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Estimation of the volatility distribution of organic aerosol combining thermodenuder and isothermal dilution measurements

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1. Estimated COA volatility distributions and properties

Table S1: Estimated volatility distributions for the COA along with estimated properties of the two experiments using both TD and isothermal dilution measurements and only TD measurements using the approach of Karnezi et al. (2014).

	Experiment 1		**Experiment 2**	
Saturation concentration ***C**** (μg m^{-3})	**TD + Dilution**	**TD - only**	**TD + Dilution**	**TD - only**
10^{-3}	0.27	0.18	0.23	0.18
10^{-2}	0.33	0.24	0.31	0.27
10^{-1}	-	-	0.23	0.22
10^{0}	0.19	0.25	0.09	0.18
10^{1}	0.06	0.11	0.07	0.09
10^{2}	0.06	0.10	0.07	0.06
10^{3}	0.09	0.12	-	-
ΔH_{vap} (kJ mol^{-1})	100 ± 14	83 ± 19	85 ± 9	79 ± 17
Accommodation coefficient	0.06 (0.01-0.3)[a]	0.14 (0.03-0.59)[a]	0.07 (0.01-0.34)[a]	0.07 (0.01-0.36)[a]
Average volatility $\log_{10}C^*$ (μg m^{-3})	0.1	0.44	0.047	0.08

[a] The values in parenthesis represent the corresponding uncertainties for the estimated accommodation coefficients

Table S2: Estimated volatility distributions for the various sensitivity tests.

	Saturation concentration (μg m^{-3})							**log$_{10}$*C**** (μg m^{-3})	**ΔH$_{vap}$** (kJ mol^{-1})	**Accommodation coefficient**
Experiment 1	10^{-3}	10^{-2}	10^{-1}	10^{0}	10^{1}	10^{2}	10^{3}			
Base case	0.27	0.33	-	0.19	0.06	0.06	0.09	0.1	100 ± 14	0.06 (0.01-0.30)[a]
Sensitivity to a_m										
a_m=0.01	0.20	0.25	-	0.30	0.09	0.07	0.09	0.25	104±20	0.01
a_m=0.1	0.29	0.40	-	0.13	0.04	0.06	0.08	0.053	98±6	0.1
a_m=1.0	0.35	0.40	-	0.06	0.03	0.06	0.10	0.04	95±8	1.0
Sensitivity to ΔH$_{vap}$										
ΔH$_{vap}$=60 kJ mol^{-1}	0.10	0.39	-	0.32	0.05	0.05	0.09	0.25	60	0.07 (0.02-0.44)[a]
ΔH$_{vap}$ = 120 kJ mol^{-1}	0.50	0.20	-	0.10	0.04	0.06	0.10	0.036	120	0.01 (0.009-0.13)[a]
Experiment 2	10^{-3}	10^{-2}	10^{-1}	10^{0}	10^{1}	10^{2}	10^{3}			
Base case	0.23	0.31	0.23	0.09	0.07	0.07	-	0.047	85 ± 9	0.07 (0.01-0.34)[a]
Sensitivity to a_m										
a_m=0.01	0.14	0.24	0.30	0.14	0.09	0.09	-	0.12	89±10	0.01
a_m=0.1	0.24	0.36	0.20	0.07	0.06	0.07	-	0.036	84±8	0.1
a_m=1.0	0.33	0.35	0.16	0.04	0.05	0.07	-	0.022	82±5	1.0
Sensitivity to ΔH$_{vap}$										
ΔH$_{vap}$ = 60 kJ mol^{-1}	0.16	0.32	0.27	0.11	0.07	0.07	-	0.066	60	0.09 (0.02-0.44)[a]
ΔH$_{vap}$ = 120 kJ mol^{-1}	0.35	0.33	0.12	0.05	0.06	0.09	-	0.026	120	0.025 (0.01-0.085)[a]

[a] The values in parenthesis represent the corresponding uncertainties for the estimated accommodation coefficients

