ChE 3063 **Project 1** Due: October 21, 2020

Use the Peng-Robinson Equation of State and data in the back of S&VNAS 8^{th} ed. to determine:

1. 10 points

The vapor pressure of pure chloroform (1) and cyclohexane (2) at 225ºC in bar.

2. 30 points

The fugacity (in bar) of pure chloroform and pure cyclohexane at 225ºC and 10 bar total pressure.

3. 30 points

The fugacity (in bar) of pure liquid chloroform and pure liquid cyclohexane at 225ºC and 40 bar total pressure. The molar volume of pure liquid chloroform is 85.63 cm^3/mole and of cyclohexane is 108.16 cm^3/mole.

4. 30 points

The fugacities (in bar) of chloroform and cyclohexane in a 40/60 mole % mixture when T = 225ºC and P = 10 bar.

Instructions for submitting the project:

1. Use Excel to solve the problem. *Each student should start with a blank worksheet in preparing their solution. Starting with another student's work or work you get elsewhere (such as the internet) is an act of academic dishonesty.*
2. **Using the hardcopy template (or a similar sheet) which is attached, turn in a paper solution. Your Excel sheet should parallel your hardcopy solution.** Be sure to include comments on the Excel sheet and include references to the parts of the problem you are working.
3. Save the Excel sheet as "Project1-FirstName-LastName.xlsx" and email it to me *before* class the date it is due with the subject line: "ChE3063 Project 1 Solution". Submit your paper solution at the beginning of class the date it is due. It should be folded lengthwise with your name on the outside just like homework.

The Peng-Robinson Equation of State:

$$P = \frac{RT}{v-b} - \frac{a}{v(v+b)+b(v-b)}$$

$$\alpha^{0.5} = 1 + \kappa(1 - T_r^{0.5})$$

$$\kappa = 0.37464 + 1.54226\omega - 0.26992\omega^2$$

$$a = \frac{0.45724 R^2 T_c^2 \alpha}{P_c}$$

$$b = \frac{0.07780 R T_c}{P_c}$$

also, for shorthand for the P-R equation, use:

$$A = \frac{aP}{R^2 T^2}$$

$$B = \frac{bP}{RT}$$

Mixing rules:

$$a = \sum_i \sum_j y_i y_j a_{ij}$$

$$b = \sum_i y_i b_i$$

$$a_{ij} = (1 - \delta_{ij}) a_i^{0.5} a_j^{0.5}$$

where δ_{ij} is an empirical constant for the chloroform/cyclohexane mixture:

$$\delta_{ii} = 0$$

$$\delta_{ij} = 0.01$$

Polynomial form:

$$z^3 - (1 - B)z^2 + (A - 3B^2 - 2B)z - (AB - B^2 - B^3) = 0$$

Fugacity coefficient for the first component in a mixture of j components:

$$\ln\left(\frac{f_1}{y_1 P}\right) = \ln(\phi_1) =$$

$$\frac{b_1}{b}(z - 1) - \ln(z - B) - \frac{A}{2\sqrt{2}B}\left(\frac{2\sum_j y_j a_{1j}}{a} - \frac{b_1}{b}\right)\ln\left(\frac{z + 2.414B}{z - 0.414B}\right)$$

Note that z in the above equation is the compressibility factor for the mixture.

Fugacity coefficient for a pure component:

$$\ln(f\ /\ P) = \ln(\phi) = (z-1) - \ln(z-B) - \left(\frac{A}{2\sqrt{2}B}\right)\ln\left(\frac{z+2.414B}{z-0.414B}\right)$$

Hardcopy Template

1. The vapor pressure of pure chloroform and cyclohexane at 225ºC in bar

P_1^S = ________ bar ; P_2^S = ________ bar

2. The fugacity (in bar) of pure chloroform and pure cyclohexane at 225ºC and 10 bar total pressure

	Chloroform	Cyclohexane
T_r		
P_r		
α		
κ		
a		
b		
A		
B		
z		
φ		
f (fugacity)		

3. The fugacity (in bar) of pure liquid chloroform and pure liquid cyclohexane at 225ºC and 40 bar total pressure

	Chloroform	Cyclohexane
T_r		
P_r		
α		
κ		
a		
b		
A		
B		
z		
φ_i^S		
f (fugacity)		

4. The fugacities (in bar) of chloroform and cyclohexane in a 40/60 mole % mixture when T = 225ºC and P = 10 bar.

	Chloroform	Cyclohexane
T_r		
P_r		
α		
κ		
a (mixture)		
b (mixture)		
A (mixture)		
B (mixture)		
z (mixture)		
φ		
f (fugacity)		