Supplementary material: Including phase separation in a unified model to calculate partitioning of vapours to mixed inorganic-organic aerosol particles†

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1 Derivation of partitioning coefficients between two liquid phases

A component i at chemical equilibrium between two liquid phases satisfies the following expression:

$$x_i^{\alpha} f_i^{\alpha} = x_i^{\beta} f_i^{\beta} \tag{1}$$

where x_i^{α} is the mole fraction in phase α and f_i^{α} the mole fraction based activity coefficient in phase α. Both are calculated using the following expressions:

$$x_i^{\alpha} = \frac{n_i^{\alpha}}{N_T^{\alpha}};\, x_i^{\beta} = \frac{n_i^{\beta}}{N_T^{\beta}} \tag{2}$$

where n_i^{α} is the number of moles of component i in phase α, N_T^{α} the total number of moles in phase α, n_i^{β} is the number of moles of component i in phase β and N_T^{β} the total number of moles in phase β. The total number of moles in each phase is simply a summation of each contributing compound in that phase:

$$N_T^{\alpha} = \sum_j n_j^{\alpha};\, N_T^{\beta} = \sum_j n_j^{\beta} \tag{3}$$

As the total number of moles of each compound remain fixed (n_i^T), the amount in each phase can be related using the following:

$$n_i^{\alpha} = n_i^T - n_i^{\beta} \tag{4}$$

which can be expressed in terms of mole fractions:

$$n_i^{\alpha} = n_i^T - x_i^{\beta} N_T^{\beta} \tag{5}$$

Using equation 1, the total amount of component i in phase α can be related to both f_i^{α} and f_i^{β} with the following expressions:

$$n_i^{\alpha} = n_i^T - \left[\frac{x_i^{\alpha} f_i^{\alpha}}{f_i^{\beta}}\right] N_T^{\beta} \tag{6}$$

$$n_i^{\alpha} = n_i^T - n_i^{\alpha}\left[\frac{N_T^{\beta}}{N_T^{\alpha}}\frac{f_i^{\alpha}}{f_i^{\beta}}\right] \tag{7}$$

$$n_i^{\alpha} = \left[1 + \frac{N_T^{\beta}}{N_T^{\alpha}}\frac{f_i^{\alpha}}{f_i^{\beta}}\right]^{-1} n_i^T \tag{8}$$

$$\tag{9}$$

Which can be further simplified to:

$$n_i^{\alpha} = \left[1 + (\frac{N_T}{N_T^{\alpha}} - 1)\frac{f_i^{\alpha}}{f_i^{\beta}}\right]^{-1} n_i^T \tag{10}$$

Hence, the partitioning coefficient between two liquid phases is given by:

$$\left[1 + (\frac{N_T}{N_T^{\alpha}} - 1)\frac{f_i^{\alpha}}{f_i^{\beta}}\right]^{-1} \tag{11}$$

