Quiz 10
Chemical Engineering Thermodynamics
April 9, 2015

1)

9.10 Estimate the fugacity of pure *n*-pentane (C_5H_{12}) at 97°C and 7 bar by utilizing the virial equation.

See equations/tables below.

2) **EXPLAIN HOW TO SOLVE.** (*Solve if you have time*)

P10.4 A mixture containing 15 mol% ethane, 35 mol% propane, and 50 mole% *n*-butane is isothermally flashed at 9 bar and temperature *T*. The liquid-to-feed ratio is 0.35. Use the shortcut *K*-ratio method to estimate the temperature and liquid and vapor compositions.

See equations/tables below.

3) **EXPLAIN HOW TO SOLVE.** (*Solve if you have time*)

10.3 The following mixture of hydrocarbons is obtained as one stream in a petroleum refinery on a mole basis: 5% ethane, 10% propane, 40% *n*-butane, 45% isobutane. Assuming the shortcut *K*-ratio model: (a) compute the bubble point of the mixture at 5 bar; (b) compute the dew point of the mixture at 5 bar; (c) find the amounts and compositions of the vapor and liquid phases that would result if this mixture were to be isothermally flash vaporized at 30°C from a high pressure to 5 bar.

See equations/tables below.

$$Z = 1 + (B^0 + \omega B^1)P_r/T_r \quad \text{or} \quad Z = 1 + BP/RT \qquad 7.6$$

$$\text{where } B(T) = (B^0 + \omega B^1)RT_c/P_c \qquad 7.7$$

$$B^0 = 0.083 - 0.422/T_r^{1.6} \qquad 7.8$$

$$B^1 = 0.139 - 0.172/T_r^{4.2} \qquad 7.9$$

$$\text{Subject to } T_r > 0.686 + 0.439P_r \text{ or } V_r > 2.0 \qquad 7.10$$

$$f = \varphi P \qquad 9.28$$

$$\ln \varphi = \frac{BP}{RT} \qquad 9.31$$

$$\ln \varphi = \frac{P_r}{T_r}(B^0 + \omega B^1) \qquad 9.32$$

$$V^{satL} = V_c Z_c^{(1-T_r)^{0.2857}}$$ 9.40

$$f = \varphi^{sat} P^{sat} \exp\left(\frac{V^L (P - P^{sat})}{RT}\right)$$ 9.39

$$K_i = \frac{P_i^{sat}}{P}$$ or $$y_i P = x_i P_i^{sat}$$ 10.6

$$K_i = \frac{P_i^{sat}}{P} \approx \frac{P_{c,i} 10^{\frac{7}{3}(1+\omega)\left(1-\frac{1}{T_{r,i}}\right)}}{P}$$ Shortcut K-ratio 10.7

$$x_i = \frac{z_i}{1 + (V/F)(K_i - 1)}$$ 10.15

$$y_i = \frac{z_i K_i}{1 + (V/F)(K_i - 1)}$$ 10.16

$$\sum_i x_i - \sum_i y_i = \sum_i (x_i - y_i) = \sum_i D_i = 0$$

For a **bubble-temperature** calculation, writing $\sum_i y_i = 1$ as $\sum_i K_i x_i = 1$

For a **dew-temperature** calculation, writing $\sum_i x_i = 1$ as $\sum_i (y_i / K_i) = 1$

$$\sum_i x_i - \sum_i y_i = \sum_i D_i = \sum_i \frac{z_i(1 - K_i)}{1 + (V/F)(K_i - 1)} = 0$$ 10.23

R = 8.314 MPa cm³/(mole K°)

PROPERTIES OF SELECTED COMPOUNDS

Heat capacities are values for ***ideal gas at 298 K*** *and should be used for* ***order of magnitude calculations*** *only. See appendices for temperature-dependent formulas and constants.*

ID	Compound	T_c (K)	P_c (MPa)	ω	ρ g/cm³	MW	C_P^{ig}/R	δ (J/cm³)^½	α (J/cm³)^½	β (J/cm³)^½
Aliphatics										
1	METHANE	190.6	4.604	0.011	*0.29*	16	4.30	11.7	0	0
2	ETHANE	305.4	4.880	0.099	*0.43*	30	6.31	13.5	0	0
3	PROPANE	369.8	4.249	0.152	*0.58*	44	8.85	13.1	0	0
4	*n*-BUTANE	425.2	3.797	0.193	*0.60*	58	11.89	13.5	0	0
5	ISOBUTANE	408.1	3.648	0.177	*0.55*	58	11.70	12.5	0	0
7	*n*-PENTANE	469.7	3.369	0.249	0.62	72	14.45	14.3	0	0
8	ISOPENTANE	460.4	3.381	0.228	0.62	72	14.28	13.9	0	0
9	NEOPENTANE	433.8	3.199	0.196	0.60	72	14.62	13.1	0	0
11	*n*-HEXANE	507.4	3.012	0.305	0.66	86	17.21	14.9	0	0
17	*n*-HEPTANE	540.3	2.736	0.349	0.68	100	19.95	15.3	0	0
27	*n*-OCTANE	568.8	2.486	0.396	0.70	114	22.70	15.5	0	0
27	ISOOCTANE	544.0	2.570	0.303	0.70	114	22.50	14.1	0	0
46	*n*-NONANE	595.7	2.306	0.437	0.71	128	25.45	15.6	0	0
56	*n*-DECANE	618.5	2.123	0.484	0.73	142	28.22	15.7	0	0
64	*n*-DODECANE	658.2	1.824	0.575	0.75	170	33.71	15.9	0	0
66	*n*-TETRADECANE	696.9	1.438	0.570	0.76	198	39.22	16.1	0	0
68	*n*-HEXADECANE	720.6	1.419	0.747	0.77	226	44.54	16.2	0	0

