B. Chemical Engineering 3rd Year 2nd Semester Examination, 2018

Chemical Reaction Engineering II

Time: Three Hours | Full Marks: 100

Answer questions covering all COs (Course outcomes)

CO1:20;CO2:25; CO3:15;CO4: 30; CO5:10

CO1 [20]

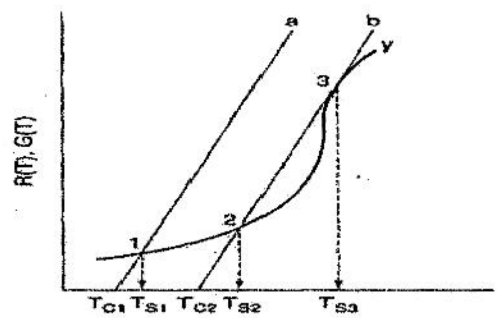
Answer Q. 1 and 2

1. a) In case of series type deactivation, $-\frac{da}{dt} =$ ____________ . Justify. [2]

1.b) Under strong control of internal pore diffusion, if the observed activation energy is 30kJ/mol, the actual activation energy is ____________. Justify. [2]

1.c) In case of competitive inhibition enzyme binds____________ and the value of MichaelisMenten constant____________. [2]

1.d)What is the significance of this plot? [1]



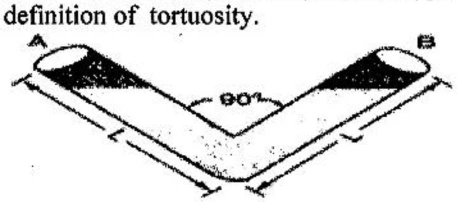
1.e) For shrinking spherical particles the time for complete conversion is proportional to __________. Justify [3]

2.Consider irreversible isomerization of $A \rightarrow B$ 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. [3]

2.(b) What is 'constriction factor'?[1]

2. (c) Calculate the tortuosity for the hypothetical pore of length "L" (as shown in figure below)from the definition of tortuosity.



[2]

2. (d) Write Mears criteria using the measured rate of reaction $-r_A'$ for (i) negligible external mass transfer resistance from the bulk gas phase to the exterior catalyst surface and (ii) negligible temperature difference between bulk fluid phase and external surface of the solid catalyst. [4]

CO2

Answer Q. 3 or 4

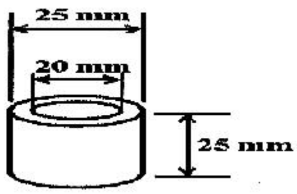
3.a) Correlate the concentration of the reactant of a first order heterogeneous catalytic reaction,

[25] A $\longrightarrow$ B with the radial position in a spherical catalyst. Derive the expression for effectiveness factor for internal mass transfer resistance controlled system. [10]

3.b) Describe the procedure by which you will determine the reaction kinetics of a first order reaction in presence of independent deactivation using a reactor with batch solid-mixed fluid modes of operation. [5]

3.c) [3]

Hydrogenation of benzene is to be carried out using Ni (density = 8910 kg/m^3) as catalyst, cast in the form of non-porous hollow cylinders, as shown below. The reaction occurs on all the surfaces of the hollow cylinder. During an experiment, one such cylinder is suspended in the reactant stream. If the observed rate of reaction is 0.39 mol (m^2 of catalyst surface)$^{-1}$ min^{-1}, then the rate of reaction in mol (kg of catalyst)$^{-1}$ min^{-1} is ________________ (rounded off to three decimal places).



3.d)

At room temperature sucrose is hydrolyzed by the enzyme sucrase follows:

$$\text{sucrose} \xrightarrow{\text{sucrase}} \text{products}$$

Starting with sucrose (C_{A0} = 1 mol/m^3) and sucrase (C_{E0} = 0.01 mol/m the following data are obtained in a batch reactor (concentrations a calculated from optical rotation measurements)

C_A, mol/m^3	0.68	0.16	0.006
t, hr	2	6	10

Find a rate equation to represent the kinetics of this reaction.

