

Supplementary Material

Estimation of secondary organic aerosol formation parameters for the Volatility Basis Set combining thermodenuder, isothermal dilution and yield measurements

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S1. Constructing Data for Evaluation

Table S1: Values of the true properties (volatility distribution of the products, vaporization enthalpy, accommodation coefficient) for three SOA systems used to generate data for pseudo-experiments A, B and C.

Exp.	“True” Properties
A	4 bins
	$C_i^* = [10^0 \ 10^1 \ 10^2 \ 10^3] \ \mu\text{g m}^{-3}$
	$\alpha_i = [0.07 \ 0.038 \ 0.179 \ 0.300]$
	$\Delta H_{\text{vap}} = 30 \ \text{kJ mol}^{-1}$
	$\alpha_m = 0.5$
B	7 bins
	$C_i^* = [10^{-2} \ 10^{-1} \ 10^0 \ 10^1 \ 10^2 \ 10^3 \ 10^4] \ \mu\text{g m}^{-3}$
	$\alpha_i = [0.001 \ 0.012 \ 0.037 \ 0.088 \ 0.099 \ 0.250 \ 0.800]$
	$\Delta H_{\text{vap}} = 30 \ \text{kJ mol}^{-1}$
	$\alpha_m = 0.5$
C	4 bins
	$C_i^* = [10^{-2} \ 10^{-1} \ 10^0 \ 10^1] \ \mu\text{g m}^{-3}$
	$\alpha_i = [0.118 \ 0.094 \ 0.116 \ 0.247]$
	$\Delta H_{\text{vap}} = 115 \ \text{kJ mol}^{-1}$
	$\alpha_m = 0.01$

Table S2: “Experimental” conditions and properties used to obtain the “measurements” of TD and isothermal dilution for pseudo-experiments A, B and C.

Exp.	Initial Concentration ($\mu\text{g m}^{-3}$)	Mean Volume Diameter (nm)	Dilution Ratio	TD Residence Time (s)	SOA Density (g cm^{-3})
A	20	200	10	17	1.5
B	20	200	10	17	1.5
C	190	145	17	50	1.3

S2. Metrics

Table S3: Relative errors (%) between the “true” and estimated parametrization.

Test	ΔH_{vap}	α_m	Stoichiometric Coefficients for each volatility bin					
			10^{-2}	10^{-1}	10^0	10^0	10^2	10^3
A1	9.7	65.8			15	87	41	15
A2	6.8	61.5			12	76	60	-
A3	6.8	61.5		-	12	76	60	-
A4	13.3	60.0			12	115	6	13
B1	12.8	77.7	-	-	42	58	277	10
B2	21.7	76.5	-	-	35	42	195	6
C1	9.1	89.7	7	23	33	13		
C2	20.7	54.1	-	-	258	42	-	-

