REACTOR DESIGN
(CHEN 4141)

Time Allotted : 3 hrs **Full Marks : 70**

Figures out of the right margin indicate full marks.

Candidates are required to answer Group A and <u>any 5 (five)</u> from Group B to E, taking <u>at least one</u> from each group.

Candidates are required to give answer in their own words as far as practicable.

Group – A
(Multiple Choice Type Questions)

1. Choose the correct alternative for the following: **10 × 1 = 10**

(i) As per the collision theory, the rate constant of a reaction is expressed as
(a) $k \propto Te^{-E/RT}$ (b) $k \propto e^{-E/RT}$
(c) $k \propto T^{1/2}e^{-E/RT}$ (d) $k \propto T^{1/2}$

(ii) For a PFR and CSTR of equal volumes, select the right statement
(a) Fractional conversion obtained from the CSTR is higher than a PFR
(b) Fractional conversion obtained from both reactors are same
(c) Fractional conversion obtained from a PFR is higher than that from CSTR
(d) For the same total volume, increasing number of CSTRs will have no effect on conversion

(iii) For a second order reaction carried out in a CSTR and PFR separately, if the fractional conversion is X, the ratio of volumetric productivities in PFR to CSTR is
(a)1-X (b) 1/(1-X) (c) X (d) 1/X.

(iv) For n CSTRs in series where a first order reaction is carried out, conversion obtained from the nth reactor is
(a) $x_n = 1 - \frac{n}{1+k\tau}$ (b) $x_n = 1 - \frac{1}{(1+k\tau)^n}$ (c) $x_n = \frac{1}{(1+k\tau)^n}$ (d) $x_n = \frac{n}{1+nk\tau}$

(v) In two-parameter model of real CSTR, the two parameters are generated considering
(a) By-passing and dead volume
(b) Recycling a portion of the exit stream and dead volume
(c) By-passing and connecting N reactors in series
(d) By-passing and recycling a portion of effluent stream.

(vi) At high substrate concentration, the rate of product formation according to Michaelis-Menten kinetics is
(a) first order (b) zero order (c) second order (d) order 0.5

(vii) In an adiabatic batch reactor
- (a) solving only mole balance equation is sufficient to determine the time taken to achieve a desired conversion
- (b) solving only energy balance equation is sufficient to determine the time taken to achieve a desired conversion
- (c) the steady state energy balance and mole balance equations are solved simultaneously to determine the time taken to achieve a desired conversion
- (d) the unsteady state energy balance and mole balance equations are solved simultaneously to determine the time taken to achieve a desired conversion

(viii) When the rate of product formation is half the maximum forward velocity, the value of Michaelis-Menten constant equals
- (a) half the substrate concentration
- (b) substrate concentration
- (c) zero
- (d) square of substrate concentration

(ix) The equation for microbial growth kinetics which incorporates carrying capacity is known as
- (a) Monod equation
- (b) logistic equation
- (c) Tessier equation
- (d) Blackmann equation.

(x) The Damköhler number is a dimensionless group representing
- (a) The ratio of rate of consumption of a species by reaction to rate of transport of the species by diffusion
- (b) The ratio of rate of consumption of a species by reaction to rate of transport of species by convection
- (c) The ratio of rate of transport of species by convection to rate of consumption of species by reaction
- (d) The ratio of rate of transport of species by convection to rate of transport of species by diffusion.

Group – B

2. (a) State the different assumptions of the transition state theory and derive the expressions for activation energy and frequency factor for a bimolecular reversible reaction**.** For the reaction set given below, perform the test for independence and determine the number of independent reactions from the set

$$Br_2 \rightarrow 2Br$$
$$Br + H_2 \rightarrow HBr + H$$
$$H + Br_2 \rightarrow HBr + Br$$
$$H + HBr \rightarrow H_2 + Br$$
$$2Br \rightarrow Br_2$$

(b) Thermal cracking of propane was studied at atmospheric pressure and 800 ^{o}C in a tubular reactor. The reaction is carried out in the presence of a diluent, steam, the diluent ratio being 0.2 moles diluent/mole hydrocarbon. The reaction can be represented as A->2P. Derive the expressions for molar flowrates of propane, products, diluent and the total molar flowrate at a certain distance inside the reactor where conversion is x_A. Using the integral method of analysis, evaluate the rate constant if a conversion of 0.63 is achieved for V/F_{A0}=50.

