# III B.Tech I Semester Examinations,November 2010 CHEMICAL REACTION ENGINEERING-I <br> Chemical Engineering 

Time: 3 hours

## Answer any FIVE Questions <br> All Questions carry equal marks

1. (a) A reaction proceeds with an equation $\mathrm{A}+\mathrm{B} \rightarrow 2 \mathrm{R}$, what is the order of reaction.
(b) For a reaction $2 \mathrm{NO}_{2}+1 / 2 \mathrm{O}_{2} \rightarrow \mathrm{~N}_{2} \mathrm{O}_{5}$, what is the relation between the components.
(c) A reaction with stoichiometric equation $1 / 2 \mathrm{~A}+\mathrm{B} \rightarrow \mathrm{R}+1 / 2 \mathrm{~S}$ has the following rate expression $-r_{A}=2 . C_{A}^{0.5} \cdot C_{B}$, what is the rate expression for the reaction written as $\mathrm{A}+2 \mathrm{~B} \rightarrow 2 \mathrm{R}+\mathrm{S}$.
(d) Discus in detail about the temperature dependency of reaction rate.

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[2+2+4+8]
$$

2. Two parallel reactions $\mathrm{A}+\mathrm{B} \rightarrow \mathrm{D} ; \mathrm{A}+\mathrm{B} \rightarrow \mathrm{U}$. have the rate expressions $k_{1} C_{A}^{a} C_{B}^{b}$ and $k_{1} C_{A}^{c} C_{B}^{d} \mathrm{CB}$ d respectively. Qritically analyse the effect of various factors on the composition as a function of time in a batch reactor.
3. At room temperature the-Second-Order irrerrsible liquid- phase reaction proceeds as follows
$\alpha \mathrm{A} \rightarrow$ Product
$-\mathrm{rA}=[0.005 \mathrm{lt} / \mathrm{mol} . \mathrm{min}] . \mathrm{CA}^{2} . \mathrm{C}_{A O}=1 \mathrm{~mol} / \mathrm{lt}$.
A batch reactor takes 18 min to till \& empty. What percent conversion \& reaction time should we use so as to maximize the daily output of product $R$ ?
4. (a) Derive the performance equation of Mixed flow reactor.
(b) A gaseous feed of pure $\mathrm{A}(2 \mathrm{~mol} /$ liter , $100 \mathrm{~mol} / \mathrm{min})$ decomposes o give variety of products in the plug flow reactor. The kinetics of conversion is represented by: $\mathrm{A} \rightarrow 2.5$ (products), $-\mathrm{r}_{\mathrm{A}}=\left(10 \mathrm{~min}^{-1}\right) \mathrm{C}_{\mathrm{A}}$
Find the expected conversion in 22-liter reactor.

$$
[6+10]
$$

5. An elementary series reactions $A \xrightarrow{k_{1}} B \xrightarrow{k_{2}} D$ take place in liquid phase in mixed flow reactor. Derive an expression for maximum concentration of B. Represent the result graphically.
6. (a) Aqueous A reacts to from $\mathrm{R}(\mathrm{A} \rightarrow \mathrm{R})$ and in the first minute in a batch reactor its concentration drops from $\mathrm{C}_{\mathrm{AO}}=2.03 \mathrm{~mol} /$ lit to $\mathrm{C}_{\mathrm{AF}}=1.97 \mathrm{~mol} / \mathrm{lit}$. Find the rate equation if the kinetics are second order with respect to A
(b) How to interpret the batch reactor data in rate equation.
7. Explain what is meant by a favourable product distribution for multiple reactor system. Describe 3 different possible series parallel reactions schemes that result in desired product through series reaction and two undesired end products through series and parallel reaction from a reactant.
8. The reaction $\mathrm{A} \rightarrow \mathrm{B}+2 \mathrm{C}$ occurs in the gas phase and is first order with respect to A. When the reaction is carried out at 1 atm pressure in a constant volume batch reactor, pressure was increased by $35 \%$ in 3 min . estimate the required for the same conversion if the reaction is carried out in constant pressure batch reactor. [16]


