

Michigan State University

DEPARTMENT OF CHEMICAL ENGINEERING AND MATERIALS SCIENCE

ChE 321: Chemical Engineering Thermodynamics

Spring 2008

Part I. April 2, 2008, CLOSED BOOK, CLOSED NOTES

General Instructions

- Submit all problems in the order of the exam.

1. Below is the output from PreosProps.m (Tref = 298.15K; Pref = 0.1MPa) at T = 295K and 1 bar, as well as documentation about how to set the array 'match'.

```
>> [Z H S U phi] = PreosProps(Tref, Pref, T, P, match);
propane Tc(K)= 369.8 Pc(MPa)= 4.249 w = 0.152
Tref= 298.15, Pref= 0.1, Zref= 0.983433
T(K)= 295 P(MPa)= 0.1
match = 0 0 0 0
Z=
    0.98294      0.00349187
V(cm^3/mol)=
    24108.8      85.6457
U (J/molK)=
   -2644.18     -16396.2
H (J/mol)=
   -233.3       -16387.6
S (J/molK)=
   -0.78665     -72.2239
fugacity (MPa)= 0.0983182  0.7307
```

---

Specify match=[i j k l] in the command window as follows

i - run match?	j - adjust	k - value	l - match which root?
0 - no matching	(ignored for	(ignored for	(ignored for i = 0,4)
1 - match U	i = 0)	i = 0,4)	1 match largest Z root
2 - match H	1 - adjust T	value to match	2 match smallest Z root
3 - match S	2 - adjust P		
4 - saturation			
(match f's)			

- (a) (15) A laboratory cylinder is 40L and holds 100% propane at 295K. The tank is 30% by volume liquid and 70% vapor. Describe how you would modify the conditions or use the printed conditions to determine the number of moles in the cylinder. If answers are not directly available from values above, provide sufficient detail to clearly indicate (using simple formulas if necessary) how you would obtain the desired results and how you would use the output values of PreosProps.m along with the tank volume.

- (b) (5) What is the numerical value of the fugacity coefficient for propane at the conditions printed above?

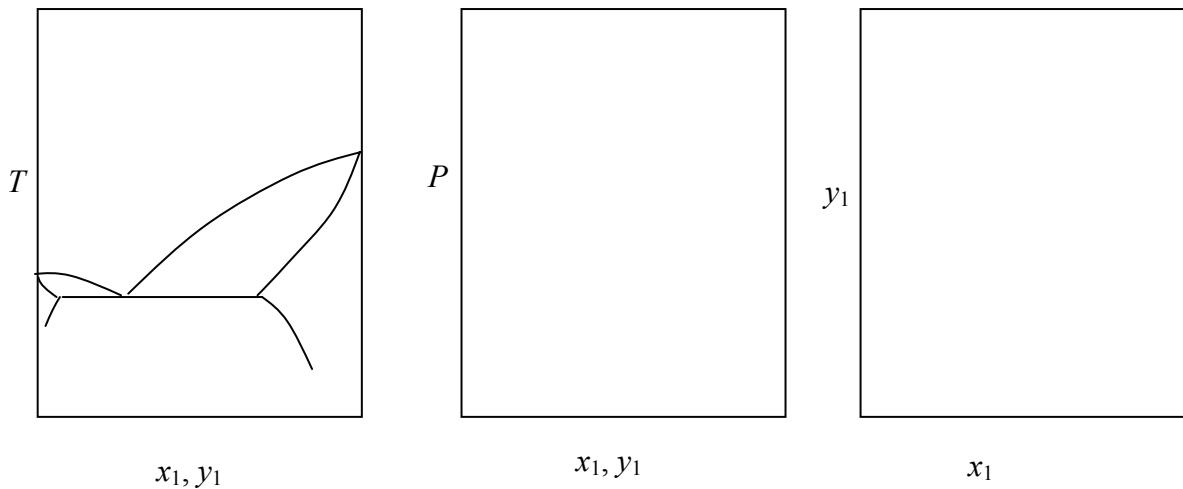
2. (5) Explain why the total kinetic energy of the sites of a multiatom molecule is different than the kinetic energy of the center of mass.

(5) Explain why the temperature fluctuates in an adiabatic simulation with attractive and repulsive potential energy using a fixed number of particles and a fixed simulation box volume.

3. (10) For each of the following mixtures, characterize the accuracy of using Raoult's law as: (I) good approximation; (II) rough approximation; (III) poor approximation.

- (a) ethyl acetate + methyl acetate \_\_\_\_\_  
 (b) isopropanol + water \_\_\_\_\_  
 (c) pentane + cyclohexane \_\_\_\_\_

4. (10) Below is a T-x-y diagram for a system that exhibits VLLE. Label the bubble line(s) on the T-x-y diagram. Sketch the expected qualitative behaviors for the P-x-y and the y-x diagrams.



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Spring 2008

Part II. April 2, 2008, OPEN BOOK, CLOSED NOTES

General Instructions

- Submit all problems in the order of the exam.

5. A fluid is described by the following equation of state:

$$Z = 1 + (a + b/T)\rho$$

where  $a = 700 \text{ cm}^3$ ,  $b = -4.46\text{E}5 \text{ cm}^3\text{K}$  and the ideal gas heat capacity is  $C_p = 98.9 \text{ J/molK}$ .

(a) (15) Derive the enthalpy departure for this fluid

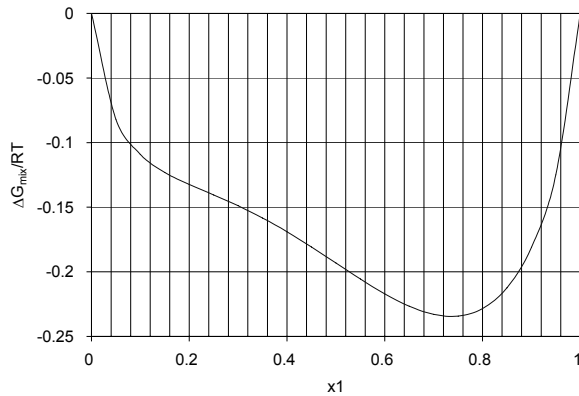
(b) (5) Calculate the value for the enthalpy departure at 400K and a density of  $3.5\text{E}-4 \text{ mol/cm}^3$ . What is the pressure in this state?

6. (15) The system ethyl acetate (1) + methanol (2) can be represented with the two parameter Margules equation using  $A_{12} = 1.138$  and  $A_{21} = .884$ . Determine the bubble temperature and coexisting vapor/liquid compositions at an overall composition of 30% ethyl acetate and 760 mmHg. If an iterative calculation is required, perform the first iteration and set forth clearly the procedure to converge the calculation.

Antoine Coefficients:

	EtOAc	methanol
A	7.10179	8.08097
B	1244.95	1582.271
C	217.881	239.726

6. The system (1) + (2) exhibits LLE and is represented by the two-parameter Margules equation with  $A_{12} = 2.5$  and  $A_{21} = 1.5$ . The behavior of the system is plotted in the figure below.



- (a) (5) Perform a hand calculation to verify the value of the plot at  $x_1 = 0.7$ .
- (b) (10) A mixture of overall composition  $x_1 = 0.2$  is fed into a decanter with a flow rate of 100 mol/min. What are the steady-state compositions and flow rates of the streams leaving the decanter?

