

# ChE 263

## Assignment #3

1. Solve the following systems of linear algebraic equations using Matrix calculations **Hint:** Remember to click and hold down <ctrl>+<shift>+<enter> when applying matrix math formulas.:

$$11x_1 + 3x_2 + x_4 + 2x_5 = 45$$

$$4x_2 + 2x_3 + x_5 = 30$$

$$3x_1 + 2x_2 + 7x_3 + x_4 = 15$$

$$4x_1 + 4x_3 + 10x_4 + x_5 = 20$$

$$2x_1 + 5x_2 + x_3 + 3x_4 + 14x_5 = 92$$

2. Determine **one** solution for x and y to the following equations (there are 4 possible solutions). (*You may want to graph the equations to see where the equations intersect and find a good guess value for solver. If you do make a plot, note that for the first equation you can only solve for y for x values between -0.7 and 0.7. For the second equation you can only solve for y with x values between -1 and 3. Also remember that when solving  $y^2=x$  for y, the solution is  $y = \pm\sqrt{x}$ .)*

$$2x^2 + y^2 = 1$$

$$(0.5x - 0.5)^2 + 2(y - 0.25)^2 = 1$$

3. The Redlich/Kwong Equation of State is

$$P = \frac{RT}{V - b} - \frac{a}{T^{1/2}V(V + b)}$$

where T is the temperature, V is the molar volume, R is the universal gas constant, and a and b are compound-specific constants. *Find the molar volume of ethane for each phase that is present at T = 77 °C and P = 1 bar. For ethane,  $a = 2.877 \times 10^8 \text{ cm}^6 \text{ bar K}^{0.5} \text{ mol}^{-2}$  and  $b = 60.211 \text{ cm}^3 \text{ mol}^{-1}$ . The Universal Gas Constant (R) is  $83.144598 \text{ cm}^3 \text{ bar / K-mol}$ .*

Hints:

- Use the ideal gas law to obtain the guess of the vapor volume and  $1.1 * b$  to obtain the guess for the liquid volume. (Graphing helps find good guesses for solver)
- Don't forget to convert temperature into Kelvin.
- You may need to include some constraints.
- IF YOU ARE STUCK ask a friend, the TA OR the instructor! Don't spent so much time feeling lost that you become discouraged.
- You should obtain something around  $28637 \text{ cm}^3/\text{mol}$  for the vapor volume and  $82.477 \text{ cm}^3/\text{mol}$  for the liquid volume. The middle root (not required but for your information) is in between.

4. Imagine mixing liquid benzene (species 1) and toluene (species 2) together in an initially empty container. At equilibrium, some of the liquid from both species will evaporate into the vapor phase and some will be left liquid phase for certain temperatures and pressures. In thermodynamics (ChEn 373), you will learn that Raoult's law may be used to describe the distribution of species in each phase. For the specific example mentioned above, Raoult's law gives the following two expressions describing the equilibrium state (following page)

$$y_1 P = x_1 P_1^{sat}(T)$$

$$y_2 P = x_2 P_2^{sat}(T)$$

where  $y_i$  is the mole fraction of species  $i$  (either 1 or 2) in the vapor phase,  $x_i$  is the mole fraction of species  $i$  in the liquid phase,  $P_i^{sat}(T)$  is the vapor pressure of species  $i$  at the system temperature  $T$ , and  $P$  is the system pressure.

The vapor pressures of benzene and toluene can be found using the Antoine Equation.

$$\ln\left(\frac{P_i^{sat}(T)}{\text{kPa}}\right) = A_i - \frac{B_i}{T/^\circ\text{C} + C_i}$$

Note that you cannot take the natural log of a number with units. Therefore,  $P_i^{sat}$  is divided by kPa or we take the ln of  $P_i^{sat}$  as it would be if it had units of kPa. Note that  $P_i^{sat}(T)$  is not  $P_i^{sat}$  times  $T$ , but is simply showing that  $P_i^{sat}$  is a function of  $T$ . Also note that  $T/^\circ\text{C}$  means that a dimensionless form of temperature is inputted as the temperature would be if it had units of  $^\circ\text{C}$ . Do not confuse  $^\circ\text{C}$  (degrees celcius) with  $C_i$  which is the constant given in the table below. The constants,  $A$ ,  $B$ , and  $C$ , are compound specific and are found in the table below.

Antoine Constants for Benzene and Toluene

Compound	A	B	C
Benzene	13.7819	2726.81	217.572
Toluene	13.9320	3056.96	217.625

If a mixture of benzene (species 1) and toluene (species 2) has  $y_1 = 0.33$  and  $P = 120$  kPa, find  $x_1$  and  $T$ . Remember that the mole fractions of each phase must sum to 1. (Hint: Follow the steps outlined in the handout from class.)

Hints:

- First figure out what you are solving for. Then figure out how many equations you have.
- You might want to set up a cell for  $P_{sat1}$  and  $P_{sat2}$  that reference your cell containing  $T$ .
- SEE THE TA OR THE INSTRUCTOR IF YOU ARE STUCK! Don't spent so much time feeling lost that you become discouraged.
- There are many right ways to do this.
- You should get about 0.17 for  $x_1$  and 109  $^\circ\text{C}$  for  $T$ .