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1. Consider a feed $\mathrm{C}_{\mathrm{A} 0}=100 \mathrm{~mol} / \mathrm{lit}, \mathrm{C}_{\mathrm{B} 0}=200 \mathrm{~mol} / \mathrm{lit}, \mathrm{C}_{\mathrm{I} 0}=100 \mathrm{~mol} / \mathrm{lit}$. to a steady flow reactor. The isothermal gas phase reaction is $A+3 B \rightarrow 6 R$ if the concentration of $A\left(C_{A}\right)$ is $40 \mathrm{~mol} /$ lit find conversion of $A\left(X_{A}\right)$, conversion of $B\left(X_{B}\right)$, and concentration of $B\left(C_{B}\right)$.
2. (a) A certain reaction has a rate $-\mathrm{r}_{\mathrm{A}}=0.005 \mathrm{C}_{\mathrm{A}}^{2} \mathrm{~mol} / \mathrm{cm}^{3}$. min . If the concentration is taken in $\mathrm{mol} / \mathrm{lit}$ and time in hrs, what would be the value and units of rate constant
(b) The pyrolysis of ethane proceeds with an activation energy of about 300 $\mathrm{KJ} / \mathrm{mol}$. How much faster is the decomposition at $650^{\circ} \mathrm{C}$ than at $500^{\circ} \mathrm{C}$.
(c) Write about activation energy and temperature dependency. $[6+4+4]$
3. A certain gas phase reaction with a stoichiometry $0.5 \mathrm{~A}+1.5 \mathrm{~B}=\mathrm{C}$ takes place in a vessel of 20 lit at $0^{\circ}$ C. Thitially the vessel contains $20 \% \mathrm{~A}, 40 \% \mathrm{~B}, 20 \% \mathrm{C}$ and rest inerts, I. The reaction attained equilibrium when the pressure is 4 bars. Find the free energy change for the reaction $2 \mathrm{C}=\mathrm{A}+3 \mathrm{~B}$.
4. (a) Find the first orderrate constant for the disappearance of A in the gas reaction $2 \mathrm{~A} \rightarrow \mathrm{R}$ if, on holding the pressure constant the volume of the reaction mixture, starting with $80 \%$ A, decreases by $20 \%$ in 3 min .
5. (a) Explain the following methods
i. Integral method
ii. Differential method
(b) Explain how one can test for irreversible bimolecular second order reaction using integral method of analysis.
6. An aqueous phase series reaction $\mathrm{R} \rightarrow \mathrm{S} \rightarrow \mathrm{U}$ is carried out in a plug flow reactor. It is desired to produce large quantities of desirable $S$ from 1.0 kilo liter per hour feed containing R only at a concentration $C_{R O} 4=0.001 \mathrm{~mol} / \mathrm{cc}$. Find the size of reactor for maximum yield of $S$. The rate constants $4 k_{1}=k_{2}=0.1$ min- 1 . [16]
7. (a) Explain different reactor combinations.
(b) Discuss rate conc curves for auto catalytic reactions.
[8+8]
8. Reactant $R$ simultaneously under goes reaction to yield $S, T$ and $U$ as per the stoichiometry
$\mathrm{A} \rightarrow \mathrm{S}, \mathrm{A} \rightarrow \mathrm{T}$ and $\mathrm{A} \rightarrow \mathrm{U}$. the rates of disappearance of A by each reaction are k 1
$\left(C_{A}\right)^{a} ; k_{2}\left(C_{A}\right)^{b}$ and $k_{3}\left(C_{A}\right)^{c}$ respectively. Sketch the fractional yield of T vs. CA for various values of rate constants and the orders of the reaction (a,b,c). [16]


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1. What is meant by relative rates of two parallel reactions? State and explain 6 various factors that effect the product distribution of two parallel reactions $\mathrm{A} \rightarrow$ $\mathrm{S}, \mathrm{A} \rightarrow \mathrm{T}$.
2. (a) Discuss the variable volume zero order reactions and how to test this reactions using Integral method of analysis
(b) Explain the integral method of analysis.
3. (a) For a gas reaction at 400 K , the rate is reported as $\frac{-\mathrm{dP}_{A}}{\mathrm{dt}}=3.66 P_{A}^{2} \cdot \mathrm{~atm} / \mathrm{hr}$.
i. What are the units of rate constant.
ii. What is the value of rate constant in this teaction,
iii. if the rate equation is expressed as $\frac{-1}{V} \frac{d N_{A}}{d t}=k \cdot C_{A}^{2} \cdot \frac{m o l}{m^{3} . \sec }$
(b) Discus in detail about the temperature dependency of reaction rate. $[8+8]$
4. Derive first order and second order reactions of equal size mixed how reactors in series.
5. Distinguish between ideal temperature profile with optimum temperature progression in non isothermal reaction. With the help of neat sketches describe the different methods of approaching the ideal temperature profile in plug flow reactor.
6. (a) Write about ideal reactors for single reaction.
(b) A plan to replace present mixed flow reactor with one having double the volume. For the same aqueous feed ( $10 \mathrm{~mol} \mathrm{~A} /$ liter ) and the same feed rate find the new conversion. The reaction kinetics are represented by $A \rightarrow R,-r_{A}$ $=\mathrm{k} C_{A}^{1.5}$. And present conversion is $70 \%$.
[8+8]
7. Find overall order of the irreversible reaction $2 \mathrm{H}_{2}+2 \mathrm{NO} \rightarrow \mathrm{N}_{2}+2 \mathrm{H}_{2} \mathrm{O}$ From the following constant volume data using equimolar amounts of hydrogen and nitric oxide.

