Ref. No.: Ex/PG/ChE/T/111B/2024

M.E. CHEMICAL ENGINEERING FIRST YEAR FIRST SEMESTER EXAM 2024

ADVANCED CHEMICAL ENGINEERING KINETICS AND REACTOR DESIGN

Full Marks 100

Use separate Answer Scripts

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

Part –I

Full Marks:60

Answer any four questions

1.a) Justify the following statements:

(i)'In a catalytic packed bed reactor, a low conversion of reactant is observed at both large and small particle sizes of the porous catalyst, while the optimal conversion being achieved in between". Elucidate the statement using a representative plot. [2]

(ii)'In a tubular catalytic packedbed 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. [2]

1. b) Consider the dissolution (pharmacokinetics) of a solid (B) particle in a liquid (A); wherein the reaction is zero-order in B and first-order in A. Derive the diameter (of the dissolving solid particle)-time relationship; and hence, find the time for complete dissolution of the solid particle. [6]

1.(c) For both slow and fast first order irreversible chemical reactions (constant density) in an isothermal CSTR with constant overflow, determine the time necessary to reach steady-state operation. [5]

2.(a) In a catalytic packed bed reactor, neglecting axial dispersion with respect to forced axial convection, derive the expression for conversion at the reactor's exit for a first order reaction. [5]

2.(b) Butane is converted to i-butane through a single site Langmuir– Hinshelwood (LH) mechanism. Derive the reaction rate equation considering surface reaction controlling. [5]

2.(c) Consider a third order isothermal gas phase catalytic cracking reaction of hydrocarbon 'A': $3A \rightarrow$ products; $(1 >> \varepsilon X)$; 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 conversion as function of catalyst weight. [5]

3. a) How can 'scale-up of packed bed reactor under constant pressure drop' be achieved ? what are the possible limitations of such 'scale-up' strategy? [6]

3.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". [6]

3.c) 'In a tubular catalytic packedbed 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]

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. [5]

4. b) How can you compute 'Dead Volume' of a reactor using 'Dispersion Model' under 'open-open' boundary condition through RTD data? Explain using pertinent equations. [5]

4. c) Elucidate the method (using diagram) of evaluating the model parameters using a step tracer input for modeling a real CSTR with dead-space and bypassing. [5]

5.(a) Defining steady state multiplicity, elucidate the 'ignition', 'extinction' and 'unstable steady state' temperatures using pertinent plots. [5]

5. b) A first order irreversible exothermic reaction (A→ products) is carried out in a CSTR with a heat exchanger. Construct the stability diagram for the first order reaction, (S_1), as a function of T_C.

Data: The ratio of inerts to A fed is 2 to 1.

$\tau = 0.1$ min
$A_0 = 1.5 \times 10^5$ mol/dm^3 • min^{-1}
$A_1 = 1.5 \times 10^5$ min^{-1}
$E = 10{,}000$ cal/mol
$R = 1.987$ cal/mol/K
$Ua = 600$ cal/min/dm^3/K
$C_{P_A} = 10$ cal/mol/K

$C_{P_I} = 20$ cal/mol/K
$T_C = \dfrac{T_0 + \kappa T_a}{1+\kappa} = T_0$
$T_0 = T_a$
$C_{P_0} = \Sigma \Theta_i C_{P_i} = 10 + 2(20) = 50$ cal/mol/K
$C_{A0} = 2.0$ mol/dm^3
$\Delta H_{Rx} = -10{,}000$ cal/mol

Find the region of stability and of runaway.. You can use non-linear equation solver and assume any missing information (if required). [10]

6. The liquid phase (high pressure) adiabatic isomerization of n-butane to i-butane (first order, reversible) is conducted in a PFR using small amounts of a liquid catalyst that provides a reaction rate constant of 31.1 h^{-1} at 360 K. Compute the PFR and CSTR volumes required to process 150 kmol/h at 95% of the equilibrium conversion of a feed (330 K) composed of 95 mol % n-butane and *5* mol% i-pentane (inert).