E.3 ANTOINE CONSTANTS

The following constants are for the equation

$$\log_{10} P^{sat} = A - \frac{B}{T + C}$$

where P^{sat} is in mmHg, and T is in Celsius. Additional Antoine constants are tabulated in Antoine.xls.

	A	B	C	T range (°C)	Source
Acetic acid	8.02100	1936.01	258.451	18–118	a
Acetic acid	8.26735	2258.22	300.97	118–227	a
Acetone	7.63130	1566.69	273.419	57–205	a
Acetone	7.11714	1210.595	229.664	−13–55	a
Acrolein (2-propenal)	8.62876	2158.49	323.36	2.5–52	b
Benzene	6.87987	1196.76	219.161	8–80	a
Benzyl chloride	7.59716	1961.47	236.511	22–180	b
Biphenyl (solid)	13.5354	4993.37	296.072	20–40	c
1-Butanol	7.81028	1522.56	191.95	30–70	d
1-Butanol	7.75328	1506.07	191.593	70–120	d
2-Butanone	7.28066	1434.201	246.499	−6.5–80	b
Chloroform	6.95465	1170.966	226.232	−10–60	a
Ethanol	8.11220	1592.864	226.184	20–93	a
Hexane	6.91058	1189.64	226.28	−30–170	a
1-Propanol	8.37895	1788.02	227.438	−15–98	a
2-Propanol	8.87829	2010.33	252.636	−26–83	a
Methanol	8.08097	1582.271	239.726	15–84	a
Naphthalene (solid)	8.62233	2165.72	198.284	20–40	e
Pentane	6.87632	1075.78	233.205	−50–58	a
3-Pentanone	7.23064	1477.021	237.517	36–102	a
Toluene	6.95087	1342.31	219.187	−27–111	a
Water	8.07131	1730.63	233.426	1–100	a

Answers Quiz 10
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1)

9.10 Estimate the fugacity of pure *n*-pentane (C_5H_{12}) at 97°C and 7 bar by utilizing the virial equation.

9.10) Estimate the fugacity of pure n-pentane…

From the Antoine equation at 97 C, the vapor pressure is 4135 mmHg/750 = 5.5 bar = 0.55 MPa

Therefore, the fugacity will be given by

$f = f^{sat} \exp(V^L(P - P^{sat})/RT) = \varphi^{sat} P^{sat} \exp(V^L(P - P^{sat})/RT)$

$\varphi^{sat} = \exp(BP^{sat}/RT)$

The virial equation can be calculated using Eqn. 6.9-6.10 at 370.15 K

B^0	B^1	BP_c/RT_c	$B(cm^3/mol)$
-0.535	-0.329	-0.617	-714.73

$\varphi^{sat} = \exp(-714.73*0.55/8.314/370.15) = 0.880 \Rightarrow f^{sat} = 0.55*0.88 = 0.484$ MPa

V^L from Rackett correlation (Eqn. 8.37) = $V_c Z_c^{(1-Tr)^{0.2857}} = 311.8(0.269)^{(1-0.788)^{0.2857}} = 134\ cm^3/mol$

$f = 0.484*\exp(134(0.7 - 0.55)/8.314/370.15) = 0.487$ MPa

2)

P10.4 A mixture containing 15 mol% ethane, 35 mol% propane, and 50 mole% *n*-butane is isothermally flashed at 9 bar and temperature *T*. The liquid-to-feed ratio is 0.35. Use the shortcut *K*-ratio method to estimate the temperature and liquid and vapor compositions.

(P10.04) A mixture containing 15 mol% ethane, 35% propane, and 50% n-butane is isothermally flashed at 9 bar and T. the liquid-to-feed ratio is 0.35. Use the shortcut K-ratio method to estimate the pressure and liquid and vapor compositions.

By short-cut vapor pressure eqn.

$$\frac{y_i}{x_i} = K_i \cong \frac{\left[10\wedge\left[\frac{7}{3}(1+\omega_i)\left(1-\frac{1}{T_{?,i}}\right)\right]\right]}{P_{r,i}}$$

$$y_i = x_i K_i$$

For the isothermal flash calculation, the P=9 bar. Equation 10.23 is programmed in the cells below the value of L/F=0.35 below the 'Flash' title. Each row holds the value of the term '$D_i = z_i(1-K_i)/[K_i + (L/F)(1-K_i)]$' from equation 10.23. The value of K_i requires T which is to the left under the 'Flash' title. These values of D_i are summed at the bottom of the column. The criteria for the isothermal flash is that T is adjusted until the sum goes to zero, as is shown at T = 319.4K. Once the value of T is found, the xi values and yi values in the last columns are generated separately using equations 10.15 and 10.16 respectively.

