

B. Chemical Engineering 3rd Year 2nd Semester Examination, 2019

Chemical Reaction Engineering II

Time: Three Hours

Full Marks: 100

Answer all questions covering all COs (Course objectives)
Assume any missing data
All symbols have usual significance, if not stated otherwise

CO1:20;CO-2:25; CO3:15;CO4: 30; CO5:10

CO1 [20]	<p>Answer Q. 1 and 2 (20)</p> <p>1. a) For an irreversible catalytic reaction, $A+B \longrightarrow M+N$, rate of reaction $r = k\theta_a\theta_b$. What will be the expression in terms of partial pressures if M and N are never adsorbed on the catalyst surface? [3]</p> <p>1. b) The true order of a catalytic reaction is 1.5. What will be the value of apparent order if the system is strongly influenced by internal mass transfer resistance? Justify. [3]</p> <p>1. c) In a continuous stirred tank bioreactor, it has been observed that at and above a particular value of residence time, no cells are present in the reactor. What might have happened? Justify your answer if the microbial growth follows Monod type kinetics. [3]</p> <p>1. d) One of the important assumptions of shrinking core model is _____ [1]</p> <p>2. (a) If C_c is the concentration (g/m^2) of carbon/coke on the catalyst surface after a reaction time, t; write typical equations relating the <i>catalyst activity</i> with C_c and t. [2]</p> <p>2. (b) Identify and briefly elucidate the types (I, II and III) of inhibition in enzymatic reaction according to the following Lineweaver-Burk plot.</p> <div style="text-align: center;"> </div> <p style="text-align: right;">[5]</p> <p>2. (c) Comment on the plausible effect of pore <i>diffusion resistance</i> for $M_w < 0.15$ and $M_w > 4.0$. Where, M_w is 'Wagner modulus' or 'Wagner-Weisz-Wheeler modulus'.</p>
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[Turn over

[3]

CO2

[25]

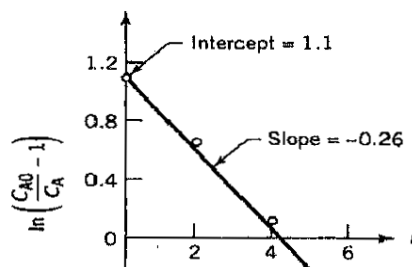
Answer 3 or 4

3.a) If C_s is plotted against $\frac{C_{E0}C_S\tau}{C_{S0}-C_S}$ for an uninhibited mixed flow enzymatic reactor, how will you determine the kinetic parameters in Michaelis-Menten equation? How will the characteristic of the plot alter if a competitive inhibitor is present? Justify your answer.

[7]

3.b) The catalytic decomposition of A ($A \rightarrow R$) is studied in a packed bed filled with 2.4mm pellets and using very high recycle rate of product gas (mixed flow assumption). It is ensured that independent deactivation of first order type has occurred. $De=5 \times 10^{-10} \text{ m}^2/\text{s}$; density= 1500 kg/m³ cat; $\tau'=4000 \text{ kg-s/m}^3$. Using the experimental data, the following plot is obtained. Determine reaction and deactivation kinetics if pore diffusion resistance is (a) negligible and b) controlling.

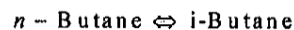
[18]



4. (a) Prove that "The specific growth rate of cells can be controlled by controlling the dilution rate in a Chemostat". Show pertinent derivations.

[5]

4. (b) Consider the isomerization of n-butane to isobutane over a solid heterogeneous catalyst.



Which can be symbolically represented as: $B \rightleftharpoons P$

Where, B: n-Butane and P: i-Butane

Considering the surface reaction step as the rate limiting step (negligible resistance to mass transfer), derive the rate equation following single site Langmuir-Hinshelwood (LH) mechanism. How would you find the observed rate constant, k and adsorption equilibrium constant, K_B ?

[7+3]

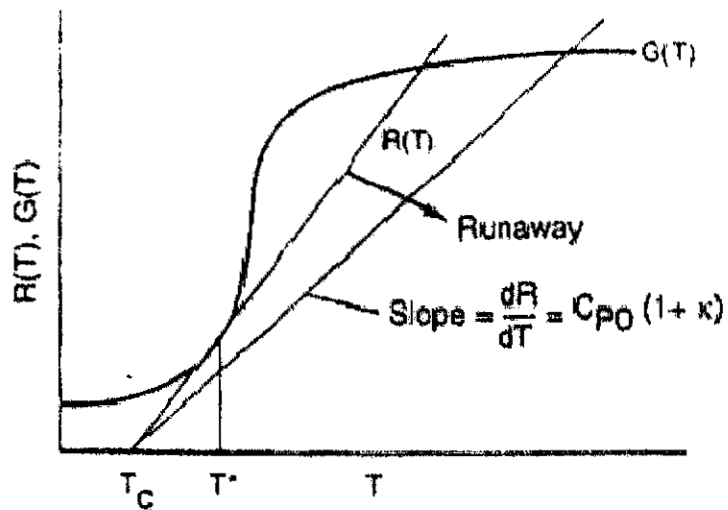
4. (c)(i) Evaluate the Michaelis-Menten parameters V_{\max} and K_M for the hydrolysis of sucrose by the enzyme sucrase (conducted in a 0.5 dm³ isothermal batch reactor) using the following data:

