Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information:

Influence of Particle Viscosity on Mass Transfer and Heterogeneous Ozonolysis Kinetics in Aqueous-Sucrose-Maleic Acid Aerosol

Frances H. Marshall,[1] Thomas Berkemeier,[2] Manabu Shiraiwa,[3]

Lucy Nandy,[4] Peter B. Ohm,[4] Cari S. Dutcher[4] and Jonathan P. Reid[1,*]

[1] School of Chemistry, University of Bristol, Bristol, BS8 1TS, UK

[2] School of Chemical & Biomolecular Engineering, Georgia Institute of Technology, Atlanta, Georgia 30332, United States

[3] Department of Chemistry, University of California, Irvine, 92697, CA, USA

[4] Department of Mechanical Engineering, University of Minnesota, Twin Cities, Minneapolis, Minnesota 55455, United States

Correspondence to: Jonathan. P. Reid j.p.reid@bristol.ac.uk

Table S1: Fitted kinetic parameters for Scenario 1.

Symbol	Unit	RH [%]	Composition (Sucrose : Maleic)	Fitting value	Parameter range*	
k_{BR}	$cm^3\ s^{-1}$	all	All	5.68×10^{-18}	3.36×10^{-18}	1.06×10^{-17}
$D_{b,O3}$	$cm^2\ s^{-1}$	10	5:1	2.16×10^{-12}	---	6.86×10^{-10}
		35	5:1	2.90×10^{-12}	---	4.52×10^{-10}
		55	5:1	4.82×10^{-11}	---	3.06×10^{-10}
		75	5:1	1.03×10^{-7}	7.76×10^{-8}	1.21×10^{-7}
		24	2:1	1.65×10^{-11}	---	7.53×10^{-9}
		40	2:1	2.00×10^{-11}	---	3.41×10^{-9}
		68	2:1	3.05×10^{-9}	4.10×10^{-10}	1.65×10^{-8}
		24	3:5	6.82×10^{-12}	---	2.01×10^{-8}
		72	3:5	4.97×10^{-7}	3.73×10^{-7}	8.23×10^{-7}
		25	1:5	1.99×10^{-12}	---	---
		40	1:5	2.52×10^{-11}	---	3.48×10^{-9}
		71	1:5	1.07×10^{-9}	---	3.66×10^{-9}
$D_{b,MA}$	$cm^2\ s^{-1}$	10	5:1	1.93×10^{-12}	1.63×10^{-12}	3.59×10^{-12}
		35	5:1	3.74×10^{-12}	2.57×10^{-12}	7.10×10^{-12}
		55	5:1	1.00×10^{-10}	---	---
		75	5:1	1.83×10^{-10}	5.90×10^{-11}	---
		24	2:1	1.16×10^{-12}	9.99×10^{-13}	1.80×10^{-12}
		40	2:1	3.90×10^{-12}	2.43×10^{-12}	7.98×10^{-12}
		68	2:1	5.49×10^{-12}	4.38×10^{-12}	9.28×10^{-12}
		24	3:5	1.07×10^{-12}	7.27×10^{-13}	2.50×10^{-12}
		72	3:5	2.31×10^{-11}	1.78×10^{-11}	3.84×10^{-11}
		25	1:5	1.20×10^{-13}	9.04×10^{-14}	5.29×10^{-13}
		40	1:5	1.93×10^{-12}	1.55×10^{-12}	3.56×10^{-12}
		71	1:5	3.51×10^{-9}	2.00×10^{-11}	---
$H_{cp,O3,org}$	$mol\ cm^{-3}\ atm^{-1}$	all	All	2.8×10^{-4}	1.87×10^{-4}	4.48×10^{-4}

*Local uncertainty at the 10 % level (changing the parameter within these boundaries leads to at most 10 % change in model – experiment - correlation).

Table S2: Fitted kinetic parameters for Scenario 2.

