Ref. No.: Ex/Che/PC/B/T/326/2024

B. Chemical Engineering 3rd Year 2nd Semester Examination, 2024

Chemical Reaction Engineering II

Time: Three Hours

Full Marks: 100

Use separate answer-scripts for Part-I and Part-II

All COs (Course objectives) are compulsory

Assume any missing data

All symbols have their usual meaning

Overall CO-wise marks distribution

CO1	CO2	CO3	CO4	CO5
10	40	10	30	10

PART-I [50 Marks]

CO1	CO2	CO3	CO4
5	20	10	15

CO1 [5 Marks]

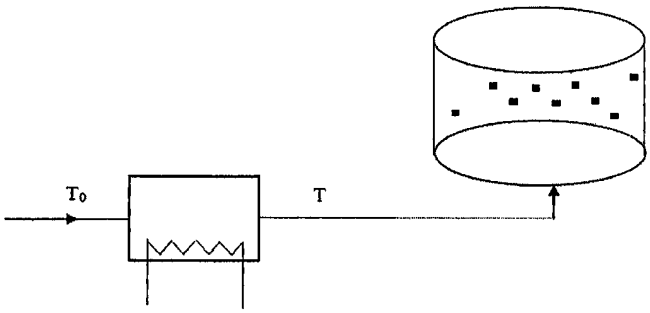
1.A) If the internal mass transfer resistance strongly dominates a catalytic reaction having true values of activation energy and order of 50kJ/mol, what would be the apparent values of activation energy?
i)50kJ/mol; ii) 30kJ/mol; iii) 25kJ/mol

1.B) If the rate of deactivation of catalyst is dependent on the concentration of product, the deactivation is
i) Series type; ii) Parallel type; iii) Side by Side type; iv) Independent type

1.C) If an enzymatic reaction is competitively inhibited, the constant K_m
i) decreases; ii) increases; iii) remains unaffected

1.D) For a slurry reactor, $\frac{C_i}{r_A} = r_b + \frac{1}{m} r_{cr}$. If r_{cr} varies linearly with particle size of catalyst which step is controlling?

1. E) For an n-th order catalytic reaction using spherical catalyst, write down the relationship between Thiele modulus (ϕ_n) and surface concentration of reactant(C_{As}),

radius of sphere (R), order of reaction (n), rate constant (k_n) and effective diffusivity (D_e).	1x5=5
CO2 **Answer any two** **[20 Marks]**	
2. For a non-catalytic reaction, $A(g) + bB(s) \rightarrow Products$, the time required for complete conversion of 400μm, 800μm and 1600μm radii particles are 40 min, 80min and 160 min respectively. What type of resistance is controlling? What relationship prevails between $\left(\frac{t}{\tau}\right), \left(\frac{r_c}{R}\right)$ and X_B under this situation? Justify with all derivations. If 60 minutes is allowed for a solid mixture having 1:1:1 size distribution for 400μm, 800μm and 1600μm solid reactant particles for reaction, what will be the conversion?	1+1+5+ 3=10
3. **Temperature time trajectory** In large scale reactors, such as those for hydrotreating and where deactivation by poisoning occurs, the catalyst decay is slow. Constant conversion with a decaying catalyst in a packed or fluidized bed is to increase the reaction rate to feed temperature.  Develop the temperature-time trajectory equation to keep conversion constant in a CSTR undergoing the reaction $A + B \rightarrow C + D$ if activation energies for reaction and deactivation are 90kCal/mol and 30kCal/mol respectively. First order independent deactivation is occurring with k_d at T_0 of $9h^{-1}$.	10
4.a) Due to deactivation of catalyst, an engineer has observed a declining trend in conversion, X_A for a catalytic reaction $A + B \rightarrow Products$ undergone in a continuous reactor. When the catalyst activity (a) is correlated with operating time (day), the following correlation is determined :$a(t) = 1 - 8.3x10^{-3}t$. The correlation between X_A and activity has been determined to be $X_A(t) = \frac{100a(t)}{1+100a(t)}$. Determine the value of average conversion, $\overline{X_A}$ over 100days operation.	6
4. b) Correlate the effectiveness factor (ɳ) relevant with internal mass transfer resistance with the overall effectiveness factor, Ω for a first order catalytic reaction using spherical catalyst.	4

CO3

10

5. For the determination of rate equation of the enzymatic hydrolysis of A, some experiments were conducted in a CSTR with and without a component B. When C_S is plotted against ($C_{E0}C_St/(C_{S0}-C_S)$), the following correlations are obtained **2+3**

Without B	**$C_S = 20(C_{E0}C_St/(C_{S0}-C_S)) - 200$**	**Slope=20** **Intercept=-200**
With B	**$C_S = 13.992(C_{E0}C_St/(C_{S0}-C_S)) - 200$**	**Slope=13.992** **Intercept=-200**

Write down the rate equation for the enzymatic reaction in absence and in presence of B. What is the role of B in the reaction? Justify your answer showing all derivations.

