Effect of aerosol volatility on the sizing accuracy of Differential Mobility Analyzers: Supplemental material

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S1 Explanation of particle evaporation equation

Evaporation or growth rate of a single-component particle in the transition regime is described by (Seinfeld and Pandis, 2006):

$$\frac{dd_p}{dt} = -\frac{4DF(d_p, \alpha)}{\rho d_p} (K(d_p, \sigma)C_{sat} - C_{env}) \quad (\text{S1})$$

in which d_p is the particle diameter, t is time, D is the diffusion coefficient of the evaporating species, C_{sat} is the saturation vapor concentration of the species, C_{env} is the concentration of the species in the surrounding environment, ρ is the density of the particle, $F(d_p, \alpha)$ is the Fuchs-Sutugin correction factor, $K(d_p, \sigma)$ is the Kelvin effect correction, α is the accommodation/evaporation coefficient, and σ is the surface tension.

The Kelvin effect correction is (Seinfeld and Pandis, 2006):

$$K(d_p, \sigma) = \exp\left(\frac{4\sigma M_w}{\rho RT d_p}\right) \quad (\text{S2})$$

in which M_w is the molecular weight of the species, R is the universal gas constant, and T is the temperature.

The Fuch-Sutugin correction is (Fuchs and Sutugin, 1971):

$$F(d_p, \alpha) = \frac{0.75\alpha(1 + Kn)}{Kn^2 + Kn + 0.283\alpha Kn + 0.75\alpha} \quad (S3)$$

in which $Kn = 2\Lambda/d_p$. Λ is the mean free path of the species in air and is equal to $3D/\bar{c}_A$, in which $\bar{c}_A$ is the air mean molecular speed.

To extend the evaporation rate expression to a general case of a multi-component particle, i.e., composed of a mixture of compounds, let us consider evaporation/condensation in terms of mass of individual species. The mass change rate be easily obtained from Eq.S1, assuming a constant particle density and ideal mixing of all components in the mixture:

$$\frac{dM_i}{dt} = -\pi d_p DF(d_p, \alpha) (K(d_p, \sigma) x_i C_{sat,i} - C_{env,i}) \quad (S4)$$

in which M_i is the mass of species i in the particle, x_i is its mole fraction in the mixture, $C_{sat,i}$ is the saturation concentration of the component i , and $C_{env,i}$ is its concentration in the gas phase.

The change of the particle mass is equal to sum of the mass change rates of individual species in the mixture. Employing a commonly-used assumption that all components in the mixture have the same M_w , the particle mass change rate is obtained:

$$\begin{aligned} \frac{dM}{dt} &= -\pi d_p DF(d_p, \alpha) \left(K(d_p, \sigma) \sum_i x_i C_{sat,i} - \sum_i C_{env,i} \right) \\ &= -\pi d_p DF(d_p, \alpha) (K(d_p, \sigma) C_{sat,av} - C_{env,t}) \end{aligned} \quad (S5)$$

in which $C_{sat,av}$ is the mole-fraction-averaged saturation vapor pressure of compounds in the mixture and $C_{env,t}$ is the total concentration of the compounds in the gas phase.

Eq.S5 can be reverted to describe the size change rate for a multi-component particle:

$$\frac{dd_p}{dt} = -\frac{4DF(d_p, \alpha)}{\rho d_p} (K(d_p, \sigma) C_{sat,av} - C_{env,t}) \quad (S6)$$

References

- Fuchs, N. and Sutugin, A.: High dispersed aerosols. In Topics in Current Aerosol Research, vol. 2, Pergamon Press, Oxford, 1971.
- Seinfeld, J. and Pandis, S. N.: Atmospheric chemistry and physics: from air pollution to climate change, Wiley & Sons, Inc., Hoboken, New Jersey, 2nd ed. edn., 2006.