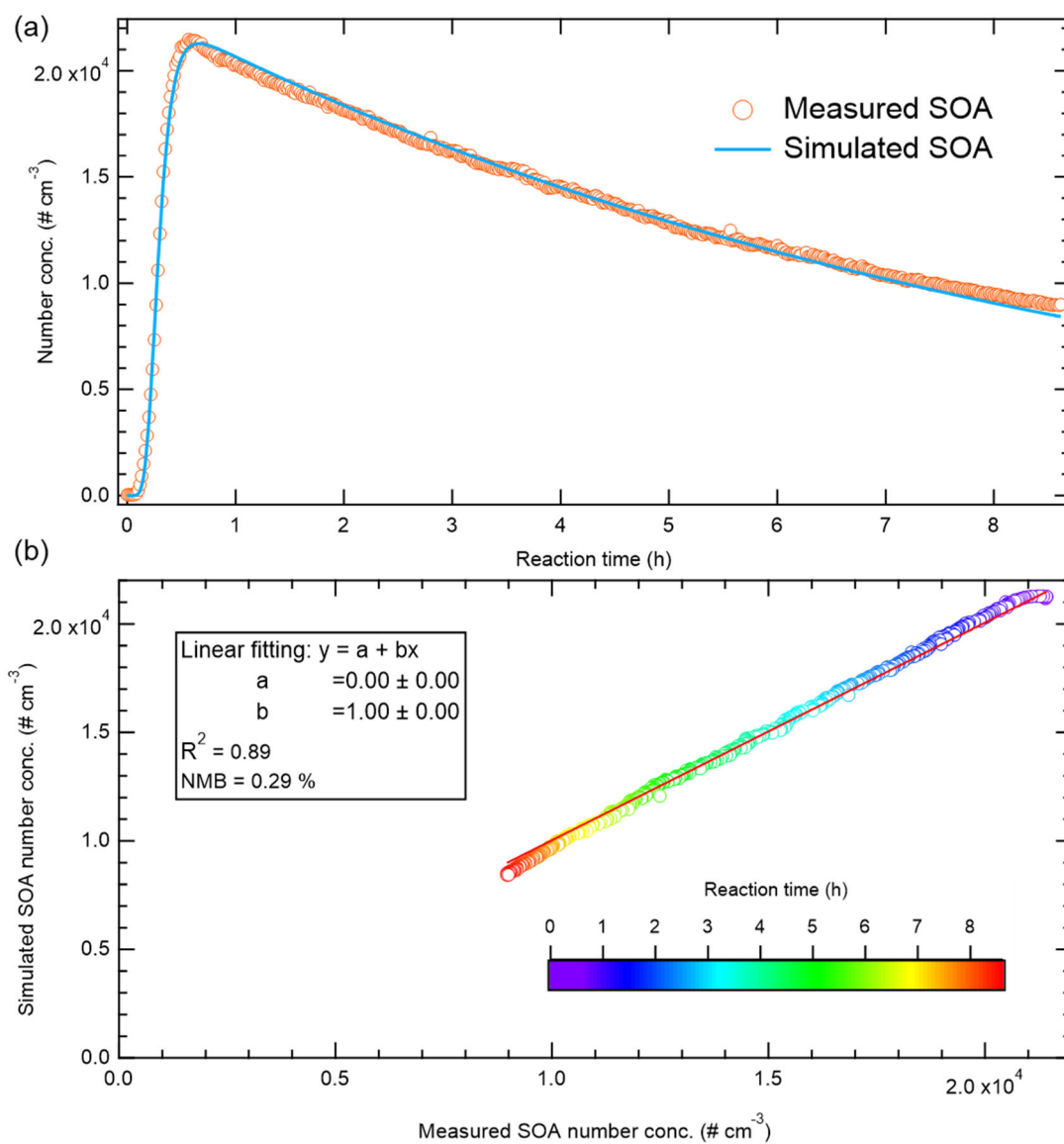


Figure S3: (a) Simulated (line) and measured (circles) SOA number concentrations (# cm^{-3}) when setting nucleation parameters. (b) Scatter plot of measured versus simulated SOA number concentrations, with a linear fit (red line). The coefficients a and b represent the intercept and slope, respectively, and R^2 denotes the correlation coefficient. Colors indicate the reaction time of the experiment. Note that the linear fitting through the origin, and NMB refers to normalized mean bias. Scatters from the initial 0.57 hours were excluded, as the number concentration during this period was fitted to CPC measurements and assumed to match measurements perfectly. Note that the coagulation is excluded.

