ChE 7023 **Homework Set 3** Due: February 20, 2019

Attached is data for Benzene and Toluene and some useful forms of the Peng-Robinson Equation of State. Use this information to determine:

1. 10 points

The vapor pressure of pure benzene and toluene at 240ºC.

2. 30 points

The fugacity of pure benzene and pure toluene at 240ºC and 10 atm total pressure.

3. 30 points

The fugacity of liquid benzene and liquid toluene at 240ºC and 30 atm total pressure

4. 30 points

The fugacities of benzene and toluene in a 40/60 mole % mixture when T = 240ºC and P=10 atm.

<u>The Peng-Robinson Equation of State:</u>

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

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

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

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

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

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

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

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

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 benzene/toluene 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 mixture:

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

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

Fugacity coefficient for the pure component:

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

Data:

	Benzene	Toluene
MW (g/mole)	78.114	92.141
T_c, K	562.1	591.7
P_c, atm	48.3	40.6
z_c	0.271	0.264
ω	0.212	0.257
constants for Antoine vapor pressure equation		
A_1	-0.3767546E2	-0.2284786E2
A_2	-0.1097523E4	-0.1874186E4
A_3	-0.9353251E2	-0.7292144E2
A_4	-0.14047730E-1	-0.1083663E-1
A_5	0.99482220E1	0.7485147E1
A_6	0.10416500E-16	0.7567229E-17
A_7	6	6

$$\ln(P) = A_1 + \frac{A_2}{T + A_3} + A_4 T + + A_5 \ln(T) + A_6 T^{A_7}$$

where:

P is in Pascals

T is in K