

Solution Manual to Chemical Reaction Engineering

By Octave Levenspiel



PREFACE

This solution manual is result of hard work done by students of B. Tech. Chemical Engineering (Batch of 2k13), Nirma University. This manual provides solution to unsolved numerical from book “Chemical Reaction Engineering” by Octave Levenspiel. We hope this will help you in solving your queries regarding numericals. For any corrections or suggestions mail us at solvecre2k13@gmail.com

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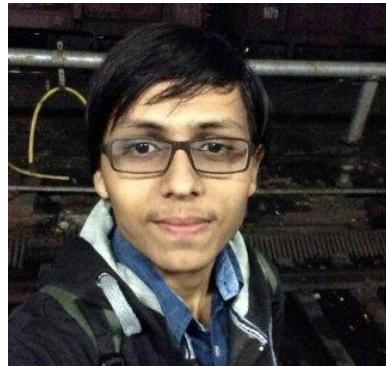
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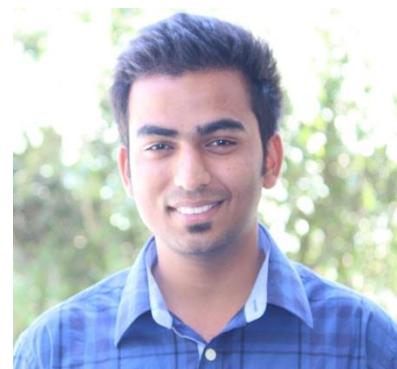
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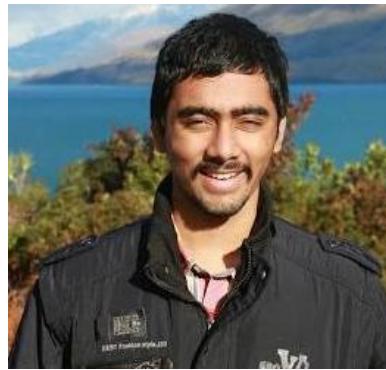
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Chapters Solved:

- ✓ **Chapter-2**
- ✓ **Chapter-3**
- ✓ **Chapter-4**
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Problem 2.1:

A reaction has the stoichiometric equation $A + B = 2R$. What is the order of reaction and rate expression?

Solution 2.1:

We require experimental kinetics data to answer this question, because order of reaction need not to match the stoichiometry, most oftenly it doesn't.

If this reaction is elementary, the order of reaction is 2. And rate expression is,

$$-r_A = K C_A C_B$$

Problem 2.2:

Given the reaction $2NO_2 + \frac{1}{2}O_2 = N_2O_5$, what is the relation between the rates of formation and disappearance of the three reaction components?

Solution 2.2:

The relation between the rates of formation and disappearance of the three reaction components is,

$$\frac{-rNO_2}{2} = \frac{-rO_2}{1/2} = \frac{-rN_2O_5}{1}$$

Problem 2.3:

A reaction with stoichiometric equation $\frac{1}{2}A + B = R + \frac{1}{2}S$ has the following rate expression,

$$-r_A = 2 C_A^{0.5} C_B$$

What is the rate expression for this reaction if the stoichiometric equation is written as $A + 2B = 2R + S$?

Solution 2.3:

It does not affect how we write the stoichiometry equation. The rate of reaction remains unchanged,

$$-r_A = 2 C_A^{0.5} C_B$$

Problem 2.4:

For the enzyme-substance $A \xrightarrow{\text{enzyme}} R$, the rate of disappearance of any substrate is given by

$$-r_A = \frac{1760[A][E_0]}{6+C_A}, \frac{\text{mol}}{\text{m}^3 \cdot \text{s}}$$

What are the units of the two constants?