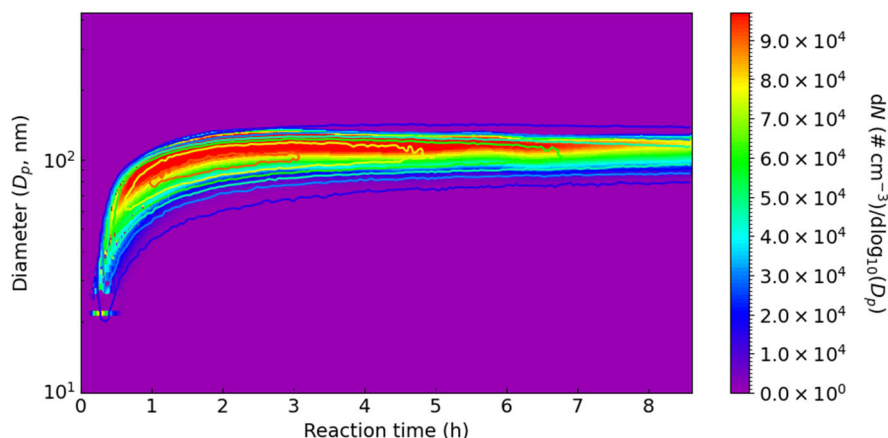



Figure S4: The time evolution of number size distributions (dN/dlog$_{10}$D$_p$) of measured (contour lines) and simulated (shaded areas) SOA when setting nucleation parameters. Note that the coagulation is excluded.

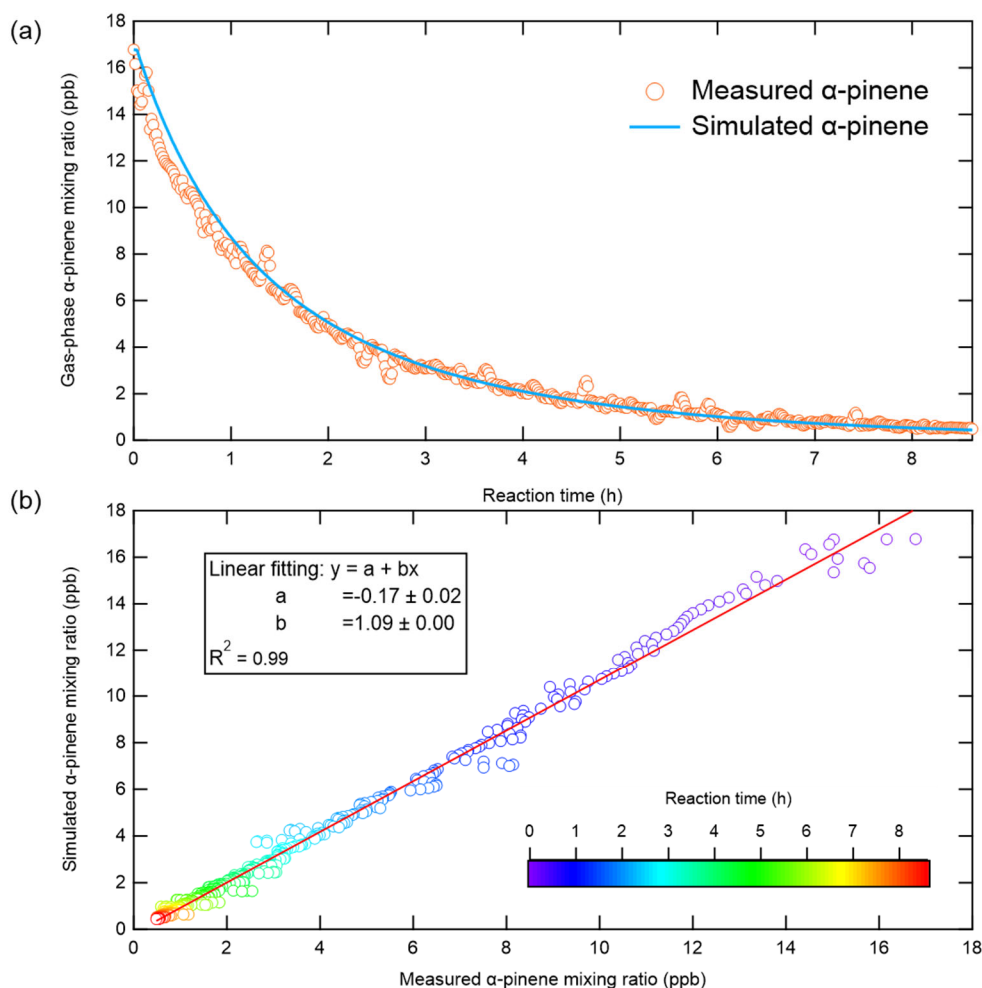
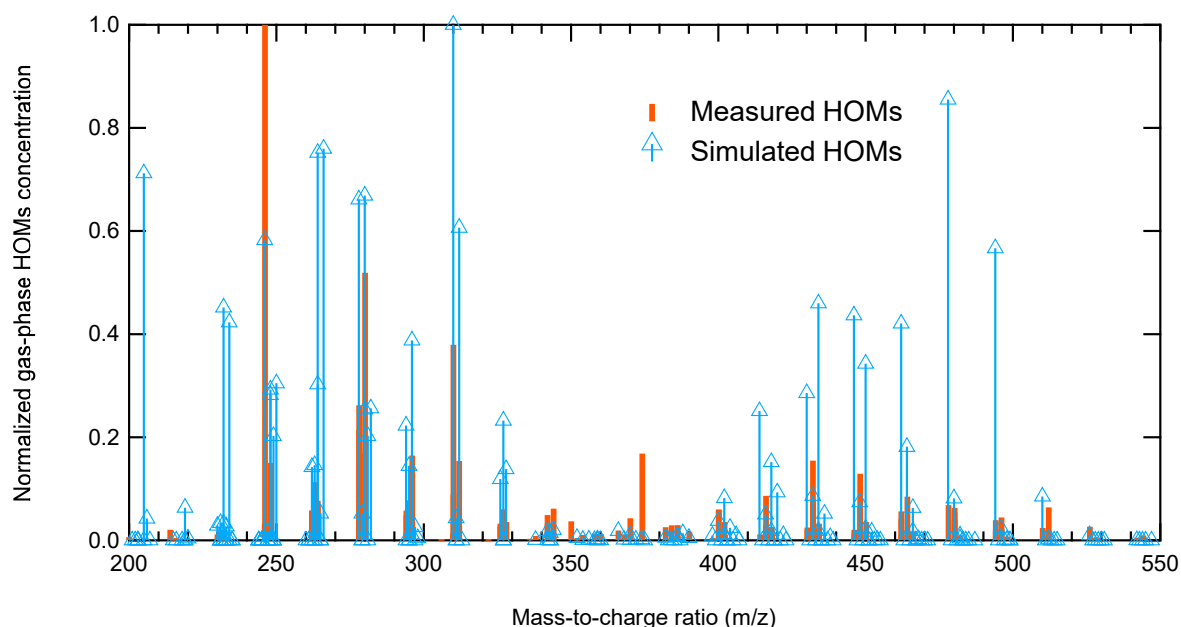