Sucrose concentration, (S); kmol/m ³	0.2	0.02	0.01	0.005	0.002
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	Hydrolysis rate, - $r_s; \text{kmol/m}^3 \cdot \text{s}$	1.08	0.55	0.38	0.2	0.09
	(ii) The initial concentration of sucrose is 0.25 mol/dm^3 and the sucrose concentration is 0.001 g/dm^3 . Calculate the time needed to convert 99% of the sucrose. [7+3]					
CO3 [15]	Answer Question 5 or 6 5.a) Analyzing the following figure, identify the controlling step. Correlate t/τ with X_B for a reaction $A(g) + bB(s) \rightarrow \text{Products}$ [7]					
	<p>The diagram shows a spherical pellet with a gas film of thickness R. Inside the pellet, there is an ash layer of thickness r_c and an unreacted core of radius r_c. The radial position is measured from the center (0) to the outer surface (R). The concentration of the gas-phase reactant is constant at $C_{Ag} = C_{As} = C_{Ac}$ in the gas film and ash layer, and drops to zero at the unreacted core boundary ($r = r_c$).</p>					
	5. b) For a slurry reactor how would you determine the controlling step? Explain with justifications. [8]					
	6. It is envisioned to mitigate the concentration of NO in an engine exhaust stream by passing it through a packed bed of spherical porous carbonaceous solid pellets. A 2% N)-98% air mix flows at a rate of $1 \times 10^{-6} \text{ m}^3/\text{s}$ via a 2 in. -ID tube packed with the pellet at a temperature of 1173 K and a pressure of 101.3 kPa. The reaction (first order in NO occurring) $\text{NO} + \text{C} \rightarrow \text{CO} + 0.5 \text{ N}_2$ follows the following rate equation: $-r'_{\text{NO}} = k_1'' S_a C_{\text{NO}}$; Use the following data:					

	<p> $S_a =$ Internal surface area $= 530 \text{ m}^2/\text{g}$ $k_1^* = 4.42 \times 10^{-10} \text{ m}^3/\text{m}^2 \cdot \text{s}$ At 1173 K, the fluid properties are $\nu =$ Kinematic viscosity $= 1.53 \times 10^{-8} \text{ m}^2/\text{s}$ $D_{AB} =$ Gas-phase diffusivity $= 2.0 \times 10^{-8} \text{ m}^2/\text{s}$ $D_e =$ Effective diffusivity $= 1.82 \times 10^{-8} \text{ m}^2/\text{s}$ The properties of the catalyst and bed are $\rho_c =$ Density of catalyst particle $= 2.8 \text{ g/cm}^3 = 2.8 \times 10^6 \text{ g/m}^3$ $\phi =$ Bed porosity $= 0.5$ $\rho_b =$ Bulk density of bed $= \rho_c(1 - \phi) = 1.4 \times 10^6 \text{ g/m}^3$ $R =$ Pellet radius $= 3 \times 10^{-3} \text{ m}$ $\gamma =$ Sphericity $= 1.0$ Compute the weight of pellet required to diminish the NO concentration to a level of 0.004% and also find the length of the tube. </p> <p style="text-align: right;">[15]</p>
<p>CO4 [30]</p>	<p>Answer any three questions</p> <p>7. A 2nd order decomposition reaction $A \rightarrow B + 2C$ is carried out in a tubular reactor packed with catalyst pellets. The system is strongly controlled by internal mass transfer resistance. Pure A enters the reactor at a superficial velocity of 3m/s, a temperature of 250°C, and a pressure of 500kPa. Experiments carried out on smaller pellets where surface reaction is limiting yielded a specific reaction rate of 0.05m⁶/mol-g cat-s. Calculate the length of bed necessary to achieve 70% conversion. Show all derivation in support of your answer. Additional information: $\eta = 0.166$; Reactor diameter=50mm; Effective diffusivity= $2.66 \times 10^{-8} \text{ m}^2/\text{s}$; Bed porosity: 0.4; Pellet density: 2000kg/m³; S_p: 400m²/g.</p> <p style="text-align: right;">[10]</p> <p>8. A countercurrent moving bed reactor with downflow of solids and upflow of gas is to be designed for the reaction $A(g) + B(s) \rightarrow C(s) + D(g)$. The reactor is to be operated at constant pressure and temperature with a feed concentration of A of 5 mol/ m³. The reactor diameter is 1m with a gas flow rate of 3m³/s. Specially prepared 0.02m diameter pellets of B are fed from the top of the reactor at a rate of 0.5kg/s. The pellets are very reactive and very porous layer of C is formed during reaction and effective diffusivity through the product layer is $1 \times 10^{-7} \text{ m}^2/\text{s}$. Neglect external diffusion resistance and the change in size of pellets with reaction. The value of reaction rate constant, k is 1mm/s. Total solid fraction in the bed is 0.5. The pellet density is 5000kg/m³. Since the molecular weights (=120) of B and C are not very different, the mass flow rate of solid may be assumed to be constant over the reactor length. Correlate the conversion with the reactor length.</p> <p style="text-align: right;">[10]</p> <p>9. A hydrocarbon oil containing thiophene (C₄H₄S) is hydrodesulfurized in a trickle bed reactor undergoing the following reaction: $\text{Thiophene} + 4\text{H}_2 \rightarrow \text{C}_4\text{H}_{10} + \text{H}_2\text{S}$. Pure hydrogen and hydrocarbon liquid are fed to the top of the catalyst bed operated at 40 bar and 300°C. Assume that the liquid is saturated with hydrogen throughout the column. Although the reaction is of</p>

