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Supplement of

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

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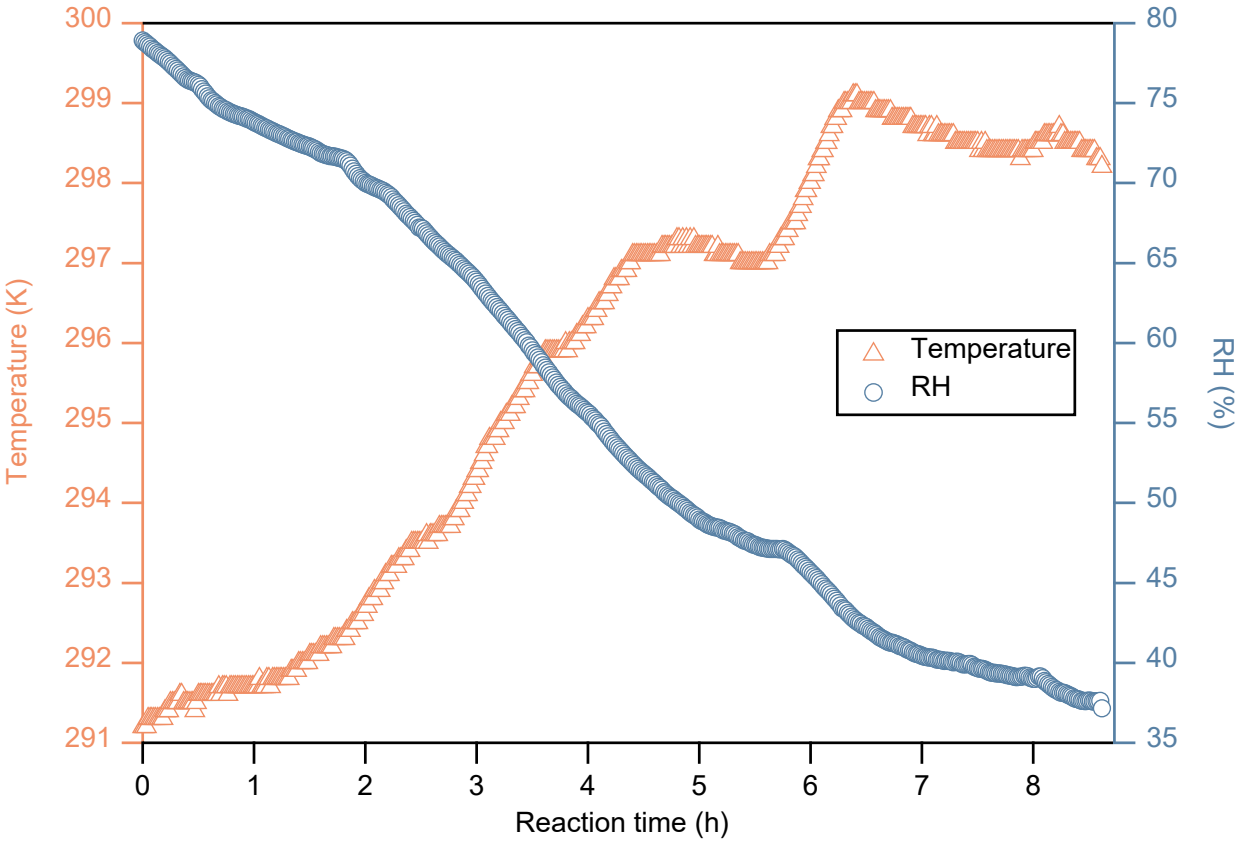


Figure S1: Time evolution of measured temperature (K) and relative humidity (RH; %) during the dark α-pinene ozonolysis experiment.

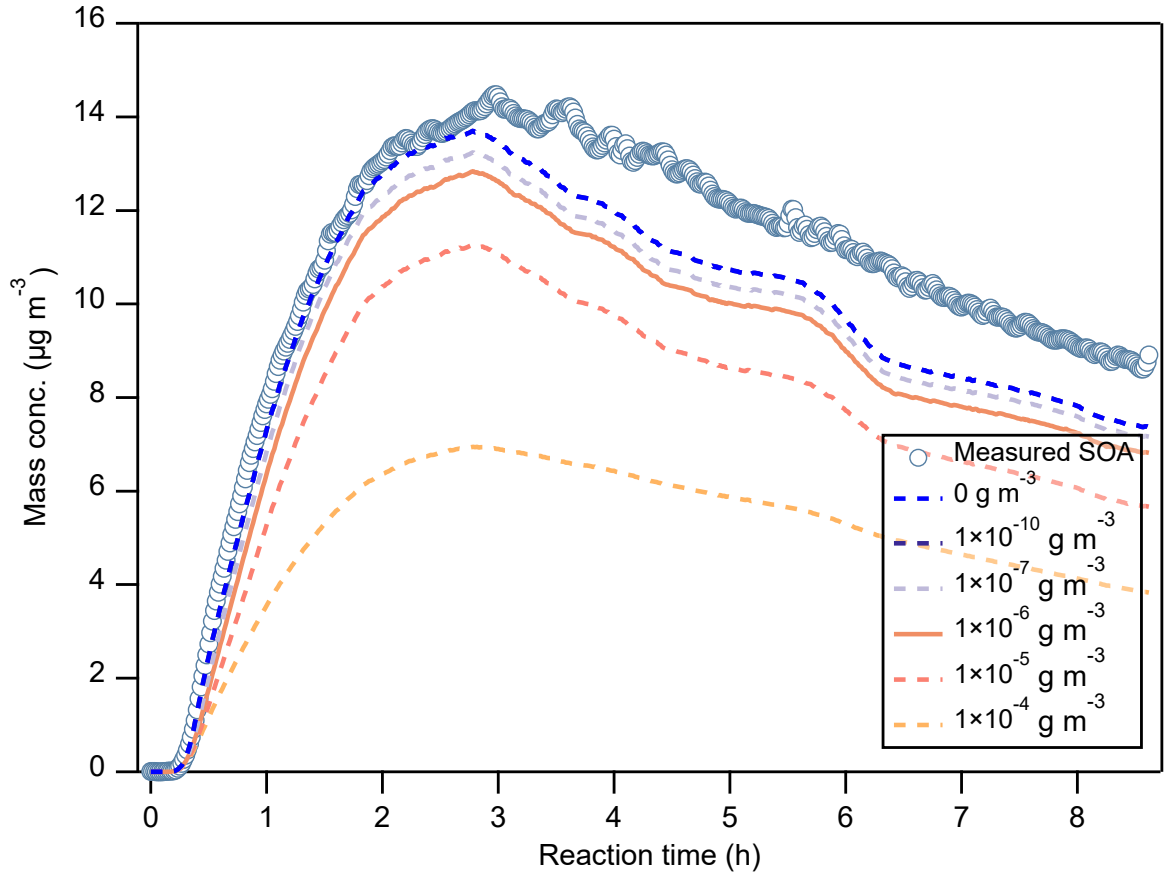


Figure S2: Sensitivity of SOA mass concentration to the parameter C_w, which represents the effective absorbing wall mass concentration (g m^{-3}). This study adopts $C_w = 1\times10^{-6}$ g m^{-3}.

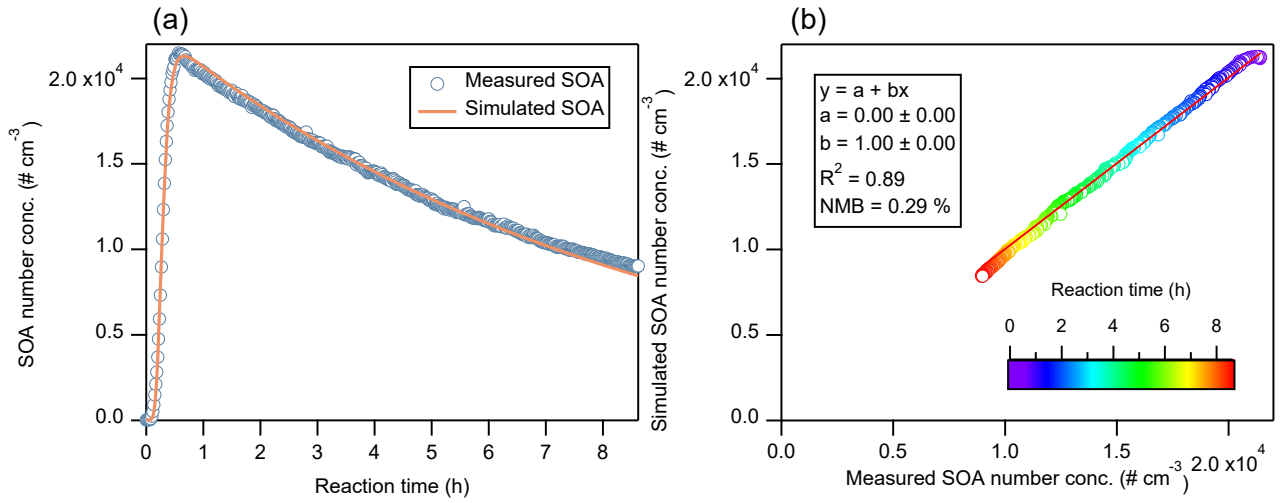


Figure S3: (a) Simulated (line) and measured (circles) SOA number concentrations (# cm^{-3}) using the nucleation parameters. (b) Scatterplot of measured versus simulated SOA number concentrations, with a linear fit (red line). The coefficients a and b represent the intercept and slope, respectively, and R^2 denotes the correlation coefficient. Colors indicate the reaction time during the experiment. Note that the linear regression is constrained through the origin. NMB refers to normalized mean bias. Data points from the initial 0.57 h are excluded because the number concentration during this period was fitted to CPC measurements and therefore assumed to match measurements exactly. Coagulation is excluded from the simulation.

