Final

Josh Whitehead
ChEn 3853

1) a) $k_a = 0.0246 \boxed{= 2.46\times10^{-2}}$

b.) $n_C^i = 1$

$n_{H_2O}^i = 1$

$n_{CO}^i = n_{H_2}^i = 0$

$n_C^f = n_i^i + v_i \xi = 1 - \xi$

$n_{H_2O}^f = 1 - \xi$

$n_{CO}^f = \xi$

$n_{H_2}^f = \xi$

$$K_a = \Pi y_i = \left(\frac{\xi}{\cancel{1+\xi}}\right)^2 \frac{\cancel{1+\xi_1}}{1-\xi_1} = \frac{\xi^2}{(1-\xi_1)^2} = 2.46\times10^{-2}$$

$\rightarrow \xi = 0.135$

$n_{CO}^f = n_{CO}^i + \nu_{CO}\xi = \xi = 0.135$

$n_C^f = 1 - \xi = 0.865$

$$\frac{n_{CO}^f}{n_C^i} = 0.135 \boxed{= 13.5\% \text{ Converted}}$$

p1_Kcalc - Excel

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L19

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Stoichiometric Number	Name	$\Delta H^o_{f,298}$ (kJ/mol)	$\Delta G^o_{f,298}$ (kJ/mol)	Constants for C_P in J/mol-K: a	b	c	d
-1	CARBON	0	0	-3.958	5.586E-02	-4.548E-05	1.517E-08
-1	H2O (g)	-241.835	-228.614	32.24	1.924E-03	1.055E-05	-3.596E-09
1	CO (g)	-110.53	-137.16	30.87	-1.285E-02	2.789E-05	-1.272E-08
1	H2 (g)	0	0	27.14	9.274E-03	-1.381E-05	7.645E-09

enter all species above line 14

Reaction T(K)	780
ΔH^o_T (kJ/mol)	135.503
ΔG^o_T (kJ/mol)	24.019
$\ln K_a$	-3.703620916
K_a	0.024634167

Intermediate Calculations, J and I defined in text

Δa	Δb	Δc	Δd
29.728	-6.136E-02	4.901E-05	-1.665E-08

R (kJ/mol-K)	0.0083145
ΔH^o_{298} (kJ/mol)	131.305
ΔG^o_{298} (kJ/mol)	91.454
$\ln K_{a,298}$	-36.892086
J (kJ/mol)	124.76876
I	5.9152294

Instructions | Ka Calculator | Rev.

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2.) a.) $y_i P = x_i \gamma_i P_i^{sat}$

Margule - 1 : $\gamma_1 = \exp(x_2^2 A)$

$\gamma_2 = \exp(x_1^2 A)$

@ azeotrope: $\frac{K_1}{K_2} = \frac{\frac{y_1}{x_1}}{\frac{y_2}{x_2}} = 1$

$\therefore \frac{y_1}{x_1} = \frac{\gamma_1 P_1^{sat}}{P}$ $\quad \frac{y_2}{x_2} = \frac{\gamma_2 P_2^{sat}}{P}$

$\therefore \frac{\gamma_1 P_1^{sat}}{\cancel{P}} = \frac{\gamma_2 P_2^{sat}}{\cancel{P}}$ $\quad \frac{\gamma_1}{\gamma_2} = \frac{P_2^{sat}}{P_1^{sat}} = \frac{3.17}{5.62}$

$\therefore \frac{\exp(x_2^2 A)}{\exp(x_1^2 A)} = \frac{3.17}{5.62}$

$\boxed{A = 1.74}$

---

b.) ~~$\gamma_2 = \exp(0.6$~~ $\gamma_1 = \exp(0.4^2 \cdot 1.74) = 1.32$

$\gamma_2 = \exp(0.6^2 \cdot 1.74) = 1.86$

~~$y_i P = x_i P_i^{sat}$~~ $\quad P = \sum x_i \gamma_i P_i^{sat} = \underbrace{0.6 \cdot 1.32 \cdot 5.62 + 0.4 \cdot 1.86 \cdot 3.1}$

$\boxed{P = 6.82 \text{ kPa}}$

$y_1 = \frac{x_1 P_1^{sat} \gamma_1}{P} = \frac{0.6 \cdot 5.62 \cdot 1.32}{6.82} = \boxed{y_1 = 0.653}$

