# BITS, PILANI – DUBAI CAMPUS

**FIRST SEMESTER 2013 – 2014**

**THIRD YEAR (Chemical)**

Course Code: CHE F311 **COMPREHENSIVE EXAMINATION**

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.

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1.(a) Differentiate elementary and non-elementary reactions. (2 m)

1.(b) The reaction $A \rightarrow B$, with 90% conversion. If $k = 0.5\ min^{-1}$, $C_{Ao} = 2.0$ moles/L, and $v = 4$ liter/min, what residence time and reactor volume will be required, if? (12 m)

(i) a PFR is used (assuming first order reaction)
(ii) a PFR used (assuming second order reaction)
(iii) a CSTR used (assuming first order)
(iv) a CSTR used (assuming second order)

2.(a) Differentiate between differential and integral method of analysis of batch rector data. (4m)

2.(b) Consider the set of elementary reactions,

$$A \xrightarrow{k_1} B;$$

$$A + B \xrightarrow{k_2} C;$$

$$A + D \xrightarrow{k_3} 2E;$$

At time t = 0, a batch reactor is filled with a mixture of A and D. Deduce the relation between the concentration of B and D after a time t? (10 marks)

3. The catalytic decomposition of hydrogen peroxide in buffered medium to water and oxygen has been studied at 25°C in presence of the enzyme catalyst by stopped flow technique. The concentration of $H_2O_2$ at various times was followed at a platinum electrode which is polarized anodically. Determine the order and rate constant from the following data. (10 m)

| Time, Sec | Con. Of $H_2O_2$ (M) $\times 10^4$ |
|---|---|
| 0 | 4 |
| 3.33 | 2.25 |
| 5 | 1.34 |
| 6.67 | 0.948 |
| 10 | 0.533 |
| 11.67 | 0.331 |
| 13.33 | 0.259 |
| 16.67 | 0.134 |

4. A PFR operating isothermally at 773 K is used to conduct the A $\rightarrow$ B + C. If a feed of pure methylacetoxy propionate (gas) enters at 5 atm and at a flow rate of 0.193 $ft^3/s$, what length of pipe with a cross-sectional area of 0.0388 $ft^2$ is necessary for the reaction to achieve 90 percent conversion? Data: $k = 7.8 \times 10^9 \exp[-19{,}200/T]\ s^{-1}$ (T in K) (10 m)

5.(a) The first order liquid phase reaction A $\rightarrow$ B is conducted isothermally in a plug flow reactor of 5 liter volume. The inlet volumetric flow rate is 1 liter/min. The inlet concentration of A is 2 mole/liter and the exit concentration of A is 0.5 mole /liter. If PFR is replaced by 4 mixed flow reactors in series, each of 2 lit volume, calculate the % conversion of A. (6 m)

5.(b) For the elementary reversible reaction, 2A $\leftrightarrow$ R + S, Derive the relation between equilibrium constant $k_1$ and $k_2$. (4 m)

6.(a) A parallel reaction scheme given below produces P and S as the desired and undesired products respectively. Propose a suitable contacting scheme for minimization of the undesired product. (4 m)

A + B with $k_1$ gives P $dC_P/dt = k_1 C_A C_B^{0.4}$

A + B with $k_2$ gives S $dC_S/dt = k_2 C_A^{0.8} C_B^{1.3}$

6.(b) Mention the steps occur in a heterogeneous catalytic reaction. (4 m)

6.(c) Discuss briefly about optimum temperature progression for various types of the reaction to minimize $V/F_{Ao}$ for a given conversion of reactant. (4 m)

7.(a) A chemical reactor for a liquid decomposing with rate $-r_A = kC_A$ ; $k = 0.307\ min^{-1}$. Find the fraction of reactant unconverted in the real reactor and compare this with the fraction unconverted in a PFR of the same size. (8 m)

| t, min | 5 | 10 | 15 | 20 | 25 | 30 |
|---|---|---|---|---|---|---|
| E | 0.03 | 0.05 | 0.05 | 0.04 | 0.02 | 0.01 |

7. (b) Define closed vessel and open vessel (2 m)

# BITS, PILANI – DUBAI CAMPUS
## FIRST SEMESTER 2013 – 2014
### THIRD YEAR (Chemical)

Course Code: CHE F311 | **TEST 2** | Date: 08.12.13

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**

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1. The desired liquid phase reaction

   A + B gives R +T  ; $dC_R/dt = dC_T/dt = k_1 C_A^{1.8} C_B^{0.1}$

   Is accompanied by the undesirable side reaction

   A + B gives S + U  ; $dC_S/dt = dC_B/dt = k_2 C_A C_B^2$

   Propose a suitable contacting scheme for minimize the concentration of the undesired product. (5 m)

2. t-Butyl alcohol (TBA) is an important octane enhancer that is used to replace lead additives in gasoline. TBA was produced by the liquid phase hydration (W) of isobutene (I) over an Amberlyst-15 catalyst. The system is normally a multiphase mixture of hydrocarbon, water and solid catalysts. However, the use of co solvents or excess TBA can achieve reasonable miscibility. Derive the rate law for the following reaction assuming the surface reaction is rate limiting. I + W ↔ TBA (10 m)

3. Sketch the any reaction path on $X_A$ Vs T plot for mixed flow reactor and plug flow reactor and also sketch to determine the volume of the above said reactors. (5 m)

## BITS, PILANI – DUBAI CAMPUS
**FIRST SEMESTER 2013 – 2014**
**THIRD YEAR (Chemical)**

Course Code: CHE F311 **TEST 1** Date: 10.10.13
Course Title: Kinetics and Reactor Design Max Marks: 25
Duration : 50 minutes (Closed Book) Weightage: 25%