Figure S5: (a) The time evolution of the measured (circles) and simulated (line) gas-phase α-pinene mixing ratio (ppb). (b) Scatter plot of measured versus simulated α-pinene concentrations, with a linear fit (red line). The coefficients a and b represent the intercept and slope, respectively, and R^2 denotes the correlation coefficient. Colors indicate the reaction time of the experiment.

45 **Figure S6: Measured and simulated gas-phase HOMs mass spectra averaged over the first 10 minutes of experiment, during which gas-phase HOMs were rapidly accumulated and particle-phase concentrations were low.**

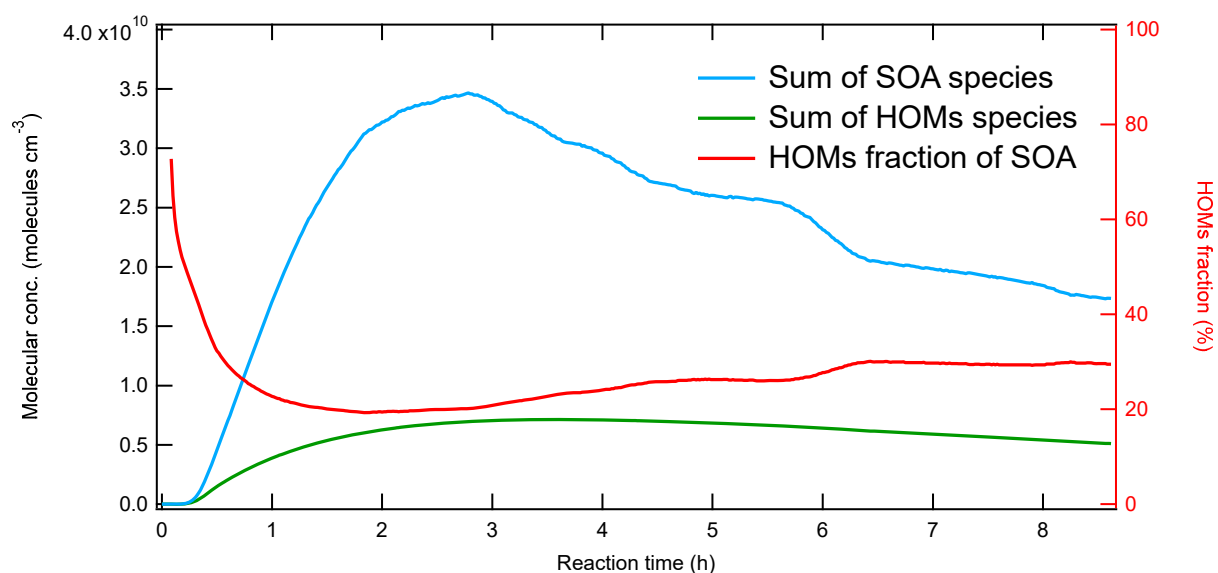



Figure S7: The time evolution of total molecular concentrations (molecules cm^{-3}) of simulated SOA and HOMs species, and HOMs fraction (%) of SOA.