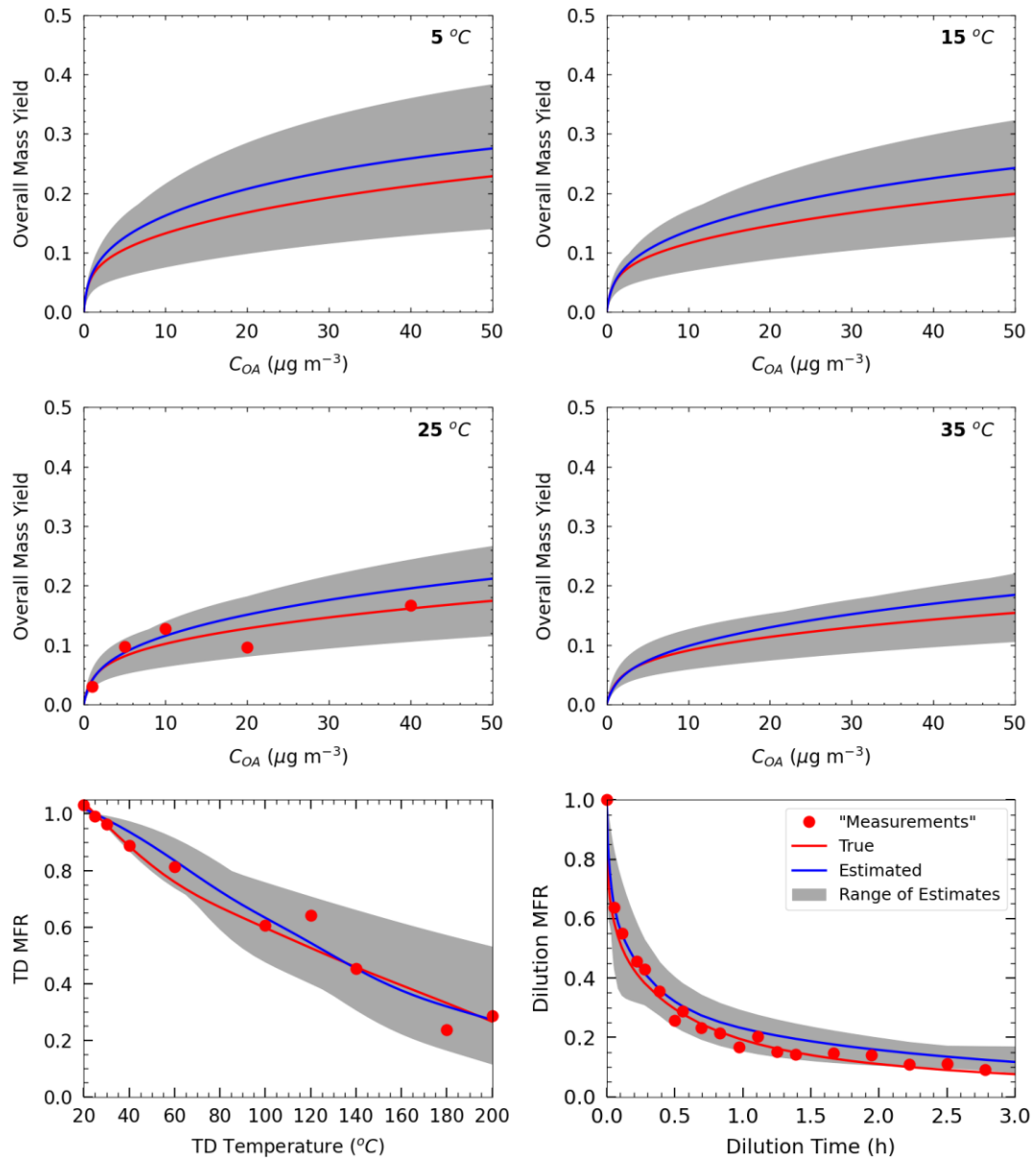


Figure S1: “Measurements” of Test A2 in Experiment A (red dots), true (red line) and estimated (blue line) yields at four temperatures (at 5 °C, 15 °C, 25 °C, and 35 °C), TD (thermogram), and dilution (areogram) values. The grey area shows the range of good solutions.

