Name ID No

BIRLA INSTITUTE OF TECHNOLOGY & SCIENCE, PILANI - HYDERABAD CAMPUS

First Semester 2022-2023

Kinetics and Reactor Design (CHE F311)

Comprehensive examination **Part-A** (Closed Book) **& Part B** (Open Book)

Date: 19/12/2022 Total marks: 80 Duration: 180 min. Weightage: 40%

PART-A Marks: 40 Max. duration: 105 min.

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1. **Write the <u>final answer</u> by pen below each question**. Use extra sheet for rough work.

[2×8 =16]

A. For a gas-solid catalytic reaction, the bulk phase diffusivity (D_A) of reactant A is 0.5 cm^2/s. The porosity and tortuosity of the catalyst is 0.5 and 5, respectively. Find the effective diffusivity of A (in cm^2/s) inside the catalyst. (assume pores are cylindrical in shape).

B. Activation energy of the ethane pyrolysis reaction is 300 kJ/mol. How much faster is decomposition at 600 °C than at 500 °C if other operating conditions are the same?

C. In a recycling reactor, the overall conversion of 'A' in an isothermal liquid phase reaction (A→B) is 80%. Find the per pass percentage conversion of 'A' if the recycling ratio is 3.

D. Liquid phase reaction $2A \rightarrow R$ follows elementary rate law with k = 0.05 L/(mol.h). The reaction is carried out in a CSTR with C_{A0}=10 mol/L and space-time 2 hours. Find the Damkohler number of the system.

E. For a constant density system, on doubling the concentration of a reactant, the rate of reaction triples. Find the reaction order.

F. A first-order gas-phase reaction $A(g) \rightarrow R(g)$ is carried out isothermally in a packed-bed reactor (PBR) containing 35 kg catalyst. Pure A enters the PBR at 20 atm. The pressure drop parameter (α) is = 0.02 per kg of catalyst. What is the total pressure (P) at the exit of the PBR?

G. A liquid phase, isothermal reaction with k =0.1 min^{-1} is being carried out in a batch reactor. What will be the time required to reach 75% conversion?

H. The Thiele Modulus for a zero-order irreversible gas-solid (slab type catalyst) catalyzed reaction is 10. Find the effectiveness factor for the reaction.

2. Write the final answer by pen below each question. Use extra sheet for rough work.

[3 ×8 =24]

i. An isothermal irreversible gas-phase elementary reaction A+2B → 4R occurring in a steady flow reactor. The inlet concentration of A, B and an inert (I) are 100, 200, and 100 mol/L respectively. If the concentration of 'A' at the exit of the reactor is 50 mol/L, find the exit conversion of 'B'.

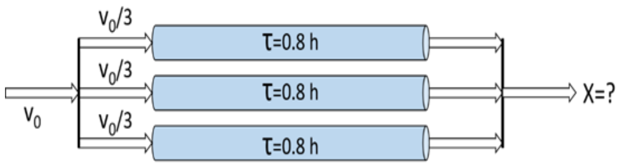
ii. For a steady flow in a tubular reactor, the dispersion number is 0.05. Find the number of tanks for the tanks-in-series model equivalent to the dispersion number.

iii. A liquid phase, autocatalytic reaction ($A + R \rightarrow R + R$) is being carried out in a CSTR operating at a steady state. The feed contains 99% A, and 1% R. The rate constant is k = 1 L/(mol.min). The total concentration of the two species is constant throughout the reaction at 1 mol/L. Determine the space-time required to obtain a product consisting of 10% A and 90% R.

iv. Liquid reactant 'A' passes in steady flow through 3 equal size of isothermal CSTRs connected in series. The total residence time (from the entry of the first reactor to the exit of the third reactor) is 3 min. The concentration of 'A' at the inlet of the first reactor is 8 mol/m^3 and at the exit of the third reactor is 1 mol/m^3. Find the reaction rate constant value for a first-order reaction.

v. The liquid-phase reaction $A + B \rightarrow C$ follows elementary rate law (k = 0.1 L/(mol.min)) and is carried out isothermally in a 200 L CSTR. A stream with a volumetric flow rate of 5 L/min and containing 2 M of reactant A is mixed with another stream of same volumetric flow rate and containing 2 M of reactant B before entering the reactor. Find the conversion percentage of A.

vi. Gas phase reaction $A \rightarrow B$ with k = 1 h^{-1} is carried out in 3 PFRs with a parallel arrangement as shown below. All the reactors are operating at the same temperature, and the space-time for each PFR is 0.8 hours. Find the percentage conversion in the final stream that combines the exit streams from all the 3 PFRs.