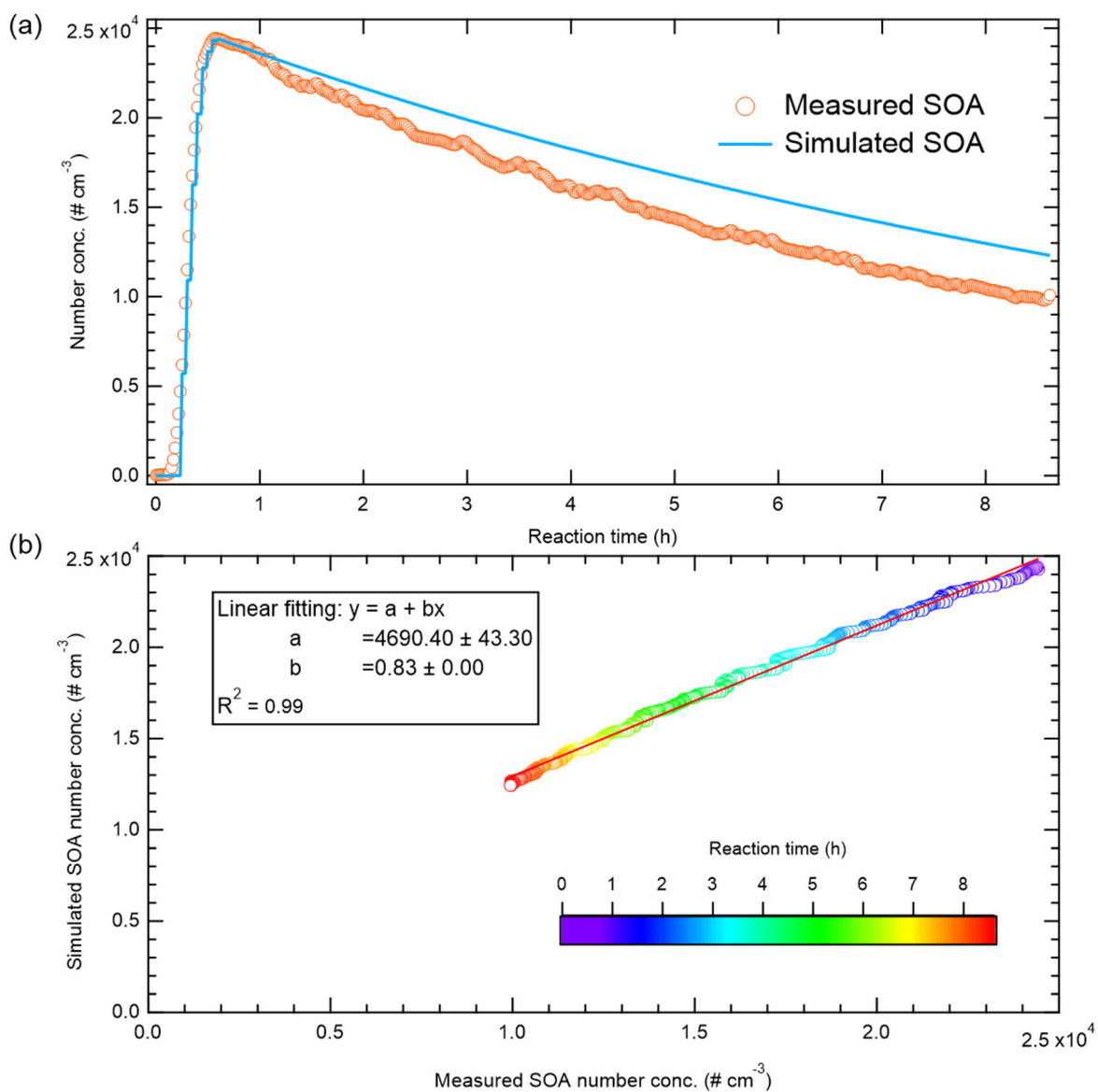



Figure S8: (a) Simulated (line) and measured (circles) SOA number concentrations (# cm⁻³) when constraining size distribution of seed particle and not considering coagulation. **(b)** Scatter plot of measured versus simulated SOA number concentrations, with a linear fit (red line). Scatters from the initial 0.6 hours were excluded, as the number concentration during this period was fitted to SMPS measurements.

