Beant College of Engineering & Technology, Gurdaspur

Department of Chemical Engineering

Tutorial Sheet No.1
Topics: Introduction to Chemical Kinetics

Subject: Chemical Reaction Engineering-I   Semester: 4th, Chemical Engineering

Q1. A reaction has the stoichiometric equation ***A + B = 2R.*** What is the order of reaction?

Q2. Given the reaction $\boldsymbol{2NO_2 + 0.5O_2 = N_2O_5}$, what is the relation between the rates of formation and disappearance of the three reaction components?

Q3. The pyrolysis of ethane proceeds with an activation energy of about 300 kJ/mol. How much faster is the decomposition at 650^0C than at 500^0C?

Q4. An 1100-K n-nonane thermally cracks (breaks down into smaller molecules) 20 times as rapidly as at 1000 K. Find the activation energy for this decomposition.

Q5. Show that the following scheme proposed by R. Ogg, J. Chem. Phys., 15, 337 (1947) is consistent with, and can explain, the observed first-order decomposition of N205.

$$N_2O_5 \underset{k_2}{\overset{k_1}{\rightleftharpoons}} NO_2 + NO_3^*$$

$$NO_3^* \xrightarrow{k_3} NO^* + O_2$$

$$NO^* + NO_3^* \xrightarrow{k_4} 2NO_2$$

Beant College of Engineering & Technology, Gurdaspur

Department of Chemical Engineering

Tutorial Sheet No.2
Topics: Introduction to Kinetics Models

Subject: Chemical Reaction Engineering-I   Semester: 4th, Chemical Engineering

Q1. Experiment shows that the homogeneous decomposition of ozone proceeds with a rate

$-r_{o3} = k\,[O_3]^2\,[O_2]^{-1}$

(a) What is the overall order of reaction?

(b) Suggest a two-step mechanism to explain this rate and state how you would further test this mechanism.

Q2.On doubling the concentration of reactant, the rate of reaction triples. Find the reaction order. For the stoichiometry A + B →R (products) find the reaction orders with respect to A and B.

Q3. Data on the tenebrionid beetle whose body mass is 3.3 g show that it can push a 35-g ball of dung at 6.5 cm/s at 27 C, 13 cm/s at 37 C, and 18 cm/s at 40 C. How fast can it push dung at 41.5 C? [B. Heinrich. The Hot-Blooded Insects Cambridge, Mass.: 1993).]

Q4. Mechanism for enzyme catalyzed reactions. To explain the kinetics of enzyme-substrate reactions, Michaelis and Menten (1913) came up with the following mechanism, which uses an equilibrium assumption

$$\left.\begin{array}{l} A + E \underset{k_2}{\overset{k_1}{\rightleftharpoons}} X \\ X \xrightarrow{k_3} R + E \end{array}\right\} \quad \text{with} \quad K = \frac{[X]}{[A][E]}, \quad \text{and with} \quad [E_0] = [E] + [X]$$

and where $[E_0]$ represents the total enzyme and [E] represents the free unattached enzyme. G. E. Briggs and J. B. S. Haldane, Biochem J., 19, 338 (1925), on the other hand, employed a steady-state assumption in place of the equilibrium assumption

$$\left.\begin{array}{l} A + E \underset{k_2}{\overset{k_1}{\rightleftharpoons}} X \\ X \xrightarrow{k_3} R + E \end{array}\right\} \text{ with } \frac{d[X]}{dt} = 0, \quad \text{and} \quad [E_0] = [E] + [X]$$

What final rate form $-r_A$ in terms of [A], $[E_0]$, k_1, k_2 and k_3 does

(a) The Michaelis-Menten mechanism gives?

(b) The Briggs-Haldane mechanism gives?

Beant College of Engineering & Technology, Gurdaspur

Department of Chemical Engineering
Tutorial Sheet No.3

Subject: Chemical Reaction Engineering-I Semester: 4th, Chemical Engineering

Topic: ***Interpretation of Batch Reactor Data***

Q1. If $-r_A = -(dC_A/dt)$ = 0.2 mol/liter.sec when C_A = 1 mol/liter, what is the rate of reaction when CA = 10 mol/ liter? Note: the order of reaction is not known.

Q2. Liquid A decomposes by first-order kinetics, and in a batch reactor 50% of A is converted in a 5-minute run. How much longer would it take to reach 75% conversion?