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Exam 2: April 4, 2007, Closed Book Portion

1. (10) The Soave-Redlich-Kwong equation is  $Z = \frac{1}{1-b\rho} - \frac{a}{bRT} \frac{b\rho}{(1+b\rho)}$ . The parameters are made dimensionless using  $A = aP/(RT)^2$  and  $B = bP/RT$ . Rearrange the equation in the form  $Z^3 + a_2Z^2 + a_1Z + a_0 = 0$ , where  $a_2$ ,  $a_1$ , and  $a_0$  are functions of  $A$  and  $B$ .

2. The spreadsheet PREOS.xls for CO2 is shown below at a particular temperature and pressure. Consider the following problems at this state.

Peng-Robinson Equation of State (Pure Fluid)

Spreadsheet protected, but no password used.

Properties			
Gas	T <sub>c</sub> (K)	P <sub>c</sub> (MPa)	
CARBON DIOX	304.2	7.382	0.228

Current State		Roots		
T (K)		Z	V	fugacity
P (MPa)			cm <sup>3</sup> /gmol	MPa
answers for three	0.690195	452.3371	2.642504	
root region	0.195595	128.1885		
	0.073541	48.19727	2.642801	
& for 1 root region	#NUM!	#NUM!	#NUM!	

Intermediate Calculations			
R(cm <sup>3</sup> MPa/molK)			
	8.314		
T <sub>r</sub>	0.897928994	a (MPa cm <sup>6</sup> /gmol <sup>2</sup> )	
P <sub>r</sub>	0.469403662	426320.8	
	0.712243759	b (cm <sup>3</sup> /gmol)	
	1.076049118	26.65342	
fugacity ratio		A	0.286441
	0.999887602	B	0.040669

(a) (10) How many moles of CO2 are contained in a 4L vessel that is half full (by volume) of liquid?

(b) (5) A piston/cylinder holds 6 moles of CO<sub>2</sub> and has a volume of 2.5L. The cylinder volume is isothermally changed such that the pressure starts to rise. Select the approximate volume of the cylinder where the pressure starts to rise: (i) P won't rise at any volume; (ii) 2.71 L; (iii) 0.05 L; (iv) 0.29 L; (v) 2.5 L; (vi) none of the choices are very close. Your answer: \_\_\_\_\_

3. Ethylene at the inlet of a reversible, adiabatic expander is at 347.3 K and 2.5 MPa, with H = 1350.2 J/mol and S = -21.546 J/mol-K. The outlet of the expander is at 0.1 MPa, and three states at this pressure are shown below.

Current State		Roots		Stable Root has a lower fugacity						
T (K)	327.898595	Z	V	fugacity	H	U	S	H-H <sup>ig</sup>	U-U <sup>ig</sup>	S-S <sup>ig</sup>
P (MPa)	0.1		cm <sup>3</sup> /gmol	MPa	J/mol	J/mol	J/molK	J/mol	J/mol	J/molK
answers for three root region		#NUM!	#NUM!	#NUM!	#NUM!	#NUM!	#NUM!	#NUM!	#NUM!	#NUM!
		#NUM!	#NUM!	#NUM!	#NUM!	#NUM!	#NUM!	#NUM!	#NUM!	#NUM!
& for 1 root region		0.9951024	27127.973	0.099512	1350.2	-1362.6	4.314232572	-39.9974	-26.6458	-0.08129

Current State		Roots		Stable Root has a lower fugacity						
T (K)	168.848791	Z	V	fugacity	H	U	S	H-H <sup>ig</sup>	U-U <sup>ig</sup>	S-S <sup>ig</sup>
P (MPa)	0.1		cm <sup>3</sup> /gmol	MPa	J/mol	J/mol	J/molK	J/mol	J/mol	J/molK
answers for three root region		0.9703226	13621.475	0.097111	-4704.63	-6066.78	-20.28496556	-103.113	-61.4515	-0.36694
		0.0238563	334.8968	0.097052	-18073.7	-18078.2	-99.45743426	-13472.1	-12072.9	-79.5394
& for 1 root region		#NUM!	#NUM!	#NUM!	#NUM!	#NUM!	#NUM!	#NUM!	#NUM!	#NUM!

Current State		Roots		Stable Root has a lower fugacity						
T (K)	161.503246	Z	V	fugacity	H	U	S	H-H <sup>ig</sup>	U-U <sup>ig</sup>	S-S <sup>ig</sup>
P (MPa)	0.1		cm <sup>3</sup> /gmol	MPa	J/mol	J/mol	J/molK	J/mol	J/mol	J/molK
answers for three root region		0.9667771	12981.283	0.096777	-4912.91	-6211.04	-21.54596271	-109.579	-64.9694	-0.40611
		0.0271973	365.18864	0.062514	-18479.3	-18483.7	-101.9131733	-13675.9	-12337.7	-80.7733
& for 1 root region		#NUM!	#NUM!	#NUM!	#NUM!	#NUM!	#NUM!	#NUM!	#NUM!	#NUM!

(a) (10) What is the outlet temperature? Explain your reasoning.

(b) (5) How much work is obtained from the turbine, J/mol?

4. (10) For Freon22 at state 1, (250 K and 0.5 MPa), the Peng-Robinson equation gives:

Current State		Roots		Stable Root has a lower fugacity			
T (K)	250	Z	V	fugacity	H-H <sup>ig</sup>	U-U <sup>ig</sup>	S-S <sup>ig</sup>
P (MPa)	0.5		cm <sup>3</sup> /gmol	MPa	J/mol	J/mol	J/molK
answers for three root region		0.8710237	3620.8456	0.442655	-721.993	-453.916	-1.87519
		0.1023876	425.62532				
		0.0150116	62.403295	0.203856	-19618.2	-17570.9	-71.0136
& for 1 root region		#NUM!	#NUM!	#NUM!	#NUM!	#NUM!	#NUM!

For Freon22 at state 2, (400K, 0.1MPa), the Peng-Robinson equation gives:

Current State		Roots		Stable Root has a lower fugacity			
T (K)	400	Z	V	fugacity	H-H <sup>ig</sup>	U-U <sup>ig</sup>	S-S <sup>ig</sup>
P (MPa)	0.1		cm <sup>3</sup> /gmol	MPa	J/mol	J/mol	J/molK
answers for three root region		#NUM!	#NUM!	#NUM!	#NUM!	#NUM!	#NUM!
		#NUM!	#NUM!	#NUM!	#NUM!	#NUM!	#NUM!
		#NUM!	#NUM!	#NUM!	#NUM!	#NUM!	#NUM!
& for 1 root region		0.9940076	33056.718	0.099403	-63.3889	-43.4607	-0.1087

What is the entropy change in going from state 1 to state 2 as predicted by the Peng-Robinson equation? The ideal gas heat capacity for Freon22 is  $C_p/R = 6.73$ , and it can be considered independent of temperature for the purposes of this calculation. For an ideal gas,  $\Delta S^{ig} = C_p \ln(T_2/T_1) - R \ln(P_2/P_1)$ .

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Spring 2007

Exam 2: April 4, 2007, Open Book, Closed Notes Portion

5. (20) A short-cut calculation for the bubble pressure of mixture of pentane(1) and heptane(2) is converged with the following results:  $T = 333.15\text{K}$ ,  $P = 0.1135\text{ MPa}$ ,  $x_i = \{0.45, 0.55\}$ ,  $y_i = \{0.854, 0.146\}$ . These results are to be used as the first estimates for a Peng-Robinson calculation. The resulting first-estimate Peng-Robinson calculations are shown below.