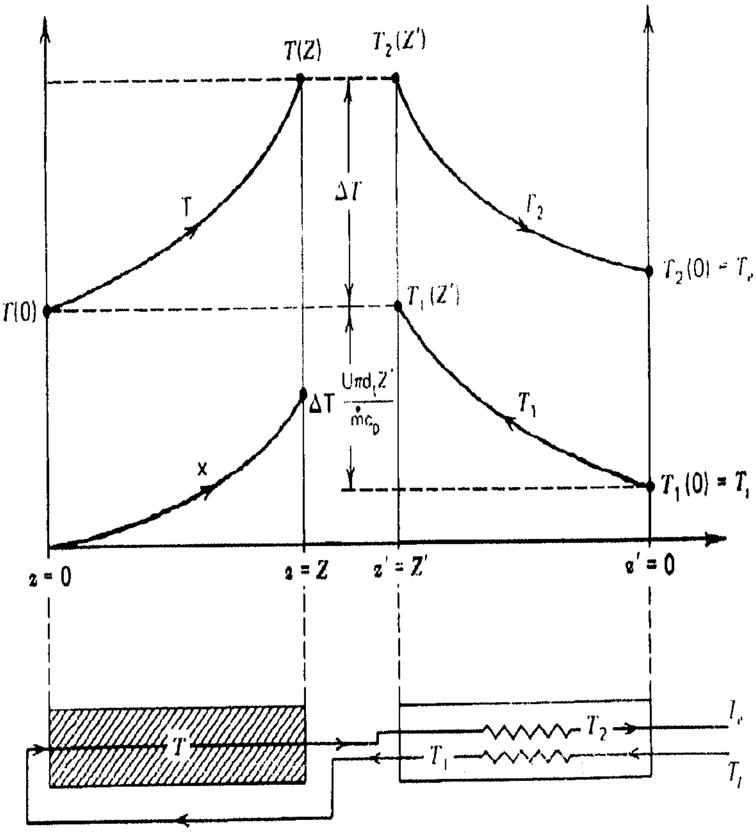
Additional data: ΔH^0_{RX} = -6900 J/mol. n-butane , Activation energy = *65.7* kJ/mol; K_c = 3.03 at 60°C. $C_{p(\text{n-butane})}$= 141 J/mol.K; $C_{p(\text{i--pentane})}$= 161J/ mol.K; $C_{p(\text{i--butane})}$= 141 J/ mol. K; Concentration of n-butane at reactor entrance= 9.3 kmol/m^3. Solve by hand calculation (showing sample results). However, if required, you may find the final answer using any ODE solver. [15]

M.E. CHEMICAL ENGINEERING FIRST YEAR FIRST SEMESTER EXAMINATION

ADVANCED CHEMICAL ENGINEERING KINETICS AND REACTOR DESIGN
Part-II

Full Marks 40
Answer question no. 3 and any two from the rest
Assume any missing data
All symbols carry usual significance

1.a) Considering an appropriate combination of reactor and heat exchanger, develop the mole and energy balance equations of an auto-thermal reactor. Explain the occurrence of multiplicity of steady state in the auto-thermal reactor.



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

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1b) Referring to the following figure for an adiabatic packed bed reactor, define parametric sensitivity.

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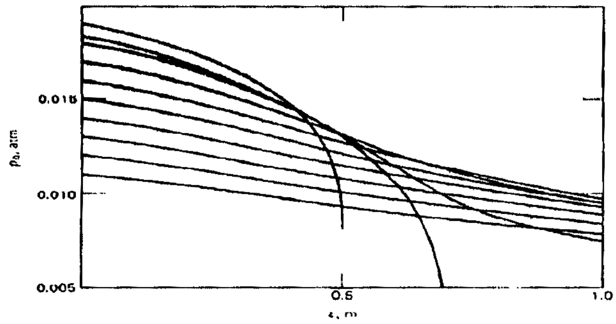
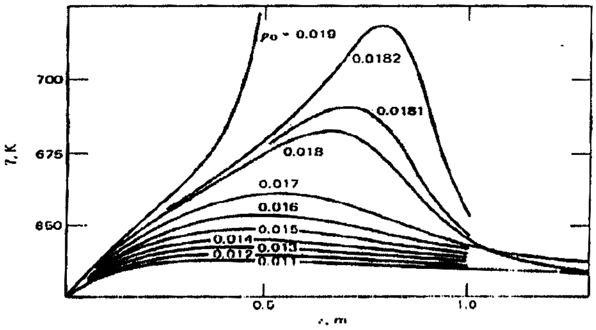


Partial pressure profiles in the reactor illustrating the sensitivity with respect to the inlet partial pressure.



