EN 315: Reaction Engineering & Combustion
Assignment -3, Due Date: 23-10-18

1. The reversible gas phase elementary reaction for ammonia production is given by

$N_2(g) + 3\ H_2(g) <=> 2\ NH_3(g)$

Ammonia production is to be carried out at constant temperature at 340°K. The feed consists of stoichiometric ratio of N_2 (g) and H_2(g) at 340°K at 2 atm. The concentration equilibrium constant, K_c, at 340°K is 0.5 $(moles/lit)^{-1}min^{-1}$.

(a) calculate the equilibrium concentration of ammonia in a constant-volume batch reactor.

(b) Calculate the equilibrium concentration of ammonia in a flow reactor.

(c) If forward rate constant K_{NH3}=0.1 $(moles/lit)^{-1}\ min^{-1}$ and total feed rate of reactants are 5 moles/(lit min) then calculate CSTR volume required to achieve 80% of the equilibrium concentration of H_2.

2. Using collision theory calculate the reaction constant at 340°K and 2 atm for pyrolysis of Ozone, which is given by following reaction

$O_3 + O \rightarrow 2O_2$

Assume activation energy of the reaction is 19 KJ/moles and diameter of O_3 and O are 4. 36 A^0 and 1.4 A^0 respectively.

3. Consider a cylindrical batch reactor that has one end fitted with a frictionless piston attached to a spring having spring constant ($h=10^5$ N/m). The other end of the spring is fixed to the wall. The spring initially at unstarched position and it is attached to cylinder surface (surface area 0.1 m^2) via piston. The initial temperature, pressure and the volume of the reactor are 400° K, 1 atm and 0.1 m^3 respectively. The force exerted by spring on cylinder surface is given by F= h*x, where 'x' is displacement of the piston from its initial position.

The gas phase reaction inside the cylinder is given by

$A + 3B \rightarrow 8\ C$

Assuming isothermal elementary reaction with rate constant, k = 0.1 $(moles/m^3)^{-}2/s$, find the total pressure and concentration of species in the reactor when 50 % of reactants are converted into product. At the beginning of the reaction assume a stoichiometric mixture of reactants.

4. Following gas phase reaction is carried out at constant temperature (500°K) using equal size (2 m^3) CSTR and PFR reactor in parallel (see figure 1).

$A + B \to 3\,C$

If equal feeds are provided in both the reactors at temperature 500°K , 1 atm pressure and the rate is given by $-r_A = C_A\, C_B$ moles/m^3. hr. Calculate the concentrations and total pressure of combined products at the exit.

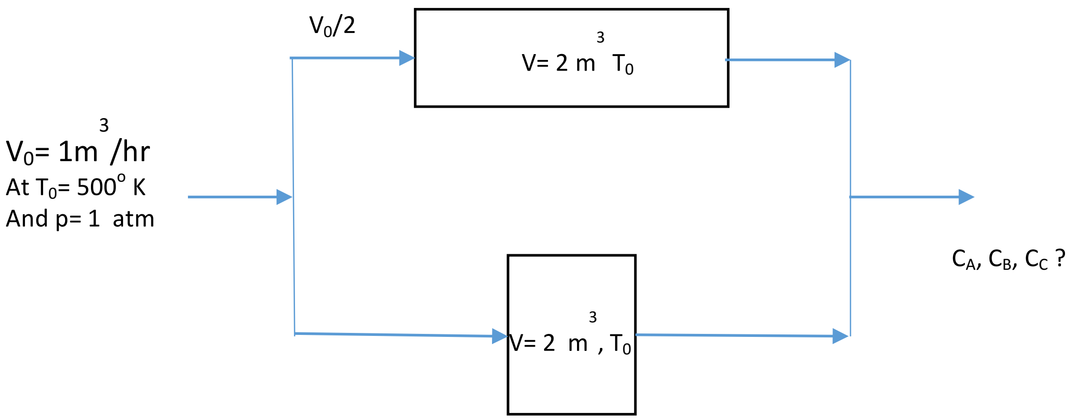

Figure 1

5. The irreversible gas-phase nonelementary reaction

$$A + B \rightarrow 3C$$

is to be carried out isothermally in a constant-pressure CSTR reactor. The feed is at a temperature of 227°C, a pressure of 1013 kPa, and its composition is 33.3% A and 66.7% B. Laboratory data taken under identical conditions are as follows (note that at X = 0, $-r_A$ = 0.00001):

r_A $mol/dm^3 sec$ x1000	X
0.01	0.0
0.005	0.2
0.002	0.4
0.001	0.6

If reactor is feed by a stoichiometric mixture of reactants with flow rate 0.1 m^3/s then find the CSTR and PFR reactor volume required for 50% conversion of A into product.

6. The butane thermally decompose to ethene, ethane, methane, propene, butene, and hydrogen at 100^oK.

(a) write a possible mechanism of the thermal decomposition of butane.

(b) Use the, *PSSH* to derive a rate law for the rate of formation of butane,

(c) Compare the PSSH solution in Part **(b)** to that obtained by solving the complete set of ODE mole balances.

7. Following gas phase reaction is carried out at constant temperature (500^oK) in a PFR reactor.

$$3A + 2B \rightarrow C$$

If stoichiometric mixture of reactants are feeds in the reactors with a rate of 1 m^3/m at temperature 500^oK , 1 atm pressure and diameter of reactor is 0.50 m. Assuming elementary reaction with rate constant k= 1.0 $(moles/lit)^{-4}$/min. Calculate the reaction volume required for 50% conversion of reactants and also calculate final total pressure in the reactor considering pressure drop in the reactor.