Chemical Engineering Thermodynamics
10.213, Fall 1996
Quiz #3, November 27

1. The following equilibrium vapor pressure data is available for a binary liquid mixture at 27°C:

x_1	0.0	0.1	0.3	0.5	0.7	0.9	1.0
p_1	0.0	0.059	0.17	0.26	0.36	0.45	0.5 bar
p_2	0.7	0.63	.50	0.37	0.23	0.082	0.0 bar

$\Delta H_1^{vap} = 25$ kJ/mol
$\Delta H_2^{vap} = 35$ kJ/mol

The heat of vaporization for species 1 is 25 kJ/mol and for species 2 is 35 kJ/mol and is fairly constant over a reasonable temperature range. One liter of species 1 contains 30 moles, while one liter of species 2 contains 20 moles.

a) What are the activity coefficients for species 1 and 2 at a composition of $x_1 = 0.1$?

b) What is the G^E for a mixture containing $x_1 = 0.3$?

c) If one mole of species 1 and one mole of species 2 is evaporated isothermally at 27 °C leaving a liquid phase with a mole fraction of $x_1 = 0.3$, what is the composition and total number of moles in the liquid phase?

d) Make a qualitative plot of pressure vs x_1, y_1. Indicate the following:

the liquid region
the vapor region
the two phase region
P_1^{sat}
P_2^{sat}
the bubble point pressure for a molar composition of $z_1 = 0.5$
the dew point pressure for a molar composition of $z_1 = 0.5$
the pressure at which one half of the mixture is in the vapor phase for a total molar composition of $z_1 = 0.5$

e) Can this mixture form an azeotrope? State the basis of your reasoning.

solution

Problem 2

At 300 K, the enthalpy, in unit of Joules per mole, of a binary solution of components 1 and 2 is given by

$$H= 200x_1 + 200x_2 + 50x_1x_2 \ .$$

A mixer operating at steady-state combines two inlets to form a single outlet stream. The following information is known about the inlet conditions.

	Flow rate (mol/s)	Mole fractions x_1	x_2	Temperature (K)
Inlet Stream F	2.0	0.2	0.8	300
Inlet Stream G	1.0	0.9	0.1	300

i) Calculate the mole fraction of component 1 in the outlet stream.

ii) Calculate the rate of heat transfer, in units of watts, required by the mixer if the outlet temperature is 300 K.

iii) The binary solution in this problem is
- a) an ideal gas mixture
- b) an ideal solution
- c) a non-ideal solution for which the temperature rises when the pure components are mixed adiabatically
- d) a non-ideal solution for which the temperature drops when the pure components are mixed adiabatically
- e) none of the above

iv) Draw a qualitative Hx diagram for this binary solution showing the
- isotherm for 300 K
- the enthalpies of pure components 1 and 2
- the partial molar enthalpies of components 1 and 2 for a solution with x_1=0.5

v) Calculate the value of the partial molar enthalpies of components 1 and 2 for a solution having x_1=0.5.

vi) Based only your knowledge of the enthalpy of the solution, if components 1 and 2 needed to mixed in a laboratory beaker, would you recommend
- a) pouring pure 1 into a beaker which initially contains pure 2
- b) pouring pure 2 into a beaker which initially contains pure 1
- c) either methods a) or b), since both are equally acceptable.
- d) mixing 1 and 2 will result in death and should not be attempted.
- e) none of the above

Quiz III Solutions

1 Data

x_1	0	.1	.3	.5	.7	.9	1.0
P_1	0	.059	.17	.26	.36	.45	.5 bar
P_2	.7	.63	.50	.37	.23	.082	0 bar

P_2^{sat} (at $x_1 = 0$), P_1^{sat} (at $x_1 = 1.0$)

a) Modified Raoult's law

$$\gamma_1 x_1 P_1^{sat} = P_1 \implies \gamma_1 = \frac{.059}{(.1)(.5)} = \boxed{1.18}$$

$$\gamma_2 x_2 P_2^{sat} = P_2 \implies \gamma_2 = \frac{.63}{(.9)(.7)} = \boxed{1.0}$$

b) $$\frac{G^E}{RT} = x_1 \ln \gamma_1 + x_2 \ln \gamma_2$$

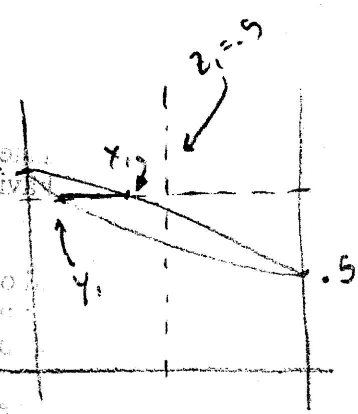
$$\frac{G^E}{RT} = (.3)\ln\frac{.17}{(.3)(.5)} + (.7)\ln\frac{.5}{(.7)(.7)} = .05$$