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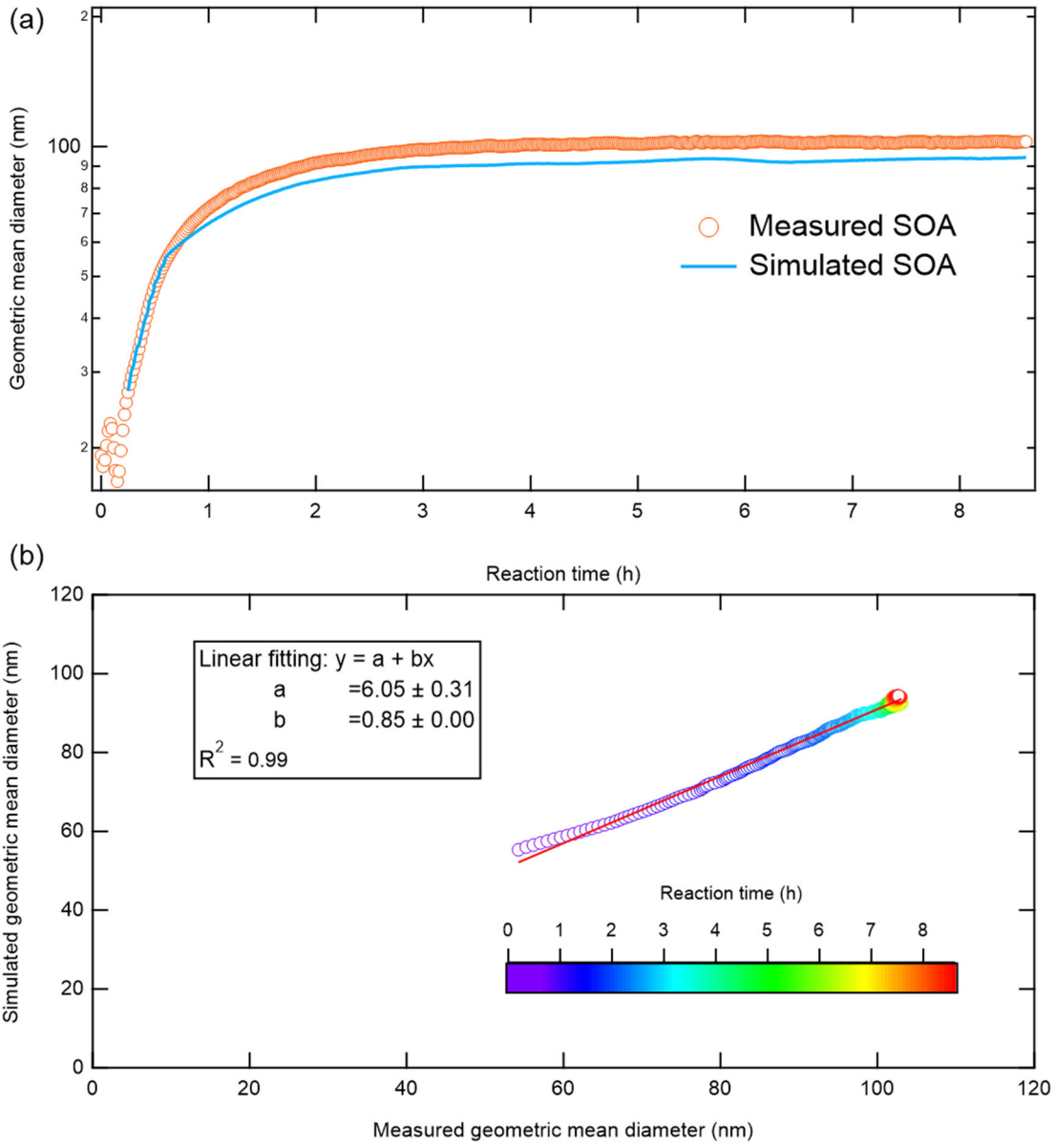


Figure S9: (a-b) Same as Fig. S8, but for geometric mean diameter (nm) of SOA. Note that the coagulation is not considered, and scatters from the initial 0.6 hours were excluded as particle size distribution during this period was fitted to SMPS measurements.