Solution 2.4:

Assume C_A is in mol/m³

Constant 6 has to be the same unit as of C_A , then and then only summation is possible.

$$\therefore 6 \text{ mol/m}^3$$

$$\frac{1760 \cdot \frac{\text{mol}}{\text{m}^3} \cdot \frac{\text{mol}}{\text{m}^3}}{\frac{\text{mol}}{\text{m}^3}} = \frac{\text{mol}}{\text{m}^3 \cdot \text{s}}$$

$$\therefore 1760 \text{ s}^{-1}$$

Problem 2.5:

For the complex reaction with stoichiometry $A + 3B \rightarrow 2R + S$ and with second order rate expression

$$-r_A = k_1[A][B]$$

are the reaction rates related as follows: $r_A = r_B = r_R$? If the rates are not so related, then how are they related? Please account for the signs, + or -.

Solution 2.5:

$$r_R = -2r_A - \frac{2}{3}r_B$$

or

$$-r_A = -\frac{1}{3}r_B = \frac{1}{2}r_R$$

Problem 2.6:

A certain reaction has a rate given by

$$r_A = 0.005C_A^2, \frac{\text{mol}}{\text{cm}^3 \cdot \text{min}}$$

If the concentration is to be expressed in mol/liter and time in hours, what would be the value and unit of the rate constant?

Solution 2.6:

Given rate expression:

$$r_A = 0.005C_A^2 \frac{\text{mol}}{\text{cm}^3 \cdot \text{min}}$$

Change the unit

$$\begin{aligned} -r_A &= 0.005C_A^2 \frac{\text{mol}}{(10^{-3})\text{lit} \cdot \frac{1}{60}\text{hr}} \\ -r_A &= 300C_A^2 \frac{\text{mol}}{\text{lit} \cdot \text{hr}} \end{aligned}$$

Value of rate constant = 300

$$\text{Unit of rate constant} = \frac{\text{mol}}{\text{lit} \cdot \text{hr}}$$

Problem 2.7:

For a gas reaction at 400 K the rate is reported as

$$-\frac{dp_A}{dt} = 3.66p_A^2, \frac{\text{atm}}{\text{hr}}$$

(a) What are the unit of the rate constant?

(b) What is the value of the rate constant for this reaction if the rate equation is expressed as

$$-r_A = \frac{-1}{V} \frac{dN_A}{dt} = kC_A^2, \frac{\text{mol}}{\text{m}^3 \cdot \text{s}}$$

Solution 2.7:

(a)

Here the rate equation is expressed in homogeneous & order of the reaction is second, so the unit of the rate constant K can be expressed by

$$K = (time)^{-1} (cons)^{1-2}$$

$$K = 3.66 (time)^{-1} (cons)^{-1}$$

(b)

here

$$-r_A = \frac{-1}{V} \frac{dN_A}{dt} = k C_A^2, \quad \frac{mol}{m^3 \cdot s}$$

$$-r_A = k C_A^2$$

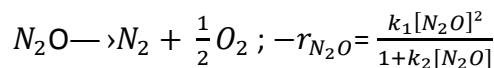
So, now using ideal gas law

$$PV = nRT$$

$$\begin{aligned} \therefore P_A &= \frac{n_A}{V} RT = C_A RT \Rightarrow \frac{-dP_A}{dt} = 3.66 P_A^2 \\ \therefore -\frac{dC_A RT}{dt} &= 3.66 (C_A RT)^2 \Rightarrow \frac{dC_A}{dt} = 3.66 C_A^2 RT \\ \therefore -r_A &= 3.66 (0.0820) * 400 * C_A^2 \left(\frac{mol}{lit. hr} \right) \\ \therefore K &= 120.13 (hr^{-1}) \left(\frac{mol}{lit} \right)^{-1} \end{aligned}$$

Problem 2.8:

The decomposition of nitrous oxide is found to be proceed as follows



What is the order of reaction WRT N_2O , and overall?

Solution 2.8:

If, k_2 concentration is low, then order of reaction is 2nd order.

If Its concentration is high, the order of this reaction is 1st order.

Overall order of reaction = 2-1 = 1.

Therefore it is of 1st order.

Problem 2.9:

The pyrolysis of ethane proceeds with an activation energy of about $300 \frac{kJ}{mol}$ How much faster is the decomposition at $650^{\circ}C$ than at $500^{\circ}C$?