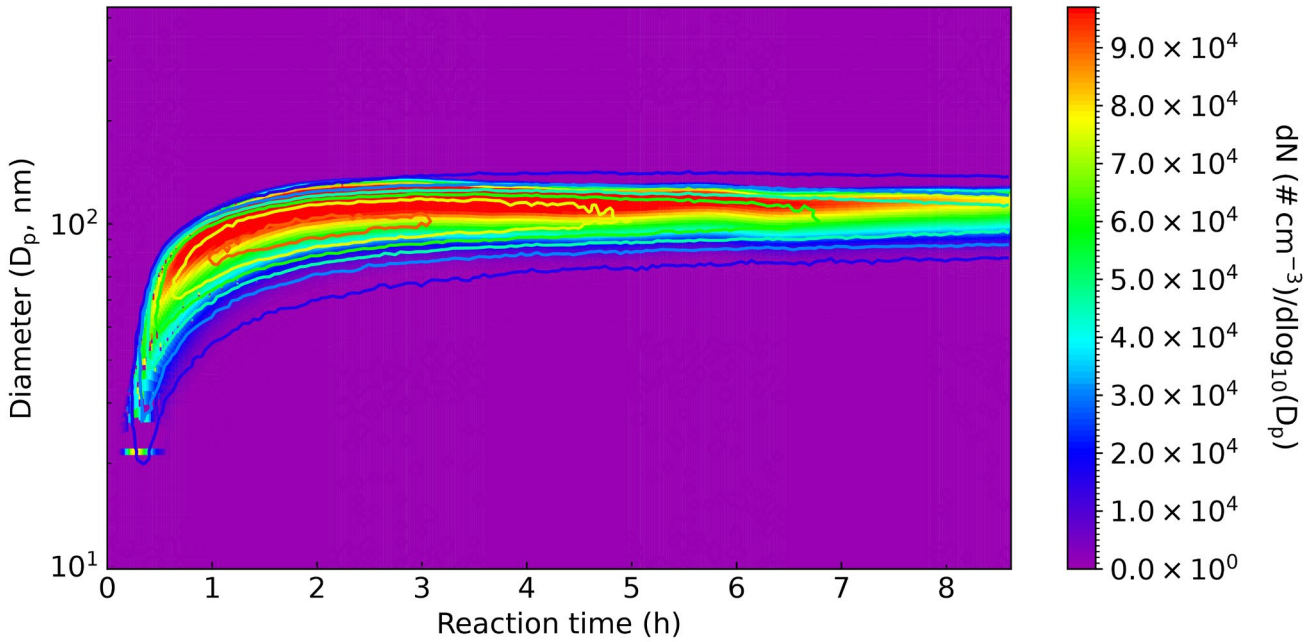


Figure S4: Time evolution of the number size distributions (dN/dlog$_{10}$D$_p$) for measured (contour lines) and simulated (shaded areas) SOA using the nucleation parameters. Coagulation is excluded from the simulation.

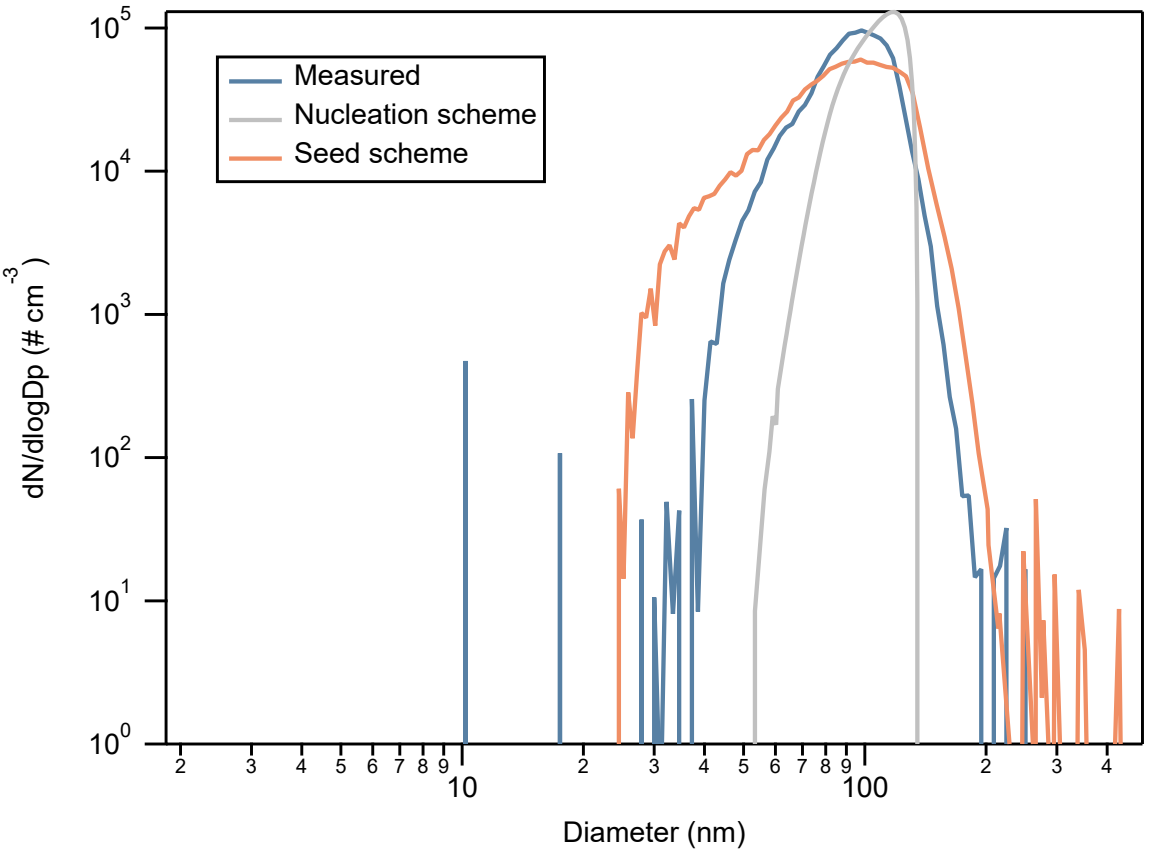
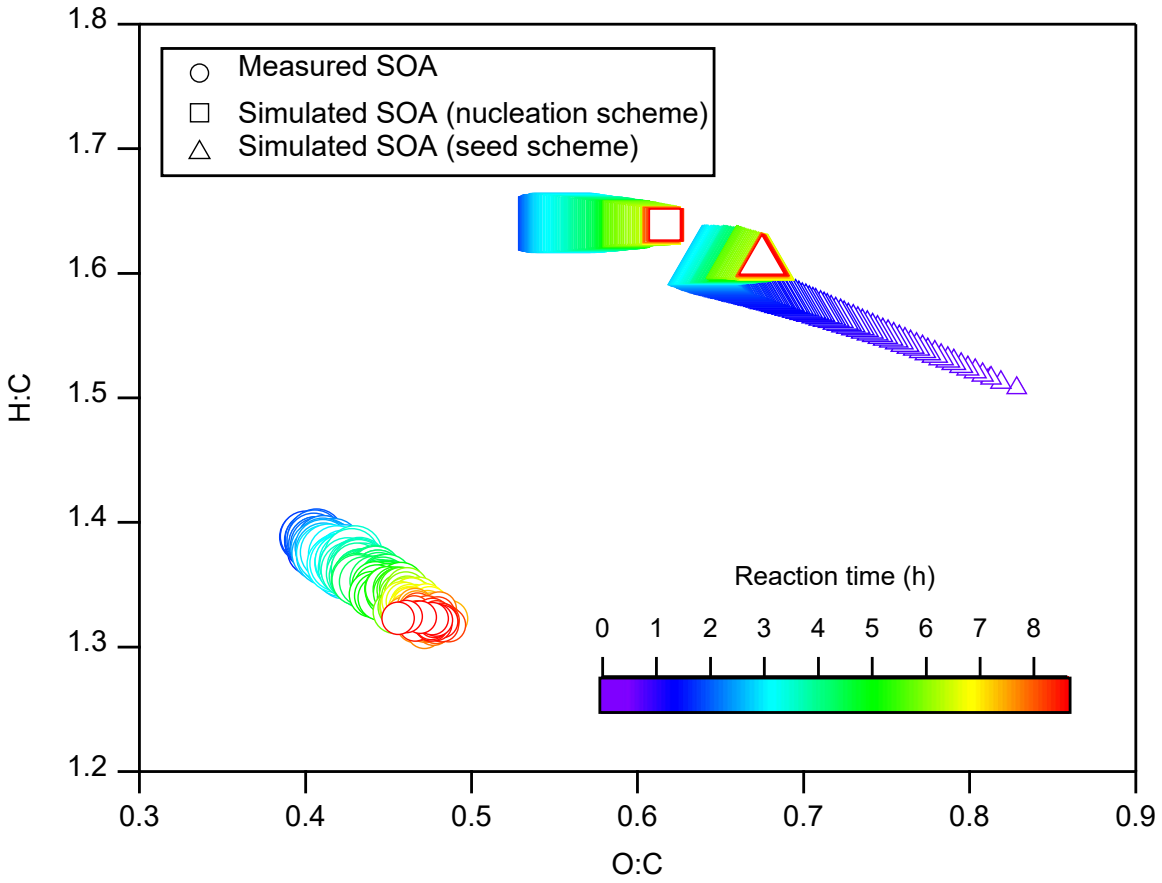


Fig. S5: Measured and simulated (by nucleation or seed schemes) particle size distribution ($dN/dlogD_p$) at the reaction time of 2 h.



20 **Figure S6: O:C and H:C ratios for measured (circles) and simulated SOA using the nucleation scheme (squares) or seed scheme (triangles).**

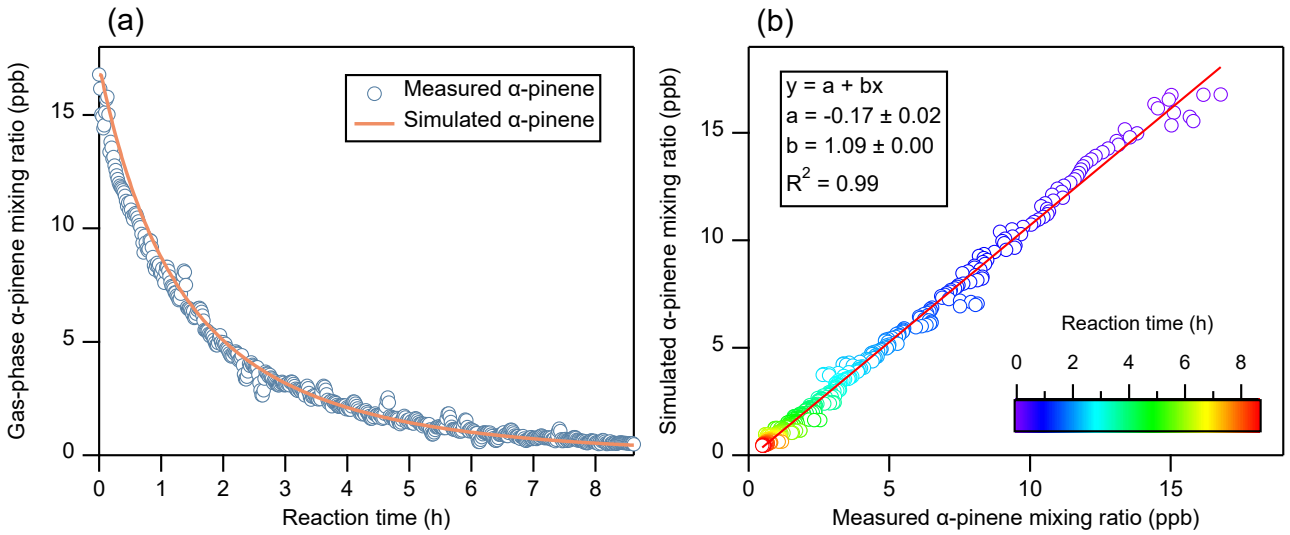


Figure S7: (a) Time evolution of the measured (circles) and simulated (line) gas-phase α-pinene mixing ratio (ppb). (b) Scatterplot of measured versus simulated α-pinene concentrations, with a linear fit (red line). The coefficients a and b represent the intercept and slope, respectively, and R^2 denotes the correlation coefficient. Colors indicate the reaction time during the experiment.

