

## Tutorial sheet 2

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

1) Estimate the fractional conversion at 1000°C and 1.5 atm

Component	$\Delta G^{\circ}_{298}(\text{kJ/mol})$	$\Delta H^{\circ}_{298}(\text{kJ/mol})$	$C_p(\text{kJ/mol.K})$
$C_2H_6$	-32.886	-84.667	$0.0096+8.73 \times 10^{-5}T$
$C_2H_4$	68.124	52.3	$0.0117+12.5 \times 10^{-5}T$
$H_2$	0	0	$0.0289+1.67 \times 10^{-5}T$

**Q.2/** A stoichiometric mixture of  $N_2$  and  $H_2$  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  $K=3.4 \times 10^{-3}$  , 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  $SO_2 + 1/2 O_2 = SO_3$  at 1000 K is  $K_p= 1.85$ . What is the ratio  $P_{SO_3} / P_{SO_2}$ :

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 °C 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

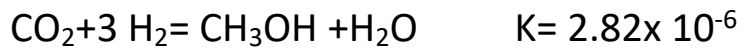


The feed to the reactor in which the above reaction takes place contains gaseous  $N_2$  and  $C_2H_2$  in their stoichiometric proportions. The reaction temperature is controlled at 300 °C. estimate the product composition if the reactor pressure is 1 atm. At 300°C  $\Delta G^{\circ}$  for the reaction is 7190cal.

## Solved Problem

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A gas mixture of 25 mol% CO<sub>2</sub> and 75 mol% CO is mixed with the stoichiometric H<sub>2</sub> for the following reactions:

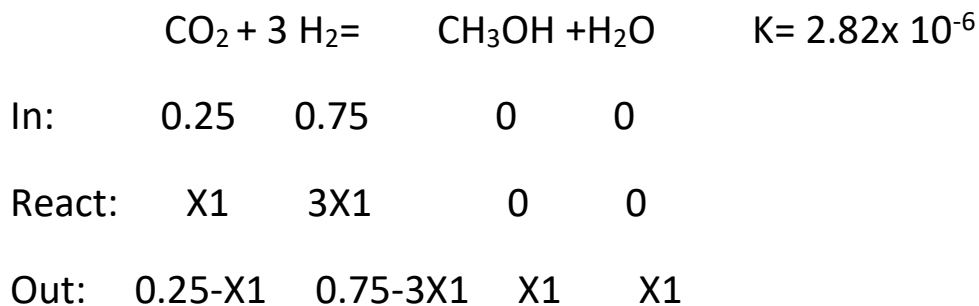


The conversion to equilibrium is affected in the presence of a catalyst at 300 atm pressure. Assuming the behavior to remain ideal, calculate the fractional conversion for each reaction and hence the composition of the equilibrium mixture.

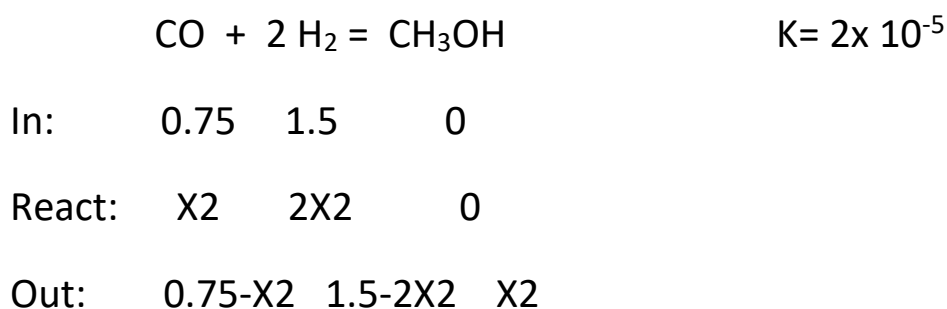
**Solution:** Basis: 1 mol feed of mix.