Solution 2.9:

$$E=300 \text{ kJ/mol.}$$

Let. Kinetic express by= $-r_A = k c_A^n$

where $k_0 e^{-e/RT}$

$-r_A \propto k_0 e^{-e/RT}$ for same can be

$$\frac{-r_{A_1}}{-r_{A_2}} = \frac{e^{-e/RT}}{e^{-e/RT}} = e^{-e/R} \left(\frac{1}{p_1} - \frac{1}{p_2} \right) = e^{-e/R} \left[\frac{T_1 - T_2}{T_1 T_2} \right]$$

$$\frac{-r_{A_{650}}}{r_{A_{500}}} = \exp \left[\frac{300}{2.314} \left(\frac{650 - 500}{650 \times 500} \right) \right]$$

= 7.58 Time faster

Problem 2.10:

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

Solution 2.10:

$$r_{1100K} = 20r_{1000K} \quad \frac{r_{1100}}{r_{1000}} = 20$$

1 Arrhenius theory

$$K = k_0 e^{-E/RT}$$

In same concentration $k_1 = k_2$

$$\frac{r_{1100}}{r_{1000}} = \frac{k_1 e^{-E/RT_{1100}}}{k_2 e^{-E/RT_{1000}}} = 20$$

$$\log 20 = \frac{-E}{R} \left(\frac{1}{1100} - \frac{1}{1000} \right)$$

$$E = \frac{\log 20 * R}{9.09 * .00001}$$

$$E = 1189.96 \frac{J}{mol}$$

Problem 2.11:

In the mid nineteenth century the entomologist henri fibre noted that French ants busily bustled about their business on hot days but rather sluggish on cool days. Checking this result with Orezon ants, I find

Running speed (m/hr)	150	160	230	295	370
Temperature °C	13	16	22	24	28

What activation represents this change in bustliness?

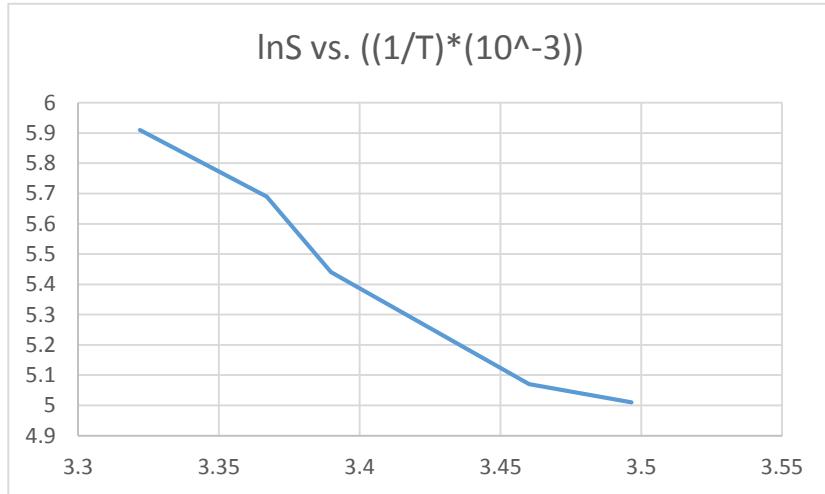
Solution 2.11:

Speed	lnS	T	$(\frac{1}{T} * 10^{-3})$
150	5.01	13	3.4965
160	5.07	16	3.4602
230	5.44	22	3.3898
295	5.69	24	3.3670
370	5.91	28	3.3220

$$\text{Slope of graph} = -\frac{E}{R} = -5420$$

$$E = (5420) * (8.314)$$

$$= 45062 \text{ J/mol}$$



Problem 2.12:

The maximum allowable temperature for a reactor is 800K. At present our operating set point is 780K. The 20-K margin of safety to account for fluctuating feed, sluggish controls, etc. Now, with a more sophisticated control system we would be able to raise our set point to 792 K with the same margin of safety that we now have. By how much can the reaction

rate, hence, production rate, be raised by this change if the reaction taking place in the reactor has an activation energy of 175 KJ/mole?

