

SUPPLEMENTARY INFORMATION:

Characterising the Evaporation Kinetics of Water and Semi-Volatile Organic  
Compounds from Viscous Multicomponent Organic Aerosol Particles

Stephen Ingram,<sup>1</sup> Chen Cai,<sup>2</sup> Young-Chul Song,<sup>1</sup> David R. Glowacki,<sup>1,3</sup>

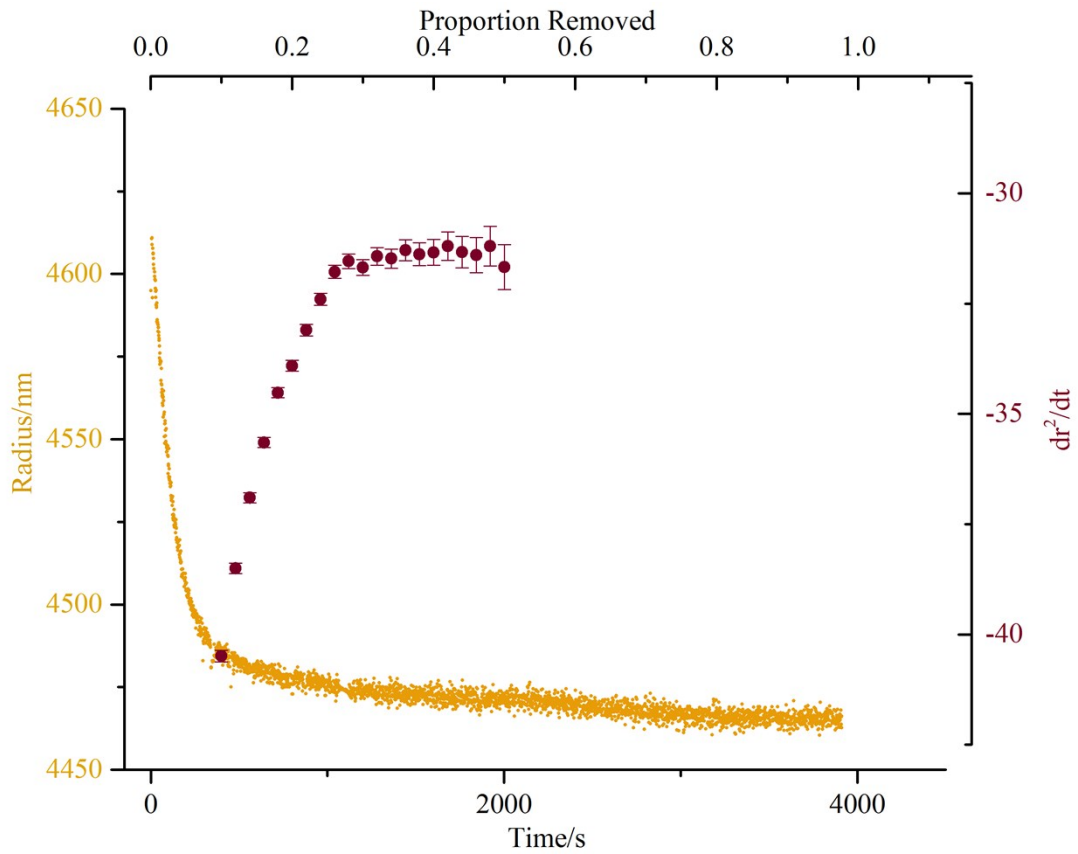
David O. Topping,<sup>4</sup> Simon O'Meara,<sup>3</sup> Jonathan P. Reid<sup>1</sup>

<sup>1</sup> *School of Chemistry, University of Bristol, Cantock's close, Bristol BS8 1TS*