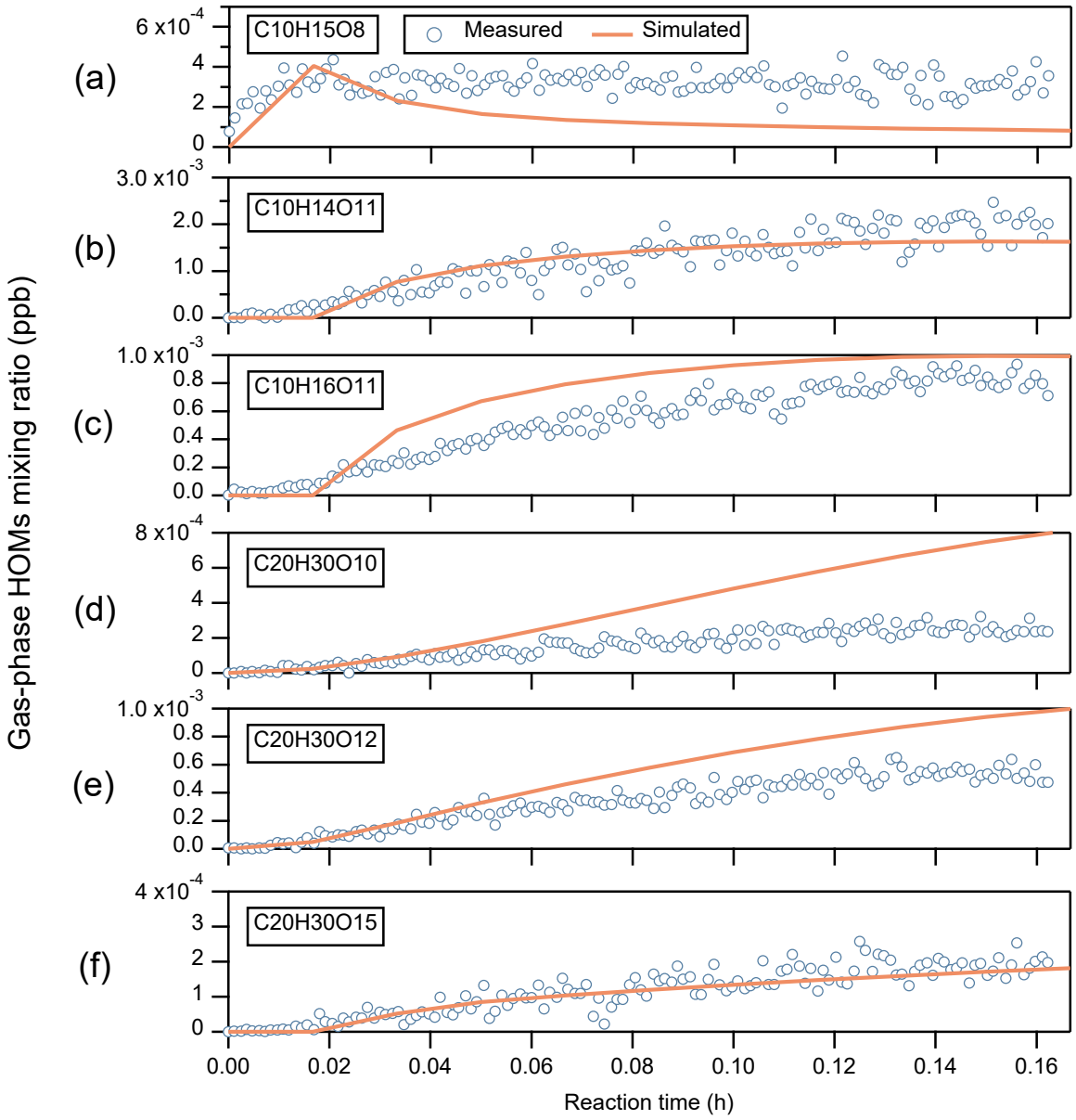


Figure S8: (a-f) Time evolution of the measured (circles) and simulated (lines) gas-phase HOMs mixing ratio (ppb) during the initial 10 min of reaction.

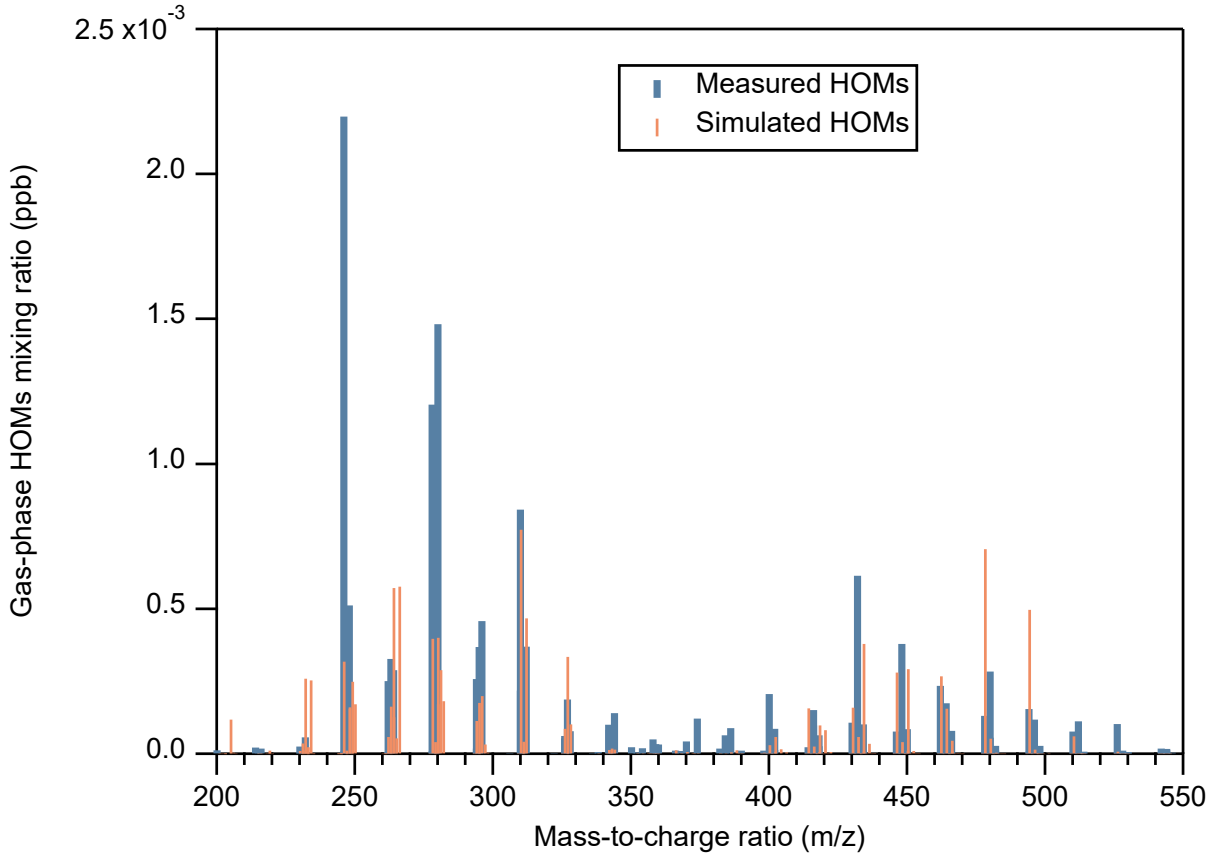


Figure S9: Measured and simulated gas-phase HOMs mass spectra averaged over the first 5 min of experiment, during which gas-phase HOMs accumulated rapidly and particle-phase concentrations remained low.

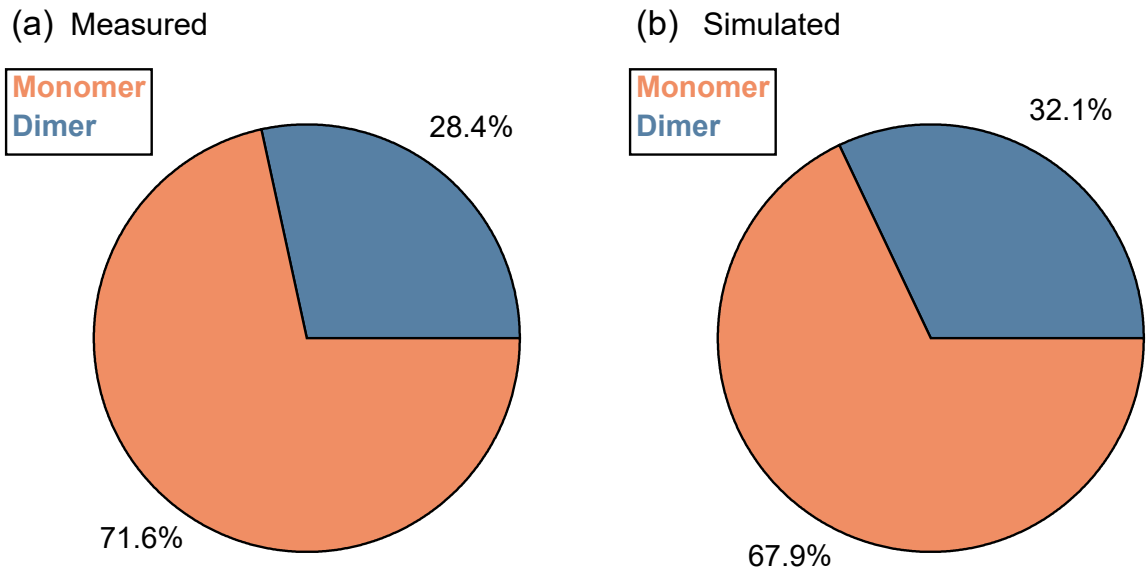


Figure S10: (a) Measured and (b) simulated fractions of HOMs monomers and dimers averaged over the first 5 min of experiment.