Temperature profiles corresponding to partial pressure profiles

2. A reaction $A(g) + B(l) \rightarrow C(l) + D(g)$ takes place in a bubble column reactor. If gas hold-up be ε, bubble diameter be d_b, k_l be mass transfer coefficient, correlate the length of the reactor with C_{B0}, X_B, P_{Ain}, P_{Aout}. F=flow rate of gaseous reactant, H=Henry's constant for A, P_t=total pressure, Hatta number. Ω=Cross sectional area.
Consider the behaviour as that of a lab-scale bubble reactor. Therefore, gas phase is in plug flow and liquid phase is in mixed flow.

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3. For a reaction network, X and Y are the major reactant and product respectively. The dynamics of concentrations of X(x_1) and Y(x_2) are represented by the following equations:

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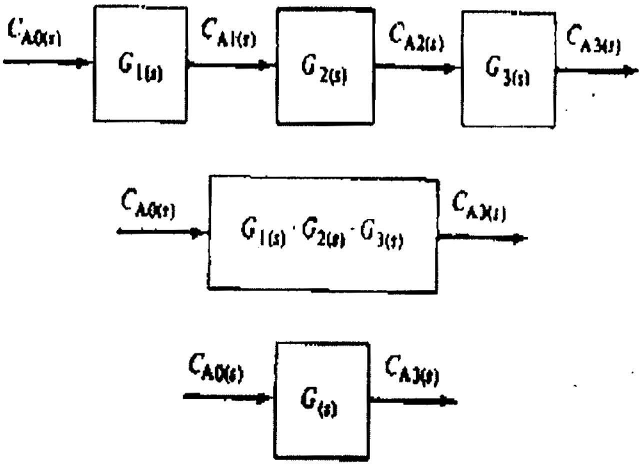
$$\frac{dx_1}{dt} = A - Bx_1 + x_1^2 x_2 - x_1$$

$$\frac{dx_2}{dt} = Bx_1 - x_1^2 x_2$$

Determining the steady state conditions, determine the condition of bifurcation.

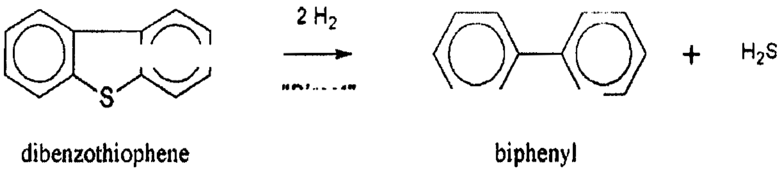
4. Referring to the following figure for three CSTRs in series, justify the following expression and state the significance of $G(s), K_p$ and all $\tau_p s$

$$G(s) = \frac{K_p}{(\tau_{p_1}s+1)(\tau_{p_2}s+1)(\tau_{p_3}s+1)}$$



If C_{A0}has a step perturbation of unity, express C_{A3} as a function of t if $\tau_{p_1} = \tau_{p_2} = \tau_{p_3}$. $L\{e^{-at}\} = \frac{1}{s+a}$; $L\{t^n e^{-at}\} = \frac{n!}{(s+a)^{n+1}}$ 15

5. a) The catalytic hydro-desulfurization of dibenzothiophene (DBT) of diesel is as follows:



Correlate the conversion of DBT with respect to axial length of a trickle bed reactor when a) the reaction is of pseudo-first order with respect to hydrogen concentration due to high concentration of DBT (5000ppm) in feed diesel, if the liquid is saturated with hydrogen. 8

5.b) Write down the system equations for a non-isothermal CSTR undergoing a first order reaction using mole and energy balance.

Convert to perturbation variables and arrange in the form

$$\frac{dC_A}{dt} = a_{11}C_A + a_{12}T + a_{13}C_{A0} + a_{14}T_0 + a_{15}F + a_{16}T_j$$

$$\frac{dT}{dt} = a_{21}C_A + a_{22}T + a_{23}C_{A0} + a_{24}T_0 + a_{25}F + a_{26}T_j$$

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