# BITS, PILANI – DUBAI CAMPUS

## FIRST SEMESTER 2012 – 2013

### THIRD YEAR (Chemical)

### COMPREHENSIVE EXAMINATION

| | | |
|---|---|---|
| Course Code: CHE C312 | | Date: 03.01.13 |
| Course Title: Kinetics and Reactor Design | | Max Marks: 80 |
| Duration: 3 hr | (Closed Book) | Weightage: 40% |

Note: Attempt ALL questions. Mention appropriate units in your answers. Without units, the answer will not be deemed as correct, even if the numerical value is correct. Cleary show all calculation steps. Use graph sheets if needed.

---

1(a) Derive the design equations for the following elementary reactions for batch reactor, MFR and tubular reactor with their assumptions, (12 m)

$A \rightarrow B$ and $A + B \rightarrow C$

1(b) Discuss working principles and its applications of any two heterogeneous reactors with a neat sketch. (2 + 2 = 4 m)

2(a) The irreversible liquid phase reaction $A \rightarrow B + C$ is carried out in a batch reactor. The following data were collected during the course of reaction:

| | | | | |
|---|---|---|---|---|
| t min | 0 | 2 | 4 | 6 |
| $C_A$ mol/dm$^3$ | 2 | 1.31 | 0.95 | 0.73 |

Determine the order of the reaction and the specific reaction rate by any method. (8 m)

2(b) It is planned to replace the present mixed flow reactor with one having double the volume. For the same aqueous feed (10 mol A /liter) and the same feed rate find the new conversion. The reaction kinetics are represented by and present conversion is 70%. (8 m)

$$A \rightarrow R \qquad -r_A = kC_A^{1.5}$$

3(a) The gaseous reaction $A \rightarrow B$ has a unimolecular reaction rate constant of 0.0015 min$^{-1}$ at 299 K. This reaction is to be carried out in parallel tubes 300 m long and 1 inch inside diameter at 399 K. A production rate of 450 kg/h of B is required. Initial reactant concentration of $1.86 \times 10^{-4}$ k mol/L. Assuming an activation energy of 25,000 cal/g mol, how many tubes are needed if the conversion of A is to be 90%? Assume perfect gas laws. A and B each have molecular weight of 58.

(R = 0.08206 L atm/ mol K = 1.987 cal/ gmol K) (12 m)

3(b) Consider a gas phase reaction 2A gives R+2S with unknown kinetics. If a space velocity of 1 $min^{-1}$ is needed for 90% conversion of A in a PFR find the corresponding space time and mean residence time or holding tome of the fluid in the reactor. (4 m)

4(a) Chemical A reacts to form R ($k_1 = 6\ hr^{-1}$) and R reacts away to form S ($k_2 = 3\ hr^{-1}$). In addition R slowly decomposes to form T ($k_3 = 1\ hr^{-1}$). If a solution containing 1.0 mol/liter of A is introduced into a batch reactor, how long would it take to reach $C_{Rmax}$ and what would be $C_{Rmax}$? (4 m)

4(b) Discuss about micro reactors with its applications. (4 m)

4(c) Sketch and discuss the following: (4 + 4 = 8 m)

i) Operating lines for minimum reactor size for different reactions types.

ii) General shape of the temperature-conversion plot for different reaction types.

5(a) The degree of backmixing in a tall slurry reactor was analyzed by injecting a pulse of methyl orange into a column. For a superficial gas velocity of 10 cm/s and a liquid velocity of 3 cm/s.

| | | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Conc PPM | 0 | 0.2 | 0.5 | 0.7 | 0.85 | 1 | 1 | 0.95 | 0.85 | 0.8 | 0.65 | 0.5 | 0.35 | 0.25 | 0.125 | 0 |
| t min | 0.3 | 0.6 | 0.9 | 1.2 | 1.5 | 1.8 | 2.1 | 2.4 | 2.7 | 3 | 4 | 5 | 6 | 7 | 8.5 | 10 |

Calculate the mean residence time of a liquid molecule in the reactor and sketch the E curve. (6 + 6 = 12 m)

5.(b) Define closed and open vessel with its boundary conditions for axial dispersion model. (4 m)

# BITS, PILANI – DUBAI CAMPUS

**FIRST SEMESTER 2012 – 2013**

**THIRD YEAR (Chemical)**

Course Code: CHE C312 **TEST 2** Date: 25.11.12

Course Title: Kinetics and Reactor Design Max Marks: 20

Duration : 50 minutes (Open Book) Weightage: 20%

**Note : only prescribed text book and own handwritten notes are allowed, physical and chemical property tables are allowed**

---

1. What reactor schemes (for semibatch and flow reactors) and conditions required to maximize the desired product for the following parallel reactions: (4 m)

$$A + C \rightarrow D \quad r_D = 800\, e^{(-2000/T)}\, C_A^{0.5} C_C$$

$$A + C \rightarrow U \quad r_U = 10\, e^{(-300/T)}\, C_A C_C$$

where D is the desired product and U is the undesired product?