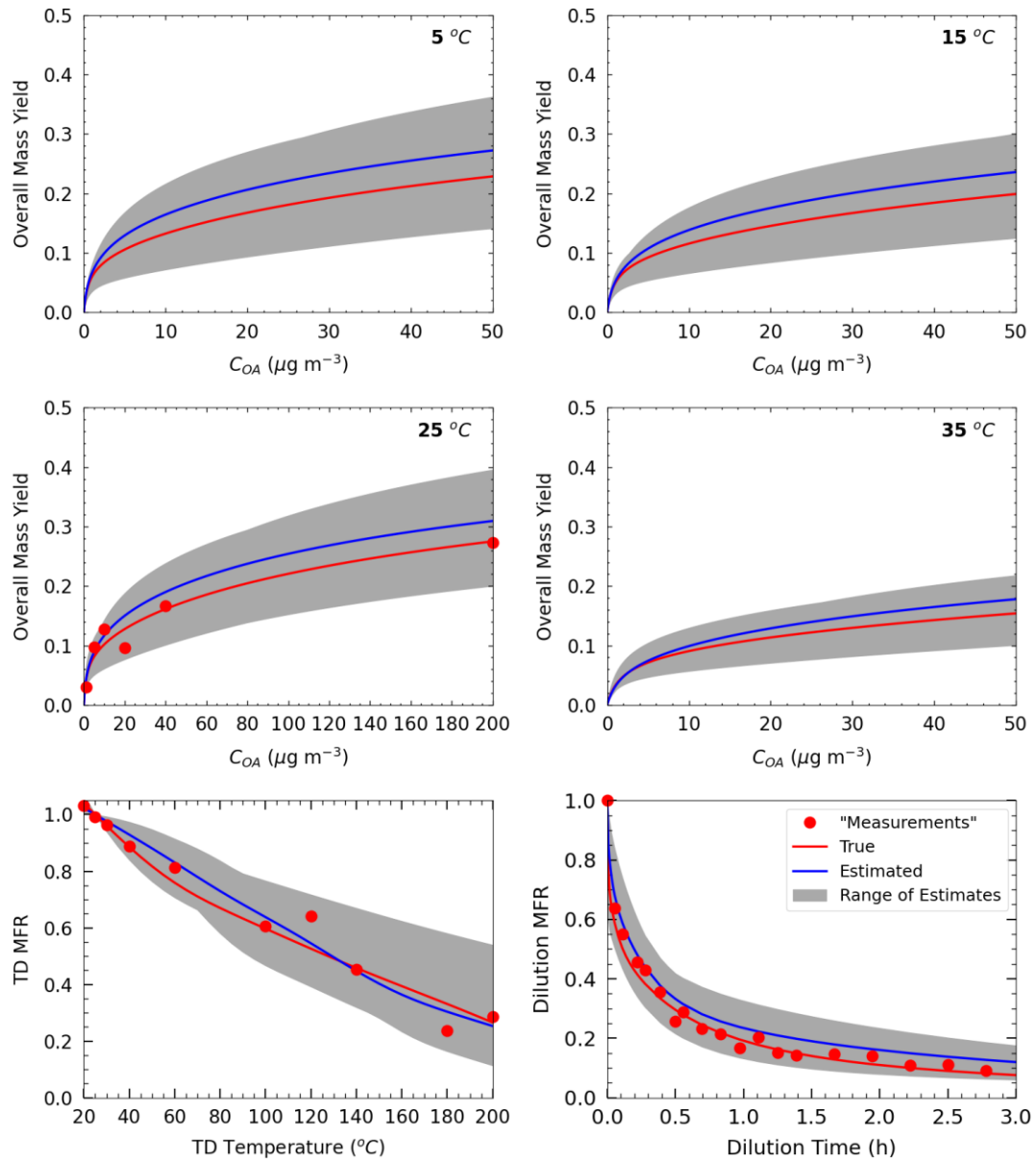


Figure S2: “Measurements” of Test A4 in Experiment A (red dots), true (red line) and estimated (blue line) yields at four temperatures (at 5 °C, 15 °C, 25 °C, and 35 °C), TD (thermogram), and dilution (areogram) values. The grey area shows the range of good solutions.

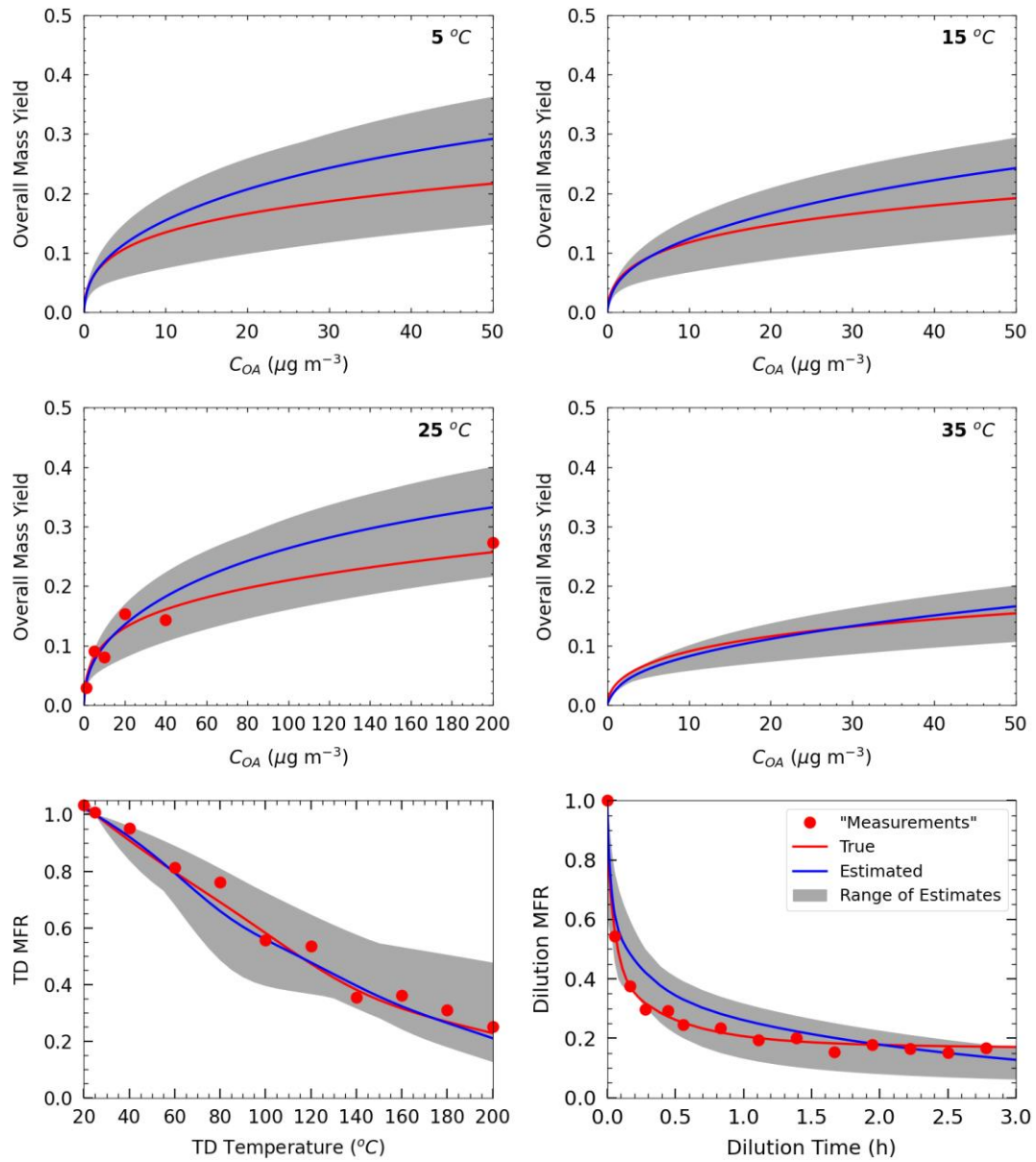


Figure S3: “Measurements” of Test B2 in Experiment B (red dots), true (red line) and estimated (blue line) yields at four temperatures (at 5 °C, 15 °C, 25 °C, and 35 °C), TD (thermogram), and dilution (areogram) values. The grey area shows the range of good solutions.