BIRLA INSTITUTE OF TECHNOLOGY AND SCIENCE (BITS) PILANI – Pilani Campus

Title: **K**inetics and **R**eactor **D**esign (CHE F311)- End-Semester Examination (2022-23)

Date: 17.12.2022 Max.Marks: 120

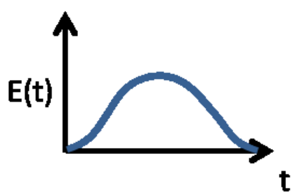
ID | **Name** |

PART- A: ***CLOSE BOOK*** **15 x 2 = 30 M**

Note: Answer the questions in the space provided.

S.No	***Question***
1.	Write the two equations (in terms of *K*, and *S**) to avoid runaway reactions in an ideal CSTR
2.	Write the *equation* for the internal effectiveness factor for a 2nd order catalytic reaction dominated by internal diffusion resistances.
3.	An impulse tracer input has been given for an ideal PFR, 5 ideal CSTRs in series, and one ideal CSTR. Draw the corresponding *E(t) versus time* responses on a single plot. Mark the type of reactors on the plot.

4.	Draw the concentration profiles inside the spherical catalyst having ϕ= 1, 100 and 10000 (C_A/C_{AS} vs r/R) for a first order system. Assume external resistances are negligible
5.	Calculate the conversion achieved by a 1.0 m length of packed reactor filled with catalyst spherical particles (surface area per unit volume, a_c= 1 m^2/m^3) and reaction is completely dominated by an external mass transfer resistance. [Data: mass transfer coefficient, k_c=1 m/s, superficial velocity, U = 1 m/s]
6.	Name the criteria's used to check the internal and external mass transfer resistances for a catalytic reaction.
7.	Do mixing patterns affect the conversion for a 1^{st} order reaction? If yes/ no, justify your answer.

8.	Write the overall effectiveness factor expression for a 1st order catalytic reaction
9.	Draw a schematic model for complete micro mixing in a tubular reactor based on the figure 
10.	What is the difference between *closed-closed* and *open-open* vessel dispersion models?
11.	Write the relationship between Tanks-in-series and the dispersion model
12.	Consider a gas phase reaction $2A \rightarrow R + 2S$ with unknown kinetics. If a space velocity of $1 \min^{-1}$ is needed for 90% conversion of A in a PFR. Find the corresponding space time and mean residence time or holding time of the fluid in the reactor.

13.	The chemical reaction $A \rightarrow B$ is carried out in a CSTR. Calculate the adiabatic temperature for 100% conversion if feed enters at 100 ^oC. [Data: The mole fraction of A in the input stream =1, The total heat capacity, Cp = 80 J mol^{-1} K^{-1}, The heat of reaction, ΔHr = - 72 kJ mol^{-1}]
14.	Explain the purpose of inter stage heating and cooling operations for the positive order adiabatic reactions with the help of neat sketches. Does this operation required for irreversible reactions?
15.	Calculate the reaction rate dominated by both external and internal mass resistances for a stagnant layer on external surface of the catalyst. [Data: reaction rate constant, k= 1.0 s^{-1}, reactant of bulk concentration C_{A}=1 mol/m^3, radius of the sphere= 1 cm, diffusivity of A in the solution is D_A=1 m^2/s, Sherwood Number=2.

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PART B: CLOSE BOOK **[6 x 15 =90 M]**

Note: *Make the appropriate assumptions by clearly stating them, if necessary*

1. A small reaction bomb fitted with a sensitive pressure-measuring device is flushed out and then filled with pure reactant A at 1-atm pressure. The operation is carried out at 25 °C, a temperature low enough that the reaction does not proceed to any appreciable extent. The temperature is then raised as rapidly as possible to 100 °C by plunging the bomb into boiling water, and the readings in Table 1 are obtained. The stoichiometry of the reaction is $2A \rightarrow B$, and after leaving the bomb in the bath over the weekend the contents are analyzed for A; none can be found. Find a rate equation in units of moles, liters, and minutes which will satisfactorily fit the data.

T, min	π, atm	T, min	π, atm
1	1.14	7	0.850
2	1.04	8	0.832
3	0.982	9	0.815
4	0.940	10	0.800
5	0.905	15	0.754
6	0.870	20	0.728

2. A first order reaction is to be carried out in a series of two mixed flow reactors. Show that the total volume of two reactors is minimum when the reactors are of equal size.

3. At 650°C phosphine vapor with 1/3 inert feed decomposes as follows: $4\,PH_3 \rightarrow P_4 + 6\,H_2, -r_{phos} = (10\ hr^{-1})C_{phos}$. What size of plug flow reactor operating at 649 °C and 11.4 atm is needed for 75% conversion of 10 mol/hr of phosphine?

4. The elementary, reversible, liquid-phase reaction $A = B$ takes place in a steadt state, wall- cooled CSTR. Pure A enters the reactor.
   a. Derive the heat generated per mole of A reacted, G(T), as a function of the reactor operating temperature (T).
   b. Multiple steady states are forming in this reactor? If forming, explain each steady state is locally stable or not?
   c. What is the conversion corresponding to the upper steady state?

Data: V= 10 m^3, v_0= 1 m^3/min, F_{A0}= 10 mol/min, UA = 3600 cal/ (min- K), Cp_A= Cp_B= 40 J/mol/K, ΔH_{Rxn}^0 = -80,000 cal/mol A, Equilibrium constant at 400 K, K= 100; forward rate constant, k 400 K = 1 min^{-1}; Feed temperature T_0= 37 ºC, Ta= 37 ºC (assume jacket is perfectly mixed). E_A/R= 20,000 K.

5. A proposed mechanism for catalytic CO oxidation, $2\,CO + O2 = 2CO2$, consists of the following steps: associative adsorption of CO, dissociative adsorption of O_2, and the bimolecular surface reaction

$$CO + S \underset{k_{-1}}{\overset{k_1}{\rightleftharpoons}} CO_{ads}$$
$$O_2 + 2S \underset{k_{-2}}{\overset{k_2}{\rightleftharpoons}} 2O_{ads}$$
$$CO_{ads} + O_{ads} \xrightarrow{k_3} CO_2 + 2S$$

Assume the O_2 and CO adsorption steps are at equilibrium and the surface reaction step is slow and irreversible. Find the production rate of CO_2 in terms of gas-phase concentrations.

6. A first order reaction $A \rightarrow B$ is carried out in a 10 cm dia tubular reactor with 6.36 m in length. k= 0.4 min-1. The results of the tracer test carried out on this reactor are provided

t(min)	**0**	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**	**12**	**14**
C(mg/L)	**0**	**1**	**5**	**8**	**10**	**8**	**6**	**4**	**3**	**2.2**	**1.5**	**0.6**	**0**

Calculate the conversion i) closed vessel dispersion model; ii) ideal PFR; iii) ideal single CSTR; iv) Tanks in series.

$$X = 1 - \frac{4q \cdot \exp(Pe_r/2)}{(1+q)^2 \exp(Pe_r q/2) - (1-q)^2 \exp(-Pe_r q/2)} \qquad q = \sqrt{1 + 4Da/Pe_r}$$

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