Ref. No. Ex/PG/ChE/T/111B/2018

MASTER OF CHEMICAL ENGINEERING EXAMINATION, 2018
(1st Semester)

ADVANCED CHEMICAL ENGINEERING KINETICS AND REACTOR DESIGN

Full Marks 100

Time: 3 hours

All symbols have usual meaning
Assume any missing data
Answer Five questions
(Any three from Group-A and Any two from Group-B)
Do not use separate Answer-scripts

Group A

Answer any three questions

1. i) State "Mears' Criteria" for negligible resistances to external diffusion and heat transfer from bulk fluid phase to external catalyst surface for heterogeneous chemical reaction .

[4+4]

1.(ii) Ethylene and oxygen are fed in stoichiometric proportions to a packed-bed reactor operated isothermally at 200°C. Ethylene is fed at a rate of 0.136 kmol/s at a pressure of 10 atm. It is proposed to use 10 banks of 1.5 inch(0.0381 m) diameter schedule 40 tubes packed with catalyst with 100 tubes per bank. Consequently, the molar flow rate to each tube is to be 0.136 gmol/s. The properties of the reacting fluid are to be considered identical to those of air at this temperature and pressure. The density of the 0.635 cm catalyst particles is 1922 kg/m^3 and the void fraction is 0.45. The rate law is

$$-r_A^{/} = k\, P_A^{1/3}\, P_B^{2/3}\ gmol/g\,cat.h \quad and \quad k = 0.0141\frac{gmol}{atm.g\,cat.h}$$

Find out the coupled differential equations(considering pressure drop) to obtain conversion of ethylene and reactor pressure as a function of catalyst weight.

[12]

2. (i) Express the following terms in RTD analyses of chemical reactor: 'Exit Age distribution Function' (for pulse and step tracer experiments), 'Mean Residence Time", 'Variance' and 'Bodenstein Number' and state their significance. **[4+2+2+2]**

2. (ii) Considering shrinking core model and quasi steady state approximation, derive the expression to determine the time for complete regeneration of a spherical catalyst pellet through removal of deposited carbon(coke) using oxygen. **[10]**

3. (i) A factor of 10 scale up in the linear dimensions of a CSTR, $S^{1/3} = 10$, requires a factor of 100,000 increase in total power and a factor of 100 increase in power per unit volume if t_{mix} is held constant. Such a scale up would be absurd. A more reasonable scale up rule is to maintain constant power per unit volume so that a 1000-fold increase in reactor volume requires a 1000-fold increase in power. What happens to t_{mix} in this case?

[10]

3.(ii) In order to increase the capacity of a tubular reactor, what are the common scaleup strategies ? Briefly state the method of scaleups for Turbulent Flow in a tubular reactor using Geometrically Similar and constant pressure drop criteria. **[4 +6]**

4. (i) Consider the second order isothermal reaction, 2A $\longrightarrow$ B which is conducted in a catalytic PBR .Find an expression relating catalyst weight and conversion of the reactant and explain graphically the effect of pressure drop on conversion/reaction rate.

[10]

4. (ii) The catalytic dehydrogenation of n-butane (R) is conducted to produce butylene (B) and hydrogen(C) in a moving-bed reactor (MBR) at 880K . The reaction may be represented as R $\longrightarrow$ Products

The lumped dehydogenation rate can be represented by a 2nd order rate law:

$$-r_R' = \mathbf{0.5}\frac{(dm)^6}{(g\,cat)\,(mol)\,(\min)}\quad C_R^2$$

The catalyst deactivation obeys a first order decay rate law, (decay constant, $k_D = 0.65$ min^{-1}). The volume changes during reaction may be neglected. The MBR contains 17 kg of catalyst that travels through the reactor at a rate of 8 kg/min. Butane is fed at the rate of 27 kmol/min at a concentration of 0.068 kmol/m^3. Determine the conversion of n-butane in the MBR. **[10]**

5.(i) Derive the equation to evaluate the conversion in a nonideal reactor by 'maximum mixedness model' considering a plug-flow reactor with side entrances. **[10]**

5. (ii) Using a pulse tracer experiment, how would you find out the number of equal volume ideal CSTRs required to model a real CSTR as per the 'Tanks-in Series " model ? Hence find out an expression for conversion in case of a first order reaction.