[7]

4. (a) Develop the kinetic rate equation for un-competitively inhibited enzymatic reaction. [5]

4. (b) Derive the expression of time required for complete regeneration of a spherical porous catalyst pellet (deactivated by coking) applying shrinking core model. Assume quasi-steady state assumption. [10]

4. (c) Thefollowing data was determined in a batch reactor for the yeast *Saccharomyces Cerevisiae*

Glucose (S) $\xrightarrow{cells(C)}$ More cells (C) + Ethanol(P)

Time (h)	Cells (g/ dm^3)	Glucose (g/ dm^3)	Ethanol (g/ dm^3)
0	1	250	0
1	1.37	245	2.14
2	1.87	238.7	5.03
3	2.55	229.8	8.96

Determine the yields: $Y_{S/C}$, $Y_{C/S}$, $Y_{S/P}$, $Y_{P/S}$, $Y_{P/C}$ and parameters of Monod equation: μ_{max} and K_s. Assume no lag and neglect maintenance at the start of the growth where there are just a few cells.[10]

CO3 [15] **Answer Q. 5 or 6**

5.a)

Liquid phase isomerization of *o*-xylene to *p*-xylene using a zeolite catalyst was carried out in a CSTR. Three sets of kinetic data at different temperatures and stirring speeds were obtained as shown below.

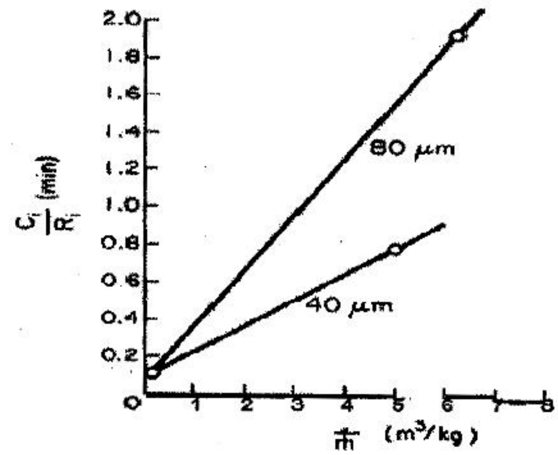
	set A			set B			set C		
temperature (K)	500	500	500	600	600	600	700	700	700
stirring speed (rpm)	1000	2000	3000	1000	2000	3000	1000	2000	3000
reaction rate (mol L^{-1} s^{-1})	0.020	0.025	0.025	0.037	0.047	0.047	0.069	0.078	0.086

The operating condition at which the reaction rate is not controlled by external mass transfer resistance is

(A) T=500K; rpm=1000 (B) T=600K; rpm=1000 (C) T=700K; rpm=2000 (D) T=600K; rpm=3000.

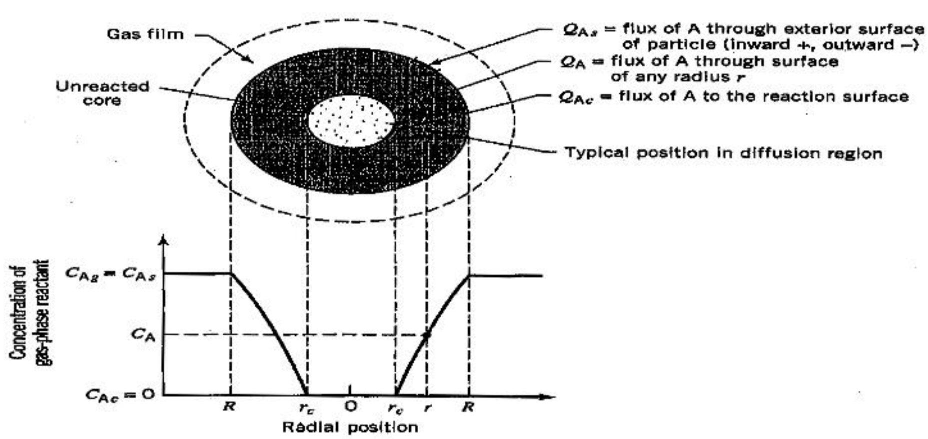
[1]