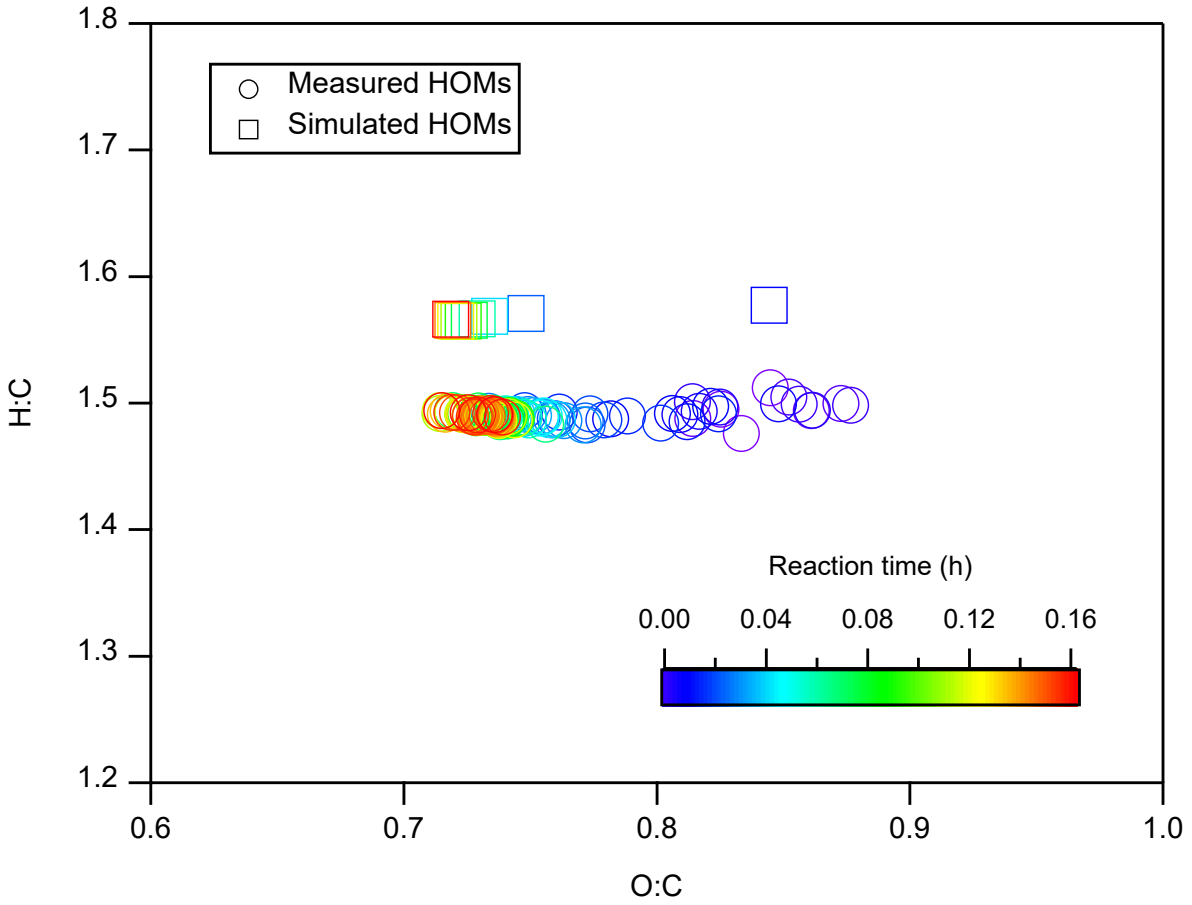


Figure S11: O:C and H:C ratios for measured (circles) and simulated (squares) gas-phase HOMs within the first 10 min of the experiment.

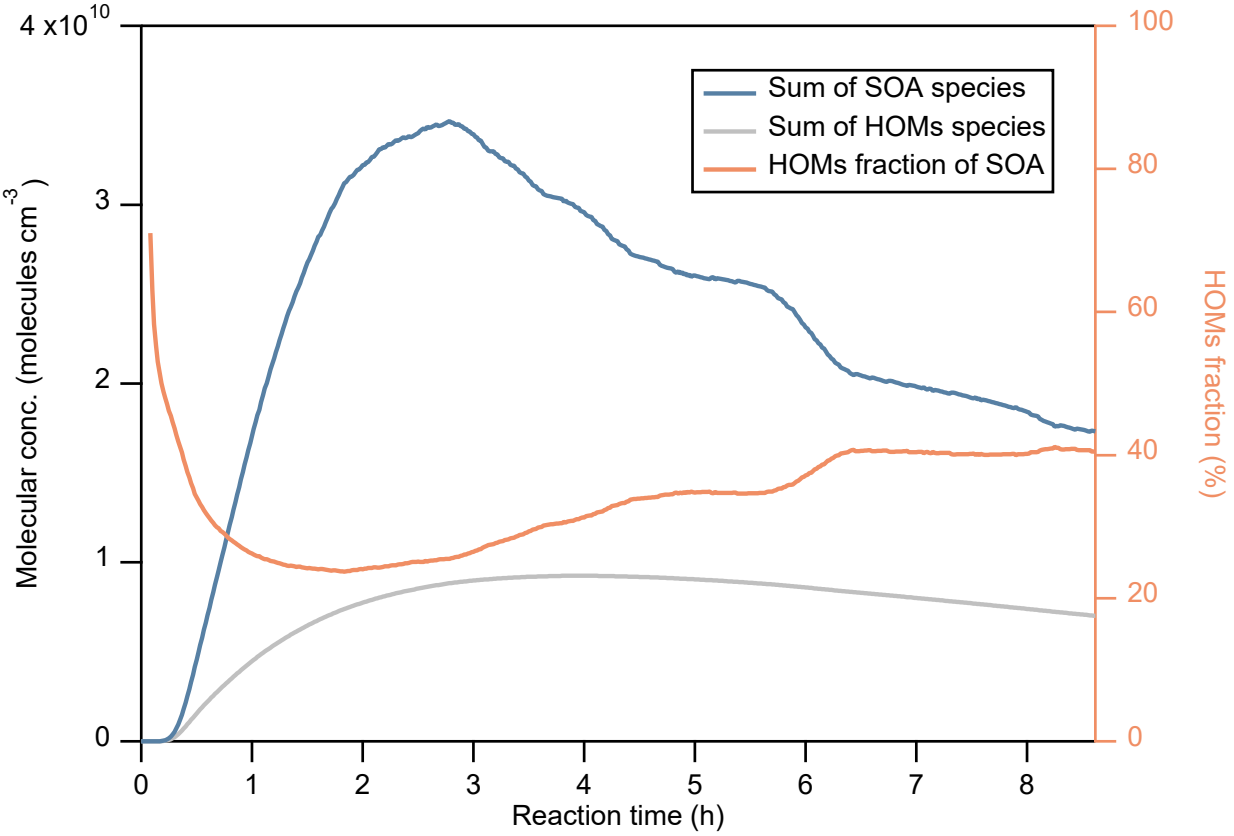


Figure S12: Time evolution of total molecular concentrations (molecules cm^{-3}) of simulated SOA and HOMs species, along with the HOMs fraction (%) of total SOA.

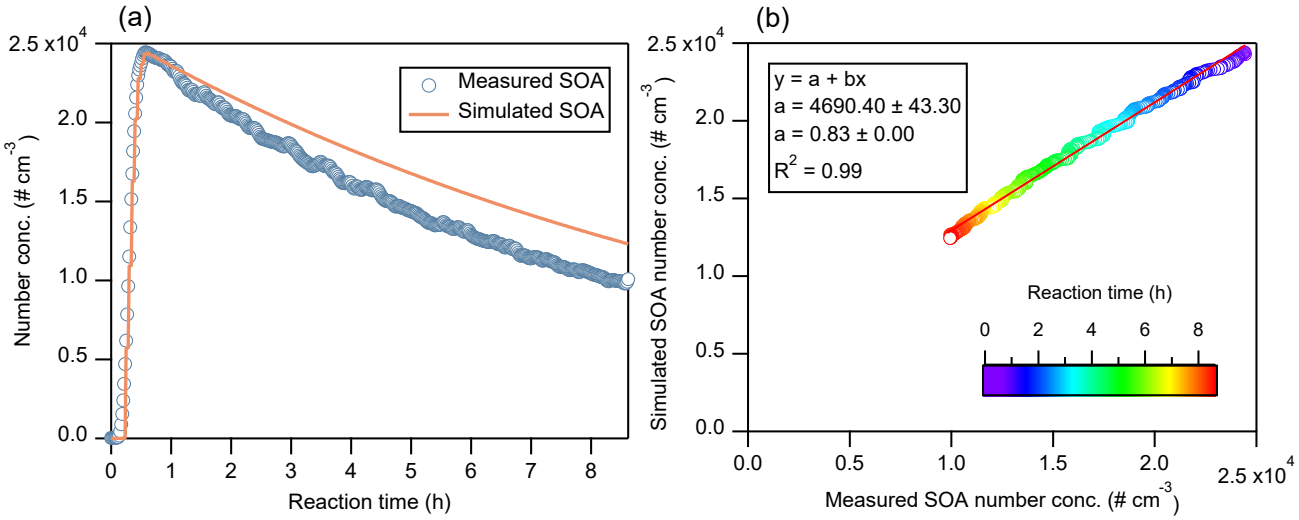


Figure S13: (a) Simulated (line) and measured (circles) SOA number concentrations (# cm^{-3}) using the SMPS-constrained seed scheme and excluding coagulation. (b) Scatterplot of measured versus simulated SOA number concentrations, with a linear fit (red line). Data points from the initial 0.6 h are excluded because the number concentration during this period was fitted to the SMPS measurements.

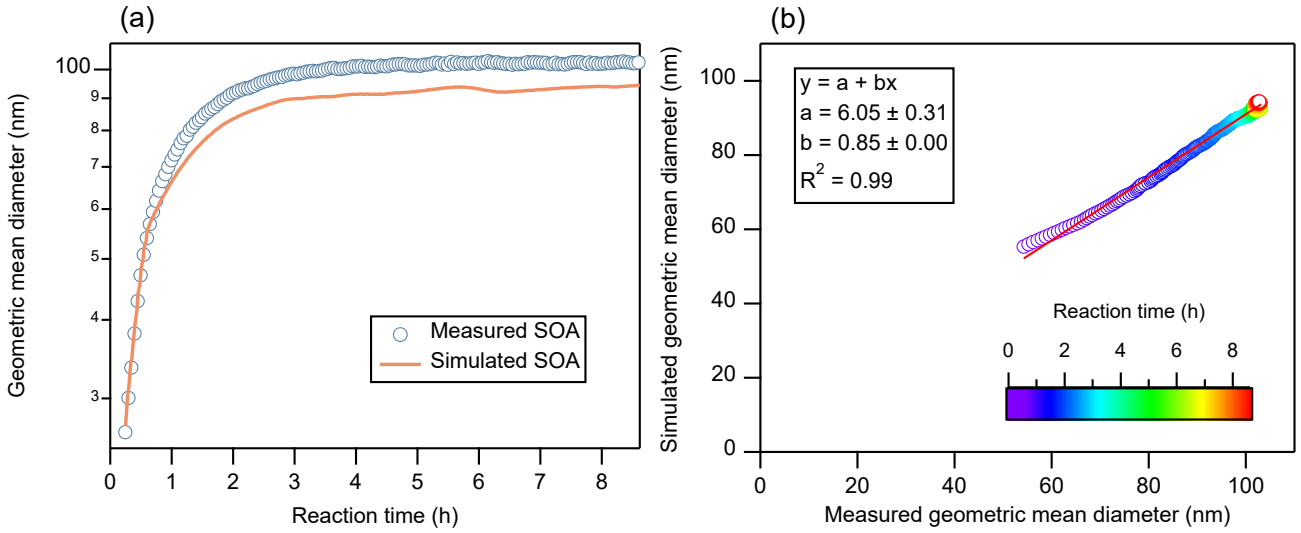


Figure S14: (a-b) Same as Fig. S13, but for the geometric mean diameter (nm) of SOA. Coagulation is excluded. Data points from the initial 0.6 h are excluded because PSD during this period was fitted to the SMPS measurements.