2. Wall loss corrections during isothermal dilution

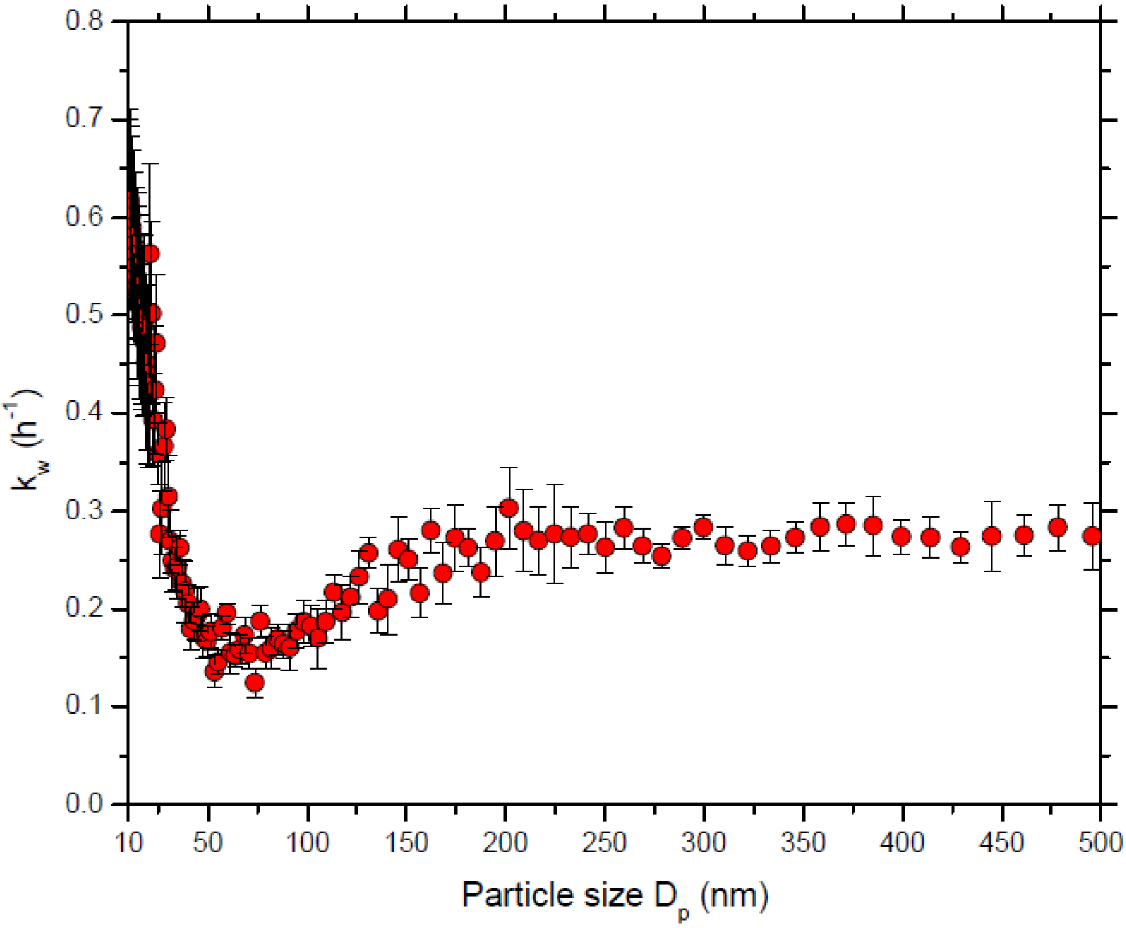

Figure S1: Wall loss rate constants as a function of particle size (red circles) for the isothermal dilution chamber during Experiment 1. The error bars represent ± 1 standard deviation.