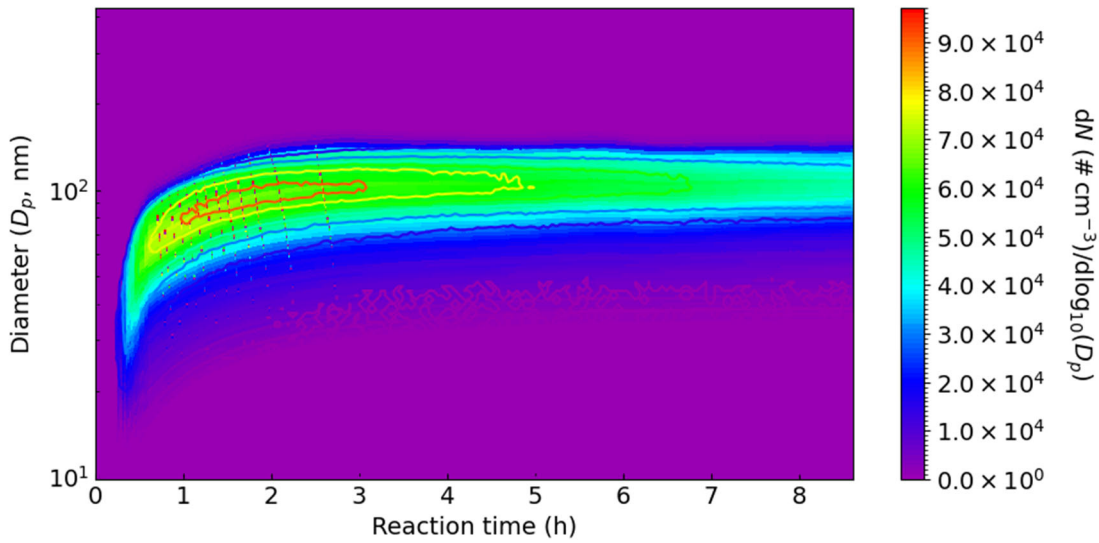



Figure S10: The time evolution of number size distributions ($dN/dlog_{10}D_p$) of measured (contour lines) and simulated (shaded areas) SOA in the case of not considering coagulation.

