Example 05.22b VLE of Hexane-Butanone-2 Via UNIFAC - as Function

Calculate the vapor-liquid equilibrium of the system n-hexane (1) - 2-butanone (2) at 60°C for a mole fraction of x_1 = 0.5 with the help of the UNIFAC method assuming ideal behavior of the vapor phase.

System: n-hexane (1) - 2-butanon (2)

Definitions: $kPa := 1000Pa$

System temperature: $T_{system} := 333.15K$

$n_{comp} := 2$

Pure component vapor pressures:

$$Antoine := \begin{pmatrix} 6.00266 & 1171.53 & 224.366 \\ 6.18846 & 1261.34 & 221.969 \end{pmatrix}$$

$$Ps(i,T) := 10^{\left(Antoine_{i,1} - \frac{Antoine_{i,2}}{Antoine_{i,3} + \frac{T}{1K} - 273.15}\right)} kPa$$

Composition:

$$x := \begin{pmatrix} .5 \\ .5 \end{pmatrix}$$

Structural information:

Components:

$$name_{comp} := \begin{pmatrix} \text{"n-hexane"} \\ \text{"2-butanone"} \end{pmatrix}$$

Groups:

$$name_{sub} := \begin{pmatrix} \text{"CH3"} \\ \text{"CH2"} \\ \text{"CH3CO"} \end{pmatrix} \qquad name_{main} := \begin{pmatrix} \text{"CH3"} \\ \text{"CH2CO"} \end{pmatrix}$$

$n_{sub} := 3$

$n_{main} := 2$

$$ID_{sub} := \begin{pmatrix} 1 \\ 2 \\ 18 \end{pmatrix} \qquad ID_{main} := \begin{pmatrix} 1 \\ 9 \end{pmatrix}$$

Subgroup i belongs to maingroup $s2m_i$:

$$s2m := \begin{pmatrix} 1 \\ 1 \\ 2 \end{pmatrix}$$

Number of subgroups of type i in component j ($\nu_{i,j}$):

$$\nu = \begin{pmatrix} 2 & 1 \\ 4 & 1 \\ 0 & 1 \end{pmatrix}$$

R- and Q-values for subgroups:

$$R := \begin{pmatrix} 0.9011 \\ 0.6744 \\ 1.6724 \end{pmatrix} \qquad Q := \begin{pmatrix} 0.848 \\ 0.540 \\ 1.488 \end{pmatrix}$$

Interaction parameters between maingroups:

$$\Delta u := \begin{pmatrix} 0 & 476.4 \\ 26.76 & 0 \end{pmatrix} K$$

$\gamma UNIFAC(x,T) :=$

for $i \in 1..n_{comp}$

$$r_i \leftarrow \sum_{j=1}^{n_{sub}} \nu_{j,i} \cdot R_j$$

$$q_i \leftarrow \sum_{j=1}^{n_{sub}} \nu_{j,i} \cdot Q_j$$

for $i \in 1..n_{comp}$

$$V_i \leftarrow \frac{r_i}{\sum_{j=1}^{n_{comp}} x_j \cdot r_j}$$

$$F_i \leftarrow \frac{q_i}{\sum_{j=1}^{n_{comp}} x_j \cdot q_j}$$

for $i \in 1..n_{comp}$

$$\ln\gamma comb_i \leftarrow 1 - V_i + \ln(V_i) - 5 \cdot q_i \cdot \left(1 - \frac{V_i}{F_i} + \ln\left(\frac{V_i}{F_i}\right)\right)$$

for $i \in 1..n_{main}$

for $j \in 1..n_{main}$

$$\psi_{i,j} \leftarrow \exp\left[\frac{-(\Delta u_{i,j})}{T}\right]$$

for $i \in 1..n_{comp}$

for $j \in 1..n_{sub}$

$$X_{j,i} \leftarrow \frac{\nu_{j,i}}{\sum_{k=1}^{n_{sub}} \nu_{k,i}}$$

for $i \in 1..n_{comp}$

for $j \in 1..n_{sub}$

$$\Theta_{j,i} \leftarrow \frac{Q_j \cdot X_{j,i}}{\sum_{k=1}^{n_{sub}} Q_k \cdot X_{k,i}}$$

for $i \in 1..n_{comp}$

for $j \in 1..n_{sub}$

$$\ln\Gamma_{j,i} \leftarrow Q_j \cdot \left(1 - \ln\left(\sum_{k=1}^{n_{sub}} \Theta_{k,i} \cdot \psi_{s2m_k, s2m_j}\right) \cdots + - \sum_{k=1}^{n_{sub}} \frac{\Theta_{k,i} \cdot \psi_{s2m_j, s2m_k}}{\sum_{l=1}^{n_{sub}} \Theta_{l,i} \cdot \psi_{s2m_l, s2m_k}}\right)$$