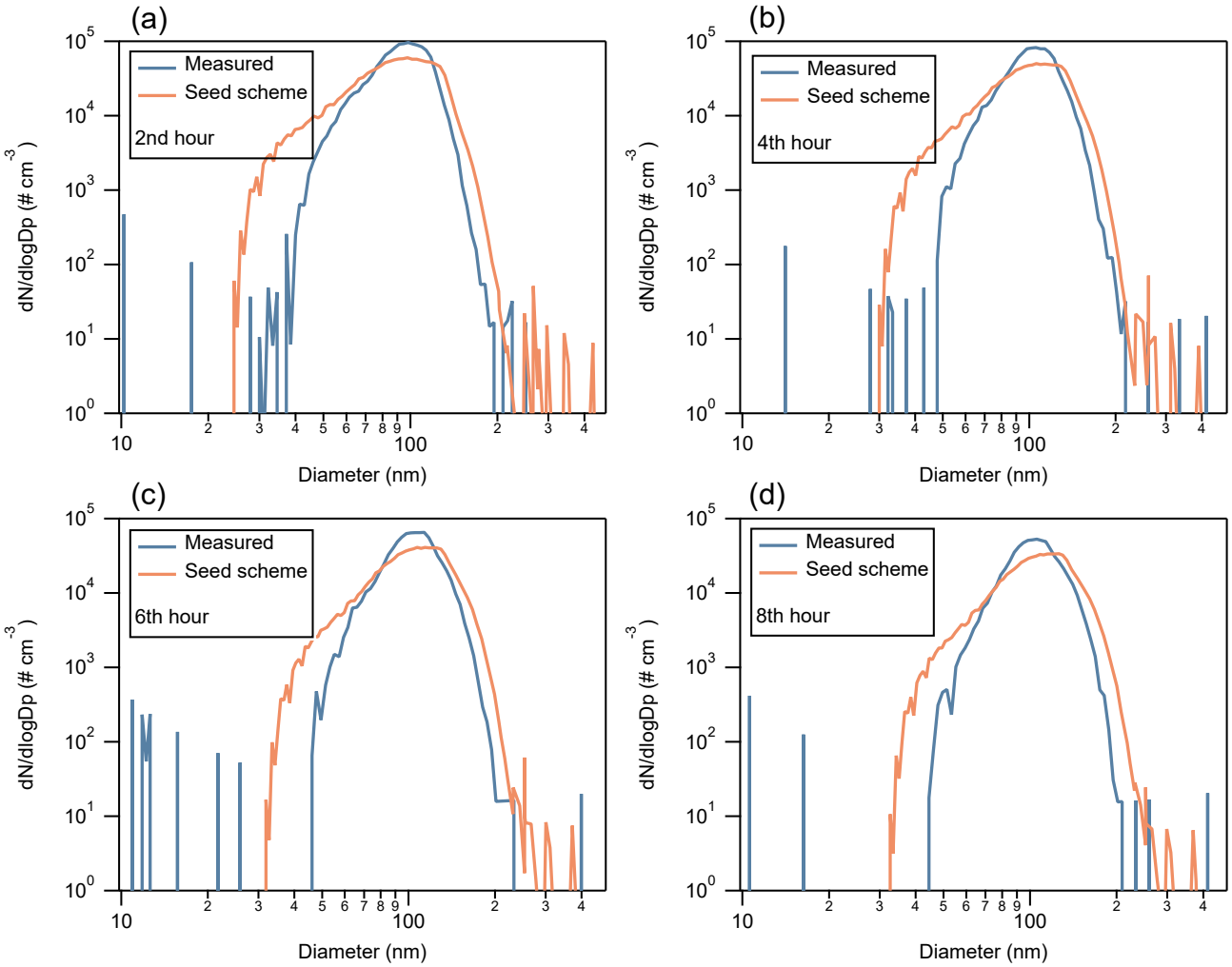


Figure S15: (a-d) Number particle size distribution ($dN/dlog_{10}D_p$) at reaction hours 2, 4, 6, and 8.

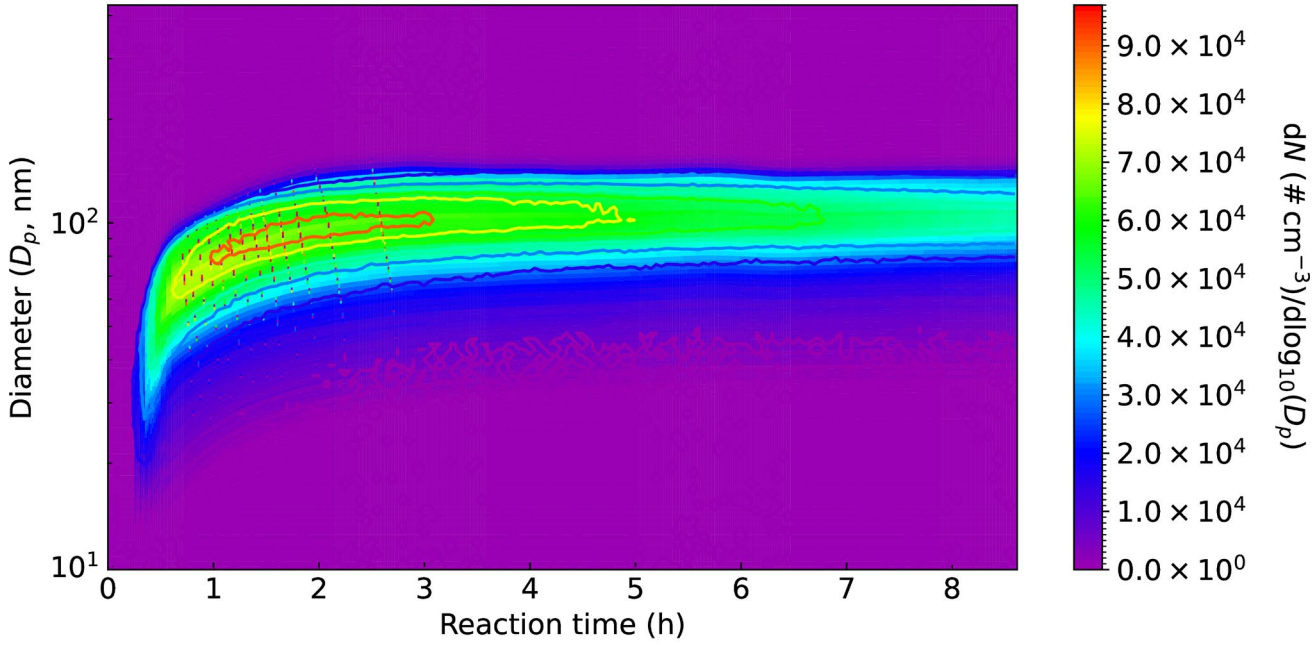


Figure S16: Time evolution of the number size distributions ($dN/dlog_{10}D_p$) for measured (contour lines) and simulated (shaded areas) SOA. Coagulation is excluded in the simulation.

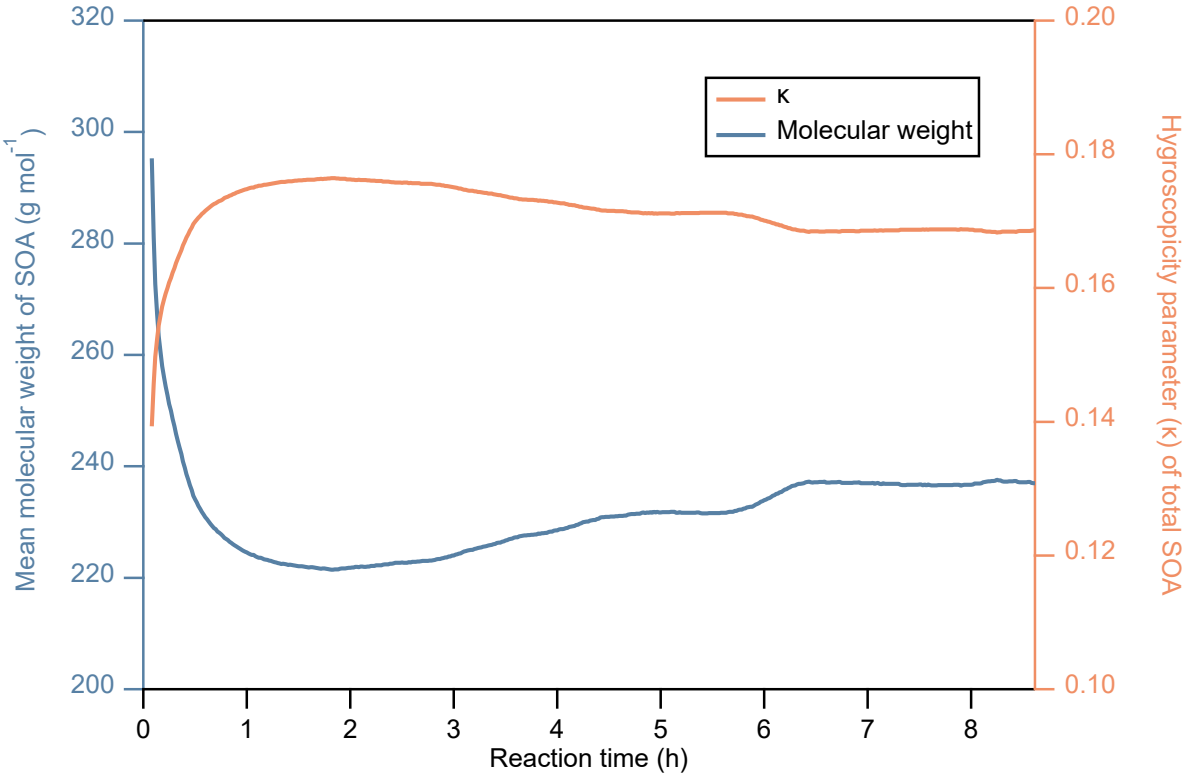


Figure S17: Time evolution of the mean molecular weight and hygroscopicity parameter (κ) of simulated SOA.

