Tutorial sheet 2

Q.1/ Assuming that ΔH is independent of temperature for the following pyrolysis reaction :$C_2H_6 = C_2H_4 + H_2$

1) Estimate the fractional conversion at 1000^oC and 1.5 atm

Component	ΔG^o_{298}(kJ/mol)	ΔH^o_{298}(kj/mol)	Cp(kJ/mol.K)
C_2H_6	-32.886	-84.667	$0.0096+8.73X10^{-5}T$
C_2H_4	68.124	52.3	$0.0117+12.5X10^{-5}T$
H_2	0	0	$0.0289+1.67X10^{-5}T$

Q.2/ A stoichiometric mixture of N2 and H2 is to be brought to equilibrium at 600 atm pressure for the reaction $1/2N_2 + 3/2H_2 = NH_3$, at 373 K. the equilibrium constant $K=3.4x\ 10^{-3}$, from the thermodynamic data. Estimate the fractional conversion assuming 1) ideal gas mixture 2) non - ideal gas.

Q.3/ The equilibrium constant for the reaction SO2 + 1/2 O2 =SO3 at 1000 K is Kp= 1.85.What is the ration P_{SO3} / P_{SO2}:
a) when the partial pressure of oxygen at equilibrium is 0.3 bar.
b) a) when the partial pressure of oxygen at equilibrium is 0.6 bar.

Q.4/ A gaseous mixture containing 60%H_2 , 20%N_2 and 20% inert gas is passed over a catalyst at 500atm pressure to produce ammonia. Estimate the maximum conversion if $K_p = 0.0125$ for the reaction $N_2 + 3H_2 = 2NH_3$, and the system behaves ideally.

Q.5/ at 400 ^oC and total pressure of 10 atm, ammonia is dissociated to extent of 98%. Calculate K_p , K_y and K_c for the reaction $2NH_3 = N_2 + 3H_2$.

Q.6/ one method for the production of hydrogen cyanide is by the gas phase nitrogenation of acetylene according to the reaction

$$N_{2\,(g)} + C_2H_{2(g)} \longrightarrow 2HCN_{(g)}$$

The feed to the reactor in which the above reaction takes place contains gaseous N2 and C_2H_2 in their stoichiometric proportions. The reaction temperature is controlled at 300 ^oC. estimate the product composition if the reactor pressure is 1 atm. At 300^{o}C ΔG^o for the reaction is 7190cal.

Solved Problem

A gas mixture of 25 mol% CO_2 and 75 mol% CO is mixed with the stoichiometric H_2 for the following reactions:

$CO_2 + 3H_2 = CH_3OH + H_2O$ K= 2.82×10^{-6}

$CO + 2H_2 = CH_3OH$ K= 2×10^{-5}

The conversion to equilibrium is affected in the presence of a catalyst at 300 atm pressure. Assuming the behavior to remain ideal, calculate the fractional conversion for each reaction and hence the composition of the equilibrium mixture.

Solution: Basis: 1 mol feed of mix.

Let X1 =moles of CO_2 reacted in the 1st reaction

X2= moles of CO reacted in the 2nd reaction

	CO_2 +	$3H_2$ =	CH_3OH +	H_2O	K= 2.82×10^{-6}
In:	0.25	0.75	0	0	
React:	X1	3X1	0	0	
Out:	0.25-X1	0.75-3X1	X1	X1	

$\Delta n = 2-4=-2$

	CO +	$2H_2$ =	CH_3OH	K= 2×10^{-5}
In:	0.75	1.5	0	
React:	X2	2X2	0	
Out:	0.75-X2	1.5-2X2	X2	

$\Delta n = 1-3=-2$

At equilibrium:

CO_2= 0.25 –X1,   CO=0.75-X2 , H_2=2.25-3X1- 2X2,

CH_3OH= X1+X2   , H_2O = X1

Tot. moles at eq$^{\underline{n}}$ = 3.25-2X1-2X2

$K_P=K_y\, P_T^{\Delta n}$

$$2.82x10^{-6} = \frac{\left(\frac{X1+X2}{3.25-2X1-2X2}\right)\left(\frac{X1}{3.25-2X1-2X2}\right)}{\left(\frac{0.25-X1}{3.25-2X1-2X2}\right)\left(\frac{2.25-3X1-2X2}{3.25-2X1-2X2}\right)^3}\ (300)^{-2}$$

$$0.2538 = \frac{(X1+X2)(X1)}{\frac{(0.25-X1)(2.25-3X1-2X2)^3}{(3.25-2X1-2X2)^2}}$$

$$\frac{0.2538(0.25-X1)(2.25-3X1-2X2)}{X1} = \frac{(X1+X2)(3.25-2X1-2X2)^2}{(2.25-3X1-2X2)^2}\text{-----(1)}$$

For The 2nd Reaction ;

$$2X10^{-5} = \frac{\frac{(X1+X2)}{(3.25-2X1-2X2)}}{\left(\frac{0.75-X2}{3.25-2X1-2X2}\right)\left(\frac{2.25-3X1-2X2}{3.25-2X1-2X2}\right)^2}(300)^{-2}$$

$$1.8 = \frac{(X1+X2)}{\frac{(0.75-X2)(2.25-3X1-2X2^2)}{(3.25-2X1-2X2\ \ )^2}}\quad \text{--------(2)}$$

$$1.8(0.75 - X2 = \frac{(X1+X2)(3.25-2X1-2X2)^2}{(2.25-3X1-2X2)^2}\text{------(3)}$$

Eq.1=Eq.3

1.8(0.75-X2)=0.2538(0.25-X1)(2.25-3X1-2X2)

5.319X1-7.09X1X2=0.5625-0.75X1-0.5X2-2.25X1+3X1^2+2X1X2

3X1^2-9.319X1+0.5625=0.5X2-9.09X1X2

$X2 = \frac{3X1^2 - 8.319X1 + 0.5625}{0.5 - 9.09X1}$-----(4)   Sub. X2 in Eq.(2) and after some steps we get

$$1.6875 - 5.4X12 + 2.7X1 = \frac{(0.5625 - 7.82X1 - 6.09X1^2)(\,0.5 - 13.9X1 + 12.18X1^2)}{0.5625 - 5.31X1 + 21.27X1^2}$$

By trial and error

Assume X1=0.1   1.9035≠ 0.882

X1=0.15   1.971 ≠ 4

X1= 0.05   1.8 ≠ -0.073

X1 = 0.11   1.91916≠1.3888

X1=0.12   1.934≠1.987

X1=0.17   1.929≠1.7995

X1= 0.119   1.932≠1.924

X1=0.1192   1.9334 ≠1.9364

so,   X1= 0.1191 which is the mole of CO_2 reacted

$$\mathrm{X2} = \frac{3(0.1191)^2 - 8.319(0.1191) + 0.5625}{0.5 - 9.09(0.1191)}$$

X2= 0.662 which is the mole of CO reacted

Fractional conversion 1st reaction= $\frac{0.1191}{0.25} = 0.4764$

Fractional conversion 2nd reaction= $\frac{0.662}{0.75} = 0.8827$

Moles at eq$^{\underline{n}}$: substitute X1 &X2 for each component:

CO_2= 0.25 –X1= 0.1309,   CO=0.75-X2=0.088 , H_2=2.25-3X1- 2X2= 0.5687, CH_3OH= X1+X2 =0.1191+0.662=0.7811 , H_2O = X1=0.1191