for $i \in 1..n_{sub}$

$$X_{M_i} \leftarrow \frac{\sum_{j=1}^{n_{comp}} \nu_{i,j} \cdot x_j}{\sum_{j=1}^{n_{comp}} \sum_{k=1}^{n_{sub}} (\nu_{k,j} \cdot x_j)}$$

for $i \in 1..n_{sub}$

for $i \in 1 .. n_{sub}$

$$\Theta M_i \leftarrow \frac{Q_i \cdot X_{M_i}}{\sum_{j=1}^{n_{sub}} Q_j \cdot X_{M_j}}$$

for $i \in 1 .. n_{sub}$

$$\ln\Gamma M_i \leftarrow Q_i \cdot \left(1 - \ln\left(\sum_{j=1}^{n_{sub}} \Theta M_j \cdot \psi_{s2m_j, s2m_i} \right) \cdots + - \sum_{j=1}^{n_{sub}} \frac{\Theta M_j \cdot \psi_{s2m_i, s2m_j}}{\sum_{k=1}^{n_{sub}} \Theta M_k \cdot \psi_{s2m_k, s2m_j}} \right)$$

for $i \in 1 .. n_{comp}$

$$\ln\gamma res_i \leftarrow \sum_{j=1}^{n_{sub}} \nu_{j,i} \cdot \left(\ln\Gamma M_j - \ln\Gamma_{j,i} \right)$$

$$\exp\left(\ln\gamma comb + \ln\gamma res \right)$$

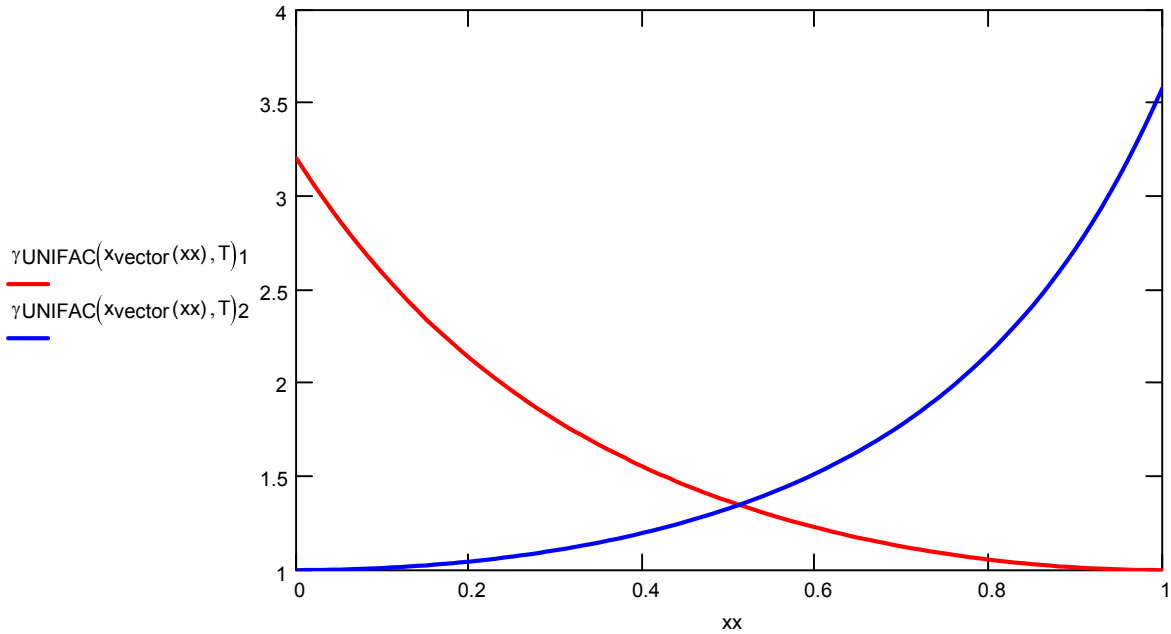
$$\gamma UNIFAC(x, T_{system}) = \begin{pmatrix} 1.428 \\ 1.365 \end{pmatrix}$$