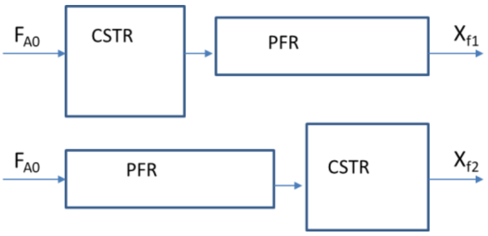


vii. A first-order gas-solid irreversible isothermal reaction (A → P) is carried out using a spherical porous catalyst. The reactant concentration at the external surface of the catalyst is 1 mol/m^3. The Thiele modulus for the system is 6. Find the concentration (in mol/m^3) of the reactant at halfway between the external surface and the center of the catalyst.

viii. The reversible gas-phase decomposition of nitrogen tetroxide (N_2O_4) to nitrogen dioxide (NO_2), is carried out isothermally in a constant-volume batch reactor. The feed consists of pure N_2O_4 at 340 K and 2 atm. The value of equilibrium constant (K_C) at 340 K is 0.1. Calculate the equilibrium conversion of N_2O_4.

Part-B (Open book) **Marks: 40**

1. A liquid-phase irreversible reaction is carried out using two equal-volume of ideal reactors (one CSTR and one PFR) in series under identical conditions as shown in the figure. Do you think that the final conversion of A (i.e, X_{f1} and X_{f2}) will be the same in both cases? Give reasons for your answer.



[4]

2. Suppose the following mechanism is proposed for the production of phosgene as per the reaction $CO + Cl_2 \rightarrow COCl_2$. Assuming step-3 is the slowest step, find the kinetic rate expression for the formation of $COCl_2$ and find the reaction order with respect to CO for a very low and very high concentration of CO.

$$Cl_2 \underset{k_{-1}}{\overset{k_1}{\rightleftharpoons}} 2Cl \qquad \text{step-1}$$

$$Cl + Cl_2 \underset{k_{-2}}{\overset{k_2}{\rightleftharpoons}} Cl_3 \qquad \text{step-2}$$

$$CO + Cl_3 \xrightarrow{k_3} COCl_2 + Cl \qquad \text{step-3}$$

[7]

3. A first-order heterogeneous irreversible isothermal reaction (A → product) was carried out using a catalyst pellet of slab geometry. The reactant concentration (C_A) at a distance of 0.04 mm inside from the external surface is equal to 77% of the external surface concentration. The concentration of the reactant at the external surface of the catalyst is 4 mol/cm^3. The length (2L) of the pellet is 0.4 mm and effective diffusivity within the catalyst is 0.1 cm^2/s.
   i) Find the concentration of the reactant at a distance of 0.1 mm from the external surface of the pellet. (show the calculation steps)
   ii) Find the effectiveness factor for the reaction
   iii) Find the value of the kinetic rate constant
   iv) Is the reaction a diffusion control or a kinetic control reaction for the given experimental conditions? Give reasons for your answer.
   v) Instead of the first-order kinetics, if it follows zero-order kinetics, find the value of Thiele modulus for the same external concentration of the reactant.

[5+2+2+2+3=14]

4. A tracer was injected as an impulse input to an isothermal mixed-flow reactor. At the exit of the reactor, the tracer concentration was measured as a function of time and the results are given in the table.
   i) Find E(t) values and fill the table.
   ii) Find F(t) values and fill the table.
   iii) Find the mean residence time(t_m).
   iv) Find the variance of the distribution
   v) If the same reactor (volume 0.2 m^3) is used for an irreversible first-order liquid phase reaction (A→B) under the identical operating condition as that of the tracer experiment with a volumetric flow rate of 0.1 m^3/min, then find the actual conversion of A. (Assume the reaction rate constant is 0.1 min^{-1}). **[3x5=15]**

t, min.	0	2	4	6	8	10
C(t), g/m^3	0	4	8	6	2	0
E(t)						
F(t)						

End