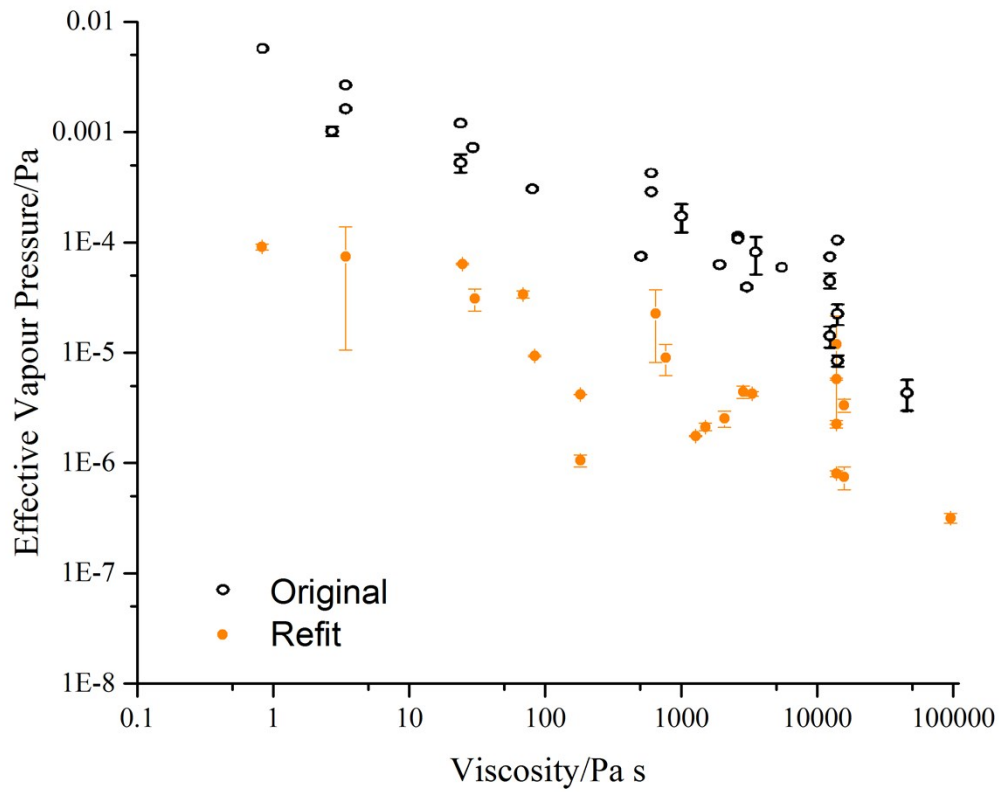
<sup>2</sup> *Department of Atmospheric and Oceanic Sciences, School of Physics, Peking University, Beijing  
100871, China*

<sup>3</sup> *Department of Computer Science, University of Bristol, BS8 1UB, UK*

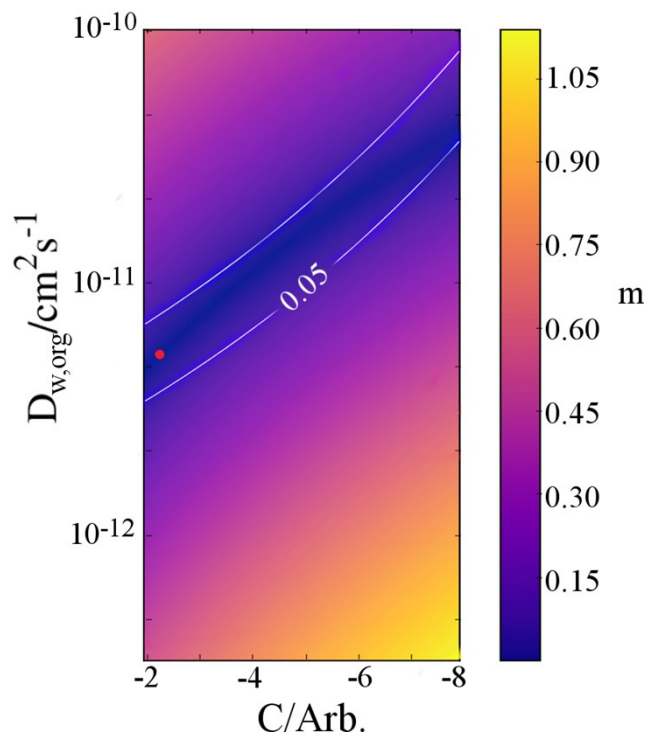
<sup>3</sup> *School of Earth and Atmospheric Sciences, University of Manchester, Manchester M13 9PL*



**Figure S1:** Retrieved gradient values  $\frac{dr^2}{dt}$  from equation 13 (red points) determined from a typical sucrose/malonic acid/water radius curve (yellow data). The fit values are found to converge as one increases the assumed length of the water loss regime, represented as the proportion of the total experimental length (top axis). Note that after a plateau in  $\frac{dr^2}{dt}$  is reached, the fit error increases each time the residual dataset is shortened.



