Supporting information

Surface equilibrium vapor pressure of organic nanoparticles measured from the Dynamic-aerosol-size Electrical Mobility Spectrometer

Ella Häkkinen[1], Huan Yang[1*], Runlong Cai[2], and Juha Kangasluoma[1]

[1]Institute for Atmospheric and Earth System Research/Physics, Faculty of Science, University of Helsinki, Helsinki, 00014, Finland

[2]Shanghai Key Laboratory of Atmospheric Particle Pollution and Prevention (LAP[3]), Department of Environmental Science & Engineering, Fudan University, 200438 Shanghai, China

* Correspondence: Huan Yang (huan.yang@helsinki.fi)

Content

Theoretical model for cases where particle evaporation in the 1st DMA is non-negligible

The theoretical model proposed in the main text assumes that particle evaporation at room temperature is negligible and particles maintain a constant size before entering the second DMA where the sheath flow is heated. This assumption is robust for less volatile chemicals such as dibutyl sebacate, PEG5, and PEG6. However, it is violated for more volatile substances like glycerol and PEG4. Consequently, we introduce an alternative theoretical model tailored for addressing the behavior of volatile chemicals that undergo observable evaporation even while traversing the 1st DMA.
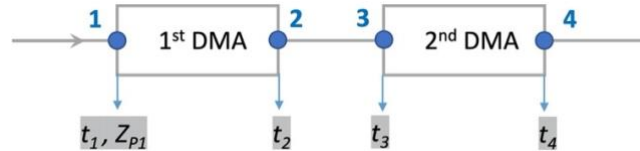
Figure S1. Positions of the four slits at which the size of particles are of interest.

The schematic diagram (Fig. S1) illustrates the transmission and evaporation processes of particles within both DMAs. Inlet and outlet slits for the two DMAs are denoted by numbers $i = 1, 2, 3$, and 4, with the corresponding times when particles reach slit i represented by t_i. Assuming particles enter the 1st DMA through slit 1 at time zero ($t_1 = 0$) with a mobility of Z_{p1}, we can establish a sequence of times: $t_2 = t_{f1}$, $t_3 = t_{f1} + t\_tube$, $t_4 = t_{f1} + t\_tube + t_{f2}$, where t_{f1}, t_{f2}, and t_tube represent the particle residence times in the 1st DMA, 2nd DMA, and the tube between the two DMAs, respectively, all of which are known quantities in the experiment. The equation governing the mobility evolution, accounting for evaporation in the transition regime, remains applicable (Eq. 2 in the main text). Hence:

$$Z_p(t) = \frac{1}{\left(Ct + Z_{p1}^{-2}\right)^{1/2}} \tag{S1}$$

In addition, the time average mobility in the 1st and 2nd DMA are both constants (Eq. 1 in the main text), thus we have:

$$\frac{1}{t_2 - t_1} \int_{t_1}^{t_2} Z_p(t)dt = \frac{(2Q_{sh1} + Q_{a1} - Q_{s1})\ln(r_2/r_1)}{4\pi L V_{c1}} \tag{S2}$$

$$\frac{1}{t_4 - t_3} \int_{t_3}^{t_4} Z_p(t)dt = \frac{(2Q_{sh2} + Q_{a2} - Q_{s2})\ln(r_2/r_1)}{4\pi L V_{c2}} \tag{S3}$$