Component	$z_i$	$T_c$ (K)	$P_c$ (MPa)	0	kij		
					n-pentane	n-hexane	n-heptane
n-pentane	0.45	469.7	3.369	0.249	-	-	-
n-hexane	0	507.4	3.012	0.305	0.00076	-	-
n-heptane	0.55	540.3	2.736	0.349	0.00171	0.00061	-

Current State		Roots		fugacity MPa	component fugacity coeff			component fugacity(MPa)		
T (K)	333.15	Z	V		n-pentane	n-hexane	n-heptane	n-pentane	n-hexane	n-heptane
P (MPa)	0.1135		$\text{cm}^3/\text{gmol}$							
answers for three		0.947612	23125.16	0.10782973	0.96731202	0.95135301	0.93614096	0.049405	0	0.0584386
root region		0.042141	1028.398							
		0.005705	139.2187	0.06813018	1.77806712	0.64432645	0.24687972	0.090815	0	0.0154115
& for 1 root region		#NUM!	#NUM!	#NUM!	#NUM!	#NUM!	#NUM!	#NUM!	#NUM!	#NUM!

Component	$z_i$	$T_c$ (K)	$P_c$ (MPa)	0	kij		
					n-pentane	n-hexane	n-heptane
n-pentane	0.854	469.7	3.369	0.249	-	-	-
n-hexane	0	507.4	3.012	0.305	0.00076	-	-
n-heptane	0.146	540.3	2.736	0.349	0.00171	0.00061	-

Current State		Roots		fugacity MPa	component fugacity coeff			component fugacity(MPa)		
T (K)	333.15	Z	V		n-pentane	n-hexane	n-heptane	n-pentane	n-hexane	n-heptane
P (MPa)	0.1135		$\text{cm}^3/\text{gmol}$							
answers for three		0.960418	23437.66	0.10916273	0.96573988	0.95204881	0.93898163	0.093608	0	0.0155599
root region		0.030535	745.1735							
		0.005127	125.1156	0.15054775	1.76304099	0.6468801	0.25107104	0.17089	0	0.0041605
& for 1 root region		#NUM!	#NUM!	#NUM!	#NUM!	#NUM!	#NUM!	#NUM!	#NUM!	#NUM!

Using the flowsheet of pg 336, and omitting the inner loop, perform calculations to determine if  $P=0.1135\text{MPa}$  is too high or too low, and provide the next guess of  $y_i$ .

6. An experiment with ethanol (1) + benzene (2) has resulted in the following VLE measurements at 45°C and 0.3871 bar:  $x_1 = 0.7087$ ,  $y_1 = 0.4751$ . The vapor pressures of the components at 45°C are  $P_1^{\text{sat}} = 0.2321$ ,  $P_2^{\text{sat}} = 0.2939$  bar.
- a. (10) fit the 2-parameter Margules equation to this experiment using modified Raoult's law.
- b. (20) from the fit of part (a), set forth the procedure to determine the dew pressure for an equimolar mixture at 45°C. Avoid unnecessary calculations in your procedure. If an iterative calculation is required, perform the first iteration and specify values for the next iteration. If an iterative calculation is not required, provide the dew pressure.

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Spring 2006

Hour Exam 2: April 12, 2006

$$R = 8.314 \text{ cm}^3\text{MPa/mol-K} = 8.314 \text{ J/mol-K}$$

$$1 \text{ bar} = 0.1 \text{ MPa}, 1 \text{ atm} = 760 \text{ mmHg} = 1.013 \text{ bar}$$

CLOSED BOOK PORTION

- (10) List the properties that are always equal in two phases at equilibrium.
- (10) Explain for what types of systems Raoult's law will be most successful. Provide some specific examples of components for which you might successfully apply the model.
- Consider propane at the state given in the figure below.

Peng-Robinson Equation of State (Pure Fluid)										Spreadsheet protected, but no password used.		
Properties				Heat Capacity constants from Appendix				ideal gas	$H^ig - H_R^ig$	$U^ig - U_R^ig$	$S^ig - S_R^ig$	
Gas	$T_c$ (K)	$P_c$ (MPa)	$\omega$	A	B	C	D	values	J/mol	J/mol	J/molK	
PROPANE	369.8	4.249	0.152	-4.224	3.06E-01	-1.59E-04	3.22E-08		2061.528	1838.297	6.509579	
Current State		Roots		Stable Root has a lower fugacity								
T (K)	325	Z	V	fugacity	H	U	S	H-H <sup>ig</sup>	U-U <sup>ig</sup>	S-S <sup>ig</sup>		
P (MPa)	0.1013	cm <sup>3</sup> /gmol	MPa	J/mol	J/mol	J/molK	J/mol	J/mol	J/mol	J/molK		
answers for three root region		0.9868082	26321.867	0.099978	2073.646	-592.759	6.550139062	-99.7836	-64.1387	-0.19779		
		0.0071903	191.79138									
		0.0038911	103.79132	1.304987	-12115.5	-12126	-58.4674714	-14288.9	-11597.4	-65.2154		
& for 1 root region		#NUM!	#NUM!	#NUM!	#NUM!	#NUM!	#NUM!	#NUM!	#NUM!	#NUM!		
				fugratio	0.076612							

(a) (10) Propane from the initial state of the figure is to be compressed adiabatically to  $P = 5$  MPa in a compressor that is 85% efficient. Explain the steps necessary to determine the actual outlet temperature using cell references from the figure. In your answer, assume that only one phase exists at the outlet.

(b) (10) Propane at the initial state in the figure is to be throttled across a valve to 0.05 MPa. Explain the steps necessary to determine the actual outlet temperature using cell references from the figure. Assume that only one phase exists at the outlet.

(c) (10) Propane at the initial state of the figure is to be expanded in a reversible expander to a pressure of 0.01 MPa. Explain how you would find the final state. Explain how you would determine if the outlet is one or two-phase. For a two phase outlet, explain clearly using cell references how you would determine the quality.

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DEPARTMENT OF CHEMICAL ENGINEERING AND MATERIALS SCIENCE

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Spring 2006

Hour Exam 2: April 12, 2006

$$R = 8.314 \text{ cm}^3\text{MPa/mol-K} = 8.314 \text{ J/mol-K}$$

$$1 \text{ bar} = 0.1 \text{ MPa}, 1 \text{ atm} = 760 \text{ mmHg} = 1.013 \text{ bar}$$

OPEN BOOK PORTION

1. (15) Simple derivative manipulations are applied to each of the starting expressions in the left column using at most three steps. The manipulations may be properly applied, or may involve errors. Indicate whether the ending expression in each row is valid. Use the workspace for scratch work for partial credit.