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3)

$$K_w = \frac{[OH^-][H^+]}{[H_2O]} = 10^{-14}$$

$$K_{H_2CO_3} = \frac{[H^+][HCO_3^-]}{[H_2CO_3]} = 10^{-6.35}$$

$$K_{HCO_3^-} = \frac{[CO_3^{2-}][H^+]}{[HCO_3^-]} = 10^{-10.33}$$

$$A = [H^+] + [Cl^-] = 6M$$

$$[H^+] = [OH^-] + [HCO_3^-] + [CO_3^{2-}] \cdot 2$$

$$[NaHCO_3] = x$$

$$[H^+] = \frac{[H_2O]10^{-14}}{[H^+]} + \frac{[H_2CO_2]10^{-6.35}}{[H^+]} + \cancel{\frac{[CO_3^{2-}][H^+]}{10^{-10.33}}} + 2\frac{10^{-10.33}[HCO_3^-]}{[H^+]}$$

$$y_i P = x_i h_i \quad \therefore \cancel{[H_2CO_3]}$$

$$10^{-7} \approx [H_2O]10^{-7} + [H_2CO_2]10^{+1.65} + 2[HCO_3^-]10^{-3.33}$$

$$10^{-1.47} = \frac{[H_2CO_3^*]}{y_{CO_2}P} \Rightarrow [H_2CO_3^*] = 10^{-1.47} \cdot 0.0004 \cdot 1 = \underline{1.36 \times 10^{-5}}$$

$$[H_2CO_3] \approx \frac{10^{-6.35} \cdot 1.36 \times 10^{-5}}{10^{-7}} = 6.054 \times 10^{-5}$$

Next Page

3 cont

$$[HCO_3^-] = \frac{10^{-6.35}\,[H_2CO_3]}{[H^+]} = 0.00027 \frac{mol}{L}$$

$$= 2.70 \times 10^{-4} \text{ mol}$$

$$\times 84 \;\; \boxed{= 2.27 \times 10^{-2} \text{ g}}$$

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4) a.) ΔH = heat input $= 50.0\ kJ$ (closed)

b.) $T_f = 415.\ K$

p4_Preos_npentane - Excel

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Peng-Robinson Equation of State (Pure Fluid)				Spreadsheet protected, but no password used.
Properties				
Gas	T_c (K)	P_c (MPa)	ω	Enter Name and Critical Properities on "Props" Worksheet.
n-PENTANE	469.7	3.369	0.249	

Reference State		For real fluid reference state identifier index	Roots Z	V cm^3/gmol	fugacity MPa	$H-H^{ig}$ J/mol	$U-U^{ig}$ J/mol	$S-S^{ig}$ J/molK	
T (K)	250								
P (MPa)	0.101325								
0 for H_R = 0, 1 for U_R = 0		1	0.930226	19083	0.094705	-370.825	-225.792	-0.9214	answers for three root region
0			0.060234	1235.668					
0 for ig, 1 for real fluid ref		2	0.005144	105.5171	0.007879	-28484.5	-26416.5	-92.6871	
1		3	#NUM!	#NUM!	#NUM!	#NUM!	#NUM!	#NUM!	& for 1 root region

Identifier Index for reference state row to use from Row 9 - Row 12 (Enter 1, 2, or 3)

YOU MUST CHOOSE A ROW WITH CALCULABLE NUMBERS, NOT ONE WITH #NUM!

2

4b ref

	Z	H(J/mol)	U(J/mol)	S(J/molK)
Reference State Values	0.005144	0	-10.6915	0
Ref State Departures		-28484.5	-26416.5	-92.6871

Solution to Cubic $Z^3 + a_2Z^2 + a_1Z + a_0 = 0$

a_2	a_1	a_0	p	q
-0.995604	0.06112599	-0.00029	-0.26928	-0.0531

$R = q^2/4 + p^3/27 =$ -1.8E-05

If Negative, three unequal real roots,

If Positive, one real root

Instructions | PVT | Props | Ref State | Crit. Props | IG Cps | rev. info p4_Preos_npentane - Excel

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M16

Peng-Robinson Equation of State (Pure Fluid)

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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)	ω	A	B	C	D	values	J/mol	J/mol	J/molK
n-PENTANE	469.7	3.369	0.249	-3.626	4.87E-01	-2.58E-04	5.31E-08		21685.43	20312.98	65.42539

Current State		Roots		Stable Root has a lower fugacity						
T (K)	415.067124	Z	V	fugacity	H	U	S	$H-H^{ig}$	$U-U^{ig}$	$S-S^{ig}$
P (MPa)	0.101325		cm^3/gmol	MPa	J/mol	J/mol	J/molK	J/mol	J/mol	J/molK
answers for three root region		0.9832661	33489.408	0.099652	50000	46606.69	157.8415	-169.902	-112.152	-0.27092
		0.0092838	316.19928		37160.1	37128.06	107.1618	-13009.8	-9590.78	-50.9507
		0.0048024	163.56563	1.019562	30412.02	30395.45	91.31439	-19757.9	-16323.4	-66.7981
& for 1 root region		#NUM!	#NUM!	#NUM!	#NUM!	#NUM!	#NUM!	#NUM!	#NUM!	#NUM!
				fugratio						
				0.09774						

4b

If thermodynamic property calculations give a #NUM! error for both root regions in the table above, fix the "reference state index indentifier" on "Ref State" page.