(3 + 4) + 5 = 12

3. (a) The following reaction was carried out at atmospheric pressure and 800 °C in a tubular reactor.

A->2B

The reaction is carried out in the presence of a diluent, steam, the diluent ratio being 0.1 mole diluent/mole hydrocarbon. Derive the appropriate rate expression and using the differential method of analysis, determine the rate constant and order of the reaction. The rate versus conversion data are as follows:

Conversion	0.49	0.63	0.69	0.71	0.76	0.78
Rate	0.01	0.0066	0.0054	0.0049	0.0041	0.0035

(Graph required)

(b) Explain what is meant by extent of a reaction. Express the mole fraction of a reacting species in an exit stream in terms of the extent of reaction. For an irreversible bimolecular second order reaction carried out in a batch reactor, derive the expression for conversion as a function of time

6 + (1 + 2 + 3) = 12

Group – C

4. (a) For the parallel reactions

$$A \to D$$
$$A \to U$$

consider all possible combinations of reaction orders and select the reaction scheme that maximizes the instantaneous rate selectivity parameter S_{DU}. Distinguish between overall and instantaneous yields from a reactor. Explain how the yield of a desired product can be obtained from yield versus reactant concentration plots for a PFR, MFR and MFR in series

(b) Substance A in liquid phase produces R and S by reactions

$$A \to R$$
$$A \to S$$

Where $r_R = k_1 C_A^2$
$r_S = k_2 C_A$

The feed C_{A0}= 1mol/m³, C_{R0}=0 and C_{S0}=0.3 mol/m³ enters the two mixed flow reactors in series where τ_1=2.5 min, τ_2=10 min. Knowing the composition in the first reactor, determine the composition of the stream leaving the second reactor.

(3 + 2 + 2) + 5 = 12

5. (a) Design a fluidized bed reactor for production of acrylonitrile by ammoxidation of propylene with air as the oxidizing agent. Required production of acrylonitrile is 40,400 tons/year (8000 h or 340 days working). The process achieves a 78% conversion of propylene at 400 °C and atmospheric pressure.

The reaction is first order with rate constant 1.44 m^3/kg cat. hr at 400 ºC. Volume fraction of propylene in feed is 0.24. Solid density is 2500 kg/m^3, specific heat 0.2 kcal/kg ºC, void fraction of the packed bed is 0.5. At minimum fluidization velocity u_{mf}= 7.2 m/h, void fraction ε_{mf} is 0.6. Gas properties are as follows:

Gas density ρ_g= 1kg/cc, specific heat Cp=0.25 kcal/kg ºC, viscosity μ=0.144 kg/m.h and effective diffusivity D_A=0.14m^2/h. Assume a bubble diameter d_b of 0.1m. The superficial feed velocity is 1800 m/h. Use Kunii and Levenspiel method for calculations.