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1. Consider a liquid-phase reaction in an isothermal CSTR $A \rightarrow 2B$ the feed concentration of A is $C_{Af} = 2$ mol/L, the residence time of the reactor is $\tau = 100$ min, and the rate constant is $k = 0.1\ \text{min}^{-1}$. Find the steady-state concentration of A in the effluent for the given feed. (4 m)

2. Consider the cumene hydroperoxide (CHP) produced in a backmix reactor

$$\text{CHP} \rightarrow \text{phenol} + \text{acetone}$$

The reaction is pseudo-first-order. Find the reactor volume to achieve 85% conversion of CHP at steady state. The flowrate into the reactor is $Q_f = 26.9\ \text{m}^3/\text{hr}$ and $k = 4.12\ \text{hr}^{-1}$

(4 m)

3. An aqueous feed of A and B (400 liter/min, 100 mmol A/liter, 200 mmol B/liter) is to be converted to product in a plug flow reactor. The kinetics of the reaction is represented by mol A+B gives R, $-r_A=200C_AC_B$ ,mol/liter .min Find the volume of reactor needed for 99.9% conversion of A to product. Derive the required equation (4 + 4 = 8 m)

4. An isothermal liquid phase reaction $A \rightarrow B$ ($k = 5\times10^{-4}$ mol/lit-s) is carried out in a batch reactor. The initial concentration of A is 2 mol/m$^3$. Determine the time (sec) at which the concentration of A depletes fully. (6 m)

5. Express the various forms of reaction rates (3 m)

# BITS, PILANI – DUBAI CAMPUS
**FIRST SEMESTER 2013 – 2014**
**THIRD YEAR (Chemical)**

Course Code: CHE F311 — **QUIZ 2** — Date: 21.11.13
Course Title: Kinetics and Reactor Design — Max Marks: 07
Duration : 20 minutes — (Closed Book) — Weightage: 7%

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

1. Sketch the concentration Vs time profile for the following reactions. (1× 4 = 4 m)

   a) $A \xrightarrow{1} R \xrightarrow{2} S$

   b) $A \xleftrightarrow{3} R \xleftrightarrow{1} S$

   c) $A \xrightarrow{1} R; A \xrightarrow{1} S$

   d) $A \xleftrightarrow{1} R; A \xleftrightarrow{1} S$

2. Sketch the contacting patterns for batch and continuous process for following conditions: (1.5× 2 = 3 m)

   a) Low $C_A$ and high $C_B$ .

   b) $C_A$, $C_B$ both high

# BITS, PILANI – DUBAI CAMPUS

**FIRST SEMESTER 2013 – 2014**

**THIRD YEAR (Chemical)**

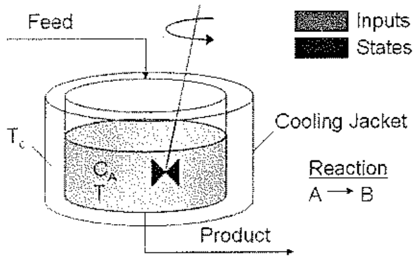
Course Code: CHE F311 **QUIZ 1** Date: 26.09.13

Course Title: Kinetics and Reactor Design Max Marks: 08

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

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

1.

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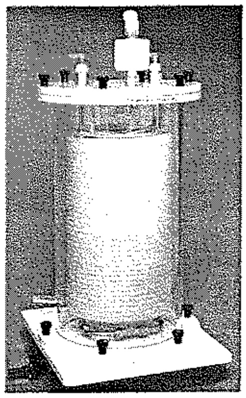

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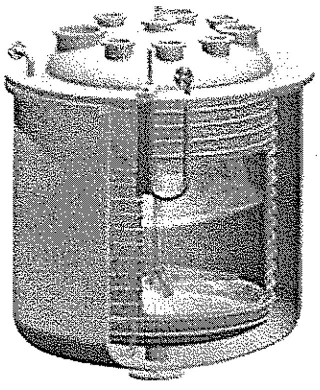

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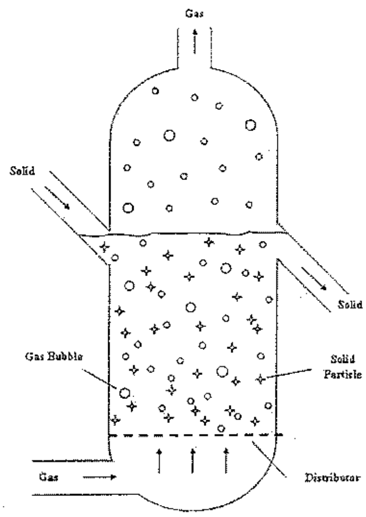


a) Combined Stirred Tank Reactor
b) None
c) Vat reactor
d) None
e) Unmixed reactor
f) Continuous Flow Reactor
g) Simple Constant Flow Reactor
h) Plume Flow Reactor
i) None
j) Fluid Packed Bed Reactor
k) Full Control Reactor
l) None
m) Simple Continuous Reactor
n) Permanent Flow Reactor

(1 ×4 = 4 m)

5. What does the mole balance for a CSTR become if -Rj = k*Cj? (2 m)

A. Cj = (Fjo-Fj)/V
B. too complicated…
C. V = (Fjo – Fj)/(k*Cj)
D. V = (Fjo-Fj)/k
E. $\tau / C_{jO} = C_{jO}$ - Cj / (k*Cj)
F. None
G. $\tau / C_{jO} = V / F_{jO}$

6. Define Transition State Theory and Collision Theory. (2 m)