Solution to Cubic $Z^3 + a_2Z^2 + a_1Z + a_0 = 0$

a_2	a_1	a_0	p	q
-0.99735226	0.01389501	-4.38E-05	-0.3176755	-0.06891

$R = q^2/4 + p^3/27 =$ -1.7E-07

If Negative, three unequal real roots,

If Positive, one real root

Intermediate Calculations			
R(cm^3MPa/molK)	8.314472		
T_r	0.883686	a (MPa cm^6/gmol^2)	
P_r	0.030076	2258142	
κ	0.741927	b (cm^3/gmol)	
α	1.090942	90.18035	
		A	0.019212
		B	0.002648

Method 1 - For region with one real root

P	Q	Root to equation in x
#NUM!	#NUM!	#NUM!

Method 2 - For region with three real roots

m	3q/pm	3*0	0	Roots to equation in x

Instructions | PVT | Props | Ref State | Crit. Props | IG Cps | rev. info

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5) @ 315.15 K and 10 mPa $V = 84.1 \frac{cm^3}{mol}$

$= 0.0841 \frac{L}{mol}$

$n = 50\cancel{L} \cdot \frac{1\,mol}{0.0841\,\cancel{L}}$

$\boxed{= 594.\ mol}$

b.) when $\frac{f^L}{f^V} = 1$ $\boxed{P = 4.49\ MPa}$

P @ 10°C < P @ 42°C

p5_Preos_CO2 - Excel

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Peng-Robinson Equation of State (Pure Fluid)

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Properties			
Gas	T_c (K)	P_c (MPa)	ω
RBON DIOX	304.2	7.382	0.228

Current State		Roots		
T (K)	315.15	Z	V	fugacity
P (MPa)	10		cm^3/gmol	MPa
answers for three root region		#NUM!	#NUM!	#NUM!
		#NUM!	#NUM!	
		#NUM!	#NUM!	#NUM!
& for 1 root region		0.32110539	84.13944	5.783614

Stable Root has a lower fugacity

Intermediate Calculations			
R(cm^3MPa/molK)		8.314472	
T_r	1.035996	a (MPa cm^6/$gmol^2$)	
P_r	1.354646	386230.9	
κ	0.712244	b (cm^3/gmol)	
α	0.97475	26.65493	
fugacity ratio		A	0.562527
	#NUM!	B	0.101724

0.084139

594.2517

To find vapor pressure, or saturation temperature, see cell A28 for instructions

5a

Solution to Cubic $Z^3 + a_2Z^2 + a_1Z + a_0 = 0$

a_2	a_1	a_0	p	q
-0.89828	0.328034	-0.045822224	0.059068	-0.00129

$R = q^2/4 + p^3/27 =$ 8.05E-06

If Negative, three unequal real roots,

If Positive, one real root

Method 1 - For region with one real root

P	Q	Root to equation in x
0.151576	-0.1299	0.021680229

Solution methods are summarized in the appendix of the text.

Method 2 - For region with three real roots

m	3q/pm	3*θ_1	θ_1	Roots to equation in x		
#NUM!	#NUM!	#NUM!	#NUM!	#NUM!	#NUM!	#NUM!

To find vapor pressure, use solver to vary B8 (P)

to find where target cell H12 = 1, for any T < T_c

Instructions PVT Props Ref State Crit. Props IG Cps rev. info

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p5_Preos_CO2 - Excel

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Peng-Robinson Equation of State (Pure Fluid)

Spreadsheet protected, but no password used.

Properties			
Gas	T_c (K)	P_c (MPa)	ω
RBON DIOX	304.2	7.382	0.228

Current State		Roots		
T (K)	283.15	Z	V	fugacity
P (MPa)	4.493669		cm^3/gmol	MPa
answers for three		0.617901944	323.7201	3.258279
root region		0.229118321	120.0356	
		0.102102043	53.49147	3.258276
& for 1 root region		#NUM!	#NUM!	#NUM!

Stable Root has a lower fugacity

Intermediate Calculations			
R(cm^3MPa/molK)		8.314472	
T_r	0.930802	a (MPa cm^6/gmol^2)	
P_r	0.608733	416364	
κ	0.712244	b (cm^3/gmol)	
α	1.050798	26.65493	
fugacity ratio		A	0.337576
	1.000001	B	0.050878

To find vapor pressure, or saturation temperature, see cell A28 for instructions

5b

Solution to Cubic $Z^3 + a_2Z^2 + a_1Z + a_0 = 0$

a_2	a_1	a_0	p	q
-0.94912	0.228055	-0.014454857	-0.07222	-0.00564

$R = q^2/4 + p^3/27 =$ -6E-06

If Negative, three unequal real roots,
If Positive, one real root

Method 1 - For region with one real root

P	Q	Root to equation in x
#NUM!	#NUM!	#NUM!

Solution methods are summarized in the appendix of the text.

Method 2 - For region with three real roots

m	3q/pm	3*θ_1	θ_1	Roots to equation in x		
0.310317	0.754622	0.715717801	0.238573	0.301528	-0.08726	-0.21427

To find vapor pressure, use solver to vary B8 (P)
to find where target cell H12 = 1, for any T < T_c

Instructions | PVT | Props | Ref State | Crit. Props | IG Cps | rev. info

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