Chapter 10 handout problems

Names: _____

1. \Excel\Virialmx.xls (pgs 320-322)

(a) Find the equations numbers from Chapter 6 programmed into cells C15:D16 . _____

(b) Equations for the cross coefficient from Chapter 10 are programmed into row 11. Find the cells that correspond to the given equations:

10.3, cell:_____; 10.4, cell: _____; 10.5, cell:_____, 10.6, cell: _____,10.7, cell: _____

(c) The programming is done using matrix multiplication, so 'looking' at some formulas does not necessarily help you 'reverse engineer' the sheet to find formulas in the text. It is better to find the cells that correspond to certain formulas. Cells F15:F17 represent the B_{ij} values. Use a hand calculation to verify that eq 10.2 is programmed into D24.

(d) Use a hand calculation to verify that eq. 10.13 is programmed into E24.

2. \PRMIX\PRMIX.exe

For the n-pentane(1) + n-hexane(2) + n-heptane(3) system the binary interaction parameters are k12=0.00076, k13 = 0.00171, k23 = 0.00061. (The components numbers in the PRMIX database are 7, 11, 17 respectively). The following table is for your results for parts (a) through (c) of the excercise:

	P(MPa)	x_1	x_2	x_3	y_1	y_2	y_3	K_1	K_2	K_3	V/F
(a)		0.097	0.3084	0.5946							0
(b)	0.5517										
(c)	0.5										
	0.6										
		0.15	0.34	0.51							0

(a) Use prmix.exe to calculate the bubble pressure at 420 K for a mixture of composition z_1 = 0.097, z_2 = 0.3084, z_3 = 0.5946. Also tabulate the values for y_i and K_i. (answer: 0.5517 MPa)

(b) Perform a flash at 420 K and P=0.5517 for z_1 = 0.15, z_2=0.34, z_3 = 0.51. Tabulate the x_i, y_i, and K_i values and compare with part (a). Record V/F. Comment on the results.

(c) Perform a flash at 420 K at the same composition as part (b) but at pressures 0.5, 0.6. Tabulate the x_i, y_i, K_i and V/F values. Also perform a bubble pressure calculation for the

composition in the last row and combine with the other results to comment on the trend of the K_i and V/F values with pressure. (This trend is generally followed except in the vicinity of a critical pressure, when the smallest K_i value curves up towards 1).

3. PRFUG.xls

Insert the values for parts 3(a) and 3(c) in the following table.

	f	$\hat{\varphi}_1$	$\hat{\varphi}_2$	$\hat{\varphi}_3$	$\hat{f}_1$	$\hat{f}_2$	$\hat{f}_3$
(a)							
(c)							

(a) Open PRFUG.xls. The sheet will open with the components and k_{ij} values used in PRMIX above. Insert the P, T, x_i and k_{ij} information from part (2a).

Tabulate the values for fugacity and fugacity coefficient in the in the table above.

(b) (skip this if you are short on time and come back later) Since $(G-G^{ig})/RT = \ln \varphi$ and also $(G-G^{ig}) = \Sigma x_i*(\mu_i-\mu^{ig}_i)$ and $(\mu_i-\mu^{ig}_i) = RT \ln \hat{\varphi}_i$, the combination should result in $\ln \varphi = \Sigma x_i \ln \hat{\varphi}_i$. Verify this calculation for the liquid phase by calculating $\ln f = \Sigma x_i \ln (\hat{f}_i / x_i)$ and comparing it to the value tabulated in the spreadsheet in E16. (There may be a slight difference due to truncation errors).

(c) Change the z_i to the vapor values found in part (2a). Record the mixture and component fugacity values found for the vapor phase in the table above. Compare the liquid and vapor fugacity values for the components and the mixture.

(d) Calculate the K_i values using fugacity coefficients ($\hat{\varphi}_i^L / \hat{\varphi}_i^V$). Compare to the values from part (2a) tabulated in the table for problem 2. Comment.

$K_1 =$ $K_2 =$ $K_3 =$

(e) Insert the P, T, x_i and k_{ij} information from part (2a). I21:I23 are pure component dimensionless parameters. K21:M23 is a matrix of A_{ij} values. Verify the value of A for the mixture (cell N13) using a hand calculation involving the A_{ij} values, $A = \sum_i \sum_j x_i x_j A_{ij}$ = =

x.1^2*A.1 + x.2^2*A.2 + x.3^2*A.3 + 2*x.1*x.2*A12 + 2*x.1*x.3*A13 + 2*x.2*x.3*A23

Solutions

1. Virial excercise

(a) 6.8-6.9
(b) C11, F11, G11, E11, D11
(c) $(0.3)^2(-0.92) + 2(0.3)(0.7)(-82.5) + (0.7)^2(-584.8) = -321.3$
(d) $\exp\{[2(0.3)(-0.92) + 2(0.7)(-82.51) + 321.3]0.1013/8.314/328\} = 1.0077$

2.

