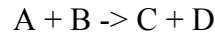


EN 315: Reaction Engineering & Combustion

Assignment -3, Due Date: 30-10-18

1. A second order reaction elementary reaction



is taking place in 20 meter long pipeline having 4 cm diameter. The pipeline is packed with the spherical catalyst of 5 mm diameter with solid fraction 0.5 and density 1900 kg/m³. The entering flow rate to the reactants is 0.25 m³/hr at 10 atm pressure and 400°K. If feed has a stoichiometric ratio of reactants and reaction rate constant $k = 10 \text{ (kmol/m}^3\text{)}^{-1}/(\text{kg of cat m}^{-3}\text{ hr})$

- (a) Calculate the conversion of A in absence of pressure drop.
 - (b) Calculate the conversion of A after accounting pressure drop due to friction.
 - (c) Calculate the conversion of A in case catalyst diameter is 1 cm while porosity is same.
2. The dehydrogenation of propane in to propylene takes place in a catalytic membrane reactor.



The equilibrium constant for these type reaction is small, here it is $K_c = 0.03 \text{ moles/lit}$. The membrane is permeable to H₂ but not to propane and propylene. Pure propane enters the reactor at 10 atm and 227°C at a rate of 10 moles/min. Here the rate of diffusion of hydrogen out of the reactor per unit volume of the reactor, R_B , is given by $R_B = K_c C_{H_2}$. Assuming constant temperature and no pressure drop

- (a) Calculate molar flow rate as a function of reactor volume.
- (b) Calculate the conversion for the reactor of volume 500 lit.

Additional information: bulk density of catalyst 1500 kg/m³, the specific reaction rate constant, k , and the transport coefficient, k_c , are 0.7 min⁻¹ and 0.2 min⁻¹, respectively.

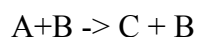
3. The gas phase reaction



follows an elementary rate law and takes place isothermally in a PBR charged with 1.5 kg of catalyst. The feed, consisting of pure A, enters the PBR at a pressure of 22 atm. The pressure and the conversion of A at the exit of the PBR is 5 atm and 0.3 respectively.

- (a) If the PBR were replaced by a “fluidized” CSTR with 1.5 kg of catalyst, what will be the conversion at the exit of the CSTR with the assumption of no pressure drop in the CSTR?
- (b) What would be the conversion in the PBR if the mass flow rate were decreased by a factor of 3 and particle size were doubled?

4. A catalyst is a material that affects the rate of a chemical reaction, yet emerges unchanged from the reaction. For example, consider the elementary reaction



where B is a catalyst. The reaction is taking place in a *semibatch reactor*, in which 1 m³ of a solution containing 50 mol/m³ of A is initially present. No B is present initially. Starting at time $t = 0$, 0.05 m³/min of a solution containing 10 mol/m³ of B is fed into the reactor. The reactor is isothermal, and $k = 10 \text{ m}^3/(\text{mol} \cdot \text{min})$.

- (a) How many moles of C are present in the reactor after half an hour?
 (b) Plot the conversion as a function of time.
 (c) Repeat parts (a) and (b) for the case when the reactor initially contains 1 m³ of B having concentration 50 mol/m³ and A is fed to the reactor at a concentration of 4 mol/m³ and at a rate of 0.05 m³/min.

5. The reaction



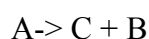
was carried out in a constant-volume batch reactor where the following concentration measurements were recorded as a function of time.

T (min)	0	5	9	15	22	30	40	60
C _A (mol/lit)	2	1.6	1.35	1.1	0.87	0.7	0.53	0.35

Table 1.

- (a) Use nonlinear least squares (i.e., regression) and one other method to determine the reaction order α and the specific reaction rate.
 (b) If you were to take more data, where would you place the points? Why?

6. The gas-phase reaction,



This reaction was carried out in the laboratory in an isothermal batch system in which the total pressure was recorded at various times during the reaction. The data given in Table 2 apply to this reaction. Only pure A was initially present in the reaction vessel, determine the reaction order, rate constant and activation energy.

Time (min)	Total Pressure (kPa)
0.0	1.0
2.5	1.4

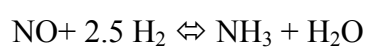
5.0	1.7
10	2.1
15	2.4
20	2.7

Table 2. Pressure time data

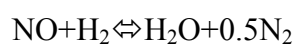
(a) *Using graphical method.*

(b) *Using fine difference method.*

7. In the production of ammonia



the following side reaction occurs:



Above catalytic reaction takes place in a differential reactor at atmospheric pressure using 2.39 g catalyst. Table 3 shows the reaction rate of the side reaction as a function of P_{H_2} and P_{NO} at a temperature of 375°C.

$P_{\text{H}_2}(\text{atm})$	$P_{\text{NO}}(\text{atm})$	Reaction rate $r_{\text{H}_2\text{O}} \times 10^5$ (mol/(min. g cat.))
0.00922	0.5	1.6
0.0136	0.5	2.56
0.0197	0.5	3.21
0.0280	0.5	3.64
0.0291	0.5	3.48
0.0389	0.00917	4.46
0.0485	0.0184	4.75
0.05	0.00917	1.41
0.05	0.0184	2.48
0.05	0.0298	3.45
0.05	0.0378	4.06
0.05	0.0491	4.15

Table 3. Formation of Ammonia.

The following rate laws for side reaction, based on various catalytic mechanisms, were suggested:

$$r_{H_2O} = \frac{k K_{NO} P_{NO} P_{H_2}}{1 + K_{NO} P_{NO} + K_{H_2} P_{H_2}}$$

$$r_{H_2O} = \frac{k K_{NO} K_{H_2} P_{H_2}}{1 + K_{NO} P_{NO} + K_{H_2} P_{H_2}}$$

$$r_{H_2O} = \frac{k K_{H_2} K_{NO} P_{NO} P_{H_2}}{(1 + K_{NO} P_{NO} + K_{H_2} P_{H_2})^2}$$

Find the parameter values of the different rate laws and determine which rate law best represents the experimental data.