**Figure S2.** Comparison of effective vapour pressure estimates determined for previously reported sucrose : maleic acid 5:1 particles, either by the method described in ref. 13 (open black circles) or via equations 13 and 14 (closed orange circles). Several of the original points have been removed due to the experiments being of insufficient length for statistically significant estimates to be retrieved by the latter method.



**Figure S3:** The map of the value of the merit function calculated from eq. 9 showing the region of the kinetic parameter space ( $D_{w,org}$ ,  $C$ ) where the model reproduces the experimental radius response for the 50 to 20 % RH transition ( $m < 0.05$ ), equivalent to 0.5 to 0.2 in mole fraction for this binary system. The original Fi-PaD fit values of  $D_{w,org}$  and  $C$  (the “bottom of the well”) is shown by the red dot.

## Derivation of Equation (14)

The mass flux of a SVOC species evaporating from a pure component droplet under isothermal conditions can be determined by the equation attributed to Maxwell:

$$\frac{dm_{MA}}{dt} = - \frac{4\pi r M_{MA} D_g}{RT} (p_{MA,\infty} - p_{MA,r})$$

As in the manuscript,  $R$  is the gas constant,  $r$  is the particle radius,  $T$  is the temperature, and  $M_{MA}$  and  $D_g$  are the molecular mass and gas phase diffusion coefficient of malonic acid respectively.

In the experiments described here, the partial pressure of malonic acid at infinite distance,  $p_{MA,\infty} = 0$ , due to the trapping cell conditions i.e. the presence of a gas flow. Thus,

$$\frac{dm_{MA}}{dt} = - \frac{4\pi r M_{MA} D_g}{RT} p_{MA,r}$$

where the partial pressure above the droplet surface  $p_{MA,r}$ . The mass fraction of SVOC in the droplet,  $F_{MA}$ , can be written as

$$F_{MA} = \frac{m_{MA}}{m_{droplet}}$$

where  $m_{droplet}$  is the mass of the droplet. The mass of the SVOC in the droplet can be written as

$$m_{MA} = \frac{4}{3} \pi r^3 \rho_{droplet} F_{MA}$$

where  $\rho_{droplet}$  is the density of the droplet. This can be written as

$$r^3 = \frac{3}{4\pi \rho_{droplet}} \frac{m_{MA}}{F_{MA}}$$

Then, using the chain rule:

$$\frac{dr^3}{dt} = \frac{dr^3}{dm_{MA}} \frac{dm_{MA}}{dt} = \frac{3r M_{MA} D_g}{\rho_{droplet} RT F_{MA}} p_{MA,r}$$

And using

$$\frac{dr^3}{dt} = \frac{dr^3 dr^2}{dr^2 dt} = \frac{3r}{2} \frac{dr^2}{dt}$$

yields

$$\frac{dr^2}{dt} = \frac{dr^2}{dm_{MA}} \frac{dm_{MA}}{dt} = \frac{2M_{MA} D_g}{\rho_{droplet} RT F_{MA}} p_{MA,r}$$

For a SVOC species in a multicomponent particle, we can assume real behaviour for the solution composition which describes the vapour pressure by

$$p_{MA,r} = p_{MA}^{\circ} x_{MA} f_{MA}$$

where  $x_{MA}$  is the mole fraction of the SVOC,  $f_{MA}$  is the activity coefficient and  $p_{MA}^{\circ}$  is the vapour pressure.

Thus,

$$p_{MA,r} = \frac{dr^2}{dt} \cdot \frac{RT\rho_{droplet}F_{MA}}{2M_{MA}D_g} = x_{MA}f_{MA}p_{MA}^{\circ}$$