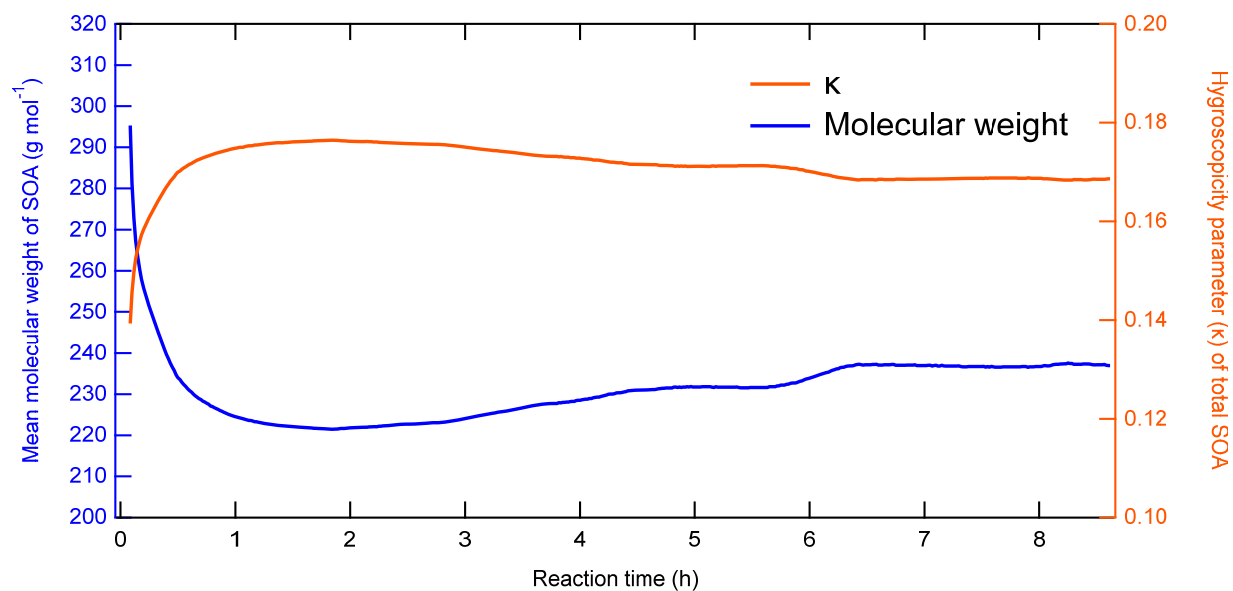
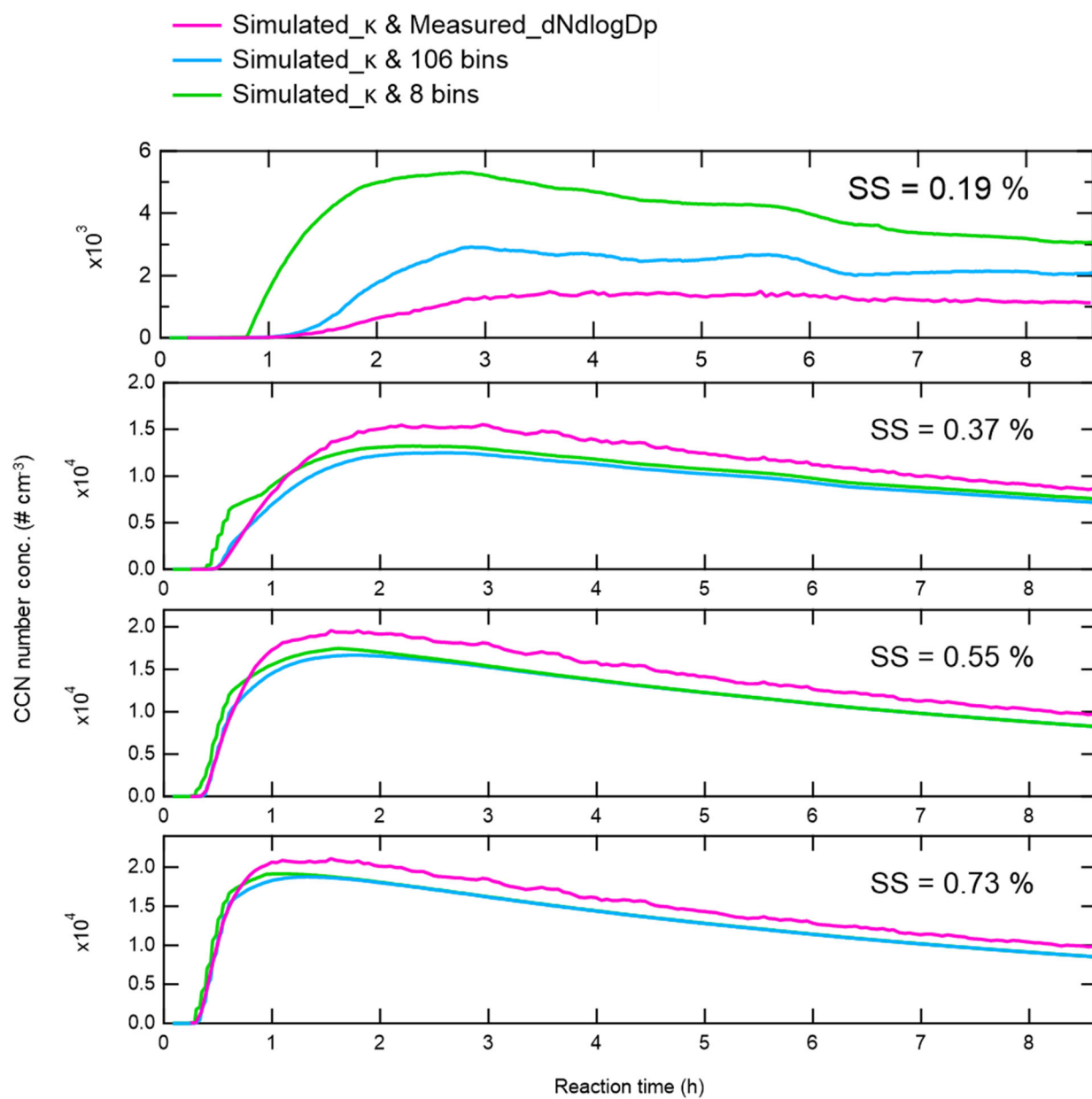



Figure S11: The time evolution of mean molecular weight and hygroscopicity parameter (κ) of simulated SOA.