Let X<sub>1</sub> = moles of CO<sub>2</sub> reacted in the 1<sup>st</sup> reaction

X<sub>2</sub> = moles of CO reacted in the 2<sup>nd</sup> reaction



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



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

At equilibrium:

$$\text{CO}_2 = 0.25 - X_1, \quad \text{CO} = 0.75 - X_2, \quad \text{H}_2 = 2.25 - 3X_1 - 2X_2,$$

$$\text{CH}_3\text{OH} = X_1 + X_2, \quad \text{H}_2\text{O} = X_1$$

$$\text{Tot. moles at eq}^n = 3.25 - 2X_1 - 2X_2$$

$$K_p = K_y P_T^{\Delta n}$$

$$2.82 \times 10^{-6} = \frac{\left(\frac{X_1 + X_2}{3.25 - 2X_1 - 2X_2}\right) \left(\frac{X_1}{3.25 - 2X_1 - 2X_2}\right)}{\left(\frac{0.25 - X_1}{3.25 - 2X_1 - 2X_2}\right) \left(\frac{2.25 - 3X_1 - 2X_2}{3.25 - 2X_1 - 2X_2}\right)^3} (300)^{-2}$$

$$0.2538 = \frac{(X_1 + X_2)(X_1)}{\frac{(0.25 - X_1)(2.25 - 3X_1 - 2X_2)^3}{(3.25 - 2X_1 - 2X_2)^2}}$$

$$\frac{0.2538(0.25 - X_1)(2.25 - 3X_1 - 2X_2)}{X_1} = \frac{(X_1 + X_2)(3.25 - 2X_1 - 2X_2)^2}{(2.25 - 3X_1 - 2X_2)^2} \text{-----(1)}$$

For The 2<sup>nd</sup> Reaction ;

$$2 \times 10^{-5} = \frac{\frac{(X_1 + X_2)}{(3.25 - 2X_1 - 2X_2)}}{\left(\frac{0.75 - X_2}{3.25 - 2X_1 - 2X_2}\right) \left(\frac{2.25 - 3X_1 - 2X_2}{3.25 - 2X_1 - 2X_2}\right)^2} (300)^{-2}$$

$$1.8 = \frac{(X_1 + X_2)}{\frac{(0.75 - X_2)(2.25 - 3X_1 - 2X_2)^2}{(3.25 - 2X_1 - 2X_2)^2}} \text{-----(2)}$$

$$1.8(0.75 - X_2) = \frac{(X_1 + X_2)(3.25 - 2X_1 - 2X_2)^2}{(2.25 - 3X_1 - 2X_2)^2} \text{-----(3)}$$

$$\text{Eq.1} = \text{Eq.3}$$

$$1.8(0.75 - X_2) = 0.2538(0.25 - X_1)(2.25 - 3X_1 - 2X_2)$$

$$5.319X_1 - 7.09X_1X_2 = 0.5625 - 0.75X_1 - 0.5X_2 - 2.25X_1 + 3X_1^2 + 2X_1X_2$$

$$3X_1^2 - 9.319X_1 + 0.5625 = 0.5X_2 - 9.09X_1X_2$$

$$X_2 = \frac{3X_1^2 - 8.319X_1 + 0.5625}{0.5 - 9.09X_1} \text{-----(4)}$$
 Sub.  $X_2$  in Eq.(2) and after some steps we get

$$\begin{aligned} & 1.6875 - 5.4X_1^2 + 2.7X_1 \\ &= \frac{(0.5625 - 7.82X_1 - 6.09X_1^2)(0.5 - 13.9X_1 + 12.18X_1^2)}{0.5625 - 5.31X_1 + 21.27X_1^2} \end{aligned}$$

By trial and error

Assume $X_1=0.1$	$1.9035 \neq 0.882$
$X_1=0.15$	$1.971 \neq 4$
$X_1= 0.05$	$1.8 \neq -0.073$
$X_1 = 0.11$	$1.91916 \neq 1.3888$
$X_1=0.12$	$1.934 \neq 1.987$
$X_1=0.17$	$1.929 \neq 1.7995$
$X_1= 0.119$	$1.932 \neq 1.924$
$X_1=0.1192$	$1.9334 \neq 1.9364$

so,  $X_1= 0.1191$  which is the mole of  $\text{CO}_2$  reacted

$$X_2 = \frac{3(0.1191)^2 - 8.319(0.1191) + 0.5625}{0.5 - 9.09(0.1191)}$$

$X_2= 0.662$  which is the mole of  $\text{CO}$  reacted

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

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

Moles at eq<sup>n</sup>: substitute  $X_1$  &  $X_2$  for each component:

$$\begin{aligned} \text{CO}_2 &= 0.25 - X_1 = 0.1309, & \text{CO} &= 0.75 - X_2 = 0.088, & \text{H}_2 &= 2.25 - 3X_1 - 2X_2 = 0.5687, \\ \text{CH}_3\text{OH} &= X_1 + X_2 = 0.1191 + 0.662 = 0.7811, & \text{H}_2\text{O} &= X_1 = 0.1191 \end{aligned}$$