	<p>2nd order, assume that the concentration of thiophene is very large relative to hydrogen and hence the reaction may be considered to be of pseudo-first order with respect to hydrogen. If η is unity, derive the expression for fractional removal of thiophene from oil. What will be the bed height to remove 80% thiophene if its feed concentration be 1000ppm, $u=0.05\text{m/s}$; 1st order rate constant $k_H=0.11\text{L/kg-s}$; $(k_c a_c)_{H_2}=0.5\text{s}^{-1}$; $\rho=0.96\text{kg/L}$; $H_{H_2} = 50(\text{kmol/L})_{\text{gas}}/(\text{kmol/L})_{\text{Liq}}$</p> <p style="text-align: right;">[10]</p> <p>10. (a) Spherical particles of zinc ore (ZnS) 0.004m in diameter are roasted in hot air (21 % O₂) at 850°C and one atmosphere pressure according to the following reaction: $2\text{ZnS (s)} + 3\text{O}_2 \text{(g)} \rightarrow 2\text{ZnO (s)} + 2\text{SO}_2 \text{(g)}$ Density of ZnS particles = 400 kg/m³; reaction rate constant $k = 0.125 \exp[-13.300/RT]$. Effective diffusivity of air in product (ZnO) layer, $D_e=0.550 \times 10^{-4} \text{ m}^2/\text{s}$; 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. [5]</p> <p>10. (b) A pure carbon (C) particle 0.010 m in diameter is to be burned in 21% oxygen at 850°C. Density of C particle = 2000 kg/m³. Reaction rate constant for the pure carbon combustion, $k=2.5 \text{ m}^3/\text{kmol.s}$. The gas film diffusion may be neglected since a considerably high gas velocity is maintained during combustion. Find the time required for complete combustion of the carbon particle, assuming chemical reaction is the controlling step.</p> <p style="text-align: right;">[5]</p> <p>11. A first-order reaction $R \rightarrow S, \Delta H_r = 0$ is being conducted at 1 atm and 609 K in a Mixed Flow (Basket-Type) Reactor with 0.01kg of 0.0012 m catalyst particles at a feed rate of $4 \times 10^{-6} \text{ m}^3/\text{s}$ of pure R. Under these conditions, 80% conversion of R can be achieved. It is envisaged to design a high capacity commercial-sized reactor with 80% conversion at the above conditions. The choice is between a fluidized bed (approximated as MFR) with 0.001 m particles and a PBR with 0.015 m particles. Which reactor type should be selected to minimize the catalyst amount?</p> <p style="text-align: right;">[10]</p> <p>12.(a) Derive the kinetic rate equation for substrate inhibited enzymatic reaction. 12. (b) Find the optimum substrate concentration corresponding to maximum enzymatic reaction rate under substrate inhibition. Show the typical plot of substrate reaction rate as a function of substrate concentration.</p> <p style="text-align: right;">[5+5]</p>
CO5 [10]	<p>Answer Q. 13 or 14</p> <p>13. Using the following figure, state the significance of runaway condition in a non-isothermal CSTR undergoing an exothermic reaction. What is the maximum limit of temperature difference $(T^* - T_c)$? Explain with all derivations.</p>



[10]

14. (a) For a first-order liquid-phase reaction, in a CSTR, express the heat-generated term as a function of temperature. Also show the variation of heat generation curve with space time.

[3+2]

14.(b) Write the heat-removed term, $R(T)$ for a CSTR and show the variation of heat removal line with inlet temperature. Comment on the effects of the molar flow rate F_{A0} or the heat-exchange area on $R(T)$.

[5]

Provide clear nomenclature and expressions for all relevant terms used in your answers.

CO1 **Define** and **describe** the basic mechanisms of non-catalytic and catalytic heterogeneous reactions and biochemical reactions **K1 and K2**

CO2 **Develop** rate equations for different types of heterogeneous reactions and biochemical reactions **K3**

CO3 **Determine** the controlling steps for heterogeneous reactions **K4**

CO4 **Formulate** design equations for heterogeneous reactors and bioreactors and **predict** their performance **K5& K6**

CO 5 **Explain** steady state multiplicity in CSTRs **K6**