Example 08.02 SLE of Different Xylenes in Benzene

problem: Calculate the solid-liquid-equilibria of benzene (1) with various xylene-isomers (2,3,4) (ideal behavior of the liquid phase)

general constants and definitions:

$kPa := 1000Pa \qquad dm := 0.1m \qquad R := 8.31433 \frac{J}{K \cdot mol}$

input data

$ncomp := 4 \qquad i := 1..ncomp$

$T := (273.15 - 10)K$

$$T_m := \begin{pmatrix} 278.68 \\ 247.65 \\ 225.35 \\ 286.45 \end{pmatrix} K \qquad \Delta h_m := \begin{pmatrix} 9952 \\ 13604 \\ 11544 \\ 16790 \end{pmatrix} \frac{J}{mol}$$

(Experimental data in collapsed area below)

1	0	0	0	278.66
0.9915	0	0	0.0085	278.04
0.983	0	0	0.017	277.62
0.9381	0	0	0.0619	274.65
0.8955	0	0	0.1045	271.75
0.8503	0	0	0.1497	268.66
0.7933	0	0	0.2067	264.54
0.7892	0	0	0.2108	264.28
0.7384	0	0	0.2616	260.55
0.6894	0	0	0.3106	256.8
0.6525	0	0	0.3475	253.91
0.6402	0	0	0.3598	252.95
0.6308	0	0	0.3692	252.19
0.6089	0	0	0.3911	253.93
0.5938	0	0	0.4062	255.09
0.5452	0	0	0.4548	258.61
0.5026	0	0	0.4974	261.47
0.4486	0	0	0.5514	264.85
0.3966	0	0	0.6034	267.89
0.3461	0	0	0.6539	270.67
0.3002	0	0	0.6998	273.08
0.2372	0	0	0.7628	276.2
0.1964	0	0	0.8036	278.12

$$data = \begin{pmatrix} 0.1525 & 0 & 0 & 0.8475 & 280.1 \\ 0.1007 & 0 & 0 & 0.8993 & 282.32 \\ 0.0585 & 0 & 0 & 0.9415 & 284.09 \\ 0.0124 & 0 & 0 & 0.9876 & 285.8 \\ 0 & 0 & 0 & 1 & 286.39 \\ 0 & 0 & 1 & 0 & 222.65 \\ 0.1145 & 0 & 0.8855 & 0 & 218.45 \\ 0.204 & 0 & 0.796 & 0 & 214.05 \\ 0.2742 & 0 & 0.7258 & 0 & 212.95 \\ 0.3107 & 0 & 0.6893 & 0 & 213.45 \\ 0.4043 & 0 & 0.5957 & 0 & 227.35 \\ 0.4632 & 0 & 0.5368 & 0 & 233.65 \\ 0.5736 & 0 & 0.4264 & 0 & 246.45 \\ 0.631 & 0 & 0.369 & 0 & 251.65 \\ 0.7969 & 0 & 0.2031 & 0 & 264.35 \\ 0 & 0 & 1 & 0 & 278.75 \\ 1 & 0 & 0 & 0 & 278.68 \\ 0.755651 & 0 & 0 & 0.244349 & 261.12 \\ 0.737258 & 0 & 0 & 0.262742 & 259.66 \\ 0.713457 & 0 & 0 & 0.286543 & 257.92 \\ 0.695453 & 0 & 0 & 0.304547 & 256.64 \\ 0.675494 & 0 & 0 & 0.324506 & 255.08 \\ 0.64773 & 0 & 0 & 0.35227 & 251.64 \\ 0.626296 & 0 & 0 & 0.373704 & 250.76 \\ 0.617945 & 0 & 0 & 0.382055 & 251.66 \\ 0.58943 & 0 & 0 & 0.41057 & 254.29 \\ 0.568171 & 0 & 0 & 0.431829 & 255.98 \\ 0.547423 & 0 & 0 & 0.452577 & 256.9 \\ 0.520047 & 0 & 0 & 0.479953 & 259 \\ 0 & 0 & 0 & 1 & 286.5 \\ 0.675494 & 0 & 0 & 0.324506 & 251.68 \\ 0.64773 & 0 & 0 & 0.35227 & 251.74 \\ 0.626296 & 0 & 0 & 0.373704 & 251.68 \end{pmatrix}$$

Solution

$$lna(T,i) := \frac{-\Delta h_{m_i}}{R \cdot T} \cdot \left(1 - \frac{T}{T_{m_i}}\right) \qquad x_i := e^{lna(T,i)}$$