Starting Expression	Ending Expression	Indicate valid or invalid
$dU = \left(\frac{\partial U}{\partial T}\right)_P dT + \left(\frac{\partial U}{\partial P}\right)_T dP$	$\left(\frac{\partial U}{\partial S}\right)_P = \left(\frac{\partial U}{\partial T}\right)_P \left(\frac{1}{C_P}\right) + \left(\frac{\partial U}{\partial P}\right)_T \left(\frac{\partial P}{\partial S}\right)_T$	
$\left(\frac{\partial T}{\partial V}\right)_U$	$-C_V \left(\frac{\partial U}{\partial V}\right)_T$	
$\left(\frac{\partial G}{\partial P}\right)_S = -S \left(\frac{\partial T}{\partial P}\right)_S + V$	$\left(\frac{\partial G}{\partial P}\right)_S = -S \left(\frac{\partial V}{\partial T}\right)_P \left(\frac{T}{C_P}\right) + V$	

Workspace:

2. Ethyl lactate is a solvent that can be produced from ethanol and lactic acid, both of which can be produced from corn. In the reaction of ethanol and lactic acid, water is produced, which must be removed from the reaction mixture. Consider the VLE measurements that have been performed at 60°C for ethyl lactate(1) + water(2). At this condition,  $P_1^{\text{sat}} = 22.7 \text{ mmHg}$ ,  $P_2^{\text{sat}} = 150.1 \text{ mmHg}$ . A liquid composition of  $x_1 = 0.6384$  coexists with a composition  $y_1 = 0.1347$  at 120.2 mmHg.

(a) (10) Fit the van Laar equation to the experimental data.

(b) (10) Use the results of part (a) to predict the vapor composition in equilibrium with a liquid of composition  $x_1 = 0.2$  at 60°C. If an iterative procedure is required, perform the first iteration and clearly indicate the steps and formulas needed to arrive at a converged solution.

3. (10) A vented tank of n-pentane at  $34.35^{\circ}\text{C}$  and 1 bar has a headspace of  $3\text{ m}^3$ . More liquid pentane is added at the same temperature until the headspace is  $2.2\text{ m}^3$ . Estimate the emission of pentane (in mols) from the tank. Antoine constants for n-pentane are:  $A = 6.85296$ ,  $B = 1064.84$ ,  $C = 232.012$ , for  $\log_{10}(P^{\text{sat}})$  where  $P^{\text{sat}}$  in mmHg

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ChE 321: Chemical Engineering Thermodynamics

Spring 2005

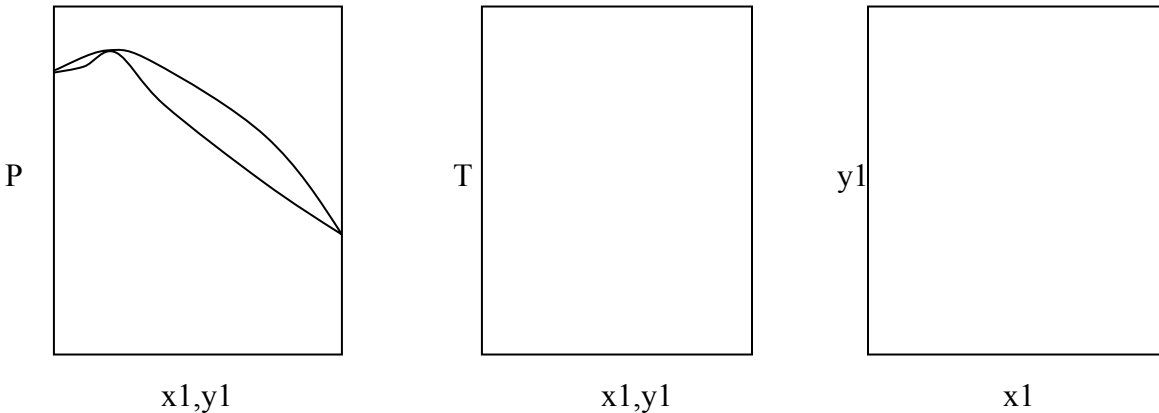
Hour Exam 2: April 5, 2005

$$R = 8.314 \text{ cm}^3\text{MPa/mol-K} = 8.314 \text{ J/mol-K}$$

$$1 \text{ bar} = 0.1 \text{ MPa}, 1 \text{ atm} = 760 \text{ mmHg} = 1.013 \text{ bar}$$

CLOSED BOOK PORTION

1. The P-x-y diagram for a binary mixture has been measured and is sketched below. To perform a distillation design, a T-x-y diagram and an x-y diagram (at constant P) is desired.
  - (a) (5) Label the L region and V region on the P-x-y diagram.
  - (b) (10) Provide qualitative sketches of the T-x-y and y-x diagrams in the provided coordinates.



2. (10) For ethane at the state  $T_2 = 325\text{K}$  and  $P_2 = 0.1013 \text{ MPa}$ , the Peng-Robinson equation gives a value of  $(S - S^{\text{ig}}) = -0.10508 \text{ J/molK}$ . For ethane at the state  $T_1 = 300\text{K}$  and  $P_1 = 3 \text{ MPa}$ , the Peng-Robinson equation gives  $(S - S^{\text{ig}}) = -5.15712 \text{ J/molK}$ . The ideal gas entropy change can be calculated using  $\Delta S = C_p \ln(T_2/T_1) - R \ln(P_2/P_1)$ , where  $C_p$  is assumed to be constant and for ethane near these temperatures has a value  $C_p = 52.1 \text{ J/molK}$ . Determine  $\Delta S$  for moving from state 1 to state 2.

3. In the system A + B, activity coefficients can be expressed by  $\ln\gamma_A = 0.65 x_B^2$ ,  $\ln\gamma_B = 0.65 x_A^2$ . The vapor pressures of A and B at 80°C are  $P_A^{\text{sat}} = 900$  mmHg,  $P_B^{\text{sat}} = 750$  mmHg.
- (15) Using Modified Raoult's law, determine the dew pressure and coexisting phase compositions for a mixture with overall composition of 30 mol% A. If an iterative solution is required, complete the first pass of the iteration, and indicate clearly the specific steps that need to be repeated to efficiently find the answer.
  - (10) Explain how you would generate a P-x-y diagram for this system in the most expeditious manner. Include equations to show how you would generate the necessary information.
4. (10) The Peng-Robinson equation of state for propylene at 300K and 1.2 MPa provides a value of  $Z = 0.801$ . Determine the number of moles that can fit into a 40L gas cylinder at this condition.

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Spring 2005

Hour Exam 2: April 6, 2005

OPEN BOOK PORTION

5. (15) Simple derivative manipulations are applied to each of the starting expressions in the left column using at most three steps. The manipulations may be properly applied, or may involve errors. Indicate whether the ending expression in each row is valid. Use the workspace for scratch work for partial credit in the event of wrong answers.

Starting Expression	Ending Expression	Indicate valid or invalid
$dA = -SdT - PdV$	$\left(\frac{\partial A}{\partial V}\right)_P = -S\left(\frac{\partial T}{\partial V}\right)_P - P$	
$\left(\frac{\partial T}{\partial V}\right)_S$	$-\frac{1}{C_V}\left(\frac{\partial S}{\partial V}\right)_T$	
$\left(\frac{\partial G}{\partial S}\right)_V = -\frac{ST}{C_V} + V\left(\frac{\partial P}{\partial S}\right)_V$	$\left(\frac{\partial G}{\partial S}\right)_V = -\frac{ST}{C_V} - V\left(\frac{\partial T}{\partial V}\right)_P$	

Workspace:

6. (10) Consider the calculation of fugacity of propylene at 300K. The vapor pressure of propylene at 300K is 1.21 MPa, where  $V^{\text{satL}} = 80.4 \text{ cm}^3/\text{mol}$  and  $V^{\text{satV}} = 1639.4 \text{ cm}^3/\text{mol}$ . Use the virial equation to represent vapor phase non-idealities. For propylene,  $T_C = 364.8\text{K}$ ,  $P_C = 4.613 \text{ MPa}$ ,  $\omega = 0.142$ . Calculate the fugacity of propylene at 300K and 2 MPa.