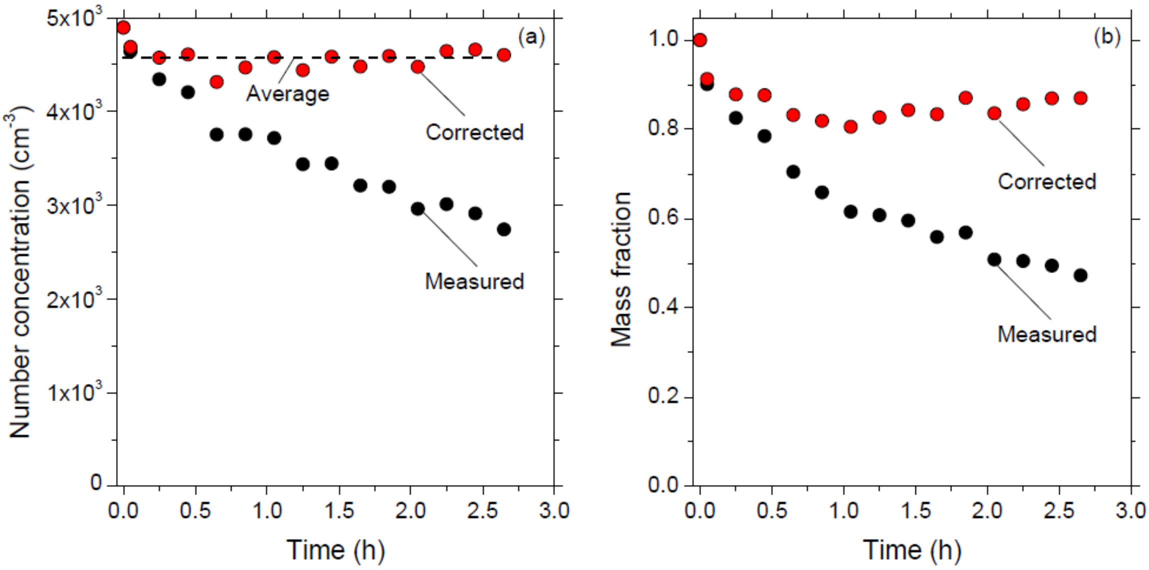

Figure S2: (a) Number concentration during isothermal dilution of Experiment 1 as a function of time measured by the SMPS. (b) Mass fraction as function of time during isothermal dilution of Experiment 1 measured by the SMPS.

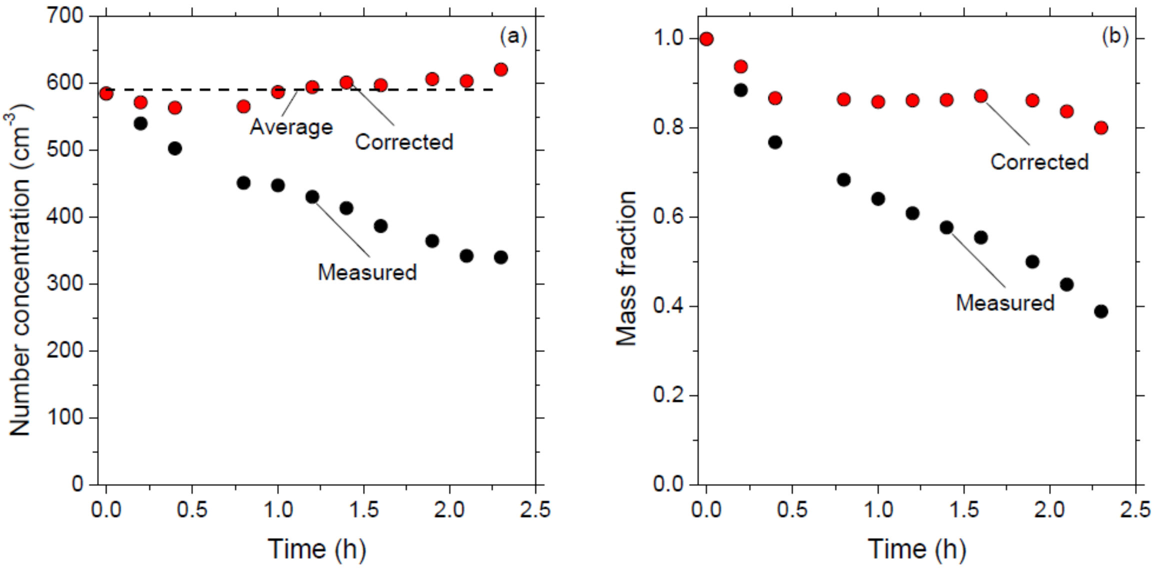

Figure S3: (a) Number concentration during isothermal dilution of Experiment 2 as a function of time measured by the SMPS. (b) Mass fraction as function of time during isothermal dilution of Experiment 2 measured by the SMPS.

