Solution

ChE 3063 **Final** **December 13, 2017**

Open Books and Notes

Your Name:________________________

answer questions and turn back in with your solution. Attach further work as needed.

I. 30 points

It is proposed to clean the oxide layer off of tungsten wire by heating it in hydrogen gas at 1 bar of pressure at 800°K. The reaction would be:

$WO_2\,(s) + 2\,H_2\,(g) \rightarrow W(s) + 2\,H_2O\,(g)$

You can use the following free energies for your calculations:

WO_2 (s) : ΔG^0_f (J/mole) = -550,640 + 153.14 T (T in Kelvin)
H_2O (g) ΔG^0_f (J/mole) = -246,449 + 54.81 T (T in Kelvin)

based upon the elements in their standard states at 1 bar pressure.

A) 10 points
Can this process work? ☑**Yes** ☐**No**

B) 20 points
What is the maximum water vapor partial pressure that can exist in the hydrogen for it to work?
0.1514 **bar**

II. 10 points

Suppose we have a series of reactions that add to an overall reaction:

$$\begin{array}{lll} & A + B \rightarrow C + D & K_{a1} \\ & C + D \rightarrow E + F & K_{a2} \\ & E + F \rightarrow G + H & K_{a3} \\ & G + H \rightarrow I + J & K_{a4} \\ + & \overline{\hspace{6em}} & \\ & A + B \rightarrow I + J & K_{a5} \end{array}$$

$K_{a1} = \frac{C*D}{A*B}$

$K_{a2} = \frac{E*F}{C*D}$

$K_{a3} = \frac{G*H}{E*F}$

$K_{a4} = \frac{I*J}{G*H}$

$K_{a1}K_{a2}K_{a3}K_{a4} = \frac{I*J}{A*B} = K_{a5}$

A) 5 points
How is K_{a5} related to the other K_a's?

$K_{a5} = K_{a1}K_{a2}K_{a3}K_{a4}$ **(write your answer here).**

B) 5 points
How many independent reactions are there? 4 **Independent Reactions**

II. 30 points

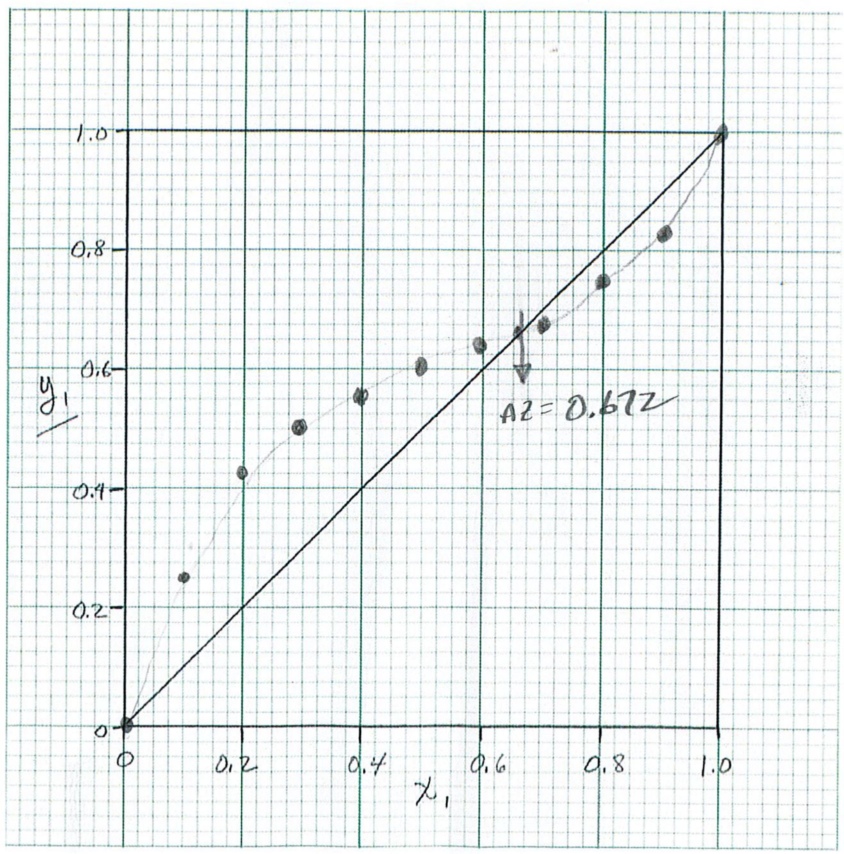
For the system n-hexane (1)/ methyl ethyl ketone (2) at 60°C, Van Laar constants are A = 1.1347, B = 1.2677 for the Van Laar equations in this form:

$$\ln(\gamma_1) = \frac{A}{\left(1+\frac{Ax_1}{Bx_2}\right)^2} \qquad \ln(\gamma_2) = \frac{B}{\left(1+\frac{Bx_2}{Ax_1}\right)^2}$$

A)

A) 10 points

For this system, plot y_1 vs x_1 below. Provide enough data points so you can determine if there is an azeotrope.