$$G^E = (.05)(8.314)(300) = \boxed{128\ J/mol}$$

c) $L + V = 2$ mol $\quad \boxed{z_1 = .5}$

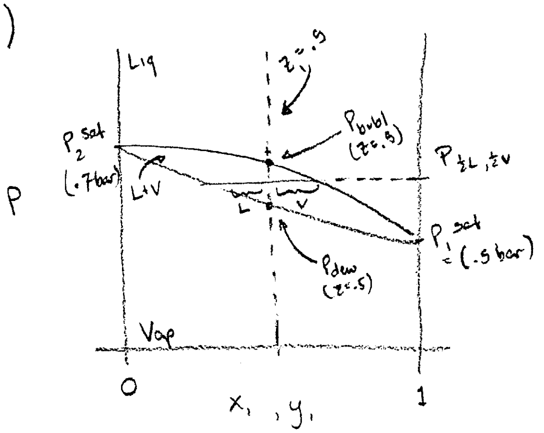
$x_1 = .3 \quad x_2 = .7$

$$y_1 = \frac{P_1}{P_{Tot}} = \frac{.17}{.67} = \boxed{.25} \qquad y_2 = \frac{.50}{.67} = \boxed{.75}$$



x_1
y_1
z_1

The desired result is not possible. See HW 8, Problem 3 d)



$P_{bubl} = P_1 + P_2$
$= .63$

$P_{\frac{1}{2}L, \frac{1}{2}V}$ = Use Lever rule, L = V (on diagram)

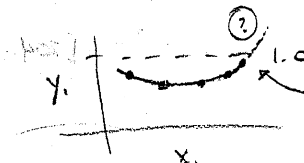
e) Azeotrope $\rightarrow$ $y_1 = x_1$

Look at x_1, y_1

From data and $\overset{mod}{\text{Raoult's}}$ law...

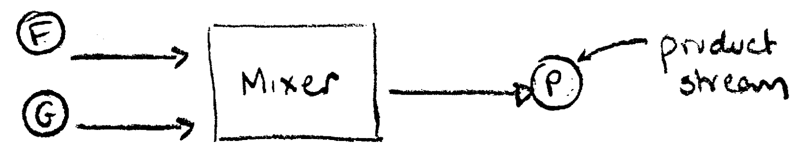
x_1	0	.1	.3	.5	.7	.9	1.0
y_1	N/A	.86	.83	.82	.87	.94	N/A

$\frac{x_1}{y_1}$ never equals 1 over the range of data. It is possible, but not likely that an azeotrope forms.



the curve is sloping up, but it may or may not reach $x_1/y_1 = 1.0$.

(2)



a) Use MB: IN = OUT (No Gen/Acc)

<u>Total</u> $F + G = P$ ⟶ $2 + 1 = \boxed{P = 3 \frac{mol}{s}}$

<u>On comp 1</u> $2(.2) + 1(.9) = 3(x_{1,product})$

$$\boxed{\begin{array}{l} x_{1,product} = .43 \\ x_{2,product} = .57 \end{array}}$$

b) Use EB: $IN - OUT + GEN = 0$ Heat transfer

$$F \cdot H_F + G \cdot H_G - P \cdot H_P + \dot{Q} = 0$$

- Calculate H's using given eqn:

$$H = 200(x_1 + x_2) + 50 x_1 x_2$$

$$H_F = 200 + 50(.2)(.8) = 208 \text{ J/mol}$$

$$H_G = 200 + 50(.9)(.1) = 204.5 \text{ J/mol}$$

$$H_P = 200 + 50(.43)(.57) = 212.3 \text{ J/mol}$$

- Solve EB for $\dot{Q}$

$$\dot{Q} = (3[212.3] - 2[208] - 1[204.5]) \frac{mol}{s} \left(\frac{J}{mol}\right)\left(\frac{W \cdot s}{J}\right)$$

$$\boxed{\dot{Q} = 16.4 \text{ W}}$$

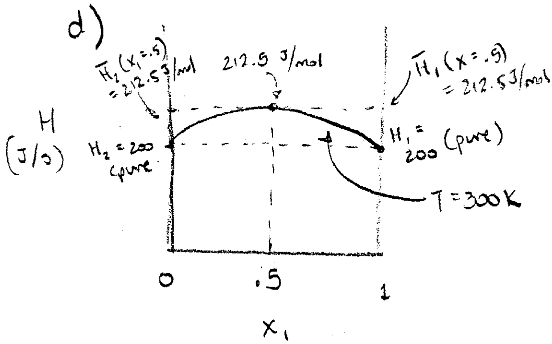
Since $\dot{Q} > 0$, heat must be added. The mixing is endothermic.

c) ⓔ (D) : Non ideal b/c heat of mixing $\neq 0$

$$H = \underbrace{200\,(x_1 + x_2)}_{H^{id}} + \underbrace{50\,x_1 x_2}_{H^E \text{ or } H^{mix}}$$

If the mixing is done adiabatically, $\dot{Q} = 0$. The temperature will drop.

d)



- Isotherm: plot H vs x using eqn
- H_1 ; H_2 : set ($x_2 = 0, 1$) respectively
- Partial molar H: find tangent intercepts (horizontal line)

e) Method 1: read off the graph

Method 2: Use SEVN eqn 10.15, 10.16

$$\bar{H}_1 = H + x_2 \frac{dH}{dx_1}$$

$$= 200 + 50\,x_1 x_2 + x_2(50 - 100\,x_1)$$

$$= \boxed{212.5 \text{ J/mol}}$$

$$\bar{H}_2 = H - x_1 \frac{dH}{dx_2}$$

$$= \boxed{212.5 \text{ J/mol}}$$

f) ⓒ : isotherm is symmetric (heat release is the same in both directions

mathematically, $\boxed{\frac{dH}{dx_1} = \frac{dH}{dx_2}}$