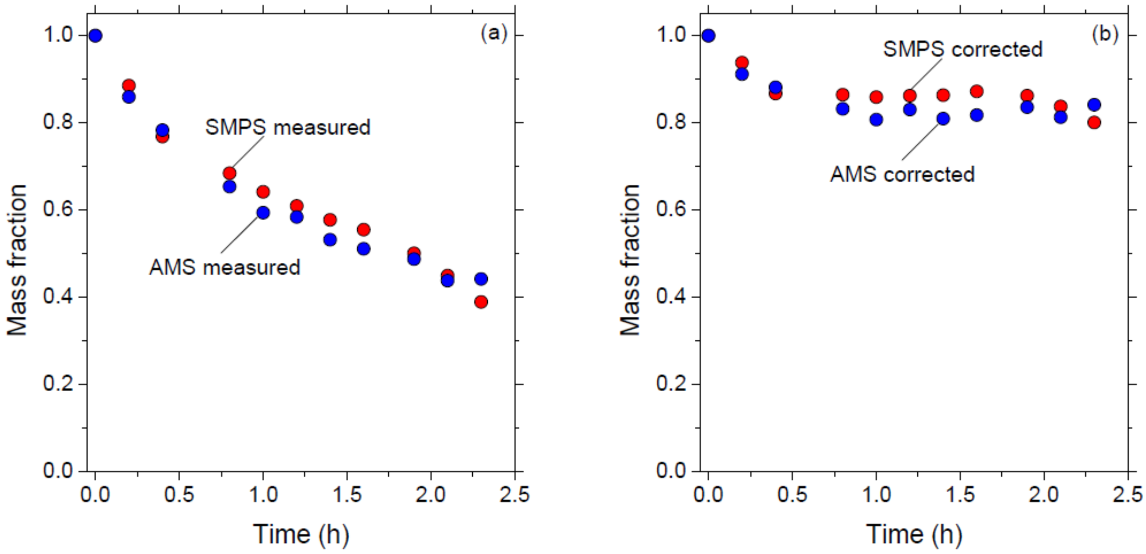

Figure S4: (a) Measured mass fractions as function of time during isothermal dilution of Experiment 2. (b) Corrected mass fractions as a function of time during isothermal dilution of Experiment 2.