For the n-pentane(1) + n-hexane(2) + n-heptane(3) system the binary interaction…
Solution:
(a) Compounds 7,11,17

P = 0.5517 MPa, y1 = 0.2189, y2 = 0.3766, y3 = 0.4046,
K1 = 2.256, K2 = 1.221, K3 = 0.6804

(b) x1 = 0.097, x2 = 0.3098, x3 = 0.5936, y1 = 0.2178, y2 = 0.378, y3 = 0.404,
K1 = 2.256, K2 = 1.221, K3 = 0.6804. The coexisting compositions are the same because the Gibbs phase rule constrains the system since there are only two degrees of freedom, which are both the same as part (a).

(c)

P(MPa)	K1	K2	K3	V/F
0.5	2.47	1.33	0.74	0.93
0.5517	2.26	1.22	0.68	0.44
0.6	2.09	1.14	0.64	0.11
0.619	2.04	1.11	0.62	0.

The trend is for K to decrease with P.

3.

comparison of fugacities

	f	$\hat{\varphi}_1$	$\hat{\varphi}_2$	$\hat{\varphi}_3$	$\hat{f}_1$	$\hat{f}_2$	$\hat{f}_3$
(a)	0.434	2.075	1.073	0.5713	0.111	0.183	0.187
(c)	0.481	0.920	0.879	0.840	0.111	0.183	0.187

(a) values tabulated above.

Component	z_i	Tc (K)	Pc (MPa)	ω	kij n-pentane	kij n-hexane	kij n-heptane
n-pentane	0.097	469.7	3.369	0.249	-	-	-
n-hexane	0.3084	507.4	3.012	0.305	0.00076	-	-
n-heptane	0.5946	540.3	2.736	0.349	0.00171	0.00061	-

Current State		Roots			component fugacity coeff			component fugacity(MPa)		
T (K)	420	Z	V	fugacity	n-pentane	n-hexane	n-heptane	n-pentane	n-hexane	n-heptane
P (MPa)	0.5517		$cm^3/gmol$	MPa						
answers for three		0.83697	5297.444	0.47372404	0.92436726	0.87946335	0.8379282	0.049467	0.149636	0.2748747
root region		0.116961	740.2796							
		0.027379	173.2889	0.43379314	2.07516065	1.07276594	0.57127008	0.111052	0.182525	0.1873999

(b) Uisng fugacity coeffients:

$\ln \varphi = 0.097*\ln(2.075) + 0.3084*\ln(1.073) + 0.5946\ln(0.5712) = -0.2404$

$\varphi = 0.7863$, $f = \varphi P = 0.7863*0.5517 = 0.4338$ MPa. QED

Using fugacity:

$\ln f = 0.097*\ln(0.11105/0.097) + 0.3084*\ln(0.18253/0.3084) + 0.5946*\ln(0.1874/0.5946)$

$= -0.8352 \rightarrow f = 0.43379$ MPa. QED

(c)

					kij		
Component	z_i	Tc (K)	Pc (MPa)	†	n-pentane	n-hexane	n-heptane
n-pentane	0.2189	469.7	3.369	0.249	-	-	-
n-hexane	0.3766	507.4	3.012	0.305	0.00076	-	-
n-heptane	0.4045	540.3	2.736	0.349	0.00171	0.00061	-

Current State		Roots								
T (K)	420	Z	V	fugacity	component fugacity coeff			component fugacity(MPa)		
P (MPa)	0.5517		$cm^3/gmol$	MPa	n-pentane	n-hexane	n-heptane	n-pentane	n-hexane	n-heptane
answers for three		0.854194	5406.46	0.48076933	0.92038635	0.87851047	0.83968749	0.111152	0.182528	0.1873869
root region		0.101235	640.7503							
		0.026805	169.6593	0.52949988	2.05978287	1.07062802	0.57343046	0.248754	0.222445	0.1279683

(d) The component fugacities are the same, but the mixture fugacities are not.

$K_1 = 2.075/0.92 = 2.255$

$K_2 = 1.073/0.879 = 1.22$

$K_3 = 0.5713/0.84 = 0.68$

values are the same by fugacity ratio as by composition ratio. This is a converged result.

(e)

		A		
A	B	n-pentane	n-hexane	n-heptane
0.101355	0.014247	0.1013545	0.119446	0.137072
0.14098	0.017215	0.1194458	0.14098	0.161839
0.186011	0.02018	0.1370716	0.161839	0.186011

mixture	
A	0.1624387
B	0.0186904

$A = x.1^2*A.1 + x.2^2*A.2 + x.3^2*A.3 + 2*x.1*x.2*A12 + 2*x.1*x.3*A13 + 2*x.2*x.3*A23$

$= 0.097^2*0.101355 + 0.3084^2*0.14098 + 0.5946^2*.186011$

$+ 2*0.097*0.3048*0.11945 + 2*0.097*0.5946*0.13707 + 2*0.3084*0.5946*0.16184$

$= 0.1624$ QED