Example 05.05 Temperature Dependence of the Activity Coefficients

problem: Estimate the activity coefficients for the system ethanol (1) - water (2) at theta = 50 °C using the experimental excess enthalpy data of Larkin assuming that the excess enthalpy is independent of temperature.

general constants and definitions:

$$R := 8.31433 \frac{J}{K \cdot mol}$$

input data

$$ncomp := 2 \qquad i := 1 .. ncomp$$

Liquid and vapor mole fractions, temperature, pressure

$$x_1 := 0.252 \qquad x_{ncomp} := 1 - \sum_{i=1}^{ncomp} x_i \qquad x = \begin{pmatrix} 0.252 \\ 0.748 \end{pmatrix}$$

Activity coefficients at theta = 70°C

$$\left(\left[\gamma^{343.15K}\right]\right)_1 := 1.891$$

$$\left(\left[\gamma^{343.15K}\right]\right)_2 := 1.198 \qquad \left(\left[\ln\gamma^{343.15K}\right]\right) := \ln\left(\left[\gamma^{343.15K}\right]\right)$$

$$T_1 := (273.15 + 70)K \qquad T_2 := (273.15 + 50)K$$

Partial molar excess enthalpies:

$$\left(\left[h^E\right]\right)_1 := 725 \frac{J}{mol}$$

$$\left(\left[h^E\right]\right)_2 := -335 \frac{J}{mol}$$

Solution

Calculation of the activity coefficients at theta = °C

$$\left[\left(\left[\ln\gamma^{323.15K}\right]\right)_i\right] := \left(\left[\ln\gamma^{343.15K}\right]\right)_i + \frac{\left(\left[h^E\right]\right)_i}{R}\left(\frac{1}{T_2} - \frac{1}{T_1}\right)$$

$$\left(\left[\ln\gamma^{323.15K}\right]\right) = \begin{pmatrix} 0.653 \\ 0.173 \end{pmatrix}$$

$$\left[\gamma^{323.15K}\right] := e^{\left[\ln\gamma^{323.15K}\right]} \qquad \left[\gamma^{323.15K}\right] = \begin{pmatrix} 1.921 \\ 1.189 \end{pmatrix}$$