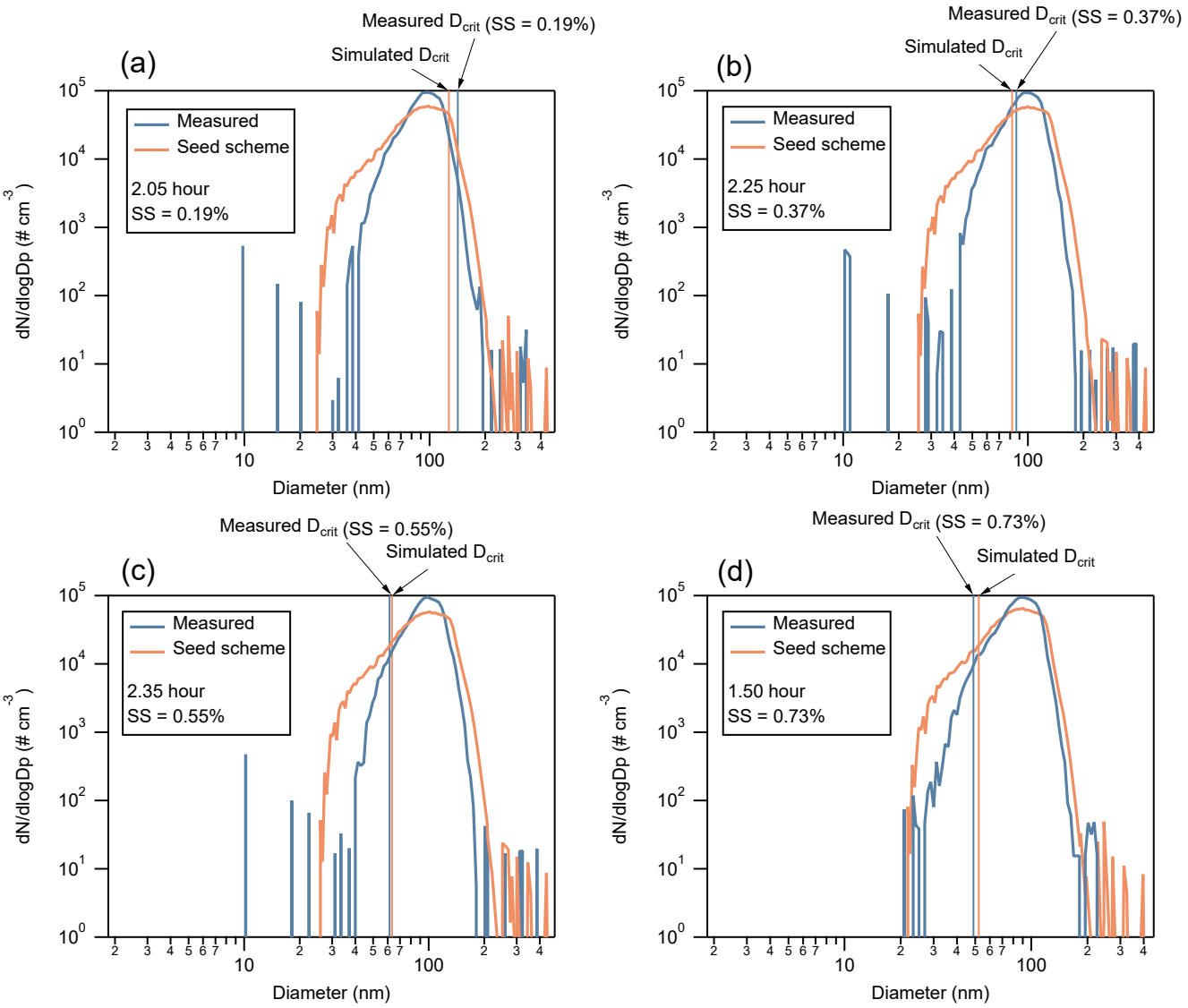


Figure S18: (a-d) Measured PSD and D_{crit}, together with those simulated using the seed scheme, at four SS corresponding to time points before and after 2 h.

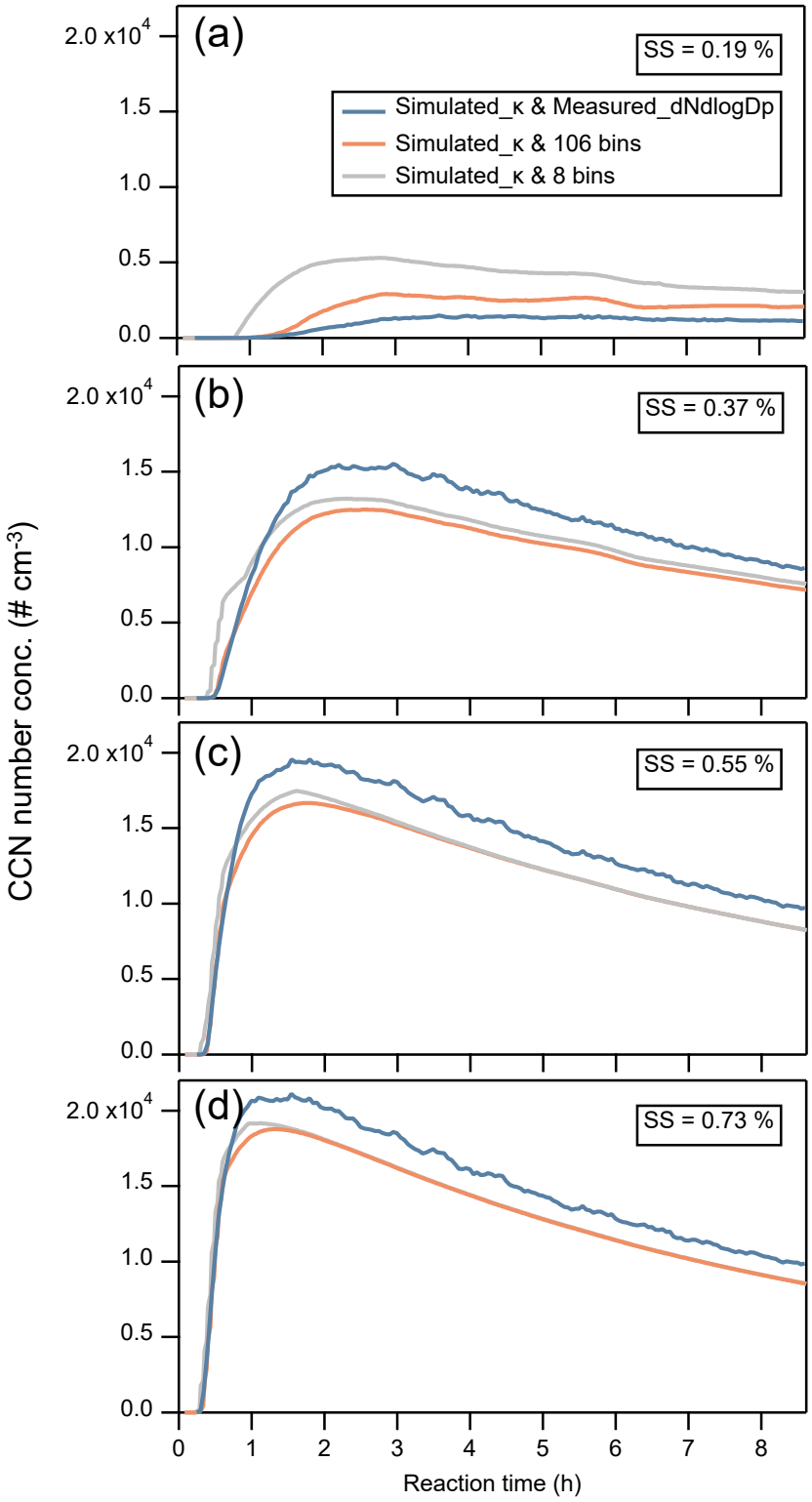


Figure S19: (a-d) CCN number concentrations (# cm^{-3}) at different SS, calculated using κ simulated by UManSysProp and three types of number PSDs: the measured PSD, and simulated PSD using the 106-bin and 8-bin size-resolution settings.

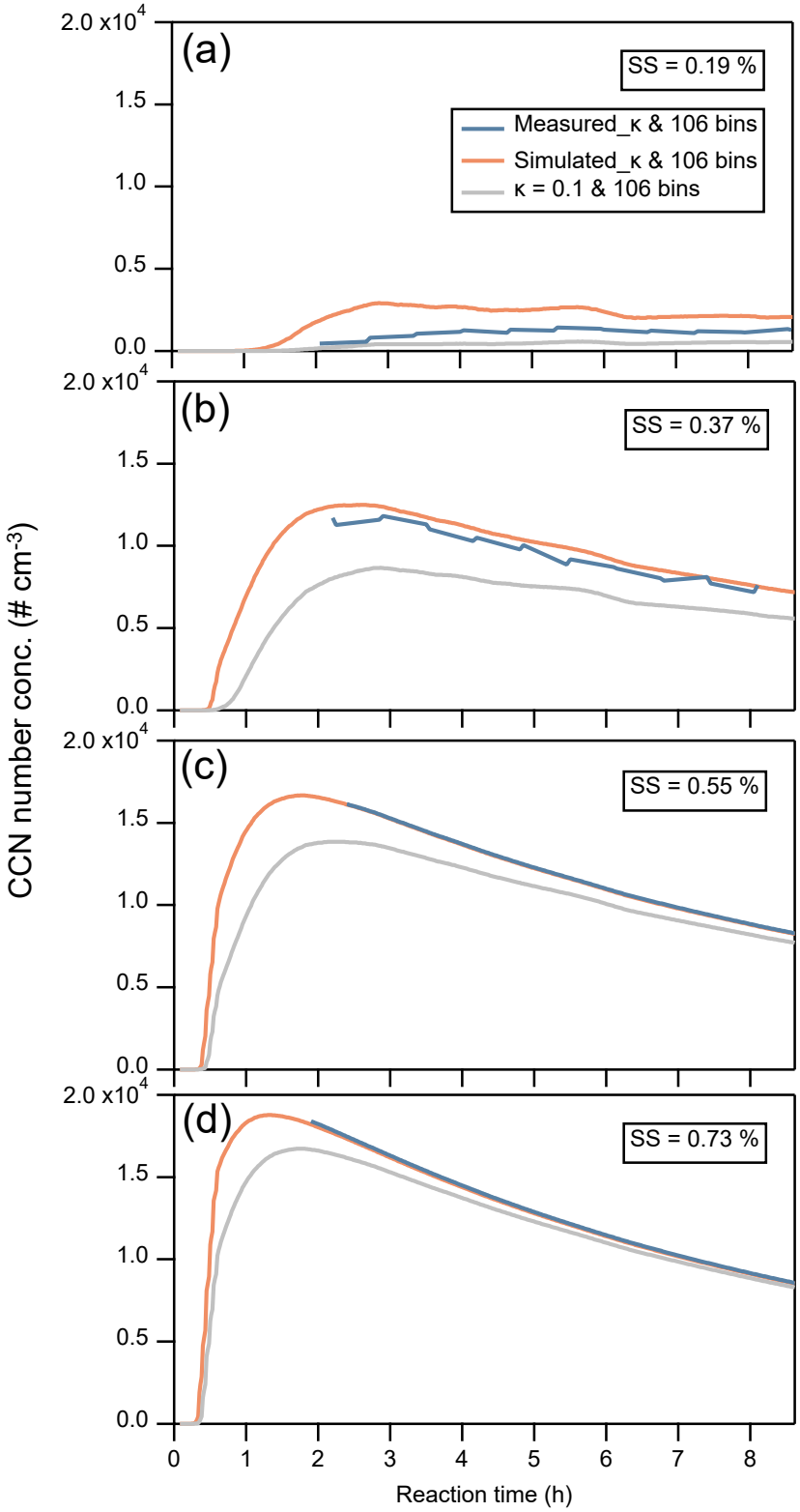
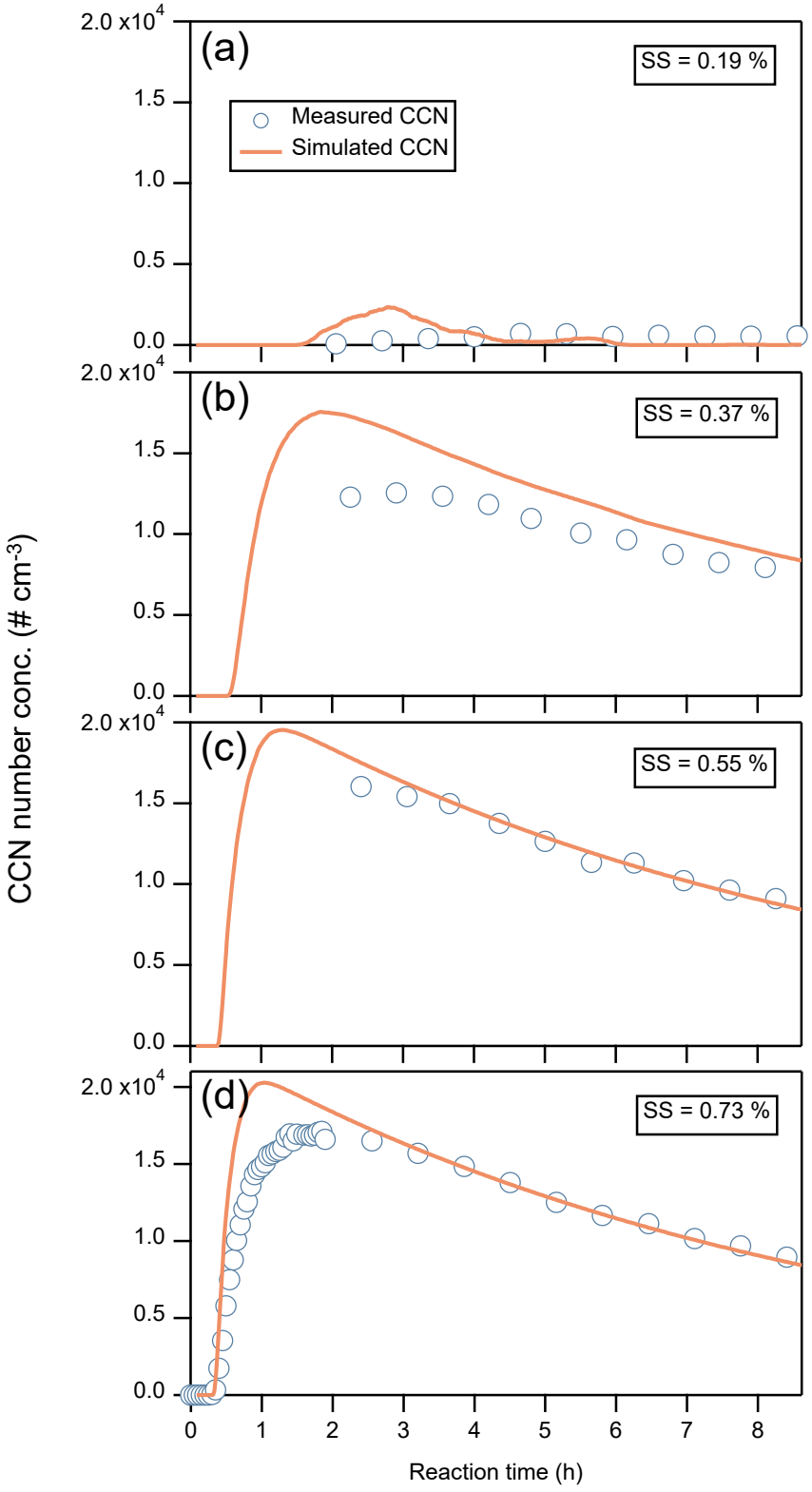