7. (15) VLE for the system ethanol(1) + benzene(2) has been measured at  $45^\circ\text{C}$ , resulting in  $x_1 = 0.3141$  and  $y_1 = 0.3625$  when  $P = 0.4124 \text{ bar}$ . The vapor pressures are  $P_1^{\text{sat}} = 0.2321 \text{ bar}$ ,  $P_2^{\text{sat}} = 0.2939 \text{ bar}$ . Obtain the van Laar parameters that represent this system.



- b. (10) From the results of part (a), provide a quantitative sketch of the  $P$ - $x$ - $y$  diagram and a qualitative sketch of the  $T$ - $x$ - $y$  diagram of the system.
4. A container holds hexane(1) and heptane(2) with an overall composition of 90 mol% hexane. At  $72^\circ\text{C}$ ,  $P_1^{\text{sat}} = 836 \text{ mmHg}$ ,  $P_2^{\text{sat}} = 326 \text{ mmHg}$ . The system pressure is  $760 \text{ mmHg}$ .
- a. (5) Beginning with Raoult's Law, determine the VLE K-ratios of the components.
- b. (10) Use the VLE K-ratios from part (a) to determine the compositions of vapor and liquid. (Hint: this can be solved without iterative calculations).
- c. (10) If the container holds 100 mol total, determine the number of moles of liquid and vapor at the stated conditions.

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ChE 321: Chemical Engineering Thermodynamics

Spring 2004

Hour Exam 2: April 9, 2004

OPEN BOOK PORTION

5. (15) Simple derivative manipulations are applied to each of the starting expressions in the left column using at most three steps. The manipulations may be properly applied, or may involve errors. Indicate whether the ending expression in each row is valid. Use the workspace for scratch work for partial credit in the event of wrong answers.

Starting Expression	Ending Expression	Indicate valid or invalid
$dH \quad TdS \quad VdP$	$\left(\frac{\partial H}{\partial V}\right)_T = T\left(\frac{\partial P}{\partial T}\right)_S + V\left(\frac{\partial P}{\partial V}\right)_T$	
$\left(\frac{\partial T}{\partial P}\right)_H$	$-C_P\left(\frac{\partial H}{\partial P}\right)_T$	
$\left(\frac{\partial S}{\partial V}\right)_P$	$\frac{C_P}{T}\left(\frac{\partial T}{\partial V}\right)_P$	

Workspace:

6. (10) Hexane flows at steady-state through a process where heat and work transfer occur. The inlet and outlet states are given below. Calculate the optimum shaft work involved, regardless of equipment configuration. The surroundings are at 295K.

Inlet State:

Properties				Heat Capacity constants from Appendix				ideal gas	$H^R - H_R^{IG}$	$U^R - U_R^{IG}$	$S^R - S_R^{IG}$
Gas	$T_c$ (K)	$P_c$ (MPa)	$\omega$	A	B	C	D	values	J/mol	J/mol	J/molK
n-HEXANE	507.4	3.012	0.305	-4.413	5.28E-01	-3.12E-04	6.49E-08		1530.104	1431.583	4.924711

Current State		Roots		Stable Root has a lower fugacity						
T (K)	310	Z	V	fugacity	H	U	S	H-H <sup>IG</sup>	U-U <sup>IG</sup>	S-S <sup>IG</sup>
P (MPa)	0.1013	cm <sup>3</sup> /gmol	MPa	J/mol	J/mol	J/molK	J/mol	J/mol	J/molK	
answers for three root region		0.9444608	24029.581	0.095954	32619.8	30185.6	96.24942431	-383.293	-240.149	-0.78566
		0.0460398	1171.3752							
		0.0052168	132.73024	0.032093	2072.585	2059.139	6.815713748	-30930.5	-28366.6	-90.2194
& for 1 root region		#NUM!	#NUM!	#NUM!	#NUM!	#NUM!	#NUM!	#NUM!	#NUM!	#NUM!

Outlet State:

Properties				Heat Capacity constants from Appendix				ideal gas	$H^R - H_R^{IG}$	$U^R - U_R^{IG}$	$S^R - S_R^{IG}$
Gas	$T_c$ (K)	$P_c$ (MPa)	$\omega$	A	B	C	D	values	J/mol	J/mol	J/molK
n-HEXANE	507.4	3.012	0.305	-4.413	5.28E-01	-3.12E-04	6.49E-08		11553.39	10872.89	28.34132

Current State		Roots		Stable Root has a lower fugacity						
T (K)	380	Z	V	fugacity	H	U	S	H-H <sup>IG</sup>	U-U <sup>IG</sup>	S-S <sup>IG</sup>
P (MPa)	0.2	cm <sup>3</sup> /gmol	MPa	J/mol	J/mol	J/molK	J/mol	J/mol	J/molK	
answers for three root region		0.9372352	14805.13	0.188118	42462.04	39501.01	119.4757852	-564.345	-366.051	-0.97591
		0.0463789	732.62969							
		0.0094882	149.88137	0.262769	15598.68	15568.71	46.0041687	-27427.7	-24298.4	-74.4475
& for 1 root region		#NUM!	#NUM!	#NUM!	#NUM!	#NUM!	#NUM!	#NUM!	#NUM!	#NUM!

7. (15) A colleague asserts that the fugacity of 1-octanol vapor at 200°C is equal to pressure at 0.1 MPa. The vapor pressure of 1-octanol at 200°C is 0.136 MPa. Evaluate the assertion using the virial coefficient correlation. Properties of 1-octanol:  $T_c = 652.5K$ ,  $P_c = 2.86$  MPa,  $\omega = 0.594$ .

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DEPARTMENT OF CHEMICAL ENGINEERING

ChE 321: Thermodynamics for Chemical Engineers

Spring 2003

$$R = 8.314 \text{ J/mol-K} = 8.314 \text{ MPa cm}^3/\text{mol-K}$$

$$1 \text{ bar} = 0.1 \text{ MPa}, \quad 1 \text{ atm} = 1.013 \text{ bar}$$

CLOSED BOOK PORTION

1. (10) (T or F)

- The compressibility factor  $Z$  is always less than or equal to unity.
- Plotting  $Z$  vs.  $P_r$  gives identical curves for all fluids at the same  $T_r$ .
- Plotting  $\ln(P_r^{\text{sat}})$  vs.  $1/T_r$  gives an almost straight line.

2. (10) Estimate with minimum calculations the values of fugacity for hexane under the following conditions. Include units. Your answer should be of the type provided by a quick estimation.

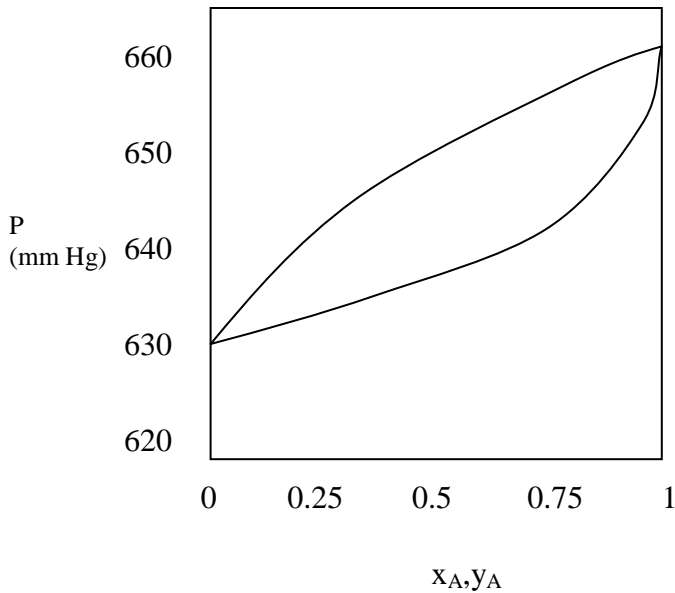
(a) Hexane is a pure vapor at 65C and 346 mm Hg. The vapor pressure of hexane at 65C is 675 mmHg.