[10]

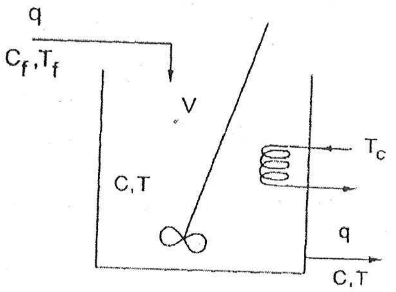
Group-B

Answer Any two

6.i) Methyl linoleate is to be catalytically converted to methyl oleate in a 2 m^3 slurry reactor. The molar feed rate of methyl linoleate is 0.7kmol/min and the diameter of the catalyst is 60μm. The saturation concentration of hydrogen in the liquid phase is 0.014kmol/m^3. The reactor is considered to be well mixed. From a laboratory experiment using the same catalyst, it has been observed that the system is internal mass transfer controlled and the value of r_b and r_{cr} with 80μm catalyst are 0.08min and 0.28min-kg/m^3. Calculate the catalyst loading necessary to achieve 30% conversion for the present reactor. Show all derivations.

[10]

6.ii) A non-adiabatic CSTR shown in Figure 1 is used for an irreversible 1st order reaction $A \rightarrow B$.



The following dimensionless material and energy balance equations are obtained

$$\frac{dx_1}{d\tau} = -x_1 - \delta(x_1 - x_{1c}) + B\,\mathrm{Da}(1 - x_2)\exp\left(\frac{x_1}{1 + x_1/\gamma}\right)$$

$$\frac{dx_2}{d\tau} = -x_2 + \mathrm{Da}(1 - x_2)\exp\left(\frac{x_1}{1 + x_1/\gamma}\right)$$

Where,

$$x_1 = \frac{T - T_f}{T_f} \frac{E}{R_g T_f}, \qquad x_2 = \frac{C_f - C}{C_f}, \qquad \theta = \frac{V}{q}, \qquad \tau = \frac{t}{\theta}$$

$$x_{1c} = \frac{T_c - T_f}{T_f} \frac{E}{R_g T_f}, \qquad \gamma = \frac{E}{R_g T_f}, \qquad \mathrm{Da} = k_0 e^{-\gamma}\theta$$

$$B = \frac{(-\Delta H) C_f}{C_p \rho T_f} \frac{E}{R_g T_f}, \qquad \delta = \frac{Ua}{q C_p \rho}$$

Make linear stability analysis of steady states and apply Hopf bifurcation method using Damkohler number, Da as a parameter.

[10]

7. i) Oxidation of o-xylene to o-methyl benzoic acid, $o - Xylene + 1.5O_2 \rightarrow o - methyl\,benzoic\,acid$ is conducted in a bubble reactor. The reaction is of pseudo first order with respect to o-xylene. The reactor has a diameter of 2m and the superficial gas velocity is considered to be constant at 0.057m/s. Using Van Dierendonck correlations, the gas hold-up, ε_g, and bubble diameter d_b,(evaluating Eotvos no.) have been determined to be 0. 11 and 1mm respectively. At the reactor condition, Van Dieren donck predicts a k_l of 0.781m/h. Determine the length of the reactor introducing Hatta number. $p_{O2,in}$ =2.898 bar , $P_{t,air}$ = 13.8bar , H=126.6 m^3 bar/kmol , $D_{O2/xylene}$ =$5.2x10^{-6}$ m^2/h, bulk concentration of O_2 is 2.04kmol/m^3 and feed rate of gas is 245kmol/h.

[12]

7.ii) The elementary irreversible liquid phase reaction $A + B \rightarrow C$ is carried out adiabatically in a CSTR. If an equimolar flow rate of A and B enters the reactor at 27°C and the volumetric flow rate is 2dm^3 /s, derive the expression for the volume of the reactor required for 60% conversion. $k = 204.8x10^3 \exp(-10000/RT)$ L/mol-s and $\Delta H^0_{RX} = -6000 Cal/mol$

[8]

8. i) A catalytic reaction $aA(g) + bB(l) \rightarrow cC(g) + dD(l)$ is conducted in a trickle bed reactor. The reactor is packed with solid catalysts. Developing relevant molar balances in all phases, correlate the conversion of A with the height of reactor when the liquid phase can be assumed to be fully saturated with A and the reaction is of pseudo first order with respect to reactant B.

[12]

8. ii)For three CSTRs in series, determine the transfer function for the system when the residence time and rate constants in 1st, 2nd and 3rd reactors are τ_1, τ_2, τ_3 and k_1, k_2, k_3 respectively. Also determine the response C_{A3} (t) when a unit step change is introduced in the feed concentration.

[8]