Figure S20: (a-d) CCN number concentrations (# cm^{-3}) at different SS, calculated using the simulated PSD with 106 size bins and three κ representations: measured κ, κ calculated using UManSysProp, and a fixed κ value of 0.1.



65 **Fig. S21: (a-d) Measured CCN number concentrations (circles; # cm⁻³) and simulated CCN (lines) using *κ* and PSD from nucleation scheme.**

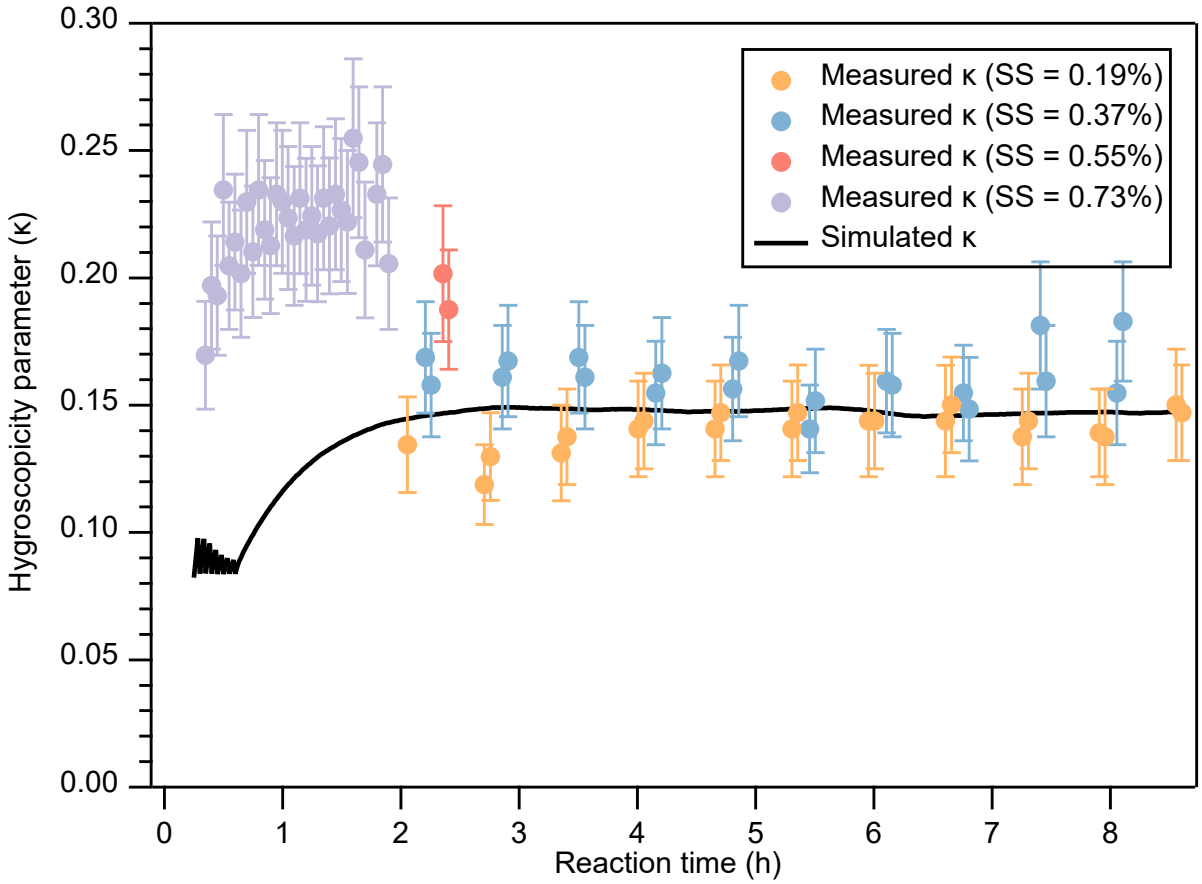


Fig. S22: Hygroscopicity parameter (κ) of simulated SOA using the seed scheme (line) and measured SOA (solid circles with standard-deviation error bars) at different supersaturation (SS).

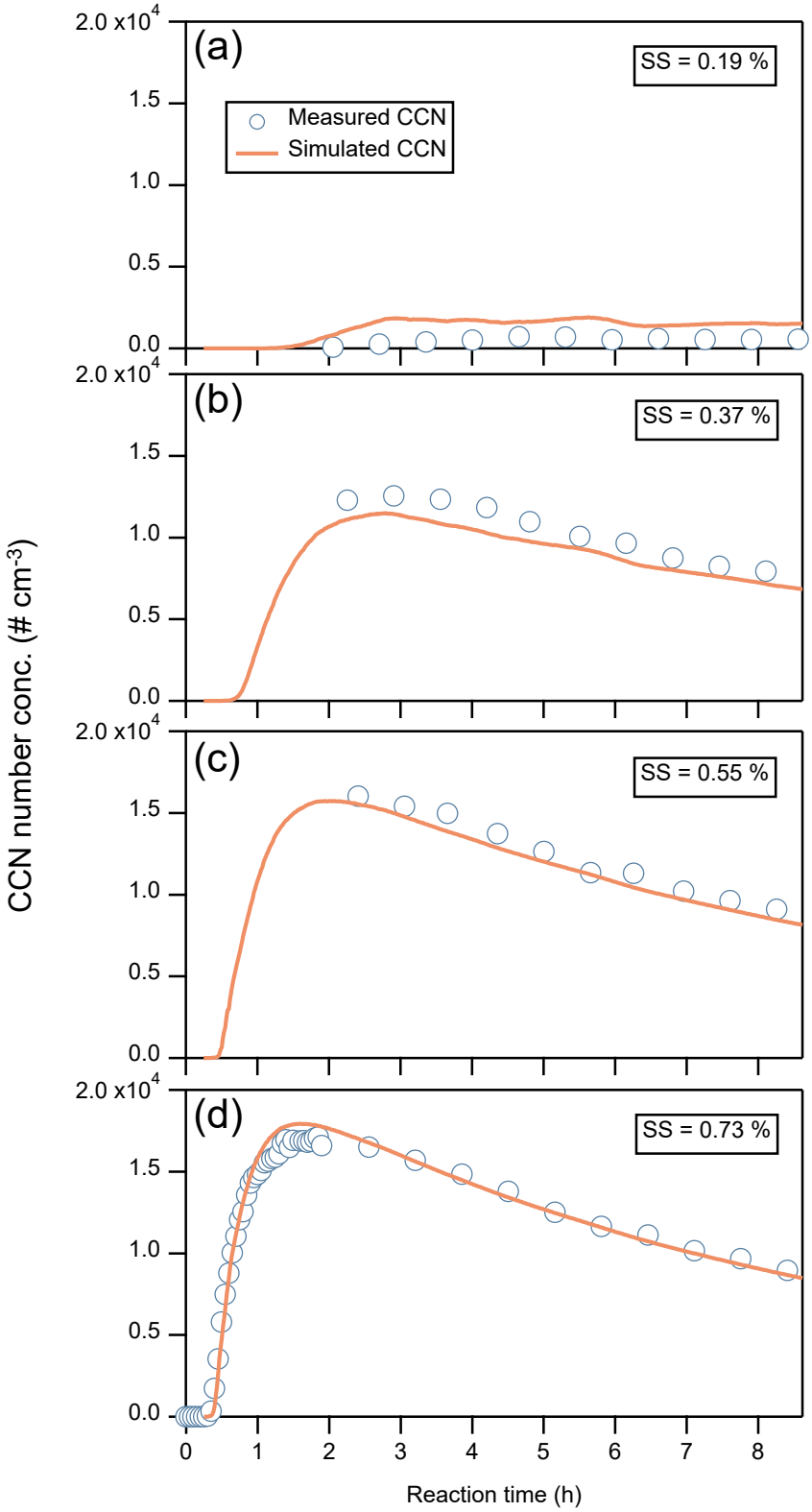


Fig. S23: (a-d) Same as Fig. S21, but for CCN simulated by κ and PSD from the seed scheme.

