Ref. No.: Ex/PG/ChE/T/111B/2025

M.E. CHEMICAL ENGINEERING FIRST YEAR FIRST SEMESTER EXAM 2025

ADVANCED CHEMICAL ENGINEERING KINETICS AND REACTOR DESIGN

Full Marks 100

Time : Three hours

Use separate Answer Scripts

All symbols have usual meaning; assume any missing data/information

Part –I

Full Marks:70

Answer any five questions

1.a) Consider the following vapour phase reaction conducted over a solid catalyst in a differential reactor : $C_6H_5CH_3 + H_2 \longrightarrow C_6H_6 + CH_4$

Assuming that the reaction between adsorbed toluene and gaseous hydrogen is reaction-rate-limited; derive a rate equation for the reaction consistent with the data (presented in the following Table) obtained from an isothermal differential reactor:

Run	$-r'_T \times 10^{10}$ $\left(\frac{\text{g mol toluene}}{\text{g cat.}\cdot\text{s}}\right)$	Partial Pressure (atm)			
		Toluene, P_T	Hydrogen (H_2),[a] P_{H_2}	Methane, P_M	Benzene, P_B
Set A					
1	71.0	1	1	1	0
2	71.3	1	1	4	0
Set B					
3	41.6	1	1	0	1
4	19.7	1	1	0	4
5	42.0	1	1	1	1
6	17.1	1	1	0	5
Set C					
7	71.8	1	1	0	0
8	142.0	1	2	0	0
9	284.0	1	4	0	0
Set D					
10	47.0	0.5	1	0	0
11	71.3	1	1	0	0
12	117.0	5	1	0	0
13	127.0	10	1	0	0
14	131.0	15	1	0	0
15	133.0	20	1	0	0
16	41.8	1	1	1	1

[a] $P_H = P_{H_2}$

[10]

1.b) State the procedure to evaluate reaction kinetic parameters for the derived rate equation.

[4]

2. a) Consider a second order isothermal gas phase chemical reaction ($\varepsilon = 0$; $1 >> \varepsilon X$), which is conducted in a catalytic PBR .Find an expression relating catalyst weight and conversion of the reactant and find the pressure profile; i.e. the total pressure (P) as a function of catalyst weight(W_c).

Hence, show the nature of the plots of (i) Pressure as function of catalyst weight; (ii) reactant concentration as function of catalyst weight; (iii) reactant conversion as function of catalyst weight.

[11]

[Turn over

2.b) 'In a tubular catalytic packed bed reactor, it is not always recommended to increase the reactor diameter to decrease the pressure drop for a specified mass flow rate of the feed'. Justify the statement.

[3]

3. (a)Briefly elucidate the mechanism of catalyst deactivation by (i) sintering and (ii) coking

3.(b)The gas-phase cracking reaction ($A \rightarrow B + C$) of hydrocarbon (A) is carried out in a fluidized reactor (approximated as a CSTR) . The feed stream contains 80% hydrocarbon (A) and 20% inert(I). The hydrocarbon contains sulfur compounds which poison the catalyst.

Assume that the cracking reaction is first-order in hydrocarbon concentration; the rate of catalyst decay is first-order in the present activity, and first-order in the reactant concentration. Model the fluid bed reactor (as a well-mixed CSTR) and determine the reactant concentration, catalyst activity, and conversion as a function of time. The volumetric feed rate to the reactor is 5000 m^3/h.

There are 50,000 kg of catalyst in the reactor and the bulk density is 500 kg/m^3.

[(3+3) +8]

4. a) How would you distinguish between "segregation model" and "maximum mixedness model" for non-ideal reactor? Write the conversion equations as per these models.

4. b) Elucidate the method of evaluating the model parameters using a step tracer input for modeling a real CSTR with dead-space and bypassing. **[6+8]**

5. a) A fully turbulent, baffled stirred vessel is to be scaled up by a factor of 512 in volume while maintaining constant power per unit volume. Determine the effects of the scale up on the impeller speed and mixing time. **[7]**

5. b) For tubular reactors operating with constant physical properties under fully turbulent flow, keeping the mean residence time and pressure drop constant, express the 'scaling factor' for diameter, length, superficial velocity in terms of throughput scale-up factor "S". **[7]**

6. For a plug flow reactor(PFR)/tubular reactor, in which heat is either added or removed through the cylindrical walls of the tubular reactor, assuming that there are no radial gradients in the reactor, carry out a steady-state energy balance to derive the energy balance equation for finding the temperature profile in the reactor. Define clearly all pertinent terms in the equations. Also, show the energy balance equation for a packed bed reactor (PBR).