Q3. Repeat the previous problem for second-order kinetics.

Q4. A 10-minute experimental run shows that 75% of liquid reactant is converted to product by a ½ order rate. What would be the fraction converted in a half-hour run?

Q5. In a homogeneous isothermal liquid polymerization, 20% of the monomer disappears in 34 minutes for initial monomer concentration of 0.04 and also for 0.8 mol / liter. What rate equation represents the disappearance of the monomer?

Q6. After 8 minutes in a batch reactor, reactant (C_{AO} = 1 mol/ liter) is 80% converted; after 18 minutes, conversion is 90%. Find a rate equation to represent this reaction.

Beant College of Engineering & Technology, Gurdaspur

Department of Chemical Engineering
Tutorial Sheet No. 4

Subject: Chemical Reaction Engineering-I Semester: 4th, Chemical Engineering

Topic: ***Design & Performance of Batch and Continuous Reactor***

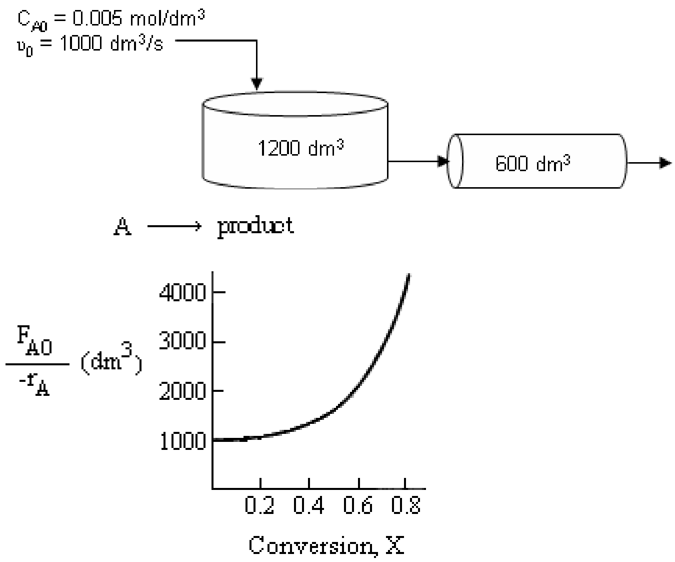
Q1. Consider a gas-phase reaction 2A →R +2 S with unknown kinetics. If a space velocity of l/min is needed for 90% conversion of A in a plug flow reactor, find the corresponding space-time and mean residence time or holding time of fluid in the plug flow reactor.

Q2. In an isothermal batch reactor 70% of a liquid reactant is converted in 13 min. What space-time and space-velocity are needed to effect this conversion in a plug flow reactor and in a mixed flow reactor?

Q3. We are planning to operate a batch reactor to convert A into R. This is a liquid reaction, the stoichiometry is A → R , and the rate of reaction is given in Table . How long must we react each batch for the concentration to drop from C_{A0} = 1.3 mol/liter to C_{Af} = 0.3 mol/liter?

C_A, mol/liter	$-r_A$, mol/liter·min
0.1	0.1
0.2	0.3
0.3	0.5
0.4	0.6
0.5	0.5
0.6	0.25
0.7	0.10
0.8	0.06
1.0	0.05
1.3	0.045
2.0	0.042

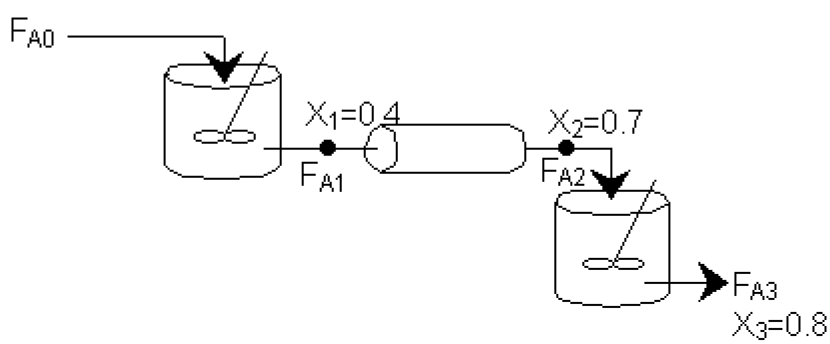
Q4. Pure A is fed at a volumetric flow rate of 1000 dm^3 /h and at a concentration of 0.005 mol/dm^3 to an existing CSTR, which is connected in series to an existing tubular reactor.