3. Sensitivity tests to accommodation coefficient

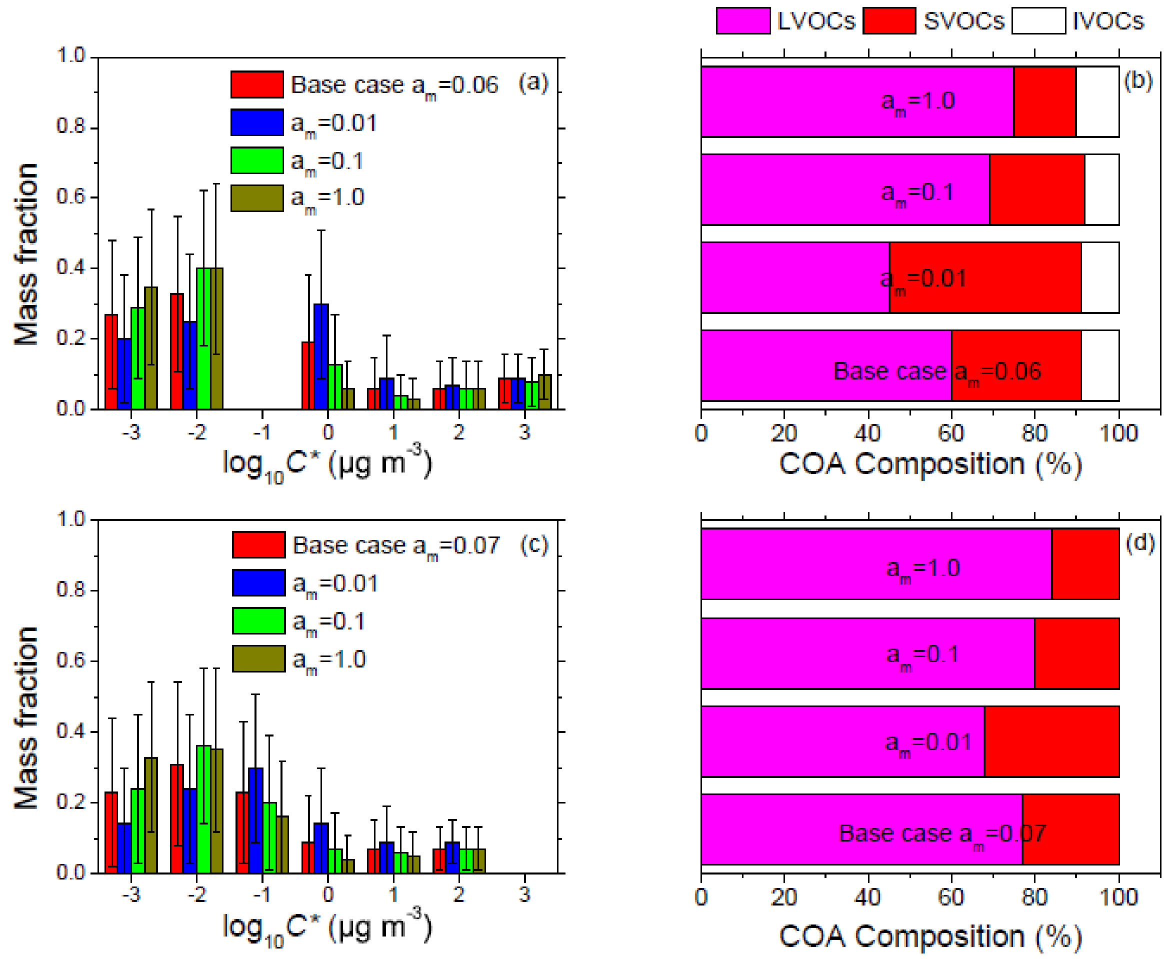

Figure S5: (a) Estimated volatility distributions assuming different accommodation coefficients for Experiment 1 using the approach of Karnezi et al. (2014). The error bars represent the corresponding uncertainty ranges. Red, blue, green, and dark yellow bars represent the estimated volatility distributions for the base case, a_m=0.01, a_m = 0.1, and a_m =1.0 respectively. (b) Corresponding COA composition of Experiment 1. LVOCs are represented in magenta, SVOCs in red, and IVOCs in white. (c) Estimated volatility distributions for different accommodation coefficients for Experiment 2 using the approach of Karnezi et al. (2014). The error bars represent the corresponding uncertainty ranges. Red, blue, green, and dark yellow bars represent the estimated volatility distributions for the base case, a_m=0.01, a_m = 0.1, and a_m =1.0 respectively. (d) Corresponding COA composition of Experiment 2. LVOCs are represented in magenta, SVOCs in red.