6. A 2 m^3 continuous stirred tank bioreactor is operated with feed concentration of substrate of 10 kg/ m^3. What feed flow is required to achieve 90% conversion of substrate under steady state? What is the biomass concentration under this condition? The growth kinetic parameters, μ_{max}, K_s *and* $Y_{X/S}$ are 0.45h^{-1}, 0.8kg/ m^3 and 0.55kg biomass/kg substrate respectively for the microorganism cultivated in the reactor. **3+2**

CO4

Answer any one

15

7.The catalytic hydro-desulfurization of dibenzothiophene (DBT) of diesel is as follows: **7.5+7.5**

dibenzothiophene biphenyl

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 (1000ppm) in feed diesel, if the liquid is saturated with hydrogen; b) the reaction is of pseudo-first order with respect to the concentration of DBT as its concentration (100ppm) is low.

8. Hydro-desulfurization of diesel containing dibenzothiophene (DBT) as the main recalcitrant sulfur compound is to be done over CoP catalyst in a trickle bed reactor. The molecular formula of DBT is $C_{12}H_8S$ (MW:184g/mol). Operating temperature and pressure of the reactor are 200°C and 40atm respectively. The reaction is as follows:

$C_{12}H_8S + 2H_2 \rightarrow C_{12}H_{10} + H_2S$

The DBT concentration in the inlet diesel is 1000mg/L. Under the operating condition, diesel is saturated with hydrogen. The reaction is of pseudo first order with respect to

hydrogen. The effectiveness factor can be considered to be unity. Calculate the catalyst bed depth required for 80% removal of DBT in the reactor. The superficial velocity of diesel in the bed is 5cm/s. The rate constant of the reaction is 0.11cm^3/(g-s), liquid to catalyst particle mass transfer coefficient $k_c a_c = 0.5 s^{-1}$; bulk density of catalyst is 0.95g/cm^3; Henry's constant for H_2 at 200°C is 50 $\frac{(\frac{\text{mol}}{cm^3}\text{gas})}{(\frac{\text{mol}}{cm^3}\text{liquid})}$.	**15**

For awareness only

CO1 **Define** and **describe** non-catalytic and catalytic heterogeneous reaction kinetics **K1 and K2**
CO2 **Develop** rate equations for different types of heterogeneous reactions **K3**
CO3 **Solve** the rate equations for heterogeneous reactions and **analyze** the controlling steps **K3&K4**
CO4 **Formulate** design equations for heterogeneous reactors and **predict** their performance **K5& K6**
CO 5 **Explain** steady state multiplicity in CSTRs **K6**

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PART-II [50 Marks]

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CO1	CO2	CO4	CO5
5	20	15	10

CO1: Answer *Q.No.1*	**Marks**
1. Consider irreversible isomerization of A→B on the surface of the pore walls within the spherical catalyst pellet of radius R. (a)Write an expression for the effective diffusivity of 'A' through the porous catalyst pellet in terms of bulk/ Knudsen diffusivity, constriction factor, tortuosity and pellet porosity.	[2]
1. (b) Explain the single-site mechanism of heterogeneous catalytic surface reaction model proposed by Langmuir-Hinshelwood.	[3]
CO2: Answer any *Two questions*	**Marks**
3. (a)Considering shrinking core model and quasi steady state approximation, derive the expression to determine the time for complete regeneration of a spherical catalyst pellet.	[6]
3.(b) Spherical particles of zinc ore (ZnS) 0.004m in diameter are roasted in hot air (21 % O_2) at 850°C and 1atm pressure according to the following reaction: $2ZnS(s) + 3O_2(g) \rightarrow 2ZnO(s) + 2SO_2(g)$ Density of ZnS particles =400 kg/m^3; reaction rate constant, k = 0.125 exp[-13.300/RT]. Effective diffusivity of air in product (ZnO) layer, $D_e=0.550\times10^{-4}$ m^2/s; Film resistance can be neglected. Compute the time required for complete reaction of ZnS particle, considering diffusion through the ash (ZnO) layer as the controlling resistance.	[4]