B) 10 points

Estimate the composition of the azeotrope: $0.672 = x_1 = y_1$

C) 10 points

What is the pressure of the azeotrope? 78.1 **kPa**

You may assume the vapor above the liquid is an ideal gas.

III. 30 points

Find the fugacity of the individual components in a chloroform (1)/dichloromethane (2) mixture at 400°C and 80 bar. The composition of the mixture is 60 mole% (1)/ 40 mole% (2). Use good practice in evaluating the fugacities, and note your assumptions. Poor assumptions will result in less than 100% credit.

f_1= 63.81 **bar**

f_2= 67.55 **bar**

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I $WO_2(s) + 2H_2(g) \longrightarrow W(s) + 2H_2O(g)$

$T = 800°K$

$G^\circ_{f,WO2} = (-550,640 + 153.14T) \times -1$ T in K

$G_{f,H2} = 0$ G in J/mole

$G^\circ_{f,W} = 0$

$G^\circ_{f,H2O} = (-246,449 + 54.81T) \times 2$

$\Delta G^\circ_R = 57742 - 43.52T$

at $T = 800K$

$\Delta G^\circ_{R,800} = 22926$ J/mole

$$K_a = \exp\left(\frac{-22926 \text{ J/mole}}{8.314 \text{ J/m K} \cdot 800 K}\right) = 0.03184$$

$$K_a = \frac{\cancel{a_W}\, a_{H2O}^2}{a_{H2}^2\, \cancel{a_{WO2}}} = \frac{f_{H2O}^2}{f_{H2O}^2}$$

$$K_a = \frac{y_{H_2O}^2}{y_{H_2}^2} = 0.03184$$

$$\frac{y_{H2O}}{y_{H2}} = 0.1784 = \frac{1 - y_{H2}}{y_{H2}}$$

$$\left.\begin{aligned} y_{H2} &= 0.8486 \\ y_{H2O} &= 0.1514 \end{aligned}\right\} @ P = 1\text{bar}$$

$$\boxed{P_{H2O} = 0.1514 \text{ bar}}$$

II. $K_{a1} K_{a2} K_{a3} K_{a4} = K_{a5}$

A	1.1347		Antoine Constants			
B	1.2677			A	B	C
T(ºC)	60		n-hexane	13.8193	2696.04	224.317
T(K)	333.15		MEK	14.1334	2838.24	218.69
P1s (kPa)	76.46138					
P2s (kPa)	51.89285					

x1	x2	gamma 1	gamma 2	P (kPa)	y1	y2
0					0	
0.1	0.9	2.557	1.010	66.73909	0.2929	0.7071
0.2	0.8	2.133	1.043	75.93477	0.4296	0.5704
0.3	0.7	1.809	1.102	81.53658	0.5089	0.4911
0.4	0.6	1.561	1.194	84.89642	0.5622	0.4378
0.5	0.5	1.372	1.327	86.86288	0.6037	0.3963
0.6	0.4	1.230	1.517	87.89273	0.6419	0.3581
0.7	0.3	1.126	1.785	88.07997	0.6844	0.3156
0.8	0.2	1.056	2.170	87.08692	0.7414	0.2586
0.9	0.1	1.014	2.727	83.92493	0.8314	0.1686
1					1.0000	

0	0
1	1

$x_1^{Az} = 0.672$

$P = x_1 \gamma_1 P_1^s + x_2 \gamma_2 P_2^s$

Azeotrope

x1	x2	gamma 1	gamma 2	P (kPa)	y1	y2
0.672	0.328	1.152	1.700	88.12255	0.6716	0.3284

T (ºC)	400
T (K)	673
P (bar)	80.000
virial coefficients	
B_{11} (cm^3/mole)	-158.442
B_{22} (cm^3/mole)	-119.106
B_{12} (cm^3/mole)	-137.706
δ_{12}	2.135993
y_1	0.600
y_2	0.400

	Tc (K)	Pc (bar)	omega	Vc (cm3/mole)	Zc
chloroform (1)	536.4	54.72	0.222	239.00	0.293
dichloromethane(2)	510.0	60.80	0.199	185.00	0.265
interaction	523.0	57.54	0.211	210.84	0.279

	Tr	B0	B1	Pr
chloroform (1)	1.255	-0.2105	0.0727	1.462
dichloromethane(2)	1.320	-0.1878	0.0853	1.316
interaction	1.287	-0.1989	0.0793	

ϕ_1	0.7977	$\phi_1 = \exp (P /RT * (B_{11} + y_2^2 * \delta_{12}))$
ϕ_2	0.8443	$\phi_2 = \exp (P /RT * (B_{22} + y_1^2 * \delta_{12}))$

f1 (bar)	~~63.81449~~	38.29
f2 (bar)	~~67.54761~~	27.02