Where V_{ci}, Q_{shi}, Q_{ai}, and Q_{si} are the voltage, sheath flow rate, aerosol flow rate, and sample flow rate for DMA i ($i = 1$ or 2). And r_1, r_2, and L are the DMA gemetrical parameters that have been given in the main text and are the same for both DMAs. Eqs. S2 and S3 hence provide enough equations to solve for the two unknown variables C and Z_{p1}. The two equations are solved numerically through a trial-and-error procedure. Once C and Z_{p1} are obtained, the mobilities at any of the four slits can be computed based on Eq. S1 by inputting the corresponding time that the particle reaches that slit. Finally, the mobility can be converted to radii according to the mobility-radius relationship (Eqs. 5a and 5b) provided in the main text.
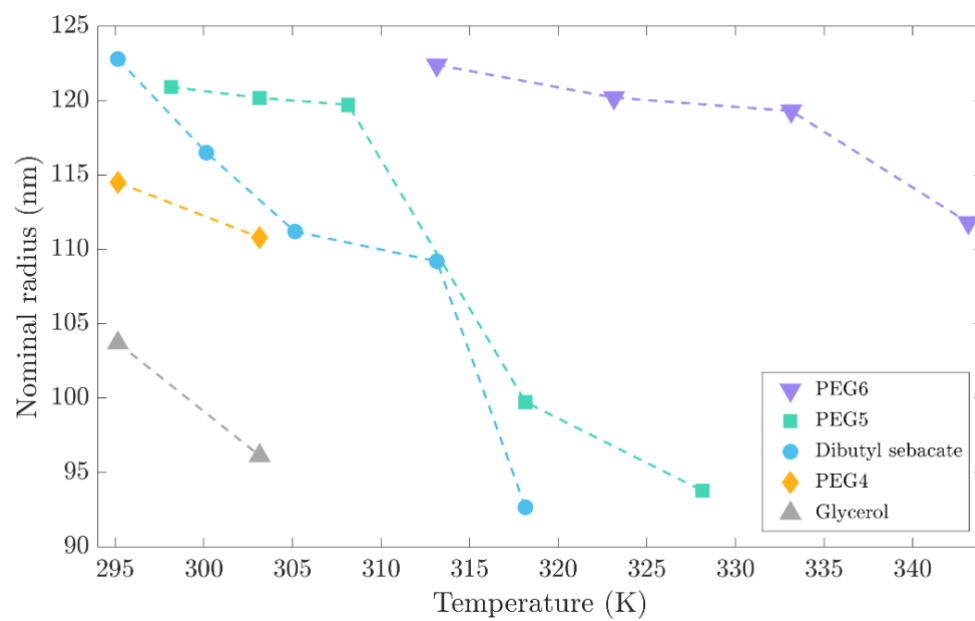
Figure S2. Nominal radius as a function of temperature with residence time of 2.23 s for each measured compound.
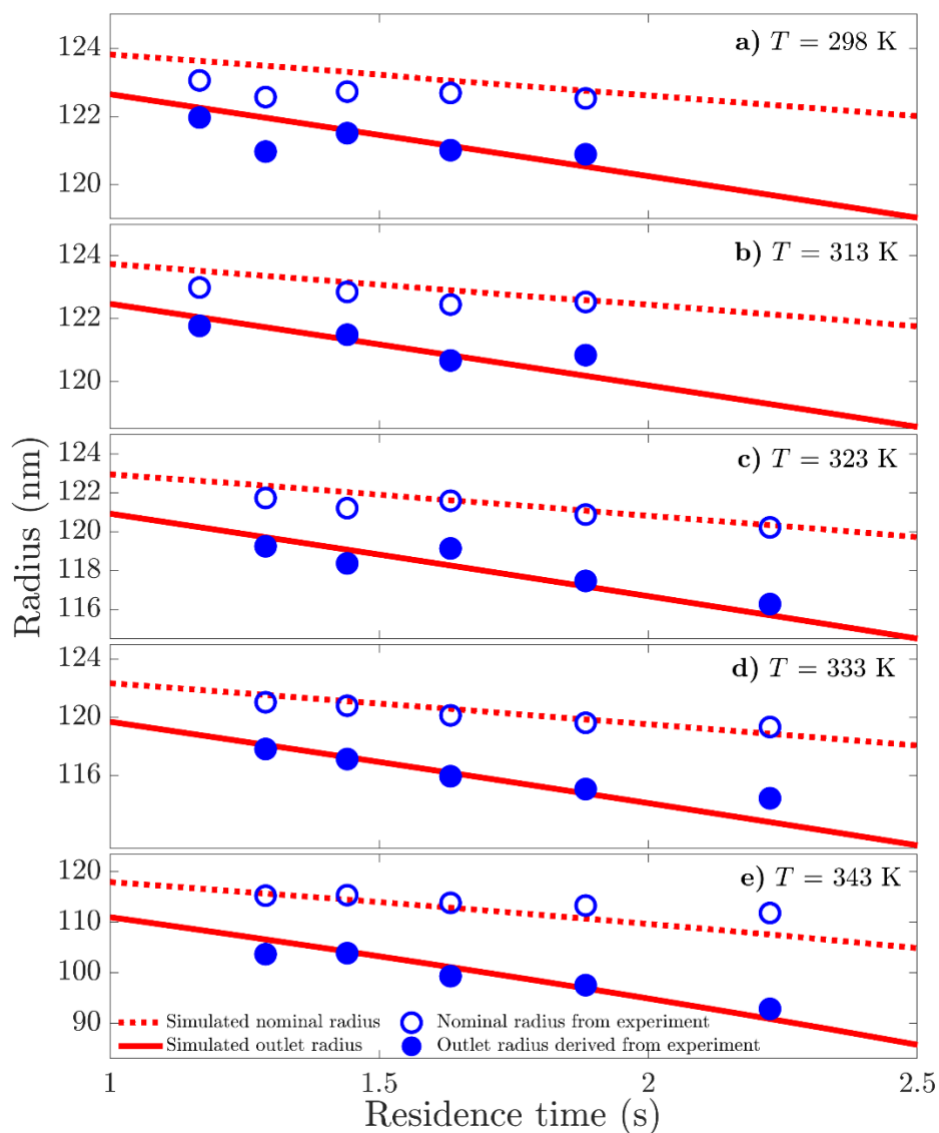
Figure S3. PEG6 particle radius as a function of residence time inside the 2nd DMA at five different temperatures. Empty circles are the measured nominal radii, filled circles are radii at the outlet of the 2nd DMA inferred from the measured nominal radii using the model. The red lines show the simulated nominal and outlet radii.
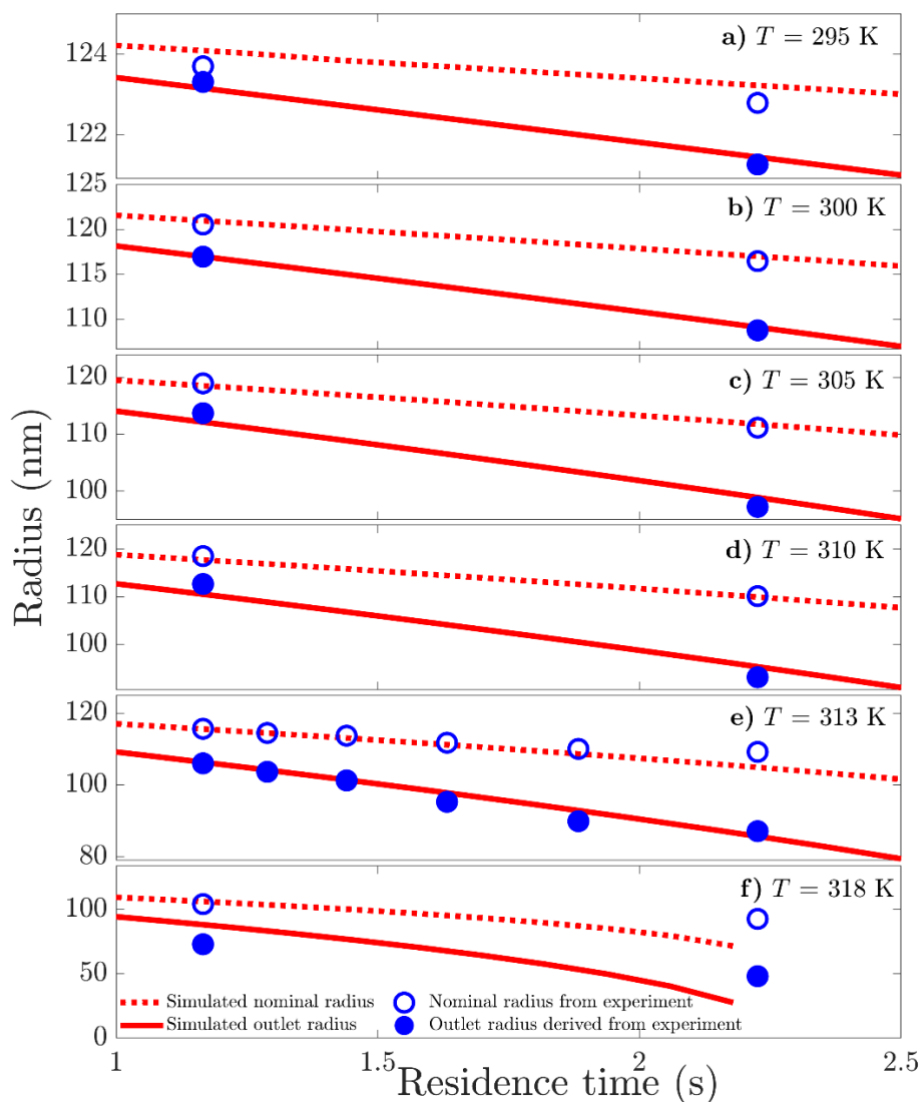