4. Consider the occurrence of a first order isomerization reaction A ➡ B in a catalytic packed bed reactor. Neglecting any radial variation in concentration and assuming the reactor is operated at steady state, find the conversion of A at the reactor exit (neglecting axial dispersion/diffusion) in terms of bulk density of the catalyst bed, k'', S_a, overall effectiveness factor, reactor length, and superficial velocity.	**[10]**
5.The gas-phase cracking reaction (A→ 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) for determination of 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.	**[10]**
CO4: Answer any *Q.No.6(a), 6(b) and any one between 6.(c) and 6.(d))*	**Marks**
6. (a) Why should you consider the effect of Pressure Drop on Performance of Packed Bed Reactor (PBR)?	**[2]**
6.(b) Plot the pressure drop in a 60 ft length of a 1.5-inch schedule 40 pipe packed with catalyst pellets of 0.25-inch diameter. There is 104.4 lb/h of gas passing through the bed at constant temperature of 260°C.The void fraction is 45% and the properties of the gas are similar to those of air at this temperature. The entering pressure is 10 atm.	**[5]**
6.(c) A second-order reaction 2A ➡ Q+R is taking place in 20 meters of the packed bed described in Q.6.(b). The flow and packed-bed conditions remain the same as in Q.6.(b) except that they are converted to SI units; ,P_o= 10 atm = 1013 kPa. and Entering volumetric flow rate: v_o=7.15m^3/h Catalyst pellet size: D_p= 0.006 m Solid catalyst density: ρ_c= 1923 kg/ m^3 Cross-sectional area of 1.5-inch schedule 40 pipe: A_c = 0.0013 m^2 Pressure drop parameter: β_0 = 25.8 kPa/m; Reactor length: L = 20 m ; The entering concentration of A is 0.1 kmol/m^3 and the specific reaction rate is k= 12 m^6/(kmol.kg_{cat}.h) a) calculate the conversion in the absence of pressure drop. (b) calculate the conversion accounting for pressure drop.	**[8]**
6.(d) The pressure drop in PBR may be computed using Ergun Equation: $\frac{dP}{dy} = \frac{-G}{\rho g_C d}\frac{(1-\psi)}{\psi^3}\left[\frac{150(1-\psi)\mu}{d} + 1.75G\right]$. If the PBR is operated under isothermal condition, (i) Find out the differential equation relating reactor pressure with catalyst weight. (ii) If ε or εX=0; find an expression for the conversion as a function of catalyst weight for a first order isothermal reaction $R \rightarrow Q$	**[4+4]**

CO5: Answer any *One question*	**Marks**
7.(a) Explain the graphical method of finding plug flow reactor (PFR) size for adiabatic operations in case of reversible first-order endothermic reaction	**[3]**
7.(b) Explain the procedure to obtain the Conversion-temperature-rate (reaction pathways) plot of a reversible first order exothermic reaction: Q⇔R	**[7]**
8. 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, (S1), as a function of TC. Data: The ratio of inert to A fed is 2 to 1. $\tau = 0.1 \text{ min}$ $A_0 = 1.5 \times 10^5 \text{ mol/dm}^3 \bullet \text{min}^{-1}$ $A_1 = 1.5 \times 10^5 \text{ min}^{-1}$ $E = 10{,}000 \text{ cal/mol}$ $R = 1.987 \text{ cal/mol/K}$ $Ua = 600 \text{cal/min/dm}^3\text{/K}$ $C_{P_A} = 10 \text{cal/mol/K}$ $C_{P_I} = 20 \text{cal/mol/K}$ $T_C = \frac{T_0 + \kappa T_a}{1+\kappa} = T_0$ $T_0 = T_a$ $C_{P_0} = \sum \Theta_i C_{P_i} = 10 + 2(20) = 50 \text{cal/mol/K}$ $C_{A0} = 2.0 \text{mol/dm}^3$ $\Delta H_{Rx} = -10{,}000 \text{cal/mol}$ Find the region of stability and of runaway. You can use non-linear equation solver and assume any missing information (if required).	**[10]**