2. Consider the following elementary reactions: (6 m)

$A + B \rightarrow R$ (with rate constant $k_1$)
$R + B \rightarrow S$ (with rate constant $k_2$)

Determine $k_2/k_1$ for the following cases using the attached figure:

**(a)** One mole A and 1 mole B are thrown together and mixed in a flask. B is entirely consumed, found 70% conversion. (2 m)

**(b)** One mole A is added bit by bit with constant stirring to 1 mole B. on completion of the reaction, 0.4 mole of R is found to be present in the mixture. (2 m)

**(c)** One mole A and 0.8 moles B are mixed together slowly. The reaction is very slow, and when B is entirely consumed. 0.2 mole S is present in the mixture.(2 m)

3. Define Damkohler number, mention its significance. (3 m)

4. Sketch the concentration-time curves for the following elementary reversible reactions, (3 m)

a) $A \underset{1}{\longleftrightarrow} R \xrightarrow{1} S$ b) $A \overset{10}{\longleftrightarrow} R \overset{1}{\longleftrightarrow} S$

5. The following liquid phase reactions are carried out in a CSTR at 325k. (4 m)

| | | |
|---|---|---|
| $3A \rightarrow B + C$ | $-r_{1A} = k_{1A} C_A$ | $k_{1A} = 0.7\ min^{-1}$ |
| $2C + A \rightarrow 3D$ | $-r_{2D} = k_{2D} C_C^{\ 2} C_A$ | $k_{2D} = 0.3\ dm^6 / mol^2\ min$ |
| $4D + 3C \rightarrow 3E$ | $-r_{3E} = k_{3E} C_D C_C$ | $k_{3E} = 0.2\ dm^3 / mol\ min$ |

The concentration measured inside the reactor are $C_A = 0.1$, $C_B = 0.93$, $C_C = 0.51$, and $C_D = 0.049$ all in mol/dm$^3$. Determine $r_{1A}$, $r_{2A}$, and $r_{3A}$?

# BITS, PILANI – DUBAI CAMPUS

**FIRST SEMESTER 2011 – 2012**

**THIRD YEAR (Chemical)**

Course Code: CHE C312 **TEST 1** Date: 11.10.12

Course Title: Kinetics and Reactor Design Max Marks: 25

Duration : 50 minutes (Closed Book) Weightage: 25%

---

1. The first order liquid phase reaction $A \rightarrow P$ is conducted isothermally in a plug flow reactor of 5 liter volume. The inlet volumetric flow rate is 1 liter/min and the inlet concentration of A is 2 mole/liter. If the exit concentration of A is 0.5 mole /liter, calculate the rate of the reaction. (4 m)

2. The liquid phase reaction A + B gives C follows an elementary rate law and is carried out isothermally in a flow system. The concentration of the A and B feed streams are 1 *M* each before mixing. The volumetric flow rate of each stream is 5 $dm^3$/min, and the entering temperature is 300K. The streams are mixed immediately before entering. Two reactors are available. One is a gray 200.0 $dm^3$ CSTR that can be heated to 77°C or cooled to 0°C, and the other is a white 800 $dm^3$ PFR operated at 300K that cannot be heated or cooled but can be painted red or black. Note k = 0.07 $dm^3$/mol min at 300K and E = 20 kcal/mol

   a) Determine the conversion for the above reactors (6 m)

   b) How long would it take to achieve 90% conversion in a 200 $dm^3$ batch reactor with $C_{Ao} = C_{Bo} = 1M$ after mixing at a temperature of 77°C? (4 m)

   c) How long would it take for the same reactor as in part (b) if the reactor were cooled to 0°C? (4 m)

