# Assignment 8

1. To remove oxides of nitrogen (assumed to be NO) from automobile exhaust, a scheme has been proposed that uses unburned carbon monoxide (CO) in the exhaust to reduce the NO over a solid catalyst, according to the reaction, $CO + NO \rightleftarrows \frac{1}{2} N_2 + CO_2$

When this reaction is carried out over copper catalyst, the reaction mechanism is believed to be

$$CO + S \underset{k_{-1}}{\overset{k_1}{\rightleftarrows}} CO.S$$

$$NO + S \underset{k_{-2}}{\overset{k_2}{\rightleftarrows}} NO.S$$

$$CO.S + NO.S \underset{k_{-3}}{\overset{k_3}{\rightleftarrows}} CO_2.S + N.S$$

$$N.S + N.S \underset{k_{-4}}{\overset{k_4}{\rightleftarrows}} N_2 + 2S$$

$$CO_2.S \underset{k_{-5}}{\overset{k_5}{\rightleftarrows}} CO_2 + S$$
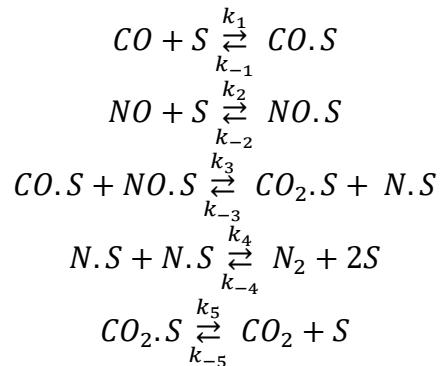
a) If surface reaction is rate controlling step, deduce the rate law.
b) If K_{CO}=2 atm^{-1} and K_{NO}=5 atm^{-1}, where K_{CO} and K_{NO} are adsorption equilibrium constant of CO and NO respectively. What is the ratio of sites containing CO to those containing NO when the conversion is 50% and 90%? The feed is equimolar in CO and NO with $P_{CO,0}$=$P_{NO,0}$=2 atm.

2. T-Butyl alcohol (C) is an important octane enhancer that is used to replace lead additives in gasoline. C was produced by the liquid-phase hydration (B) of isobutene (A) over an Amberlyst-15 catalyst. The system is normally a multiphase mixture of hydrocarbon, water, and solid catalysts. However, the use of co-solvents or excess C can achieve reasonable miscibility.

The reaction mechanism is believed to be

$$A + I \leftrightarrow A - I$$

$$B + I \leftrightarrow B\text{-}I$$

$$B - I + A - I \leftrightarrow C - I + I$$

$$C - I \leftrightarrow C + I$$
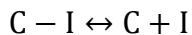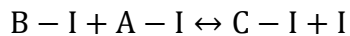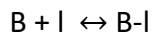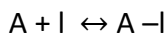
Derive a rate law assuming:
(a) The surface reaction is rate-limiting.
(b) The adsorption of isobutene is limiting.

(c) The reaction follows Langmuir –Hinshelwood models.

$$A+B \to C$$
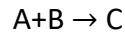
and the surface reaction is limiting.

3. At 30^0C, the amount of acetone adsorbed at partial pressure of 10 and 100 mmHg are 0.1 and 0.4 kg acetone /kg activated carbon, respectively. Assume Langmuir isotherm describe the adsorption of acetone on activated carbon. What is the amount of acetone adsorbed (in kg per kg of activated carbon) at a partial pressure of 50 mmHg and 30^0C?

4. The first order reaction $A \to B$ was carried out over two different-sized pellets. The pellets were contained in a spinning basket reactor that was operated at sufficiently high rotation speeds that external mass transfer resistance was negligible. The result of two experimental runs made under identical conditions are given in table 1. **(Folger 4th edition, Example 12-3)**

   a) Estimate the Thiele modulus and effectiveness factor for each pellet.
   b) How small should the pellets be made to virtually eliminate all internal diffusion resistance,$\acute{\eta} = 0.95$?

   Table 1 DATA FROM A SPINNING BASKET REACTOR.

	Measured rate (obs) (Mol/g-cat .s)*10^5	Pellet Radius (m)
Run 1	3	0.03
Run 2	15	0.003

5. A second-order gas phase reaction, $A \to R$, occurs in a spherical catalyst pellet with radius 9mm, and has a rate coefficient, k = 3.86 m^3/kmol s. The reactant pressure is 1 bar, the temperature is 600 K, the molecular diffusivity is D_{AR} = 0.10 cm^2/s, and the reactant molecular weight is M_A = 60. The catalyst pellets have the following properties:

$$\text{Porosity, e} = 0.6$$
$$\text{Tortuosity, t} = 3$$
$$\text{Mean pore size,r} = 100 \text{ Å}$$

   a) Estimate the effective diffusivity.
   b) Determine if there may be pore diffusion limitations.