BIRLA INSTITUTE OF TECHNOLOGY AND SCIENCE, PILANI

SECOND SEMESTER 2017-2018

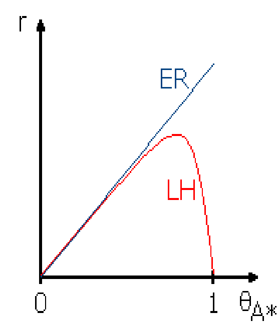
CHE 641 Reaction Engineering

Comprehensive Exam (Close Book) Date: 12.05. 2018

Duration: 3:00 PM – 06:00 PM Maximum Marks: 80

PART- A (10 x 1.5 = 15 M)

1. Answer the following in ***sequence*** with maximum 2 sentences.
   a. What is the limit on reaction temperature to prevent catalyst sintering for dry and steam reforming of hydrocarbons?
   b. At high temperatures the rate limiting step is usually diffusion rather than surface reaction control. Explain.
   c. Explain the purpose of inter stage heating and cooling operations for the positive order reactions with the help of neat sketches. Is this operation required for irreversible reactions?
   d. Tortuosity of a porous catalyst is always greater than 1. Why?
   e. When the multiple steady states were observed in solid catalytic reactions?
   f. Define Hatta number
   g. Name the criteria's for external and internal mass transfer controlled catalytic reactions
   h. Write the rate expression for gas- liquid – solid catalytic reaction.
   i. RTD in batch and packed bed reactors?
   j. Figure shows the reaction rate versus fractional coverage of A in a catalytic reaction A + B-> products. Why the rate increases in Eley-Rideal and decreases in Langmuir- Hinshelwood kinetics. Why?



2. Design a packed bed reactor in which 2nd order reaction $A \rightarrow B + 2\,C$ is conducted under negligible external mass transfer resistance. The gas is flowing at a temperature 260 °C, pressure 4.9 atm and with a superficial velocity of 4 m/s. Find the length of the reactor to achieve 81% conversion. Neglect the diffusion (10 M)

   Data: k^1 = 51 x 10^6 m^2/mol.s; D_p = 0.38 cm; S_a= 410 m^2/g cat; density of the bed = 2.1 x 10^6 g/m^3

3. Normal butane C_4H_{10}, is to be isomerized to isobutne in a plug-flow reactor. Isobutane is a valuable product that is used in the manufacture of gasoline additives. The reaction is to be carried out adiabatically in the liquid phase under high pressure using essentially trace amounts of a liquid catalyst which gives a specific reaction rate of 31.1 h-1 at 360 K. Write the MATLAB code to calculate the PFR volume necessary to process 105 gal/day (163 kmol/h) at 70% conversion of a mixture 90 mol % n-butane and 10 mol% i-pentane, which is considered an inert. The feed enters at 330 K.

$\Delta H_{Rx} = -6900 \text{ J/mol} \cdot \text{butane}$

Butane

$C_{P_{n\text{-B}}} = 141 \text{ J/mol} \cdot \text{K}$

$C_{P_{i\text{-B}}} = \mathbf{141} \text{ J/mol} \cdot \text{K}$

i-Pentane

$C_{P_{i\text{-P}}} = 161 \text{ J/mol} \cdot \text{K}$

Activation energy $= 65.7 \text{ kJ/mol}$

$K_C = 3.03$ at 60°C

$C_{A0} = 9.3 \text{ g mol/dm}^3 = 9.3 \text{ kg mol/m}^3$ (15 M)

4. The first-order reaction A→ B was carried out and the following experimental data were obtained (Table 1). All other conditions for these experiments were same. Assuming negligible external mass transfer resistance, (a) estimate the Thiele modulus and effectiveness factor for each pellet and (b) how small should the pellets be made to eliminate nearly all internal diffusion resistance? (10 M)

Table 1: Experimental data

	Measured Rate (obs) (mol/g cat s) x 10^5	*Pellet Radius (m)*
Run 1	3.0	0.01
Run 2	15.0	0.001

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PART: B 3 x 10 = 30 M

1. For a simple stoichiometry reaction $A \rightarrow B$, the reaction rate is given by

$$r = \frac{kC_A}{(1 + KC_A)^2}$$

(a) What are the units of k and K? Draw a sketch of $r(C_A)$ as a function of C_A. Show what happens at both low C_A concentration and high C_A concentration.

(b) Draw a sketch of $1/r(C_A)$ as a function of C_A. Find the minimum of $1/r(C_A)$. Draw this point also on your sketch.

(c) Assume we run this reaction in liquid phase in a CSTR and also in a PFR. To achieve a conversion of A of 50 percent, and with the following parameter values, which reactor has more volume, the CSTR or the PFR? C_{Af} = 1.4 mol/L K = 2.0

Justify your answer. You might find your sketch of $1/r(C_A)$ in the previous part useful.

(d) To achieve the same 50 percent conversion of A and with the following parameter values, which reactor has more volume, the CSTR or the PFR?

C_{Af} = 0:6 mol=L K = 1.0

Justify your answer. You might find your sketch of $1/r(C_A)$ in the previous part useful.

2. A particular catalyst has a surface area S= 100 m2/g, a density ρ= 3 g/cm3 and a void fraction ε= 0.3.

   (a) The pseudo homogeneous rate of the irreversible reaction A -> B in a test of this catalyst was 1×10^{-2} moles/liter sec when the reactant concentration was 1 mole/liter and 2.5×10^{-3} when the reactant concentration was 0.5 moles/liter. What is the surface reaction rate expression in moles/cm^2 sec?

   (b) What reactor volume will be necessary to process 100 liters/set of 2 molar A to 90% conversion in a packed-bed reactor?

3. It is planning to remove about 90% of the A present in a gas stream by absorption in water which contains reactant B and the reaction is carried out in a tower column. Chemicals A and B react in the liquid as follows:

$$A(g \to l) + B(l) \to R(l), \qquad -r_A = kC_AC_B$$

B has a negligible vapor pressure, hence does not go into the gas phase.

(a) What volume of contactor is needed?

(b) Where does the resistance of absorption reaction lie?

Data: Henry's Law constant: $H_A = 10^5$ Pa. $k = \infty$

For the gas stream:

$F_g = 90\,000$ mol/hr at $\pi = 10^5$ Pa

$p_{Ain} = 1000$ Pa

$p_{Aout} = 100$ Pa

Physical data

$\mathscr{D} = 3.6 \times 10^{-6}\ m^2/hr$

$C_U = 55\,556$ mol H_2O/m^3 liquid, at all C_B

For the packed bed

$F_l = 900\,000$ mol/hr

$C_{Bin} = 55.56\ mol/m^3$

$k_{Ag}a = 0.36\ mol/hr \cdot m^3 \cdot Pa$

$k_{Al}a = 72\ hr^{-1}$

$a = 100\ m^2/m^3$

$f_l = V_l/V = 0.08$