$lna(T,i) =$

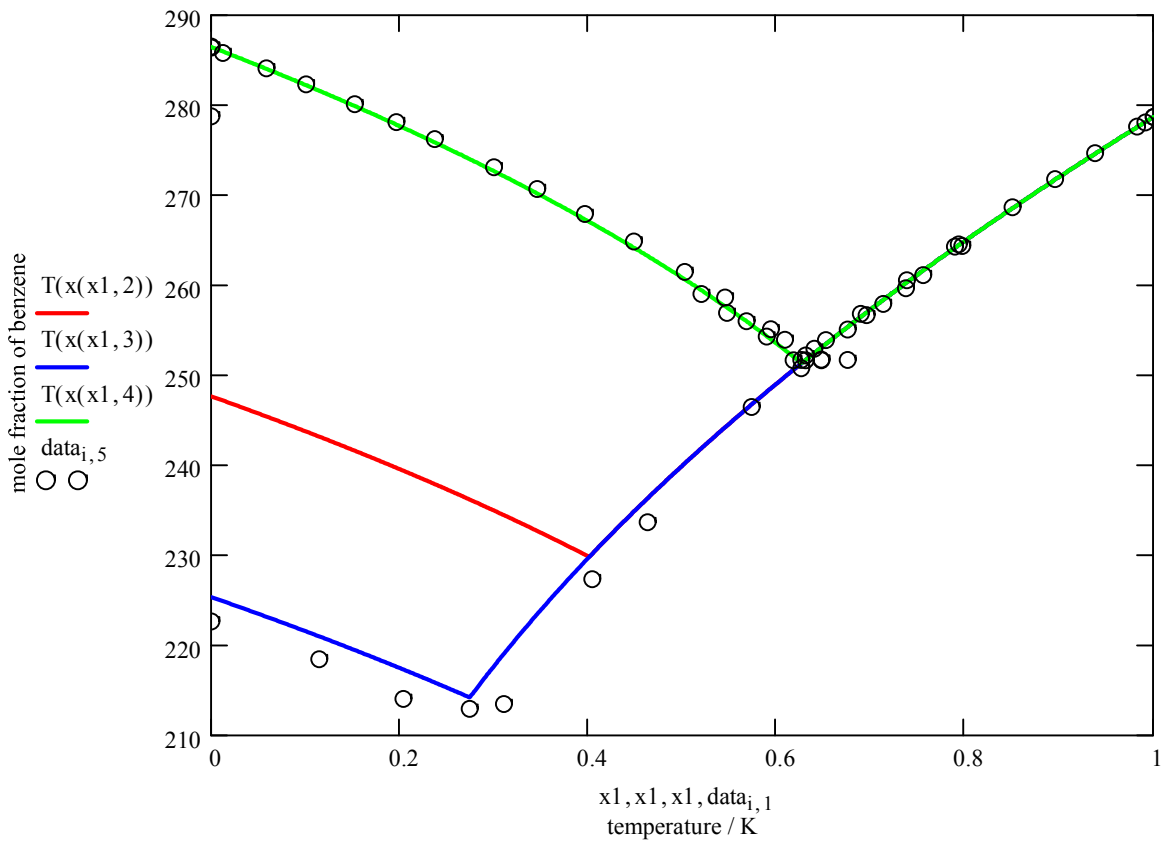
-0.253
0.389
0.885
-0.624

$x_i =$

0.7761
1.4757
2.4231
0.5357

$$T(x) := \left| \begin{array}{l} \text{for } i \in 1..ncomp \\ \quad \left| \begin{array}{l} T_i \leftarrow 0 \ \text{ if } x_i < 10^{-10} \\ \text{otherwise} \\ \quad \left| \begin{array}{l} \ln x_i \leftarrow \ln(x_i) \\ T_i \leftarrow \left(-\Delta h_{m_i}\right) \cdot \dfrac{T_{m_i}}{\left[\left(-\Delta h_{m_i}\right) + \ln x_i \cdot R \cdot T_{m_i}\right]} \end{array} \right. \end{array} \right. \\ T_{SLE} \leftarrow \max(T) \\ T_{SLE} \end{array} \right.$$

$$x(x1, j) := \left| \begin{array}{l} x_1 \leftarrow x1 \\ \text{for } i \in 2..ncomp \\ \quad \left| \begin{array}{l} x_i \leftarrow 1 - x1 \ \text{ if } i = j \\ x_i \leftarrow 0 \ \text{ otherwise} \end{array} \right. \\ x \end{array} \right.$$

$$T\left(\begin{pmatrix} .2 \\ .8 \\ 0 \\ 0 \end{pmatrix}\right) = 239.559\ \mathrm{K}$$

$i := 1..rows(data)$