Symbol	Unit	RH [%]	Composition (Sucrose : Maleic)	Fitting value	Parameter range*	
$D_{b,O3}$	$cm^2\ s^{-1}$	10	5:1	8.21×10^{-7}	6.75×10^{-7}	9.85×10^{-7}
		35	5:1	1.08×10^{-6}	8.08×10^{-7}	1.40×10^{-6}
		55	5:1	2.40×10^{-6}	2.01×10^{-6}	2.82×10^{-6}
		75	5:1	1.23×10^{-5}	1.03×10^{-5}	1.48×10^{-5}
		24	2:1	1.11×10^{-6}	9.18×10^{-7}	1.33×10^{-6}
		40	2:1	2.12×10^{-6}	1.46×10^{-6}	3.05×10^{-6}
		68	2:1	1.15×10^{-6}	8.97×10^{-7}	1.48×10^{-6}
		24	3:5	1.85×10^{-6}	1.25×10^{-6}	2.60×10^{-6}
		72	3:5	2.69×10^{-5}	2.00×10^{-5}	3.81×10^{-5}
		25	1:5	6.64×10^{-7}	4.72×10^{-7}	8.92×10^{-7}
		40	1:5	3.19×10^{-6}	2.47×10^{-6}	4.03×10^{-6}
		71	1:5	5.10×10^{-6}	4.30×10^{-6}	6.11×10^{-6}
$H_{cp,O3,org}$	$mol\ cm^{-3}\ atm^{-1}$	all	All	4.6×10^{-5}	3.8×10^{-5}	5.47×10^{-5}

*Local uncertainty at the 10 % level (changing the parameter within these boundaries leads to at most 10 % change in model – experiment - correlation).

Table S3. Parameters for the Vignes-type description of diffusion coefficients, following Eqs. (1) and (2). The free fit to experimental data is labelled "Fit 1" and diffusion coefficients of both ozone and maleic acid have been parameterized. The fit with fixed diffusion coefficients of maleic acid is labelled "Fit 2".

Symbol	Unit	Fit 1 D_{O3}	Fit 1 D_{MA}	Fit 2 D_{O3}
$D_{w,0}$	$cm^2\ s^{-1}$	1.00×10^{-5}	3.53×10^{-13}	1.30×10^{-6}
B		1.00×10^{-10}	3.10×10^{-2}	2.47×10^{-2}
C		6.96×10^{-3}	5.88×10^{-2}	4.07×10^{-2}
$D_{s,0}$	$cm^2\ s^{-1}$	5.58×10^{-12}	1.00×10^{-7}	1.00×10^{-3}

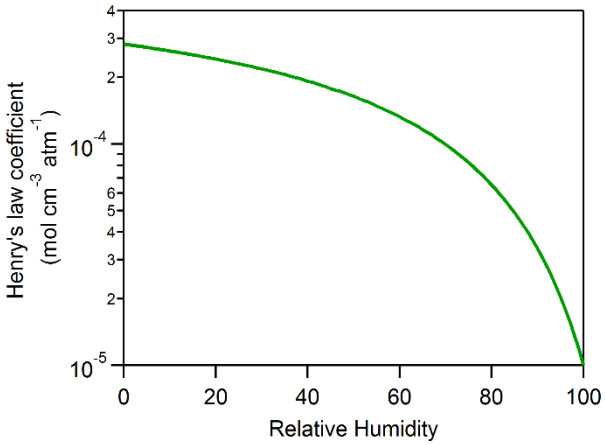

Figure S1: RH dependence of the Henry's law solubility coefficient of ozone in the aqueous organic particles $H_{cp,O3}$ obtained from global optimization for scenario 1. The solubility at 100 % RH was fixed to $H_{cp,O3,w} = 1 \times 10^{-5}$ mol cm^{-3} atm^{-1}; at 0 % RH, $H_{cp,O3,org}$ was used as a fit parameter; intermediate values are interpolated via equation (2) in the main article (solid line). Note that no composition-dependence (sucrose:maleic acid ratio) was assumed in both scenarios 1 and 2.