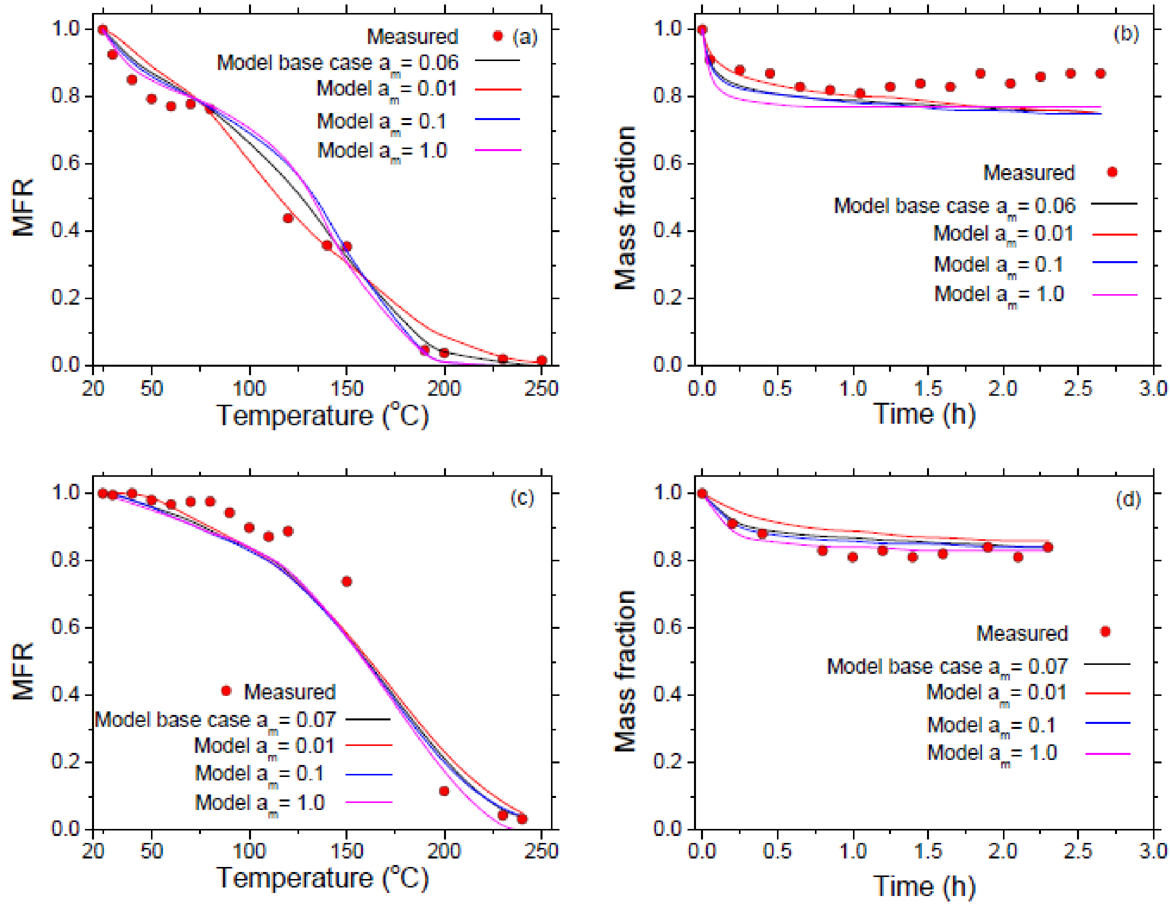

Figure S6: (a) Thermogram of the OA TD measurements of Experiment 1. Red circles represent the loss corrected measurements and the black line represents the best fit for the base case estimated by the model of Karnezi et al. (2014). Red, blue, and magenta lines represent the model predictions for a_m = 0.01, a_m =0.1, and a_m =1.0 respectively. (b) Mass fraction during isothermal dilution as a function of time of Experiment 1. Red circles represent the loss corrected measurements and the black line represents the best fit for the base case estimated by the model of Karnezi et al. (2014). Red, blue, and magenta lines represent the model predictions for a_m = 0.01, a_m =0.1, and a_m =1.0 respectively. (c) Thermogram of the OA TD measurements of Experiment 2. Red circles represent the loss corrected measurements and the black line represents the best fit for the base case estimated by the model of Karnezi et al. (2014). Red, blue, and magenta lines represent the model predictions for a_m = 0.01, a_m =0.1, and a_m =1.0 respectively. (d) Mass fraction during isothermal dilution as a function of time of Experiment 2 Red circles represent the loss corrected measurements and the black line represents the best fit for the base case estimated by the model of Karnezi et al. (2014). Red, blue, and magenta lines represent the model predictions for a_m = 0.01, a_m =0.1, and a_m =1.0 respectively.