3. An aqueous reactant stream (4 mol A/ liter) passes through a mixed flow reactor followed by a plug flow reactor. Find the concentration at the exit of the plug flow reactor if in the mixed flow reactor C, = 1 mol/liter. The reaction is second-order with respect to A, and the volume of the plug flow unit is three times that of the mixed flow unit. (7 m)

# BITS, PILANI – DUBAI CAMPUS

**FIRST SEMESTER 2012 – 2013**

**THIRD YEAR (Chemical)**

**QUIZ 2**

Course Code: CHE C312 | Date: 29.10.12

Course Title: Kinetics and Reactor Design | Max Marks: 07

Duration : 20 minutes | (Closed Book) | Weightage: 7%

**Name:** .......................... **ID No:** ...................... **Sec / Prog:** ..........

---

1. Rate of a gaseous phase reaction is given by, $-\frac{dp_A}{dt} = k\,p_A^2$. The unit of rate constant is (1 m)

   a) $(atm)^{-1}$ b) $(hr)^{-1}$ c) $(atm)^{-1}.(hr)^{-1}$ d) $atm.(hr)^{-1}$ e) none f) $atm^{-1}$ (hr) g) $atm^{-2}\,hr^{-2}$

2. A large CSTR, small CSTR and PFR are available. In general, how would you arrange them for getting maximum conversion for reactions of order n >1, n <1 and n=1 Why? (1.5 m)

3. For a certain gas phase reaction, $-\frac{dC_A}{dt} = k\,C_A^n$ The rate of reaction in terms of partial pressure may be expressed as (1 m)

   a) $-\frac{dp_A}{dt} = k\,p_A^n$ b) $-\frac{dp_A}{dt} = k\,RT\,p_A^n$ c) $-\frac{dp_A}{dt} = k\,(RT)^{-n}\,p_A^n$

   d) $-\frac{dp_A}{dt} = k\,(RT)^{1-n}\,p_A^n$ e) $-\frac{dp_A}{dt} = k\,(RT)^{n}\,p_A^{1-n}$ f) none

4. A homogeneous gas phase decomposition reaction 4A → B + 7S takes place in an isothermal plug flow reactor. The reaction rate is, $-r_A = k_1C_A$ with $k_1 = 0.17\ s^{-1}$; feed concentration of A ($C_{AO}$) = 0.1 mol/m$^3$. Feed flow rate ($F_{AO}$) = 0.17 mol/s. Determine the size of the reactor in order to achieve 50% conversion. (3.5 m)

# BITS, PILANI – DUBAI CAMPUS

**FIRST SEMESTER 2012 – 2013**

**THIRD YEAR (Chemical)**

Course Code: CHE C312 **QUIZ 1** Date: 24.09.12

Course Title: Kinetics and Reactor Design Max Marks: 08

Duration : 20 minutes (Closed Book) Weightage: 8%

**Name:** . . . . . . . . . . . . . . . . . . . . . . . . . **ID No:** . . . . . . . . . . . . . . . . . . . . . . **Sec / Prog:** . . . . . . . . . . .

---

1. The reaction : 2A + 3B → 5C is carried out in a reactor. If at a particular point, the rate of disappearance of A is 10 mol/dm$^3$s, what are the rates of B and C? (4 m)

2. The half life equation defined as (1 m)

a) $t_{1/2} = \frac{(1-2^{n-1})C_{Ao}^{\ 1-n}}{K\,(1-n)}$ b) $t_{1/2} = \frac{(2^{1-n}-1)C_{Ao}^{\ 1-n}}{K\,(n-1)}$

c) $t_{1/2} = \frac{(2^{n-1}-1)C_{A}^{\ 1-n}}{K\,(1-n)}$ d) $t_{1/2} = \frac{(1-2^{n-1})C_{Ao}^{\ 1-n}}{K\,(n-1)}$

3. Which equation is used in arriving at the design equation for a batch reactor? (1m)

A. Gj = VRj

B. dNj/dt = 0

C. Fjo = Fj = 0

D. $\tau/C_{Ao} = X_A/-r_A$

4. What does the mole balance for a CSTR become if Rj = -kCj? (1m)

A. $\tau$/Cj = $X_A$/(k×Cj)

B. too complicated...

C. V = (Fjo – Fj)/(k×Cj)

D. V = (Fjo-Fj)/k Fjo

5. What is the rate of appearance of B in the reaction A → B? (1m)

A. very slow B. $r_b = -r_a$ C. $r_b = r_a$ D. $r_b = (r_b-r_a)$