If the volume of the CSTR is 1200 dm^3 and the tubular reactor volume is 600 dm^3 , what are the intermediate and final conversions that can be achieved with the existing system? The reciprocal rate is plotted in the figure below as a function of conversion for the conditions at which the reaction is to be carried out.

Q5. Using either the data in Table, calculate the reactor volumes V_1, V_2, and V_3 for the CSTR/PFR/CSTR reactors in series sequence shown in Figure along with the corresponding conversion.

X	0	0.2	0.4	0.6	0.8
$-r_A$(mol/dm^3.s)	0.010	0.0091	0.008	0.005	0.002
$-1/r_A$(dm^3.s/mol)	100	110	125	200	500
$F_{A0}/-r_A$ (dm^3)	200	220	250	400	1000



Beant College of Engineering & Technology, Gurdaspur

Department of Chemical Engineering
Tutorial Sheet No.5

Subject: Chemical Reaction Engineering-I Semester: 4^{th}, Chemical Engineering

Topic: Design of Single reactions

Q1. At present 90% of reactant A is converted into product by a second-order reaction in a single mixed flow reactor. We plan to place a second reactor similar to the one being used in series with it.

(a) For the same treatment rate as that used at present, how will this addition affect the conversion of reactant?

(b) For the same 90% conversion, by how much can the treatment rate be increased?

Q2. The reactor setup consists of three plug flow reactors in two parallel branches. Branch D has a reactor of volume 60 liters followed by a reactor of volume 30 liters. Branch E has a reactor of volume 50 liters. What fraction of the feed should go to branch D?

Q3. 100 liters/hr of radioactive fluid having a half-life of 20 hr is to be treated by passing it through two ideal stirred tanks in series, V = 40 000 liters each. In passing through this system, how much will the activity decay?

Q4. The kinetics of the aqueous-phase decomposition of A is investigated in two mixed flow reactors in series, the second having twice the volume of the first reactor. At steady state with a feed concentration of 1 mol A/ liter and mean residence time of 96 sec in the first reactor, the concentration in the first reactor is 0.5 mol A/ liter and in the second is 0.25 mol A/ liter. Find the kinetic equation for the decomposition.

Q5. Using a color indicator which shows when the concentration of A falls below 0.1 mol/ liter, the following scheme is devised to explore the kinetics of the decomposition of A. A feed of 0.6 mol A/ liter is introduced into the first of the two mixed flow reactors in series, each having a volume of 400 cm3. The color change occurs in the first reactor for a steady-state feed rate of 10 cm^3/ min, and in the second reactor for a steady-state feed rate of 50 cm^3/min. Find the rate equation for the decomposition of A from this information.

Department of Chemical Engineering

Tutorial Sheet No.6

Subject: Chemical Reaction Engineering-I   Semester: 4^{th}, Chemical Engineering

Topic: **Recycle Reactors**

Q1. At present conversion is 2/3 for our elementary second-order liquid reaction $2A \rightarrow 2R$ when operating in an isothermal plug flow reactor with a recycle ratio of unity. What will be the conversion if the recycle stream is shut off?

Q2. For an irreversible first-order liquid-phase reaction (C_{A0} = 10 mol/liter) conversion is 90% in a plug flow reactor. If two-thirds of the stream leaving the reactor is recycled to the reactor entrance, and if the throughput to the whole reactor-recycle system is kept unchanged, what does this do to the concentration of reactant leaving the system?

Q3. We wish to explore various reactor setups for the transformation of A into R. The feed contains 99% A, 1% R; the desired product is to consist of 10% A, 90% R. The transformation takes place by means of the elementary reaction having rate constant k = 1 liter/mol.min.

$$A+R \rightarrow R+R$$

The concentration of active materials is throughout. $\mathbf{C_{AO}+C_{RO}=C_A+C_R=C_O=1}$ **mol/lit.** What reactor holding time will yield a product in which C_R = 0.9 mol/liter (a) in a plug flow reactor, (b) in a mixed flow reactor, and (c) in a minimum-size setup without recycle?