4. Sensitivity tests to vaporization enthalpy

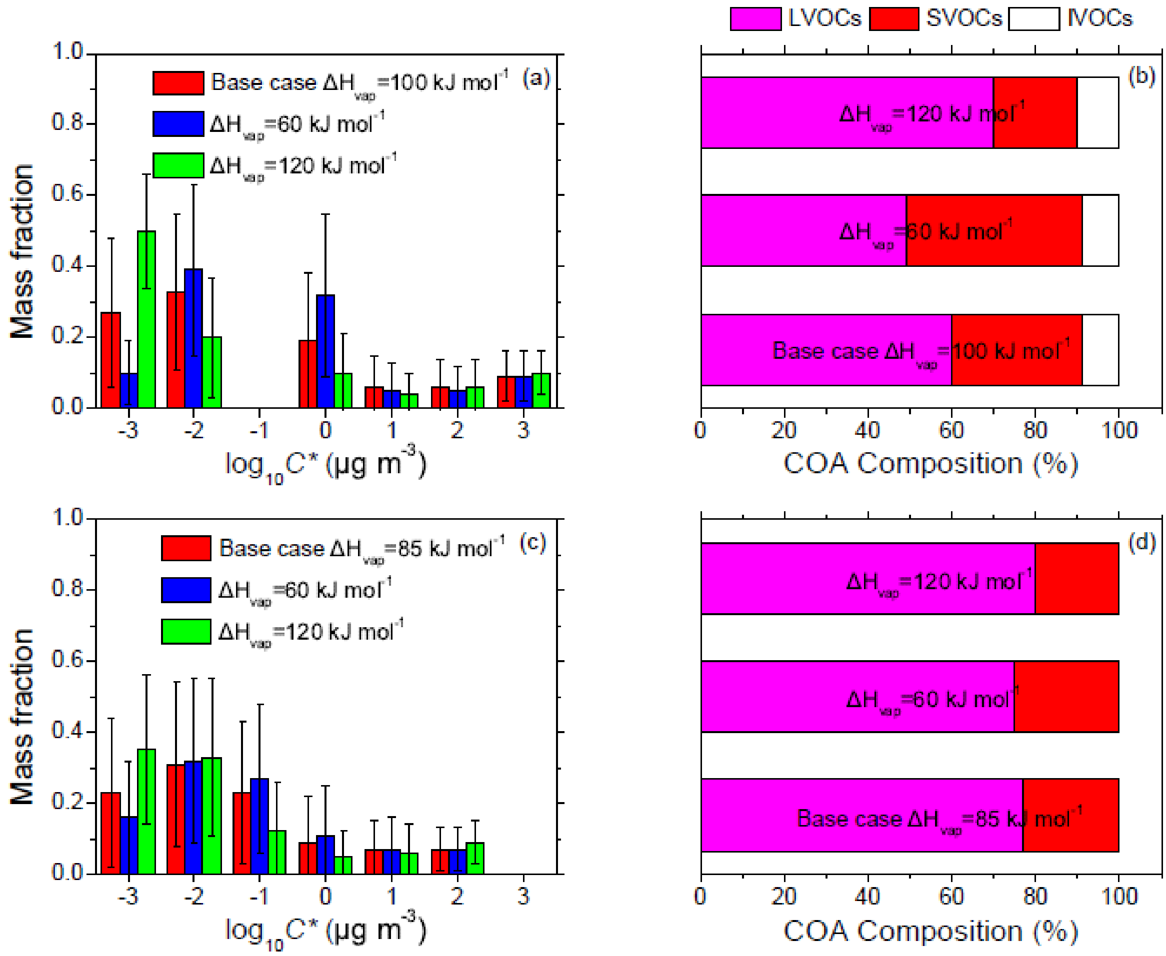

Figure S7: (a) Estimated volatility distributions assuming different vaporization enthalpies for Experiment 1 using the approach of Karnezi et al. (2014). The error bars represent the corresponding uncertainty ranges. Red, blue, and green bars represent the estimated volatility distributions for the base case, ΔH_{vap}=60 kJ mol^{-1}, and ΔH_{vap}=120 kJ mol^{-1} respectively. (b) Corresponding COA composition of Experiment 1. LVOCs are represented in magenta, SVOCs in red, and IVOCs in white. (c) Estimated volatility distributions assuming different vaporization enthalpies for Experiment 2 using the approach of Karnezi et al. (2014). The error bars represent the corresponding uncertainty ranges. Red, blue, and green bars represent the estimated volatility distributions for the base case, ΔH_{vap}=60 kJ mol^{-1}, and ΔH_{vap}=120 kJ mol^{-1} respectively. (d) Corresponding COA composition of Experiment 2. LVOCs are represented in magenta, SVOCs in red.