Figure S4. Dibutyl sebacate particle radius as a function of residence time inside the 2nd DMA at five different temperatures. Empty circles are the measured nominal radii, filled circles are radii at the outlet of the 2nd DMA inferred from the measured nominal radii using the model. The red lines show the simulated nominal and outlet radii.
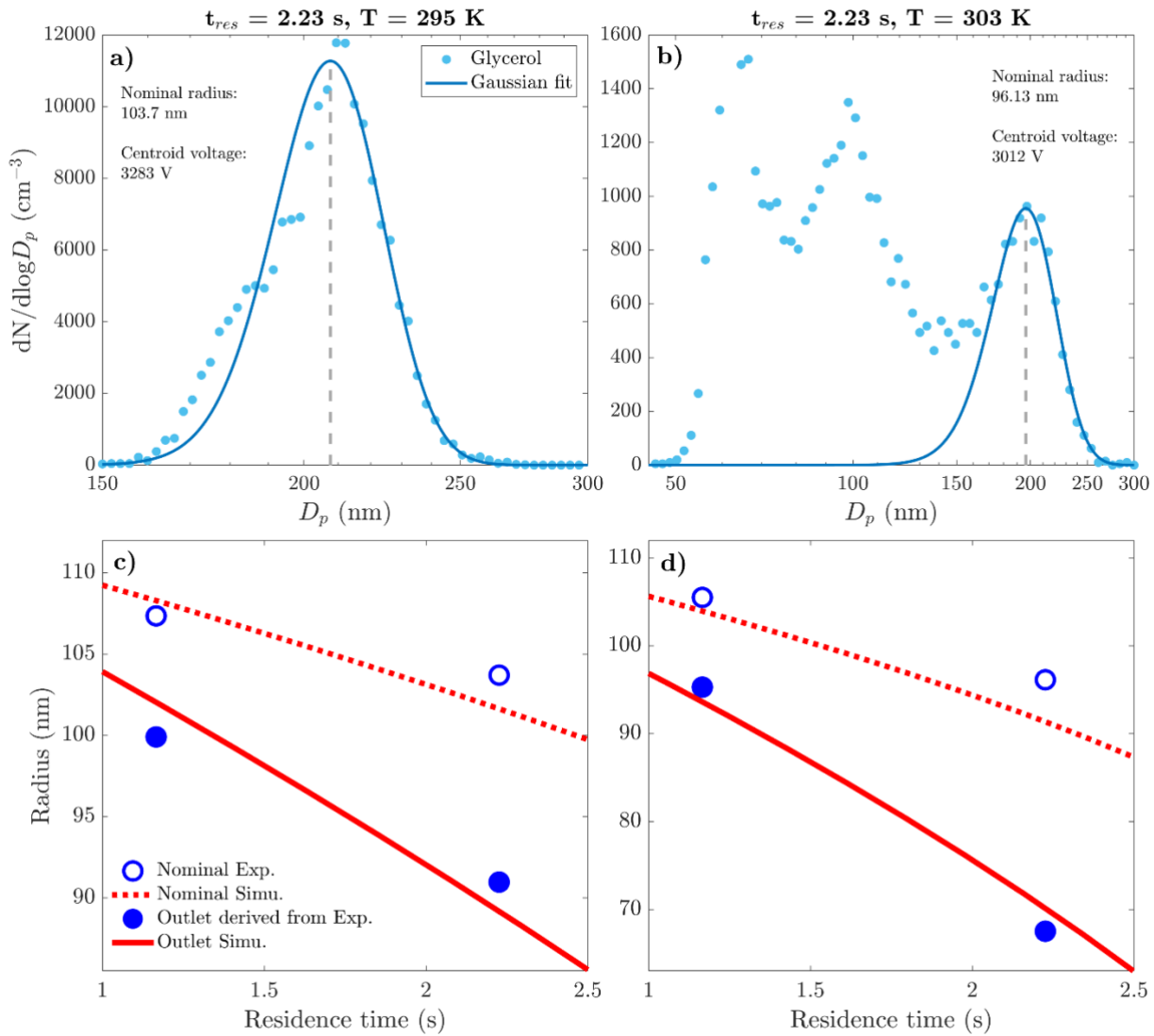
Figure S5. Figures on top: Glycerol particle number concentration as a function of voltage at 2nd DMA sheath flow rate of 10 L min^{-1} and at temperature of 295 K and 303 K. Figures on bottom: Glycerol particle radius as a function of residence time inside the 2^n DMA at temperature of 295 K and 303 K. Empty circles are the measured nominal radii, filled circles are radii at the outlet of the 2nd DMA inferred