| Total pressure (mmHg) | 200 | 240 | 280 | 320 | 360 |
| :---: | :---: | :---: | :---: | :---: | :---: |
| Half - life (sec) | 265 | 186 | 115 | 104 | 67 |

8. Define and explain the fractional yield of D in the set of reactions $2 \mathrm{~A} \rightarrow A_{2} / 2 \mathrm{~B} \rightarrow B_{2}$ and $\mathrm{A}+\mathrm{B} \rightarrow \mathrm{D}$ that take place in mixed flow reactor. Assuming the elementary reactions, sketch the fractional yield of D as a function of $\mathrm{C}_{A}$.

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1. Find the first - order rate constant for the disappearance of A in the gas reaction $2 \mathrm{~A} \rightarrow \mathrm{R}$ if, on holding the pressure constant the volume of the reaction-mixture, starting with $75 \%$ A, decreases by $30 \%$ in 3 min .
2. (a) Define rate of reaction? What are the variables affecting the rate of reaction.
(b) At 500 K the rate of bimolecular reaction is 10 times that of the rate at 400 K. Find the activation energy from
i. Arrhenious law
ii. collision theory
3. If one of the products of 2 parallel reactions is desired and is targeted for maximization explain different factors that can be controlled relative to the system intrinsic factors such as activation energy, order of reaction. Sketch the composition. [16]
4. Reactant A undergoes elementary reversible series reactions $A \underset{k_{2}}{\stackrel{k_{1}}{\longrightarrow}} B \underset{k_{4}}{\stackrel{k_{3}}{4}} C$ Draw the concentration- time curves for various relative values of rate constants in a batch reactor.
5. The data in the table given below have been obtained on the decomposition of gaseous reactant A in a constant volume batch reactor at $100^{\circ} \mathrm{C}$.the stoichiometry of the reaction is $2 \mathrm{~A} \rightarrow \mathrm{R}+\mathrm{S}$

| t, sec | 0 | 20 | 40 | 60 | 80 | 100 | 140 | 20 | 260 | 330 | 420 |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $\mathrm{P}_{\mathrm{A}}, \mathrm{atm}$ | 1 | 0.80 | 0.68 | 0.56 | 0.45 | 0.37 | 0.25 | 0.14 | 0.08 | 0.04 | 0.02 |

What size of plug flow reactor operating at $100^{\circ} \mathrm{C}$ and 1 atm can treat $100 \mathrm{molA} / \mathrm{hr}$ in a feed consisting of $20 \%$ of inerts to obtain $95 \%$ conversion of A?
6. (a) Explain how one can test for irreversible reactions in parallel using integral method of Analysis.
(b) Aqueous A reacts to from $\mathrm{R}(\mathrm{A} \rightarrow \mathrm{R})$ and in the first minute in a batch reactor its concentration drops from $\mathrm{C}_{\mathrm{A} 0}=2.03 \mathrm{~mol} / \mathrm{lit}$ to $\mathrm{C}_{\mathrm{AF}}=1.97 \mathrm{~mol} / \mathrm{lit}$. Find the rate equation if the kinetics are second order with respect to A. $[8+8]$
7. Show that for an exothermic reaction more than one reactor composition may satisfy the material and energy balance. Stating all conditions describe such a situation.
8. A speatic Enzyme E, which act as a homogenious catalyst a harm full organic A is present in industries waste water degrades into harmly chemicals at a given Enzyme conc. EE test in a laboratory mixed flow react gives the following res as

| $\mathrm{C}_{A O} \mathrm{~m} \mathrm{~mol} / \mathrm{m}^{3}$ | 2 | 5 | 6 | 6 | 11 | 14 | 16 | 24 |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $\mathrm{C}_{A} \mathrm{~m} \mathrm{~mol} / \mathrm{m}^{3}$ | 0.5 | 3 | 1 | 2 | 6 | 10 | 8 | 4 |
| $\tau$-min | 30 | 1 | 50 | 8 | 9 | 20 | 20 | 4 |

We wish to treat $0.1 \mathrm{~m}^{3} / \mathrm{min}$ of this waste water having $\mathrm{C}_{A O}=10 \mathrm{~m} \mathrm{~mol} / \mathrm{m}^{3}$ to $90 \%$ conv with that Enzyme at conc $\mathrm{C}_{E}$. Assume PFR with possible recycle exit fluid. What design do you recommend? Calculate size of the reactor Ecu if it should be used with recycle and if so determine the recycle flow rate in $\mathrm{m}^{3} / \mathrm{min}$. Sketch the recomeded design.

