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:

$$ x_i^\alpha f_i^\alpha = x_i^\beta f_i^\beta $$

where $x_i^\alpha$ is the mole fraction in phase $\alpha$ and $f_i^\alpha$ the mole fraction based activity coefficient in phase $\alpha$. Both are calculated using the following expressions:

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

where $n_i^\alpha$ is the number of moles of component $i$ in phase $\alpha$, $N_T^\alpha$ the total number of moles in phase $\alpha$, $n_i^\beta$ is the number of moles of component $i$ in phase $\beta$ and $N_T^\beta$ the total number of moles in phase $\beta$. The total number of moles in each phase is simply a summation of each contributing compound in that phase:

$$ N_T^\alpha = \sum_j n_j^\alpha; N_T^\beta = \sum_j n_j^\beta $$

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:

$$ n_i^\alpha = n_i^T - n_i^\beta $$
which can be expressed in terms of mole fractions:

\[ n_i^\alpha = n_i^T - x_i^\beta N_i^\beta \]  

(5)

Using equation 1, the total amount of component \( i \) in phase \( \alpha \) can be related to both \( f_i^\alpha \) and \( f_i^\beta \) with the following expressions:

\[ n_i^\alpha = n_i^T - \left( x_i^\beta f_i^\alpha \right) N_i^\beta \]  

(6)

\[ n_i^\alpha = n_i^T - n_i^\alpha \left[ \frac{N_i^\beta}{N_i^\alpha} f_i^\alpha \right] \]  

(7)

\[ n_i^\alpha = \left[ 1 + \frac{N_i^\beta}{N_i^\alpha} f_i^\alpha \right]^{-1} n_i^T \]  

(8)

\[ n_i^\alpha = \left[ 1 + \frac{N_i^\beta - 1}{N_i^\alpha} \frac{f_i^\alpha}{f_i^\beta} \right]^{-1} n_i^T \]  

(9)

Which can be further simplified to:

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

(10)

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

\[ \left[ 1 + \left( \frac{N_i^\beta}{N_i^\alpha} - 1 \right) \frac{f_i^\alpha}{f_i^\beta} \right]^{-1} \]  

(11)