$i := 1 .. n_{comp}$

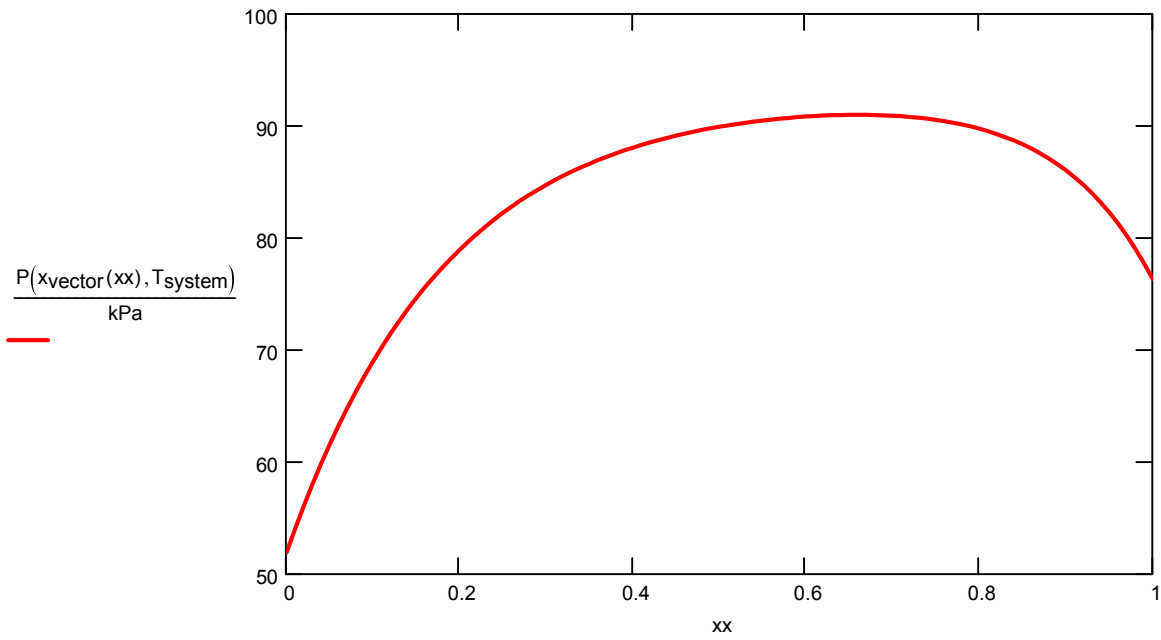
$j := 1 .. n_{comp}$

$$x_{vector}(xx) := \begin{pmatrix} xx \\ 1 - xx \end{pmatrix}$$

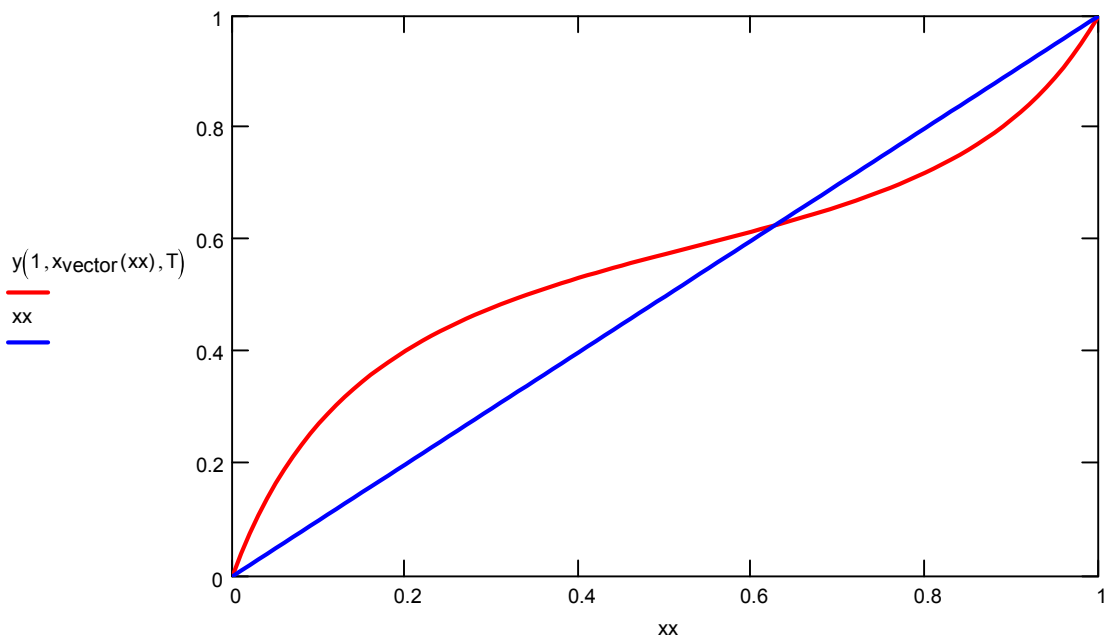
$xx := 0, 0.01 .. 1$ $\quad T := 373K$

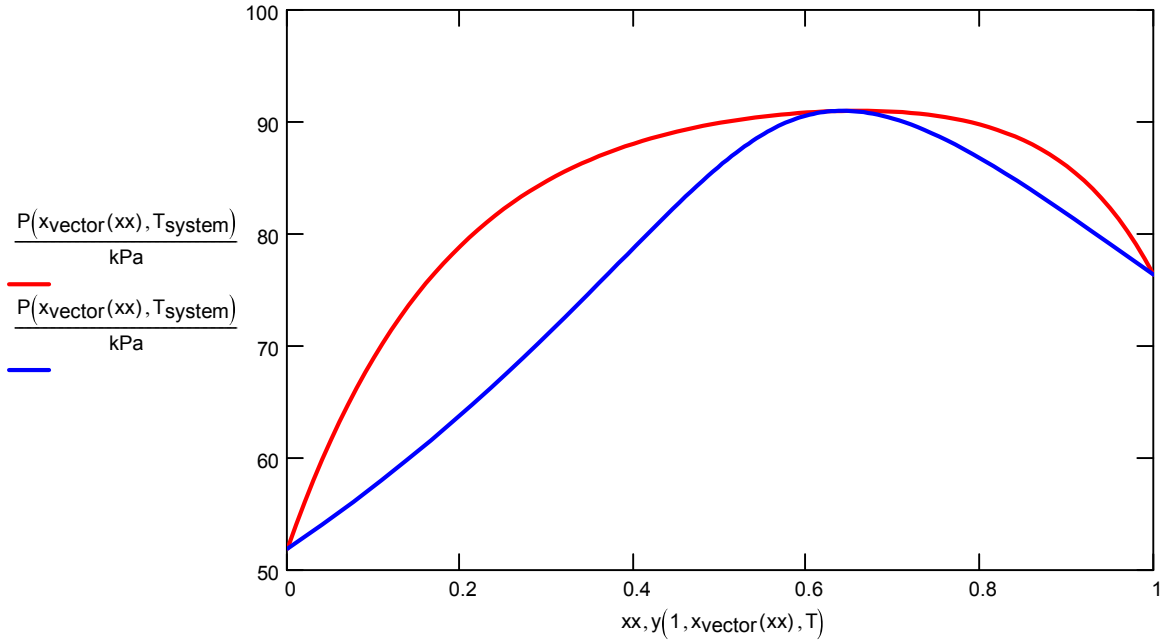


Calculation of the total pressure: $P(x,T) := \sum_i x_i \cdot \gamma UNIFAC(x,T)_i \cdot Ps(i,T)$ $P(x, T_{system}) = 89.915\,kPa$



Calculation of the vapor composition: $y(i,x,T) := \frac{x_i \cdot \gamma UNIFAC(x,T)_i \cdot Ps(i,T)}{P(x,T)}$ $y(1, x, T_{system}) = 0.606$





Calculation of the K-factors:

