Example 08.04 SLE in the Ternary Mixture of o-, m- and p-Xylene

problem: Construct the SLE diagram for the ternary system o-xylene-m-xylene-p-xylene assuming eutectic behavior. Since isomer compounds are considered, ideal behavior can be assumed.

general constants and definitions:

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

input data

$n_{comp} := 3 \qquad i := 1 .. n_{comp}$

$T := (273.15 - 10)K$

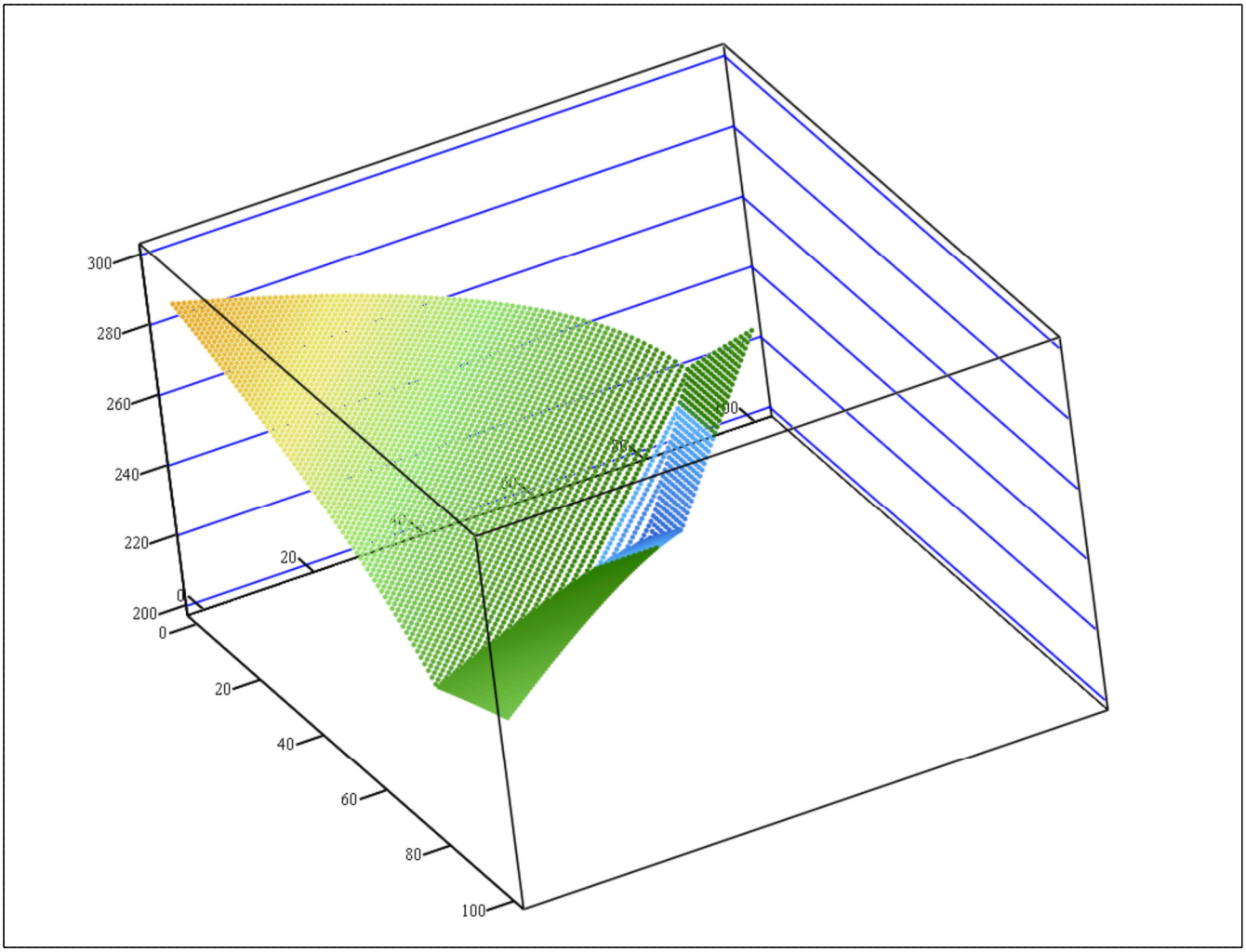
$$T_m := \begin{pmatrix} 247.65 \\ 225.35 \\ 286.45 \end{pmatrix} K \qquad \Delta h_m := \begin{pmatrix} 13604 \\ 11544 \\ 16790 \end{pmatrix} \frac{J}{mol} \qquad components := \begin{pmatrix} \text{"o-xylene"} \\ \text{"m-xylene"} \\ \text{"p-xylene"} \end{pmatrix}$$

Solution

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

$$T_{SLE}\left(\begin{pmatrix} .2 \\ .4 \\ .4 \end{pmatrix}\right) = 253.501\ K$$

$$
x_{mat} := \left| \begin{array}{l}
x_{mat} \leftarrow 0 \\
n_{max} \leftarrow 100 \\
\text{for } i \in 0..n_{max} \\
\quad \text{for } j \in 0..n_{max} - i \\
\qquad x_{mat_{i+1,\,j+1}} \leftarrow T_{SLE}\left(\begin{pmatrix} \dfrac{i}{n_{max}} \\ \dfrac{j}{n_{max}} \\ 1 - \dfrac{i}{n_{max}} - \dfrac{j}{n_{max}} \end{pmatrix}\right) \\
x_{mat}
\end{array} \right.
$$



x_{mat}