ChE 3063 | **EXAM II** | **October 20, 2017**

Open Books and Notes

YOUR NAME: Solution

I. 50 points

A. 30 points

Using the data in the table below for the binary system Acetone (1), Cyclohexane (2) at 308.15 K, compute γ_1, γ_2 (activity coefficients), and the function G^E/RTx_1x_2 and enter the numbers directly in the data table.

P (kPa)	x_1	x_2	y_1	y_2	γ_1	γ_2	$G^E/(RT*x_1*x_2)$
19.625	0.000	1.000	0.000	1.000	----	1.0	----
37.877	0.098	0.902	0.482	0.518	4.062	1.108	2.604
45.476	0.198	0.802	0.601	0.399	3.010	1.153	2.092
49.489	0.387	0.613	0.665	0.335	1.854	1.378	1.836
50.969	0.598	0.402	0.709	0.291	1.318	1.820	1.742
50.196	0.895	0.105	0.841	0.159	1.028	3.873	1.780
45.863	1.000	0.000	1.000	0.000	1.0	----	----

B. 5 points

Plot the values of $G^E/(RT*x_1*x_2)$ on the graph below. Be sure to include the axis scale numbers for the vertical axis.

C. 15 points

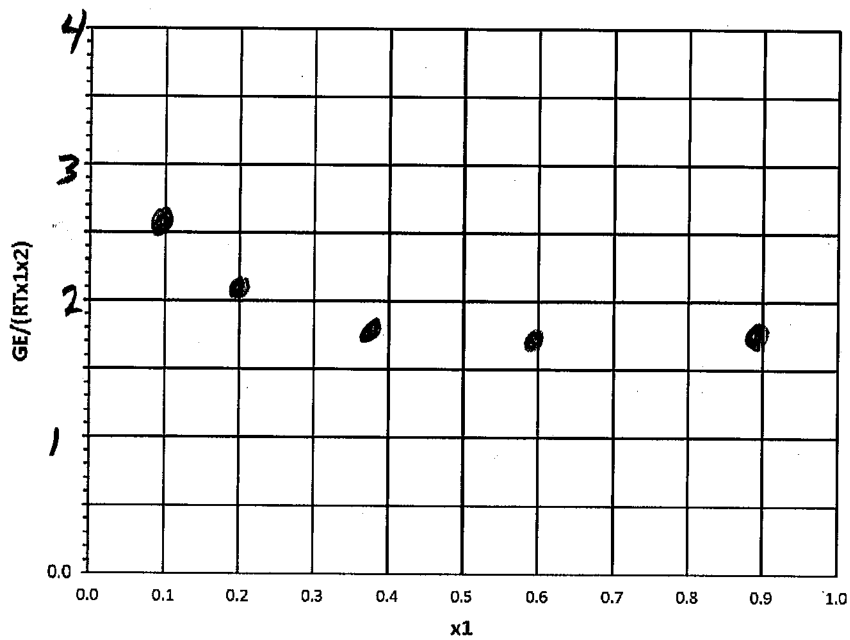
Of the three below, which activity coefficient correlation do you think would model this set of data best? Check off your answer. Briefly explain why you chose the one you did.

☐ Regular Solution

☐ Margules 3-suffix

☑ Van Laar

Why? Not linear & not constant



II. 50 points

The Berthelot equation of state can be written:

$$\mathbf{P(v-b)=RT} \qquad \text{where b is a constant which can be computed as } \mathbf{b}=\frac{\mathbf{RT_C}}{\mathbf{8P_C}}$$

in terms of total moles, this equation can be written:

$$\mathbf{V}=\frac{\mathbf{n_T RT}}{\mathbf{P}}+\mathbf{n_T b} \qquad \text{where } n_T \text{ is total moles, and V is total volume (of course)}$$

<u>Using the Berthelot equation of state</u>, find:

A. 20 points

An expression for the fugacity coefficient of a pure gas

B. 20 points

An expression for the fugacity coefficient of component (1) in a binary gas mixture using the mixing rule:

$$\mathbf{b}=\mathbf{y_1b_1}+\mathbf{y_2b_2} \qquad \text{or:} \qquad \mathbf{n_Tb}=\mathbf{n_1b_1}+\mathbf{n_2b_2}$$

C. 10 points

Find the fugacity of ethane in a 30 mole% /70 mole% ethane (1)/propane(2) mixture at 40 bar and 400K using the result from part B.

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II. a) $V = \frac{n_T RT}{P} + n_T b$ For binary: $V = \frac{n_T RT}{P} + n_1 b_1 + n_2 b_2$

for pure gas, $\overline{V}_i = V_i^0 = V/n_T$

$$RT \ln \phi = \int_0^P \left[\frac{RT}{P} + b - \frac{RT}{P}\right] dP$$

$$RT \ln \phi^{PURE} = \int_0^P b\, dP = bP$$

$$\boxed{\ln \phi^{PURE} = bP/RT} = \frac{\frac{RT_c}{8P_c} P}{RT} = \frac{P_r}{8T_r}$$

b) $\left.\frac{\partial V}{\partial n_1}\right)_{T,P,n_2} = \overline{V}_1 = \frac{RT}{P} + b_1$

$P(V-b) = RT$
$PV - Pb = RT$
$\frac{PV}{RT} - \frac{Pb}{RT} = 1$
$\frac{PV}{RT} = z = 1 + \frac{Pb}{RT}$

$$RT \ln \phi_1 = \int_0^P b_1 dP = b_1 P$$

$$\boxed{\ln \phi_1 = b_1 P/RT}$$

c) Ethane $T_c = 305.3\,K$, $P_c = 48.72$ bar

$$b_1 = \left(83.14 \frac{cm^3\text{-bar}}{mole\,K}\right)\left(\frac{305.3\,K}{8 \times 48.72\,bar}\right) = 65.12\ cm^3/mole$$

$$\phi_1 = \exp\left(\frac{65.12 \cdot 40\,bar}{83.14 \cdot 400\,K}\right) = 1.081$$

$$\boxed{f_1 = (1.081)(0.3)(40\,bar) = 12.972\ bar}$$