Given: Bubble relative velocity U_{br}=0.711×(g × d_b)$^{0.5}$,

Mass transfer coefficients are calculated from the following correlations :

$(k_{bc})_b = 4.5\left(\frac{u_{mf}}{d_b}\right) + 5.85\left(\frac{D_A^{1/2} g^{1/4}}{d_b^{5/4}}\right)$ and $(k_{ce})_b = 6.78\left(\frac{\varepsilon_{mf} D_A u_b}{d_b^{\,3}}\right)^{1/2}$

The equation for concentration profile in the bed is

$$-u_b \frac{dC_{Ab}}{dz} = k\left[\rho_b + \cfrac{1}{\cfrac{k}{(k_{bc})_b} + \cfrac{1}{\rho_c \cfrac{V_{iz}}{V_b} + \cfrac{1}{\cfrac{k}{(k_{ce})_b} + \cfrac{1}{\rho_e \cfrac{1-f_b}{f_b}}}}}\right] C_{Ab} = K_r C_{Ab}$$

Moreover $\frac{\bar{C}_A}{C_{Ai}} = \exp\left(\frac{-K_r L_f}{u_b}\right)$

(b) Discuss the uses of slurry reactors in different chemical engineering applications

8 + 4 = 12

Group – D

6. (a) Develop the design equation of a chemostat where cell growth and product formation are the two processes contributing to substrate utilization

(b) Derive the Michaelis-Menten kinetics using quasi steady state assumption. Explain the significance of critical oxygen concentration in fermentation

7 + (3 + 2) = 12

7. (a) In a fed-batch bioreactor, prove that the total amount of cells in the culture increase with time. What is the necessary assumption behind this derivation?

(b) Consider scale-up of a fermenter from a 10 litre to 10,000 litre vessel. The small fermenter has a height to diameter ratio 3. Impeller diameter is 40% of the tank diameter. Agitator speed is 500 rpm and three Rushton impellers are used. Determine the dimensions of the large fermenter and agitator speed for

(i) Constant P/V
(ii) Constant impeller tip speed
(iii) Constant Reynolds number.

(5 + 1) + (3 × 2) = 12

Group – E

8. (a) The elementary irreversible organic liquid phase reaction $A+B \rightarrow C$ is carried out adiabatically in a flow reactor. An equal molar feed in A and B enters at 27ºC and the volumetric flow rate is 2 dm^3/s. Calculate the PFR and CSTR volumes necessary to achieve 85% conversion. Calculate the conversion that can be achieved in a 500 dm^3 CSTR. Given: $H_A^o(273)$=-20 kcal/mol, $H_B^o(273)$=-15 kcal/mol, $H_C^o(273)$=-41 kcal/mol, C_{A0}=0.1 kmol/m3, Cp_A=Cp_B=15 cal/mol K, Cp_C=30 cal/mol K, k=0.01 dm3/mol. s at 300 K, E=10000 cal/mol.

(b) For a first order reaction carried out in a non-isothermal CSTR, derive the expressions for heat generation and heat removal terms and explain the multiplicity of steady states. What necessary information can be obtained from an ignition extinction curve? Explain the runaway criteria.

(4 + 2) + (2 + 2 + 2) = 12

9. (a) The first order reaction A->B is carried out in a 10 cm diameter tubular reactor 6.36 m long. The specific reaction rate is 0.25 min^{-1}. Results of a tracer test carried out in the reactor are given below. Calculate conversion using (i) closed vessel dispersion model from the following

expression $X = 1 - \dfrac{4q\exp(Pe_r/2)}{(1+q)^2\exp(Pe_r q/2) - (1-q)^2\exp(-Pe_r q/2)}$

where $q = \sqrt{1+4Da/Pe_r}$

(i) tank in series model.

The reactor Peclet number can be calculated from

$$\frac{\sigma^2}{\tau^2} = \frac{2}{Pe_r} - \frac{2}{Pe_r^2}\left(1-e^{-Pe_r}\right)$$

Here $\tau = \int_0^\infty tE(t)dt$ and $\sigma^2 = \int_0^\infty t^2E(t)dt - \tau^2$

The effluent tracer concentration time data (tracer test results) are as follows

t(s)	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

(b) Explain the use of segregation model for predicting conversion in a reactor.

9 + 3 = 12

Department & Section	Submission Link
CHE	https://classroom.google.com/c/MTQyODQ1NTUyNDE3/a/MjcxMjE2MjY5NTg5/details