Table S1: The chemical formulas of all organic species, including HOMs, formed during dark α-pinene ozonolysis.

Chemical species in MCM and PRAM			
CH3O2	C9PAN2	C721PAN	C18H26O4
CH3O	C85CO3H	C721CO3H	C88O2
CH3NO3	C85OOH	NORPINIC	C718CO3
HCHO	C86OOH	C721OOH	C87O2
CH3O2NO2	C511OOH	C722OOH	NC826O2
CH3OOH	C7PAN3	C44OOH	C18H27O6NO3
CH3OH	C235C6CO3H	C811NO3	C20H30O8
CO23C4CHO	CO235C6OOH	C516O	C20H31O6NO3
BIACETO2	APINBO	C516OOH	C19H28O9
CH3CO3	APINBNO3	C10H15O2O2	C19H29O6NO3
HCOCH2CO3	APINBOOH	LIMOOA	C18H26O9
CO23C4CO3	APINBCO	LIMALAO2	C18H27O7NO3
C5PAN9	NAPINAO2	LIMALBO2	C20H30O9
CO23C4CO3H	NAPINBO2	C10H17O3O2	C20H31O7NO3
CO23C3CHO	NAPINAO	BPINENE	C19H28O10
HCOCH2CHO	NAPINAOOH	LIMONENE	C19H29O7NO3
HCOCH2O2	NAPINBO	CARENE	C18H26O10
C3PAN2	NC101CO	C10H15O4O2	C18H27O8NO3
HCOCH2CO3H	NAPINBOOH	C10H15O3O2	C20H30O10
HCOCH2CO2H	NC101O2	C10H15O5O2	C20H31O8NO3
GLYOX	NC101O	C10H15O6O2	C19H28O11
BIACETO	NC102O2	C10H15O7O2	C19H29O8NO3
BIACETOOH	NC102O	C10H15O8O2	C18H26O11
BIACETOH	NC71O2	C10H15O9O2	C18H27O9NO3
HOCH2CO3	NC71O	C10H15O10O2	C20H30O11
HOCH2CHO	NC71CO	C10H15O11O2	C20H31O9NO3
PHAN	NC101OOH	C10H15O12O2	C19H28O12
HOCH2CO3H	NC102OOH	C10H15O2O	C19H29O9NO3
HOCH2CO2H	NC71OOH	C10H15O3O	C18H26O12
ACETOL	NC72O2	C10H15O4O	C18H27O10NO3
MGLYOX	NC72O	C10H15O5O	C20H30O12
CH3COCH2O2	NC61CO3	C10H15O6O	C20H31O10NO3
CH3COCH2O	NC72OOH	C10H15O7O	C19H28O13
HCOCO	NC6PAN1	C10H15O8O	C19H29O10NO3
HCOCO3	NC61CO3H	C10H15O9O	C18H26O13
HCOCO3H	APINCO	C10H15O10O	C18H27O11NO3
HCOCO2H	APINCNO3	C10H15O11O	C20H30O13
HMVKAO2	C720O2	C10H15O12O	C20H31O11NO3
HMVKAO	APINCOOH	C10H14O3	C19H28O14

HMVKANO3	APINCOH	C10H14O4	C19H29O11NO3
HMVKAOOH	HCC7CO	C10H14O5	C18H26O14
HO12CO3C4	C720O	C10H14O6	C18H27O12NO3
CO2H3CHO	C720NO3	C10H14O7	C20H30O14
CO2H3CO3	C720OOH	C10H14O8	C20H31O12NO3
C4PAN6	C720OH	C10H14O9	C19H28O15
CO2H3CO3H	C719O2	C10H14O10	C19H29O12NO3
PAN	C719O	C10H14O11	C18H26O15
CH3CO3H	C719NO3	C10H14O12	C18H27O13NO3
CH3CO2H	C719OOH	C10H14O13	C20H30O15
HCOCH2O	C719OH	C10H15O2NO3	C20H31O13NO3
HCOCH2OOH	APINOOA	C10H15O3NO3	C19H28O16
CH3COCH3	APINOOB	C10H15O4NO3	C19H29O13NO3
HYPERACET	C107O2	C10H15O5NO3	C18H26O16
CHOC3COCO3	C109O2	C10H15O6NO3	C18H27O14NO3
CHOC3COO2	C107O	C10H15O7NO3	C20H30O16
CHOC3COO	C108O2	C10H15O8NO3	C20H31O14NO3
CHOC3COPAN	C108O	C10H15O9NO3	C19H28O17
CHOC3COOOH	C108NO3	C10H15O10NO3	C19H29O14NO3
C413COOOH	C717O2	C10H15O11NO3	C18H26O17
C4CODIAL	C717O	C10H15O12NO3	C18H27O15NO3
C312COCO3	C717NO3	C10H16O4iso1	C20H30O17
CHOCOCH2O2	C107OOH	C10H16O5iso1	C20H31O15NO3
CHOCOCH2O	C107OH	C10H16O6iso1	C19H28O18
C312COPAN	C108OOH	C10H16O7iso1	C19H29O15NO3
C312COCO3H	C108OH	C10H16O8iso1	C18H26O18
ALCOCH2OOH	C717OOH	C10H16O9iso1	C18H27O16NO3
C33CO	C717OH	C10H16O10	C10H16O3
H1CO23CHO	C109O	C10H16O11	C10H17O5O2
APINENE	C89CO3	C10H16O12	C10H17O4O2
APINAO2	C920CO3	C10H16O13	C10H17O6O2
APINBO2	C109OOH	C10H16O14	C10H17O7O2
APINCO2	C109OH	C20H30O5	C10H17O8O2
APINAO	C109CO	C20H30O6	C10H17O3O
APINANO3	C920O2	C20H30O7	C10H17O4O
PINAL	C920O	C923CO3	C10H17O5O
APINAOOH	C921O2	LIMAO2	C10H17O6O
APINBOH	C921O	LIMCO2	C10H17O7O
C96O2	C922O2	LIMALO2	C10H16O4iso2
C96CO3	C922O	LIMBO2	C10H16O5iso2
PINALO2	C621O2	C20H31O4NO3	C10H16O6iso2
C96O	C621O	BPINAO2	C10H16O7iso2

C96NO3	H1C23C4CHO	BPINBO2	C10H16O8iso2
C97O2	H1C23C4O2	BPINCO2	C10H16O9iso2
C97O	H1C23C4CO3	C918CO3	C10H17O3NO3
C98O2	H1C23C4O	C20H31O5NO3	C10H17O4NO3
C98O	H1C23C4PAN	NLIMO2	C10H17O5NO3
C98NO3	HC23C4CO3H	NLIMALO2	C10H17O6NO3
C614O2	H1C23C4OOH	NC91CO3	C10H17O7NO3
C614O	C920PAN	NBPINAO2	C10H17O8NO3
C614NO3	C920CO3H	NBPINBO2	C10H18O5
PINALO	HOPINONIC	C19H28O5	C10H18O6
PINALNO3	C920OOH	C19H28O6	C10H18O7
C106O2	C921OOH	C19H28O7	C10H18O8
C106O	C922OOH	C19H28O8	C10H18O9
C106NO3	C621OOH	C923O2	C10H18O10
C716O2	APINBOO	C924O2	C20H34O6
C716O	C89CO2	C816CO3	C20H34O7
CO13C4CHO	C89O2	NORLIMO2	C20H34O8
C10PAN2	C89O	LMKAO2	C20H35O5NO3
PERPINONIC	C89NO3	LMKBO2	C20H35O6NO3
PINONIC	C810O2	C926O2	C19H32O6
C96OOH	C810O	C817CO3	C19H32O7
C96OH	C810NO3	LMLKAO2	C19H32O8
NORPINAL	C514O2	LMLKBO2	C19H32O9
C97OOH	C514O	C823CO3	C19H33O6NO3
C97OH	C514NO3	C925O2	C18H30O6
C98OOH	C89PAN	NOPINAO2	C18H30O7
C98OH	C89CO3H	NOPINBO2	C18H30O8
C614OOH	C89CO2H	NOPINCO2	C18H30O9
C614OH	C89OOH	NOPINDO2	C18H30O5
C614CO	C89OH	C918O2	C18H31O7NO3
PINALOOH	C810OOH	C9DCO2	C20H34O9
PINALOH	C810OH	C915O2	C20H35O7NO3
C106OOH	C514OOH	C917O2	C19H32O10
C106OH	C514OH	C919O2	C19H33O7NO3
C716OOH	C811CO3	C914O2	C18H30O10
C716OH	C811O2	C916O2	C18H31O8NO3
CO235C6CHO	C811O	C88CO3	C20H34O10
H3C25C6O2	C812O2	C87CO3	C20H35O8NO3
H3C25C6CO3	C812O	C822CO3	C19H32O11
H3C25C6O	C813O2	NLMKAO2	C19H33O8NO3
H3C2C4CO3	C813O	C19H29O5NO3	C18H30O11
H3C2C4PAN	C813NO3	C18H26O5	C18H31O9NO3

H3C2C4CO3H	C516O2	C18H26O6	C20H34O11
H3C2C4CO2H	C811CO3H	C18H26O7	C20H35O9NO3
H3C25C6PAN	PINIC	C729CO3	C19H32O12
H3C25C5CHO	C811PAN	C816O2	C19H33O9NO3
H3C25CCO3H	C811OOH	C817O2	C18H30O12
H3C25CCO2H	C811OH	C826O2	C18H31O10NO3
H3C25C6OOH	C721CHO	C822O2	C20H34O12
H3C25C6OH	C812OOH	C818O2	C20H35O10NO3
C85O2	C812OH	C823O2	C19H32O13
C85CO3	C813OOH	C819O2	C19H33O10NO3
C85O	C813OH	C727CO3	C18H30O13
C86O2	CO13C3CO2H	C731CO3	C18H31O11NO3
C86O	C721O2	C824O2	C20H34O13
C511O2	C721CO3	C820O2	C20H35O11NO3
C511O	C721O	C18H26O8	C19H32O14
CO235C5CHO	C722O2	C825O2	C19H33O11NO3
CO235C6CO3	C722O	C821O2	C18H30O14
CO235C6O2	C44O2	C732CO3	C18H31O12NO3
CO235C6O	C44O	C8BCO2	C10H18O4

Table S2: Simulated hygroscopicity parameter (κ) of SOA calculated from different chemical compositions and the corresponding particle sizes (nm).

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