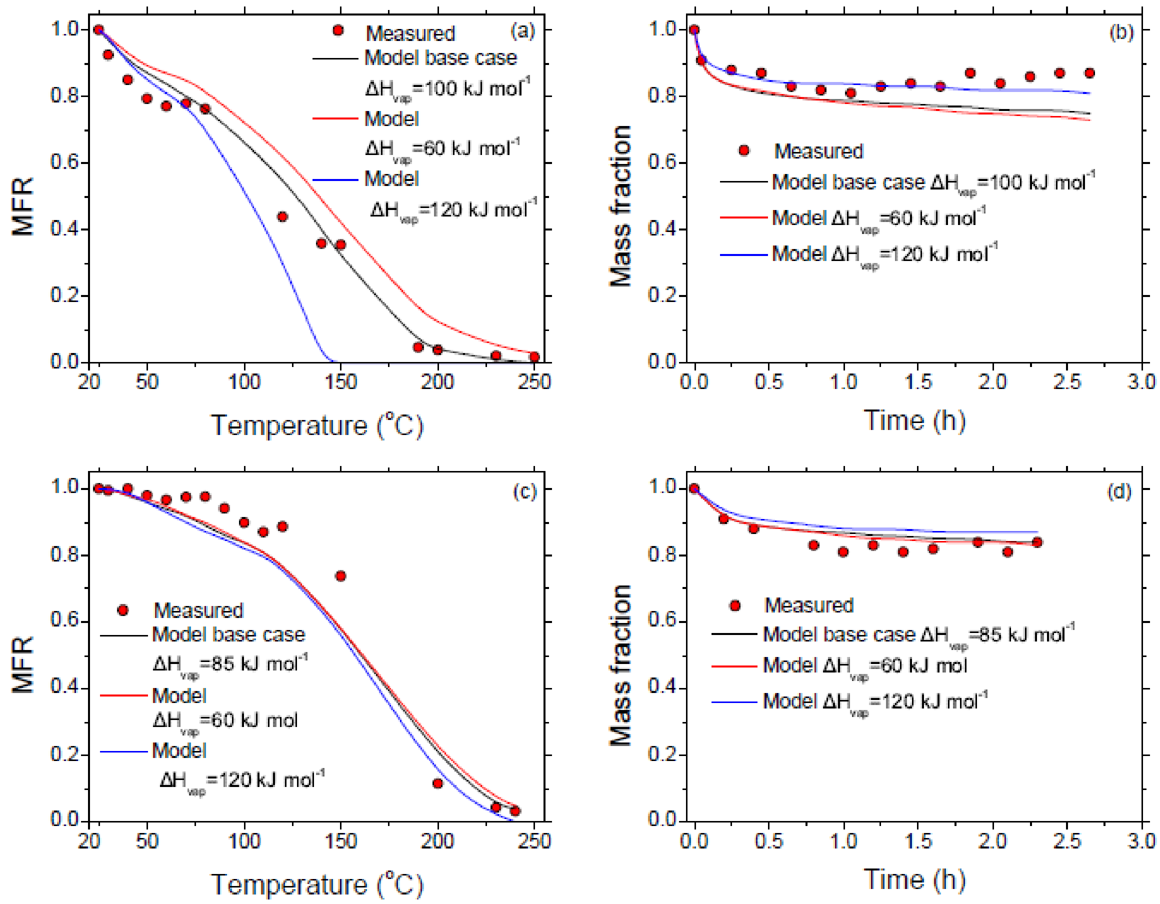

Figure S8: (a) Thermogram of the OA TD measurements of Experiment 1. Red circles represent the loss corrected measurements and black line represents the best fit for the base case estimated by the model of Karnezi et al. (2014). Red, and blue lines represent the model predictions for ΔH_{vap} = 60, and ΔH_{vap} = 120 kJ mol^{-1} respectively. (b) Mass fraction during isothermal dilution as a function of time of Experiment 1. Red circles represent the loss corrected measurements and black line represents the best fit for the base case estimated by the model of Karnezi et al. (2014). Red, and blue lines represent the model predictions for ΔH_{vap} = 60, and ΔH_{vap} = 120 kJ mol^{-1} respectively. (c) Thermogram of the OA TD measurements of Experiment 2. Red circles represent the loss corrected measurements and black line represents the best fit for the base case estimated by the model of Karnezi et al. (2014). Red, and blue lines represent the model predictions for ΔH_{vap} = 60, and ΔH_{vap} = 120 kJ mol^{-1} respectively. (b) Mass fraction during isothermal dilution as a function of time of Experiment 2 Red circles represent the loss corrected measurements and black line represents the best fit for the base case estimated by the model of Karnezi et al. (2014). Red, and blue lines represent the model predictions for ΔH_{vap} = 60, and ΔH_{vap} = 120 kJ mol^{-1} respectively.

References

Karnezi, E., Riipinen, I. and Pandis, S. N.: Measuring the atmospheric organic aerosol volatility distribution: A theoretical analysis, Atmos. Meas. Tech., 7, 2953–2965, 2014.