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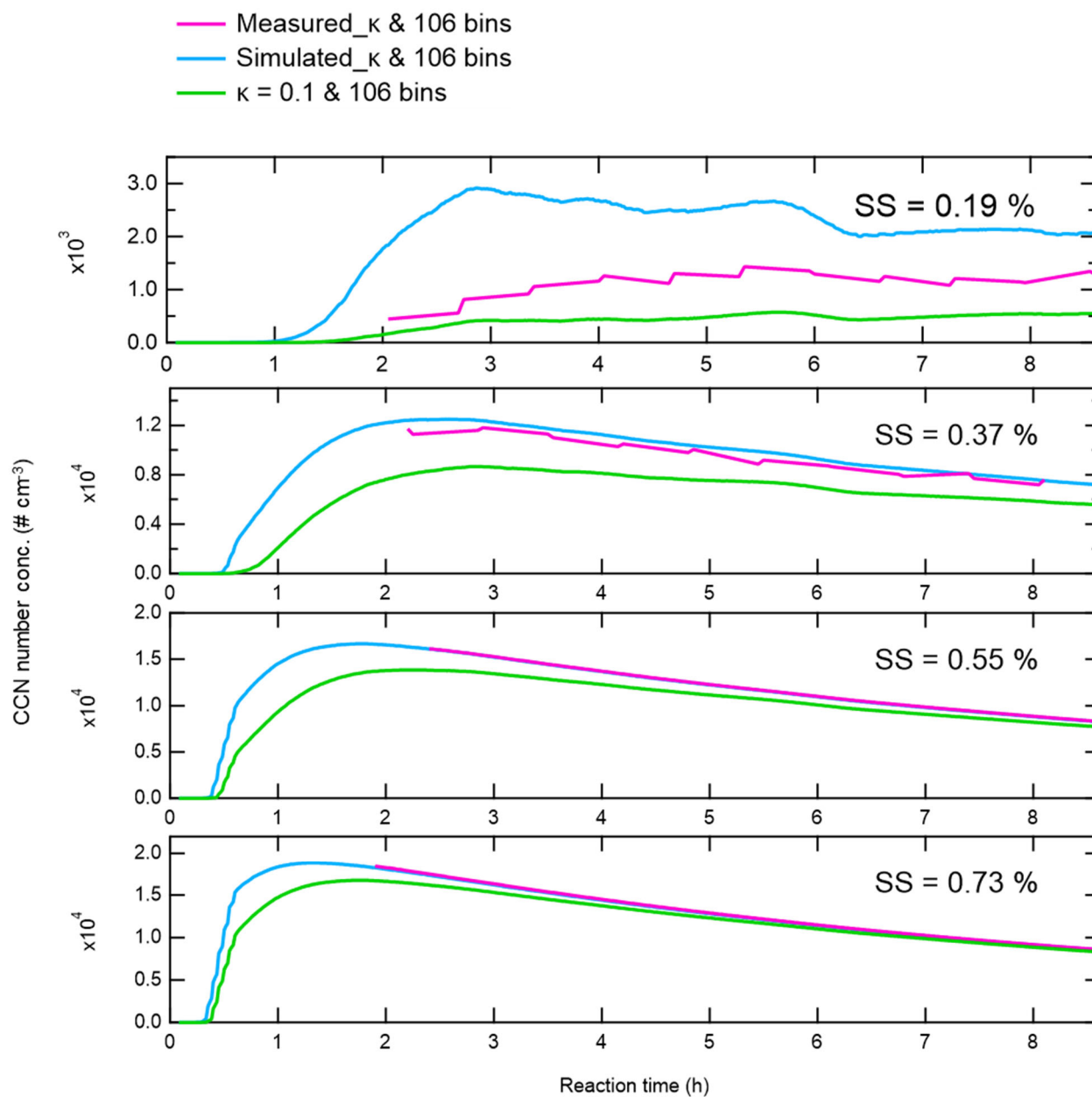
Figure S13: (a-d) The CCN number concentrations (# cm⁻³) at different SS based on simulated particle number size distribution of 106 size bins setting and three kinds of κ, including measurement (purple line), calculation of UManSysProp (blue line), and a fixed value (0.1) (green line).