(b) Hexane is in a vapor mixture with acetone at 65C and 480 mmHg. The mole fraction of hexane is  $y_{\text{hexane}} = 0.4$ . The vapor pressures are  $P_{\text{hexane}}^{\text{sat}} = 675$  mmHg,  $P_{\text{acetone}}^{\text{sat}} = 1020$  mmHg.

(c) Hexane is a pure liquid at 65C and 760 mmHg. The vapor pressure of hexane at 65C is 675 mmHg.

3. (20) For the system 1-butanol (1) + 2-propanol (2) at 90C, the vapor pressures are  $P_1^{\text{sat}} = 257 \text{ mmHg}$  and  $P_2^{\text{sat}} = 1026 \text{ mmHg}$ . Using Raoult's law, estimate the dew pressure and coexisting phase compositions for an overall composition of 70 mol% butanol. If an iterative solution is required, perform the first iteration, and indicate clearly the specific steps used to efficiently find the answers.

4. A P-x-y diagram is shown below for the system A+B. From the diagram, mark the answers to the following questions, label them as '(a)', '(b)', etc., and provide numerical values.



- (a) (5) The dew pressure and coexisting phase compositions (use  $x$  for liquid,  $y$  for vapor) and  $L/F$  for an overall composition  $z_A = 0.5$ .
- (b) (5) The phase compositions (use  $x$  for liquid,  $y$  for vapor) and calculated  $L/F$  for an overall composition  $z_A = 0.5$  at 645 mm Hg.

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5. (25) The (1) + (2) system exhibits vapor liquid equilibria at 24.95 kPa and 50C. The compositions of the coexisting phases are  $x_1 = 0.36$  and  $y_1 = 0.62$  and  $P_1^{\text{sat}} = 69.4$  kPa,  $P_2^{\text{sat}} = 15.8$  kPa.

(a) fit the two parameter Margules equation to the experimental data.

(b) use the results of part (a) to calculate the bubble pressure and coexisting phase compositions for a mixture of overall composition at  $z_1 = 0.8$  at 50C.

(c) calculate  $G^E/RT$  for the liquid mixture of composition  $x_1 = 0.8$ .

6. (10) Estimate the vapor pressure of methyl ethyl ketone at 333 K without using Antoine coefficients.

7. (15) Propane passes through a reversible expander. The inlet conditions are 380 K and 5 MPa.

	A	B	C	D	E	F	H
7	T (K)	380	Z	V	fugacity	H	S
8	P (MPa)	5		cm <sup>3</sup> /gmol	MPa	J/mol	J/molK
9	answers for three		#NUM!	#NUM!	#NUM!	#NUM!	#NUM!
10	root region		#NUM!	#NUM!	#NUM!	#NUM!	#NUM!
11			#NUM!	#NUM!	#NUM!	#NUM!	#NUM!
12	& for 1 root region		0.3500705	221.19692	3.091485	-1177.28	-29.5211617

Several possible outlet states are given below (note that one state is on the next page).

Calculate the work done by the expander in J/mol.

(state 1)

	A	B	C	D	E	F	H
6	Current State		Roots		Stable Root has a lower fugacity		
7	T (K)	281.943934	Z	V	fugacity	H	S
8	P (MPa)	0.1		cm <sup>3</sup> /gmol	MPa	J/mol	J/molK
9	answers for three		0.9806874	22988.116	0.0981	-1177.28	-4.05906683
10	root region		0.0134418	315.08611			
11			0.0034694	81.324746	0.534207	-17946	-77.6250711

(state 2)

	A	B	C	D	E	F	H
7	T (K)	183.073417	Z	V	fugacity	H	S
8	P (MPa)	0.1		cm <sup>3</sup> /gmol	MPa	J/mol	J/molK
9	answers for three		0.9395331	14300.373	0.094287	-7086.69	-29.5211996
10	root region		0.0524708	798.64357			
11			0.0042977	65.414722	0.006712	-27263.8	-117.764806
12	& for 1 root region		#NUM!	#NUM!	#NUM!	#NUM!	#NUM!

(state 3)

	A	B	C	D	E	F	H
7	T (K)	230.609012	Z	V	fugacity	H	S
8	P (MPa)	0.1		cm <sup>3</sup> /gmol	MPa	J/mol	J/molK
9	answers for three		0.9669301	18538.79	0.09679	-4522.41	-17.1171082
10	root region		0.0264368	506.86756			
11			0.0036971	70.883116	0.09679	-23226.5	-98.2244172
12	& for 1 root region		#NUM!	#NUM!	#NUM!	#NUM!	#NUM!

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ChE 321: Thermodynamics for Chemical Engineers

Spring 2002

$$R = 8.314 \text{ J/mol-K} = 8.314 \text{ MPa cm}^3/\text{mol-K}$$

$$1 \text{ bar} = 0.1 \text{ MPa}, \quad 1 \text{ atm} = 1.013 \text{ bar}$$

CLOSED BOOK PORTION

1. (5) The fundamental relation for  $U$  is  $dU = TdS - PdV$ . The definition of Helmholtz energy is  $A \equiv U - TS$ . Derive the relation for  $dA$ .
  
2. (5) The van der Waals equation is  $Z = 1/(1 - b\rho) - a\rho/RT$ . The parameters are made dimensionless using  $A = aP/(RT)^2$  and  $B = bP/RT$ . Rearrange the equation in the form  $Z^3 + a_2Z^2 + a_1Z + a_0 = 0$ , where  $a_2$ ,  $a_1$ , and  $a_0$  are functions of  $A$  and  $B$ .
  
3. At 1 MPa and 300K pure component (1) is a vapor with a fugacity coefficient of 1.0 and pure component (2) is a vapor with a fugacity coefficient of 0.83.
  - (a) (5) Gaseous components (1) and (2) are mixed at 1 MPa and 300K, such that  $y_1 = 0.4$  and  $y_2 = 0.6$ . Provide the values of the component fugacities in the mixture if the mixture is assumed to be an ideal gas mixture.

(b) (5) Gaseous components (1) and (2) are mixed at 1 MPa and 300K, such that  $y_1 = 0.4$  and  $y_2 = 0.6$ . Provide the values of the component fugacities in the mixture if the mixture is assumed to be an ideal solution of vapors.

4. The equation of state for a simple fluid has been correlated to the equation  $Z = 1 + aP/RT$ , where  $a = -2540 \text{ cm}^3/\text{mol}$ , and  $C_p = 56 \text{ J/mol-K}$ .