Though not required, the table below also shows the bubble T and dew T calculations for P = 0.9 MPa.

For the bubble calculations, in each column, the temperature at the top of the column is used to calculate the K-ratio. Then $y_i = x_i K_i$. The temperature is adjusted until the sum of y's is unity. This is an iterature calculation.

For the dew T calculations, in each column, the temperature at the top of the column is used to calculate the K-ratio. Then $x_i = y_i/K_i$. The temperature is adjusted until the sum of x's is unity. This is an iterative calculation.

pMPa=	0.900				BUBT		DEWT		FLASH			
	z	Tc	Pc	w	290	y	326.9	x	319.4	0.35	x	y
C1	0	190.6	4.6	0.011	32.92	0.000	49.257	0.000	45.74	0	0.000	0.000
C2	0.15	305.4	4.88	0.099	3.963	0.594	7.9952	0.019	7.027	-0.184	0.031	0.214
C3	0.35	369.8	4.25	0.152	0.86	0.301	2.0955	0.167	1.779	-0.181	0.232	0.413
nC4	0.5	425.2	3.8	0.193	0.213	0.106	0.614	0.814	0.505	0.3648	0.737	0.372
						1.0016		1.0002		6E-08	1.000	1.000

Equation 7.7 given below with other useful expressions.

3)

10.3 The following mixture of hydrocarbons is obtained as one stream in a petroleum refinery on a mole basis: 5% ethane, 10% propane, 40% *n*-butane, 45% isobutane. Assuming the shortcut *K*-ratio model: (a) compute the bubble point of the mixture at 5 bar; (b) compute the dew point of the mixture at 5 bar; (c) find the amounts and compositions of the vapor and liquid phases that would result if this mixture were to be isothermally flash vaporized at 30°C from a high pressure to 5 bar.

(10.03) The following mixture of hydrocarbons …

a) By short-cut vapor pressure eqn.

$$\frac{y_i}{x_i} = K_i \equiv \frac{\left[10^\wedge\left[\frac{7}{3}(1+\omega_i)\left(1-\frac{1}{T_{r,i}}\right)\right]\right]}{P_{r,i}}$$

$y_i = x_i K_i$

Find T when $\sum_i y_i \equiv \sum_i x_i K_i = 1$

For given liquid composition, at $P = 0.5$ MPa

Bubble point temperature = 293.376 K

OR

By Antoine Vapor Pressure Equation,

$$y_i = x_i \frac{P_i^{sat}}{P} \; ; \; P_i^{sat} = 10^\wedge\left[A_i - \frac{B_i}{T+C_i}\right]$$

Find T when $\sum y_i = 1$

A_i, B_i, C_i from tabulated in appendix or ACTCOEFF.xls

bubble point temperature = 294.68 K

b) Dew Point

Short-cut method: $x_i = \frac{y_i}{K_i}$

Find T when $\sum x_i = 1$

$T_{dew.pt} =$ 312.479 K

Dew pt. By Antoine Eqn, $x_i = y_i \frac{P}{P_i^{sat}}$.

Find T when $\sum x_i = 1$

$T_{dew.pt} =$ 313.116 K

c) Isothermal Flash

Shortcut	L/F	Antoine
L/F = 0.827		L/F = 0.852
$x = 0.02047$ $y = 0.19122$	ethane	$x = 0.02336$ $y = 0.20341$
$x = 0.08305$ $y = 0.18100$	propane	$x = 0.085735$ $y = 0.182122$
$x = 0.43173$ $y = 0.24829$	n-butane	$x = 0.42751$ $y = 0.24166$

$x = 0.46475$ iso-butane $x = 0.46340$

$y = 0.37949$ $y = 0.37281$

N.B: Choose the initial guess for L/F as between zero and unity.

Summary of shortcut calculations:

Problem 10.3				Part (a)		Part (b)		Part c	
				BUBT		DEWT		FLASH	
				293.376 =T		312.479 =T		303.15 =T	
								L/F=	0.826613
	Tc	Pc	w	K	y	K	x	K	
0.05	305.4	48.8	0.099	7.662148	0.383107	11.15689	0.004482	9.341512	-0.17049
0.1	369.8	42.49	0.152	1.694715	0.169471	2.730432	0.036624	2.179405	-0.09792
0.4	425.2	37.97	0.193	0.426258	0.170503	0.752168	0.531796	0.575108	0.183473
0.45	408.1	36.48	0.177	0.615371	0.276917	1.053624	0.427097	0.817164	0.08497
					0.999999		1		3.47E-05

Comparing with the PREOS, PREOS⇒: a)298K (b) 312K (c) L/F=.874, K={6.1,1.9,.61,.83}