5.b) The $\frac{C_i}{r_i}$ versus $\frac{1}{m}$ plot for a slurry reactor is as follows. Which is the limiting step? [2]



5. c) Methyl linoleate is to be hydrogenated to methyl oleatein a $4m^3$ slurry reactor. The molar feed rate of methyl linoleateto the reactor is 0.7 kmol/min. The saturation concentration of hydrogen at the gas-liquid interface is $0.014 kmol/m^3$. From lab scale experiment it has already been established that the system is internal mass transfer controlled. The values of resistance to gas absorption, r_b and the combined resistance, r_{cr} to transport to surface of catalyst and diffusion and reaction in the catalyst pellet for 60mm catalyst are 0.08 min and 0.21 min-kg/m3 respectively. Determine the catalyst charge necessary for 60% conversion using 80mm catalyst pellets. [11]

5.d) Using the following figure, state which resistance is controlling. **[1]**

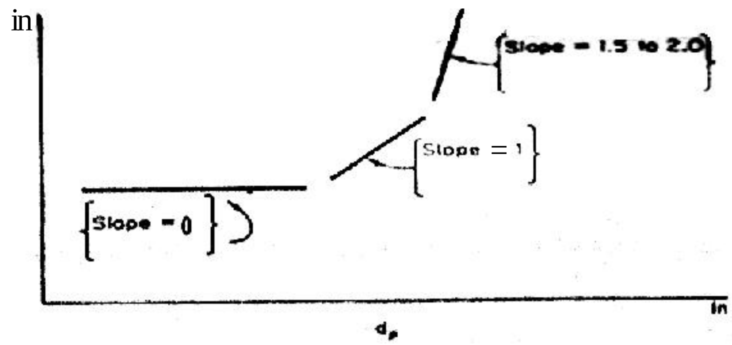


6. (a) Derive the relation between time and radius of unreacted core and hence, find the time required for completion of a fluid –solid(spherical, unchanging size) non-catalytic reaction when the chemical reaction

is the major resistance following shrinking-core model. **[6]**

6.(b)A packed bed reactor converts A to R by a first- order catalytic reaction, $A \rightarrow R$. With 0.009 m pellets the reactor operates in the strong pore diffusion resistance regime and gives 63.2% conversion. In order to reduce pressure drop, if the 0.009 m pellets were replaced by 0.018 m pellets; what would be the new conversion. [5]

6.(c)From the following plot obtained for a slurry reactor, explain the different controlling regimes for hydrogenation of methyl linoleate to produce methyl oleateover a suitable heterogeneous solid catalyst.



Effect of particle size on controlling resistance.

[4]

CO4 [30]

Answer any three from questions 7-12

7. a) To avoid wash-out condition in a continuous stirred tank bioreactor undergoing microbial reaction, the value of dilution rate should be kept below ______________________________. Derive. [3]

7. b) A reaction 4A(g)+B(l)⟶ cC(g)+dD(l) is occurring in a trickle bed catalytic reactor. Both axial and radial dispersions are negligible in gas and liquid phases. The condition is such that the reaction is pseudo first order with respect to the concentration of A. If the liquid phase is not saturated with A and both internal and external mass transfer resistances play important role, correlate the conversion of B and the length of the reactor assuming the constancy of gas phase concentration of A. [7]

8. A non-catalytic heterogeneous reaction $2NaCl+H_2O + SO_3$ Na_2SO_4+2HCl is occurring in an up-flow reactor. In a laboratory test, 85% conversion of 88-105μm particle has been observed to take 10 s. Solid hold-up is 0.01. Chemical reaction is controlling. The RTD data and size analysis data are as follows:

Particle size (μm)	Weight fraction	Residence time t/τ
50-60	0.4	0.6
70-80	0.4	0.9
105-125	0.2	1.3

Determine the average conversion of NaCl to Na_2SO_4. Will there be any change in the conversion if a down-flow reactor is used? Justify your answer. Data: Solid feed rate: 450 kg/min; D=0.6m; H=9.1m and ρ_b= 2100 kg/m^3. Show all derivations, wherever necessary. [10]

9. a)Develop the design equation for the fluidized bed reactor to correlate conversion with the length of the reactor undergoing first order reaction. [5]

9.b) The lumped cracking kinetics of a hydrocarbion present in gas oil is given by a 2nd order rate law $-r_A = 0.6\dfrac{dm^3}{g\,cat.mol\,\min}C_A^2$. Rate constant for independent deactivation, Kd=0.72min^{-1}. W=20kg; us=10kg/min; hydrocarbon feed rate gas oil =30mol/min; CA_0=0.075mol/dm^3. Determine the conversion. [5]

10.The catalytic dehydrogenation of ethylbenzene (R) is conducted to produce styrene (**B**) and hydrogen(C) in a moving-bed reactor (MBR) at 880K.The reaction may be represented as :

ethylbenzene $\longrightarrow$ Products; The lumped dehydogenation rate can be represented by a 2[nd] order rate law:

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

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. Ethyl benzene is fed at the rate of 27 kmol/min at a concentration of 0.068 kmol/m^3. Determine the conversion of ethyl benzene in the MBR. [10]

11.A specific microbial reaction obeying Monod Kinetics(without inhibitory effect)is being conducted in a continuous stirred tank bioreactor undergoing, correlate the cell production rate per unit volume and cell concentration as a function of dilution rate. Hence, find the expression of dilution rate corresponding to the maximum cell production.[10]

12. 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,

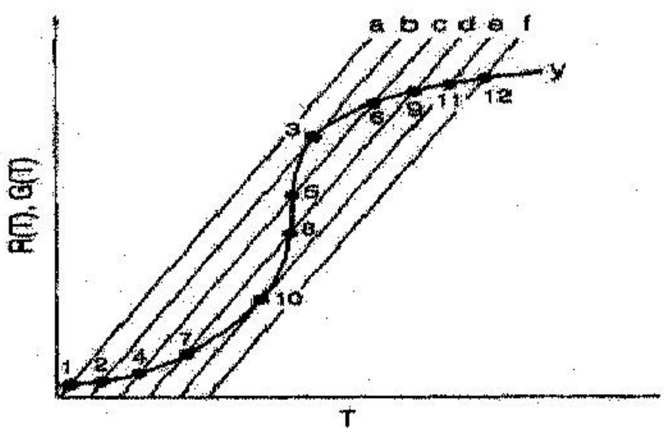
(a) Find out the differential equation relating reactor pressure with catalyst weight.

(b) If εor εX=0; find an expressionfor the conversion as a function of catalyst weight for first order isothermal reaction $R \rightarrow Q$. **[5+5]**

CO5 [10]

Answer Q. 13 or 14

13. Defining steady state multiplicity, determine the ignition –extinction diagram using the following plot. How can you modulate the inlet temperature to avoid runaway condition? Show all derivations.



[10]

14. (a) For a first order irreversible chemical reaction, assuming thatthe concentrations of the reacting

	species are weak functions of temperature, explain the construction of the stability diagram of a CSTR. [5] 14.(b) Using pertinent plot , elucidate the conditions for run-away of an exothermic chemical reaction being conducted in a non-adiabatic CSTR. Provide clear nomenclature and expressions for all relevant terms used in your answer. [5]

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 heterogeneousreactions **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**