ECHE 363 – Thermodynamics of Chemical Systems
Homework #11

This problem set is intended to serve as extra practice on Chapter 8 material (vapor–liquid equilibrium). It will not be collected or graded.

1. Consider a mixture of species (1) and (2) in vapor–liquid equilibrium at 25 °C and 90 bar. The following equation of state is available for the *vapor* phase.

$$Pv_{\mathrm{m}} = RT + P^2[Ay_1y_2 + B]$$

where

$$\frac{A}{RT} = -2.0\times10^{-4} \ [=] \ 1/\mathrm{bar}^2$$

and

$$\frac{B}{RT} = 8.0\times10^{-5} \ [=] \ 1/\mathrm{bar}^2$$

and y_1 and y_2 are the mole fractions of species (1) and (2), respectively. Species (2) is dilute in the *liquid* phase and may be described by Henry's Law with the following values at 25 °C.

$$\mathrm{H}_2 = 7000 \text{ bar}$$

$$\ln \gamma_2^{\mathrm{H}} = -7(1 - x_1^2)$$

   a. Consider a vapor mixture of 5 moles of species (1) and 10 moles of species (2). Calculate the following: v_{m}, V, $v_{\mathrm{m},2}$, $\bar{V}_2$.

   b. Calculate an expression for the pure species fugacity coefficient, ϕ_2^{vap}, and the mixture fugacity coefficient, $\hat{\phi}_2^{\mathrm{vap}}$, of species (2) in the vapor.

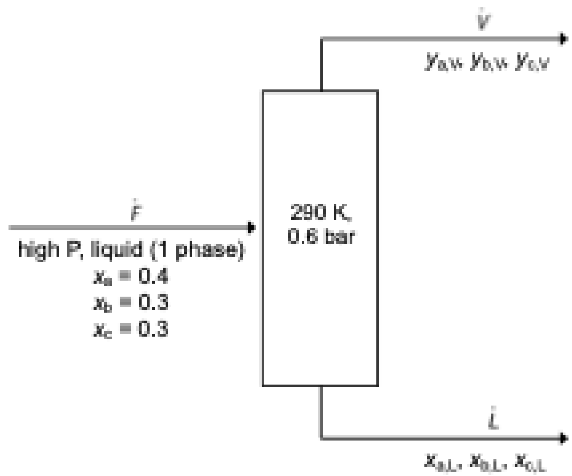
   c. In the liquid, are like interactions stronger or weaker than unlike interactions? Explain.

   d. Find the mole fraction of species (2) in the liquid in equilibrium with the vapor in part (b).

2. Consider the flash separation of a ternary mixture depicted below. In this steady-state process, a high-pressure liquid feed with molar flow rate of $\dot{F} = 1$ mol/s flows into a drum, where there is vapor–liquid equilibrium at 290 K and 3 bar. The vapor exits the top of the drum with an unknown molar flow rate $\dot{V}$, and the liquid exits the bottom of the drum with an unknown molar flow rate $\dot{L}$.

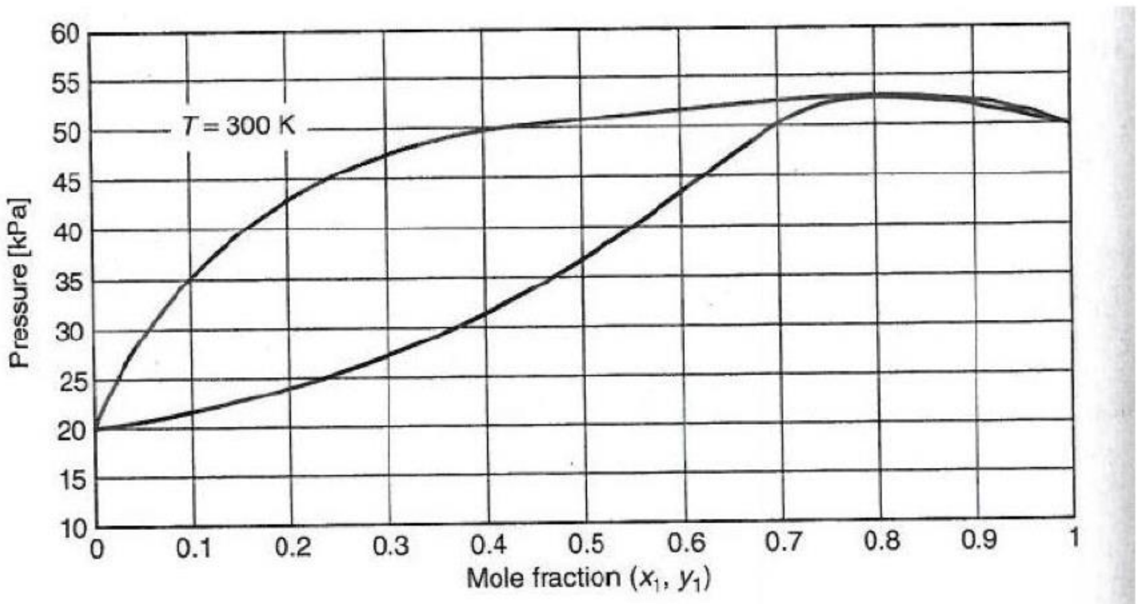
   Here, the mixture components are: a = *n*-butane, b = *n*-pentane, c = *n*-hexane. You may assume that, because the mixture contains chemically similar linear alkanes, the liquid streams are ideal Lewis–Randall solutions. You may treat the vapor as an ideal gas.

   Find the molar flow rates $\dot{V}$ and $\dot{L}$, and the compositions of the outlet streams: $y_{a,V}$, $y_{b,V}$, $y_{c,V}$, $x_{a,L}$, $x_{b,L}$, $x_{c,L}$.



3. A mixture with the following average composition is at 25 °C: 40 % cyclohexane (a), 20% benzene (b), 25% toluene (c), 15% n-heptane (d). Assuming that the liquid behaves as an ideal mixture, find P^{bubble} and P^{dew}.

4. The *Pxy* phase diagram for a binary mixture of species (1) and (2) at 300 K is shown in the following figure.



a. On the graph, identify the single-phase vapor region, the single-phase liquid region, and the two-phase region.

b. On the graph, identify the azeotrope. What is the composition of the azeotrope?

5. At 60 °C, ethanol (1) and ethyl acetate (2) exhibit an azeotrope at a pressure of 0.64 bar and $x_1 = 0.4$.

a. You wish to use the two-suffix Margules equation as a model for g_m^E. From these data, determine, as accurately as you can, the Margules parameter, A.

b. At 60 °C, what is the composition of the vapor in equilibrium with a liquid of composition of $x_1 = 0.8$?