(a) (10) Evaluate the enthalpy departure for the fluid. The enthalpy departure can be calculated from

$$\frac{(H - H^{ig})}{RT} = \int_0^P -T \frac{\partial Z}{\partial T} \frac{d\rho}{\rho} + Z - 1 \quad \text{or} \quad \frac{(H - H^{ig})}{RT} = \int_0^P -T \frac{\partial Z}{\partial T} \frac{dP}{P}$$

(b) (10) The fluid state changes from 100K and 1 MPa to 300K and 10MPa. Calculate  $\Delta H$ .

5. (15) The system (1) + (2) can be modeled with Modified Raoult's law, using the one parameter Margules equation,  $\ln \gamma_1 = 1.6 x_2^2$ ,  $\ln \gamma_2 = 1.6 x_1^2$ . The vapor pressures are  $\log_{10} P_1^{\text{sat}} = 8.4 - 1800 / (T + 230)$ ,  $\log_{10} P_2^{\text{sat}} = 7.3 - 1300 / (T + 170)$ , where T is in Celsius. Calculate the bubble pressure and coexisting phase compositions using Modified Raoult's Law for a mixture that is overall 75 mol% (1) and 25 mol% (2) at 60 °C. If an iterative solution is required, perform the first iteration, and indicate clearly the specific steps used to find the answers.

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OPEN BOOK, CLOSED NOTES PORTION

Spring 2002

6. (20) The system ethyl acetate (1) + methanol (2) forms an azeotrope at  $x_1 = 0.278$ ,  $62.1^\circ\text{C}$ , and  $760\text{ mmHg}$ . The component vapor pressures at  $62.1^\circ\text{C}$  are  $P_1^{\text{sat}} = 452\text{ mmHg}$ ,  $P_2^{\text{sat}} = 690\text{ mmHg}$ . Fit the two parameter Margules equation parameters.

7. Benzene (1) and tetralin (2) are to be modeled with the Peng-Robinson EOS. A bubble pressure calculation is to be performed at 523 K for  $x_i = \{0.273, 0.727\}$ . To start the calculation, the shortcut K-ratio method is used to find  $y_i = \{0.822, 0.178\}$  and  $P = 1$  MPa. Results from these initial guesses provide:

Component	$z_i$	$T_c$ (K)	$P_c$ (MPa)	$\omega$	kij		
					benzene	tetralin	n-heptane
benzene	0.822	562.2	4.898	0.211	-	-	-
tetralin	0.178	720.2	3.3	0.286	0	-	-
n-heptane	0	540.3	2.736	0.349	0	0	-

Current State		Roots			component fugacity coeff			component fugacity(MPa)		
T (K)	523	Z	V	fugacity	benzene	tetralin	n-heptane	benzene	tetralin	n-heptane
P (MPa)	1		cm <sup>3</sup> /gmol	MPa						
answers for three		0.864985	3761.145	0.8791683	0.90799846	0.75746031	0.85351025	0.746375	0.134828	0
root region		0.079939	347.5934							
		0.035263	153.3315	1.400344	2.03591419	0.24871339	1.64961924	1.673521	0.044271	0
& for 1 root region		#NUM!	#NUM!	#NUM!	#NUM!	#NUM!	#NUM!	#NUM!	#NUM!	#NUM!

Component	$z_i$	$T_c$ (K)	$P_c$ (MPa)	$\omega$	kij		
					benzene	tetralin	n-heptane
benzene	0.273	562.2	4.898	0.211	-	-	-
tetralin	0.727	720.2	3.3	0.286	0	-	-
n-heptane	0	540.3	2.736	0.349	0	0	-

Current State		Roots			component fugacity coeff			component fugacity(MPa)		
T (K)	523	Z	V	fugacity	benzene	tetralin	n-heptane	benzene	tetralin	n-heptane
P (MPa)	1		cm <sup>3</sup> /gmol	MPa						
answers for three		0.700231	3044.758	0.77326292	0.96168985	0.71246394	0.86643342	0.262541	0.517961	0
root region		0.231551	1006.835							
		0.039956	173.7394	0.42737395	2.1066805	0.23477628	1.91009436	0.575124	0.170682	0
& for 1 root region		#NUM!	#NUM!	#NUM!	#NUM!	#NUM!	#NUM!	#NUM!	#NUM!	#NUM!

- (a) (15) Determine the  $y_i$  for the next iteration using only the outer loop in Figure 10.2.

- (b) (10) Should the next P guess be higher or lower? (Use calculations to justify your answer).

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DEPARTMENT OF CHEMICAL ENGINEERING

ChE 321: Thermodynamics

Spring 2001

Exam 2: April 13, 2001, Open Book, Closed Notes

1. Calculations for methane are shown in Figure 8.7 on pg 274.
  - a. (5) verify by hand calculation the value shown in cell I10.
  
  - b. (5) verify by hand calculation the value shown in cell J12.
  
  - c. (10) the enthalpy departure at the conditions of Fig 8.7 is desired for liquid methane as calculated by the Peng-Robinson equation. Provide the eq number from the textbook that would lead to the value most expeditiously and provide the values of the variables used in the equation. Calculation of the final value is not required.
  
2. (15) A calculation of the dew point temperature of a ternary mixture is shown in part (b) of Example 9.1 on pg 307. Verify by hand calculation the value of  $K_i$  and  $x_i$  for propane ( $C_3$ ) at 325 K.

3. (20) A tank of liquid 70 mol% ethanol(1) + 30 mol% water (2) initially has a headspace of 3 m<sup>3</sup> at 50°C. After pumping more liquid of the same composition and temperature into the tank at 50°C, the headspace is 0.5 m<sup>3</sup>. Estimate the emission of ethanol due to the filling process at P = 760 mmHg. The vapor pressures of the pure components at 50°C are P<sub>1</sub><sup>sat</sup> = 221.2 mmHg, P<sub>2</sub><sup>sat</sup> = 92.3 mmHg.

4. (20) A short-cut calculation for the bubble temperature of mixture of Example 9.1, part (a) is converged with the following results: T = 317.59K, P = 0.8 MPa, x<sub>i</sub> = {0.23, 0.67, 0.1}, y<sub>i</sub> = {0.442, 0.504, 0.054}. These results are to be used as the first estimates for a Peng-Robinson calculation. The resulting first-estimate Peng-Robinson calculations are shown below.

Component	z <sub>i</sub>	T <sub>c</sub> (K)	P <sub>c</sub> (MPa)	ω	k <sub>ij</sub>		
					propane	i-butane	n-butane
propane	0.23	369.8	4.249	0.152	-	-	-
i-butane	0.67	408.1	3.648	0.177	0	-	-
n-butane	0.1	425.2	3.797	0.193	0	0	-

Current State		Roots			fugacity MPa	component fugacity coeff			component fugacity(MPa)		
T (K)	317.59	Z	V	cm <sup>3</sup> /gmol		propane	i-butane	n-butane	propane	i-butane	n-butane
P (MPa)	0.8										
answers for three		0.820871	2709.328		0.67748176	0.89754918	0.83392963	0.82124969	0.165149	0.446986	0.0657
root region		0.127364	420.371								
& for 1 root region		0.03096	102.1855		0.61920974	1.48505645	0.66072037	0.49928732	0.27325	0.354146	0.039943
		#NUM!	#NUM!		#NUM!	#NUM!	#NUM!	#NUM!	#NUM!	#NUM!	#NUM!