$$K_{yx}(i,x,T) := \frac{y(i,x,T)}{x_i}$$

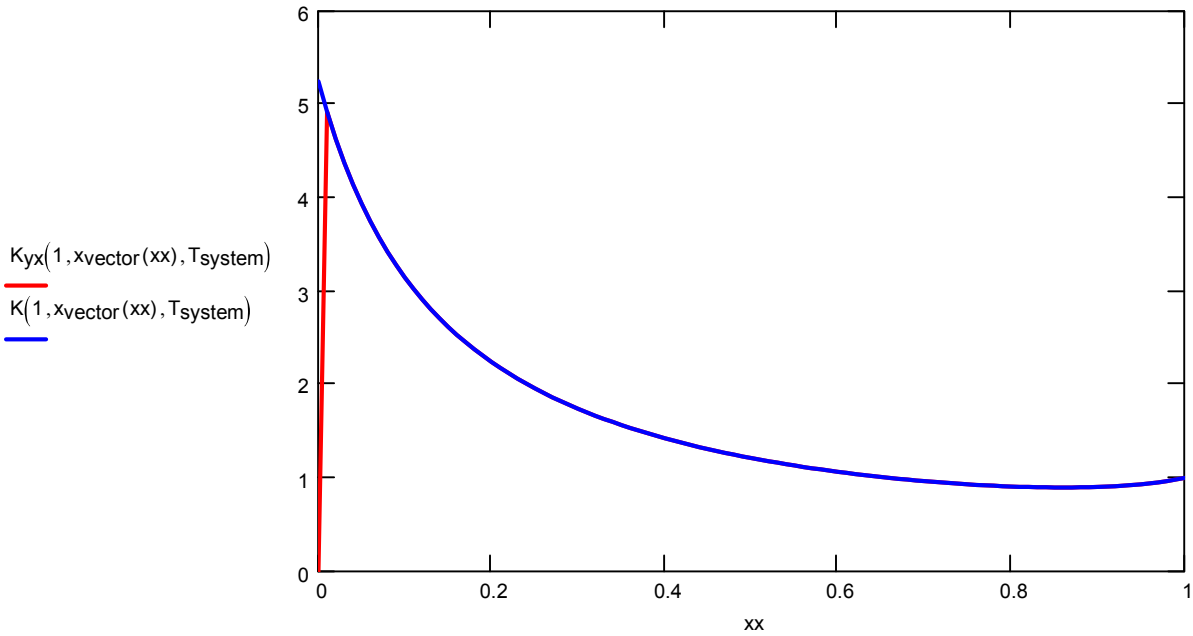
$K_{yx}(1,x,T_{system}) = 1.212$

$K_{yx}(2,x,T_{system}) = 0.788$

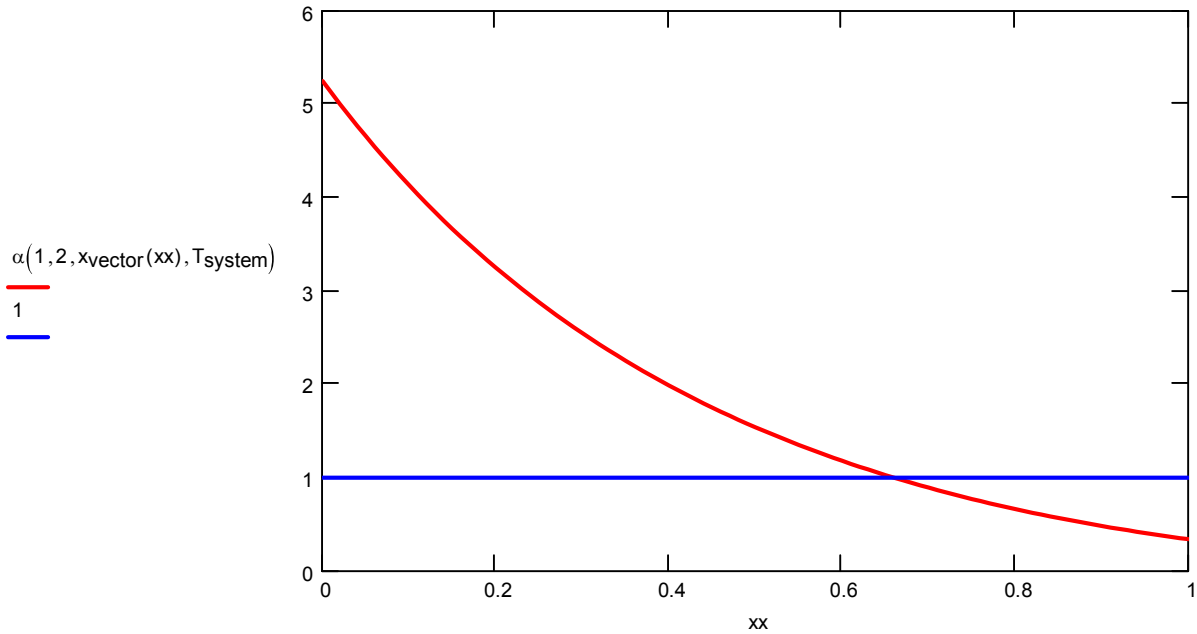
$$K(i,x,T) := \frac{\gamma UNIFAC(x,T)_i \cdot Ps(i,T)}{P(x,T)}$$

$K(1,x,T_{system}) = 1.212$

$K(2,x,T_{system}) = 0.788$



Calculation of the separation factors:

$$\alpha(i,j,x,T) := \frac{\gamma_{UNIFAC}(x,T)_i \cdot Ps(i,T)}{\gamma_{UNIFAC}(x,T)_j \cdot Ps(j,T)}$$

$$\alpha(1,2,x,T_{system}) = 1.539$$