CHE221A

Assignment 7

(To be submitted on Friday, 10th April 2023)

Q1. Calculate the dew point and bubble point temperatures of a 30% octane, 30% heptane and 40% methamphetamine mixture at 1 bar.

$$\ln P_O^{vap} = 10.422 - \frac{26799}{RT} \quad \delta_O = 7.02(cal/cc)^{1/2}$$

$$\ln P_H^{vap} = 10.456 - \frac{29676}{RT} \quad \delta_H = 7.27(cal/cc)^{1/2}$$

$$\ln P_M^{vap} = 11.431 - \frac{35200}{RT} \quad \delta_M = 7.43(cal/cc)^{1/2}$$

for T in K and P in bar. δ is the solubility parameter. The subscripts O, H and M represent octane, heptane and methamphetamine, respectively. (Hint: You can use the Solver function in MS Excel in place of carrying out manual iterations.)

Q2. In Heisenberg's production plant, a ash drum is used to separate a feed stream consisting of an equimolar mixture of 2 hydrocarbons H1 & H2. At steady state 60% of the feed stream remains unvaporised and leaves the drum as liquid. If the ash drum is operated at 1 bar, determine:
a) the operational temperature of the ash unit.
b) the composition of both liquid and vapor streams.
(Take H1 to be n-butane and H2 to be iso-butane. The parameters for Antoine's equation can be obtained from the appendix of any standard textbook.)

Q3. VLE data for methyl *tert*-butyl ether (1)/ dichloromethane (2) at 308.15 K are as follows:

P/ kPa	x_1	y_1		P/ kPa	x_1	y_1
85.265	0.0000	0.0000		59.651	0.5036	0.3686
83.402	0.0330	0.0141		56.833	0.5749	0.4564
82.202	0.0579	0.0253		53.689	0.6736	0.5882
80.481	0.0924	0.0416		51.620	0.7676	0.7176
76.719	0.1665	0.0804		50.455	0.8476	0.8238
72.422	0.2482	0.1314		49.926	0.9093	0.9002
68.005	0.3322	0.1975		49.720	0.9529	0.9502
65.096	0.3880	0.2457		49.624	1.0000	1.0000

The data are well correlated by the three- parameter Margules equation :

$$\frac{G^E}{RT} = \left(A_{21}x_1 + A_{12}x_2 - Cx_1x_2\right)x_1x_2$$

Implied by this equation are the expressions:

$$\ln \gamma_1 = x_2^2 \left[A_{12} + 2\left(A_{21} - A_{12} - C \right) x_1 + 3C x_1^2 \right]$$

$$\ln \gamma_2 = x_1^2 \left[A_{21} + 2\left(A_{12} - A_{21} - C \right) x_2 + 3C x_2^2 \right]$$

a) Find the values of parameters $A_{12,}$ $A_{21,}$ and C that provide the best fit of G^E/RT to the data.
b) Prepare a plot of $\ln\gamma_1$, $\ln\gamma_2$ and G^E/x_1x_2RT vs x_1 showing both the correlation and experimental values.
c) Prepare a *P-x-y* diagram that compares the experimental data with the correlation determined in (a).