from the measured nominal radii using the model. The red lines show the simulated nominal and outlet radii.
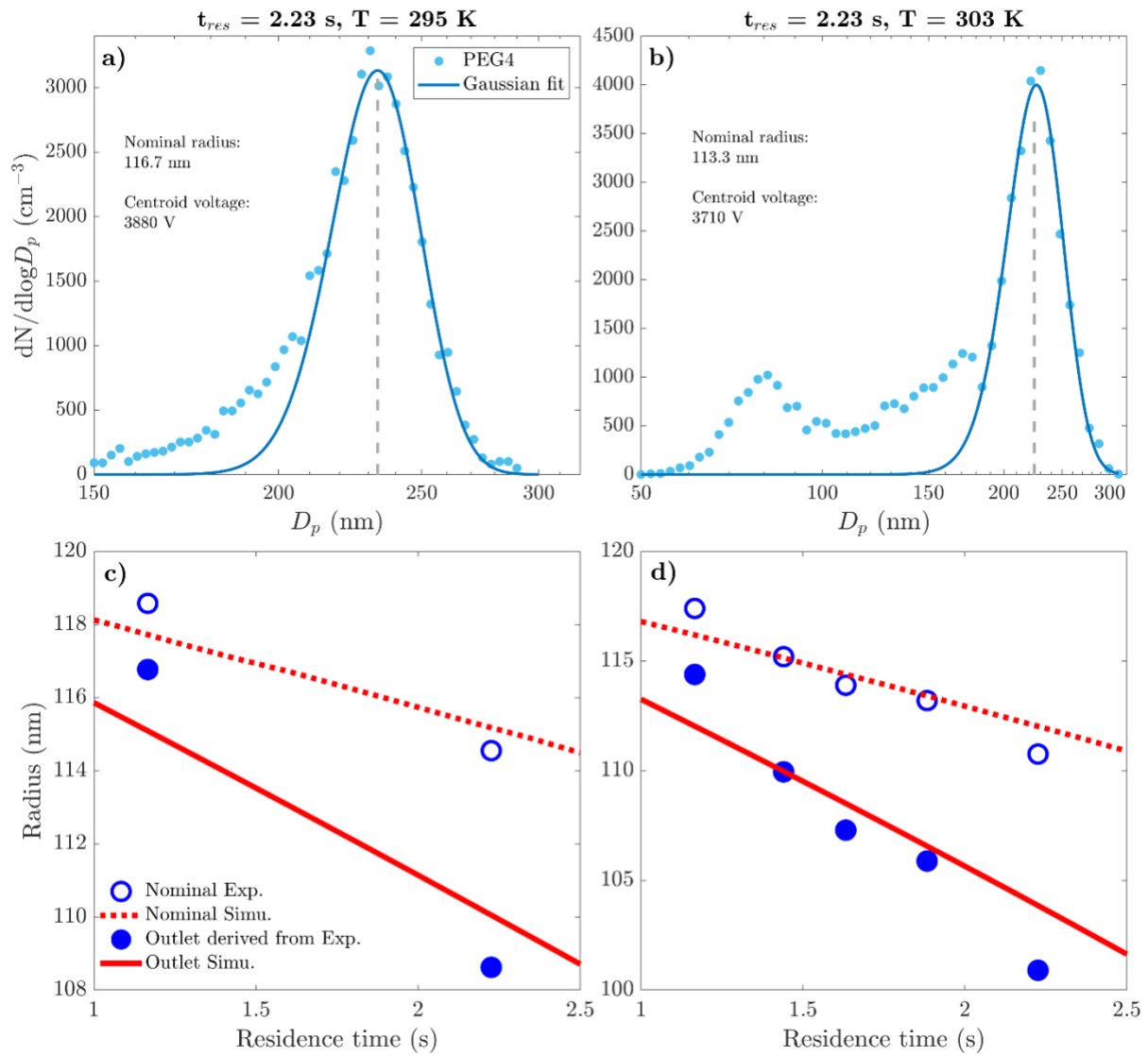
Figure S6. Figures on top: PEG4 particle number concentration as a function of voltage at 2nd DMA sheath flow rate of 10 L min^{-1} and at temperature of 295 K and 303 K. Figures on bottom: PEG4 particle radius as a function of residence time inside the 2nd DMA at temperature of 295 K and 303 K. Empty circles are the measured nominal radii, filled circles are radii at the outlet of the 2nd DMA inferred from the measured nominal radii using the model. The red lines show the simulated nominal and outlet radii.

Compound	Maximum vapor pressure (Pa)				Minimum vapor pressure (Pa)			
	Theoretical		Simulation		Theoretical		Simulation	
	$rp_l = 125$ nm	$rp_l = 220$ nm	$rp_l = 125$ nm	$rp_l = 220$ nm	$rp_l = 125$ nm	$rp_l = 220$ nm	$rp_l = 125$ nm	$rp_l = 220$ nm
Glycerol	0.036	0.10	0.037	0.10	0.0011	0.0020	0.0011	0.0018
PEG4	0.019	0.058	0.019	0.058	0.00060	0.0010	0.00060	0.00104
PEG5	0.017	0.053	0.017	0.052	0.00053	0.00095	0.00054	0.00096
PEG6	0.015	0.048	0.015	0.048	0.00049	0.00087	0.00050	0.00088
Dibutyl sebacate	0.014	0.045	0.014	0.045	0.00046	0.00083	0.00047	0.00084

Table S1. The DEMS measurable vapor pressure range for the different sample compounds at temperature of 295 K, residence time of 1.17 s and inlet particle radius of 125 and 220 nm.