[10+4]

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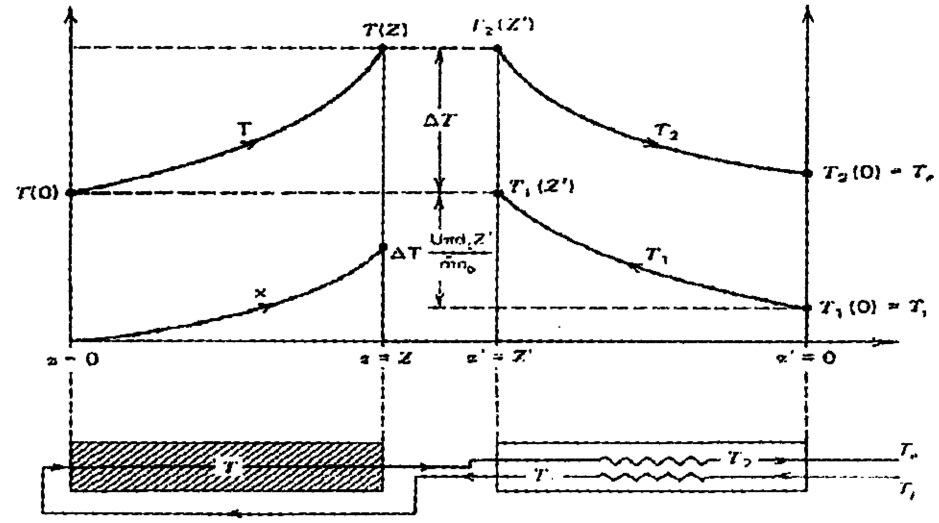
Part-II (30 Marks)

Answer Question no. 3 and any two from the rest

1. An irreversible 1st order reaction, $A \rightarrow B$ is carried out in an ideal CSTR. Write down the mole and energy balance equations in terms of perturbation variables using the concept of Taylor series expansion. The variation of heat of reaction, ΔH_r with temperature can be neglected. Determine the time dependence of concentration of A, i.e., $C_A(t)$, under isothermal condition using the principle of Laplace transformation when a step change in input concentration has been made from zero to C_{A0}. Defining steady state gain and open loop time constant of the process, determine their values if rate constant, $k = 1 min^{-1}$ and residence time, $\tau = 5\ min$. $\mathcal{L}[e^{-at}] = \frac{1}{s+a}$	10
2. The catalytic reaction, A $(g) + 3B(l) \rightarrow C(g) + D(l)$occurs in an isothermal trickle bed reactor. The concentration of B is very high and the rate of reaction is of pseudo first order with respect to A. If the liquid is saturated with A, correlate the conversion of B with the length of reactor.	10
3.a) What do you mean by bifurcation with respect to steady state stability? For a reaction network, P and Q are the major reactant and product respectively. The dynamics of concentrations of P(C_p) and Q(C_q) are represented by the following equations: $\frac{dC_p}{dt} = X - YC_p + C_p^2 C_q - C_p$ $\frac{dC_q}{dt} = YC_p - C_p^2 C_q$ X and Y are two non-zero constants. Determine the locus (C_{ps}, C_{qs})of steady state and the condition leading to bifurcation.	7
3. b) Describe the operation of an autothermal reactor using the following diagram:	3

[Turn over



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Single adiabatic bed with preheat of reactants by means of effluent.

The reaction, $A \rightarrow B$is occurring in the cylindrical packed bed reactor with diameter of d_r.

4. For a bubble reactor, correlate $N_A = -D_A \frac{dC_A}{dy}\|_{y=0}$with the bulk and interfacial concentration of reactant, A, and the Hatta number. A reaction $aA(g) + bB(l) \rightarrow cC(l) + dD(g)$ is occurring in a bubble reactor. The volumetric flow rate of liquid feed is L and the molar flow rate of gas phase is F. Correlate the required axial length with F, L, partial pressure of A, liquid phase concentration of A at the outlet, Hatta number and other important parameters, H, gas hold-up, ε, bubble diameter, d_p, D_A and k_l.	10