Component	z <sub>i</sub>	T <sub>c</sub> (K)	P <sub>c</sub> (MPa)	ω	k <sub>ij</sub>		
					propane	i-butane	n-butane
propane	0.442	369.8	4.249	0.152	-	-	-
i-butane	0.504	408.1	3.648	0.177	0	-	-
n-butane	0.054	425.2	3.797	0.193	0	0	-

Current State		Roots			fugacity MPa	component fugacity coeff			component fugacity(MPa)		
T (K)	317.59	Z	V	cm <sup>3</sup> /gmol		propane	i-butane	n-butane	propane	i-butane	n-butane
P (MPa)	0.8										
answers for three		0.8396	2771.145		0.68824379	0.89465877	0.83519174	0.82327736	0.316351	0.336749	0.0355656
root region		0.110322	364.1244								
& for 1 root region		0.030305	100.0243		0.74438071	1.48094328	0.66134127	0.50188495	0.523662	0.266653	0.0216814
		#NUM!	#NUM!		#NUM!	#NUM!	#NUM!	#NUM!	#NUM!	#NUM!	#NUM!

Using the flowsheet of pg 614, and omitting the inner loop, perform calculations to determine if is T=317.59K is too high or too low, and provide the next guess of y<sub>i</sub>.

5. An experiment with ethanol (1) + benzene (2) has resulted in the following VLE measurements at 45°C and 0.3871 bar:  $x_1 = 0.7087$ ,  $y_1 = 0.4751$ . The vapor pressures of the components at 45°C are  $P_1^{\text{sat}} = 0.2321$ ,  $P_2^{\text{sat}} = 0.2939$  bar.
- a. (10) fit the 2-parameter Margules equation to this experiment using modified Raoult's law.
- b. (15) from the fit of part (a), set forth the procedure to determine the dew pressure for an equimolar mixture at 45°C. Avoid unnecessary calculations in your procedure. If an iterative calculation is required, perform the first iteration and specify values for the next iteration. If an iterative calculation is not required, provide the dew pressure.

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DEPARTMENT OF CHEMICAL ENGINEERING

ChE 321: Thermodynamics, Open Book, Closed Notes

Spring 2000

1. (10) For the Gibbs energy,  $dG = -SdT + VdP$ . For each of the following manipulations, indicate if the result is correct (T) or incorrect (F).

Expression	Indicate T or F
(a) $\left(\frac{\partial G}{\partial S}\right)_P = -S \left(\frac{\partial T}{\partial S}\right)_P + V$	
(b) $\left(\frac{\partial G}{\partial S}\right)_V = \frac{-ST}{C_V} - V \left(\frac{\partial T}{\partial V}\right)_P$	
(c) $\left(\frac{\partial G}{\partial T}\right)_S = -S + V \frac{C_P}{T} \left(\frac{\partial T}{\partial V}\right)_P$	

(d) Given that  $\left(\frac{\partial H}{\partial T}\right)_V = C_V + V \left(\frac{\partial P}{\partial T}\right)_V$ , provide the expression that is followed for a fluid that follows the equation of state  $P = RT/(V-b) - a/T^{3/2}$  where  $a$  and  $b$  are T-independent parameters.

2. The spreadsheet PREOS.xls for methane at 111.4K and 0.1 MPa is shown on pg. 274. Consider the following problems at this state.

(a) (10) How many moles of methane are contained in a 4L vessel that is half full (by volume) of liquid?

(b) (5) A piston/cylinder holds 3 moles of methane and has a volume of 25L. The cylinder volume is isothermally changed such that the pressure starts to rise. Select the volume of the cylinder where the pressure starts to rise: (i) P won't rise at any V; (ii) 26.88 L; (iii) 25 L; (iv) 13.49 L; (v) 0.1 L; (v) none of the choices are very close. Your answer: \_\_\_\_\_

3. Propane at the inlet of a reversible, adiabatic expander is at 295 K and 0.8 MPa, with  $H = -1143 \text{ J/mol}$  and  $S = -20.117 \text{ J/mol-K}$ . The outlet of the expander is at 0.1 MPa, and two states at this pressure are shown below.

T (K)	218.992531	Z	V	fugacity	H	U	S
P (MPa)	0.1	cm <sup>3</sup> /gmol		MPa	J/mol	J/mol	J/molK
answers for three root region	0.962117	17517.301	0.09634	-5196.78	-6948.51	-20.11700041	
	0.0309848	564.14124	0.057114	-24279	-24285.9	-102.9064011	
& for 1 root region	#NUM!	#NUM!	#NUM!	#NUM!	#NUM!	#NUM!	

T (K)	230.609007	Z	V	fugacity	H	U	S
P (MPa)	0.1	cm <sup>3</sup> /gmol		MPa	J/mol	J/mol	J/molK
answers for three root region	0.9669301	18538.79	0.09679	-4522.41	-6376.29	-17.11710935	
	0.0264368	506.86758	0.09679	-23226.5	-23233.6	-98.22441894	
& for 1 root region	#NUM!	#NUM!	#NUM!	#NUM!	#NUM!	#NUM!	

(a) (10) What is the outlet temperature? Explain your reasoning.

(b) (5) How much work is obtained from the turbine, J/mol?

4. The fugacities for a ternary mixture are shown below.

Component	z <sub>i</sub>	T <sub>c</sub> (K)	P <sub>c</sub> (MPa)	ω	k <sub>ij</sub>		
					n-pentane	n-hexane	n-heptane
n-pentane	0.8168	469.7	3.369	0.249	-	-	-
n-hexane	0.1501	507.4	3.012	0.305	0.00076	-	-
n-heptane	0.0331	540.3	2.736	0.349	0.00171	0.00061	-

Current State	Roots								
T (K)	Z	V	fugacity	component fugacity coeff			component fugacity (MPa)		
P (MPa)	cm <sup>3</sup> /gmol		MPa	n-pentane	n-hexane	n-heptane	n-pentane	n-hexane	n-heptane
answers for three root region	0.962378	25449.9	0.09763912	0.96647503	0.9532928	0.9407281	0.079988	0.014499	0.0031551
	0.029472	779.3856	0.11717831	1.4519173	0.50220106	0.18514646	0.120164	0.007638	0.000621
& for 1 root region	#NUM!	#NUM!	#NUM!	#NUM!	#NUM!	#NUM!	#NUM!	#NUM!	#NUM!

(a) (10) What is the value of  $\hat{f}_{n\text{-hexane}}$  that should be used for phase equilibria calculations?

(b) (5) Verify the value shown in cell I14 using the values from other cells in the spreadsheet.

5. (10) Suppose you were to solve problem 10.16 using the Peng-Robinson equation. Would a bubble P, dew P, bubble T, dew T, or isothermal flash be the routine you would choose to use? What would you use as the specified state variables and composition to obtain a solution?

6. (10) Consider problem 10.22. What type of calculation would prove that the container isn't 100% vapor? Be sure to provide the composition that you would use for the calculation.

7. Problem 11.34 presents data for the methanol(1) + benzene(2) system. At a temperature of 58.64°C the vapor pressures of the components are  $P_1^{sat} = 600$  mmHg and  $P_2^{sat} = 373.2$  mmHg.

(a) (10) Using the vapor pressures above and the data at  $x_1 = 0.333$ , fit the two-parameter Margules equation to the data from this single composition.

(b) (5) Determine the experimental value of  $G^E/RT$  at 58.64°C and  $x_1 = 0.333$ .

(c) (10) Use the results from part (a) to calculate the bubble pressure for a mixture with overall composition of 80% methanol.