Solution 2.12:

As we know according to Arrhenius Law

$$(-r_a) = k_o T^o e^{-E_a/RT}$$

Here $T^o = 1$

$$\ln(r_1/r_2) = \ln(k_1/k_2) = (E_a/R)[1/T_1 - 1/T_2] \quad \text{Here}$$

$$T_1 = 780\text{ K}$$

$$T_2 = 800\text{ K}$$

$$E_a = 175000\text{ J/mol}$$

$$R = 8.314$$

Put in formula we get

$$r_2 = .51 r_1 \quad \text{equation 1}$$

similarly

for temperature

$$T_3 = 792\text{ K}$$

$$T_2 = 800\text{ K}$$

We get

$$r_3 = .77 r_1 \quad \text{equation 2}$$

Hence from Eq. 1 and 2 we get

$$r_3 = 1.509 \text{ times of } r_2$$

Problem 2.13:

Every May 22 I plant one watermelon seed. I water it, I fight slugs, I pray, I watch my beauty grow, and finally the day comes when the melon ripens, I then harvest and feast. Of course, some years are sad, like 1980, when blue jay flew off with the seed. Anyway, 6 summers were a pure joy and for this I have tabulated, the number of growing days vs. the mean day time temperature, during the growing season. Does the temperature affect the growth rate? If so, represent this by an activation energy.

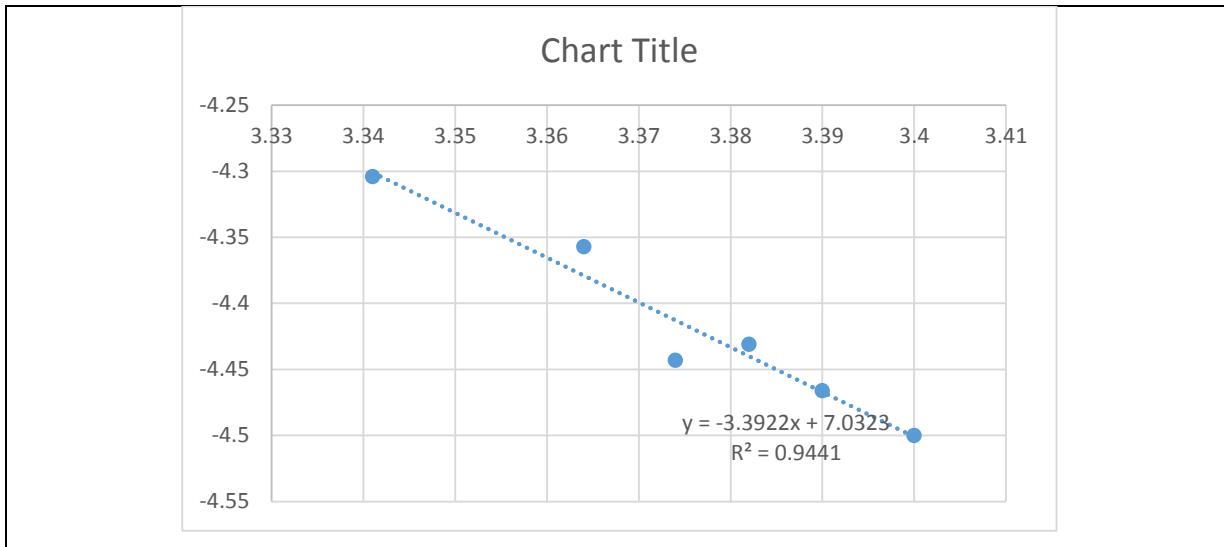
Year	1976	1977	1982	1984	1985	1988
Growing days	87	85	74	78	90	84
Mean temp °C	22.0	23.4	26.3	24.3	21.1	22.7

Solution 2.13:

Temperature	$\left(\frac{1}{T} * 10^{-3}\right)$	Days	$\ln(\text{rate}) = \ln\left(\frac{1}{\text{days}}\right)$
22	3.390	87	-4.466
23.4	3.374	85	-4.443
26.3	3.341	74	-4.304
24.3	3.364	78	-4.357
21.1	3.400	90	-4.500
22.7	3.382	84	-4.431

$$\text{Slope of graph} = -\frac{E}{R} = 3392$$

$$E = 3392 * 8.314 = 28201 \text{ J/mol}$$



Example 2.14:

On typical summer days, field crickets nibble, jump, and chirp now and then. But at night, when great numbers congregate, chirping seems to become a serious business and tends to be in [unison](#). In 1897, A.E. Dolbear reported that this social chirping rate was dependent on the temperature as given by

$$(\text{Numbers of chirps in 15 s}) + 40 = (\text{temperature } ^\circ\text{F})$$

Assuming that the chirping rate is directly measured of the metabolic rate, find the activation energy in kJ/mol of these crickets in the temperature range 60-80°F.

Solution 2.14:

$$(\text{Numbers of chirps in 15 s}) + 40 = (\text{temperature } ^\circ\text{F})$$

$$(\text{Numbers of chirps in 15 s}) = (\text{temperature } ^\circ\text{F}) - 40$$

For 60 °F

$$(\text{Numbers of chirps in 15 s}) = 20$$

For 80 °F

(Numbers of chirps in 15 s) = 40

$dN = k * (\text{metabolism rate})$

after integration we get

$$40 - 20 = k(80 - 60)$$

$k = 1 \text{ Numbers of chirps/}^{\circ}\text{F}$

$(-r_A = \text{metabolism rate}) = k_0 T^0 e^{-E_a/RT}$

Here $T^0 = 1$

For 60 °F

$(-r_A = \text{metabolism rate}) = 60$

For 80 °F

$(-r_A = \text{metabolism rate}) = 80$

$$\ln(r_1/r_2) = (E_a/R)[1/T_1 - 1/T_2]$$

$$\ln(60/80) = (E_a/8.314)[1/60 - 1/80]$$

$$E_a = -69.04 \text{ KJ/mol}$$

Problem 2.15:

On doubling the concentration of the reactant, the rate of reaction triples. Find the reaction order.

For the stoichiometry $A + B \rightarrow \text{products}$ find the reaction order with respect to A and B.

Solution 2.15:

$$-r_A = kC_A^n$$

$$\frac{r_2}{r_1} = \frac{k(C_A)^n}{kC_A^n} = 2^n$$

$$\therefore n=1.585$$

CHAPTER NO. :- 2

UNSOLVED EXAMPLE: - 2.16 to 2.23

Submitted by:-

11BCH044 (SUREJA VISHAL)

13BCH044 (NAGPARA KUMAR)

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2.16

C_A	4	1	1
C_B	1	1	8
-r_A	2	1	4

Solution

Guess that,

$$-r_A = K * C_A^p * C_B^q$$

In this Equation, There are three unknown k, p and q

From question we can make three equations

$$2 = K (4)^p (1)^q \quad \dots \quad (1)$$

$$1 = K (1)^p (1)^q \quad \dots \quad (2)$$

$$1 = K (1)^p (8)^q \quad \dots \quad (3)$$

Now Equation (3) divided by Equation (2),

$$\frac{4}{1} = \frac{K (1)^p (8)^q}{K (1)^p (1)^q}$$

$$4 = (8)^q$$

$$(2)^2 = (2)^{3q}$$

$$\text{So, } 3q = 2$$

$$q = 2/3$$

Now Equation (1) divided by Equation (2),

$$\frac{2}{1} = \frac{K (4)^p (1)^q}{K (1)^p (1)^q}$$

$$2 = (4)^p$$

$$2 = (2)^{2p}$$

$$\text{So, } 2p = 1$$

$$p = \frac{1}{2}$$

Put the values of p , q in Equation (2),

$$1 = K (1)^{1/2} (1)^{2/3}$$

$$1 = K(1)^{1/3}$$

K = 1

So, from value of p , q , and K we get rate equation,

$$-r_A = C_A^{1/2} C_B^{2/3}$$

2.17

C_A	2	2	3
C_B	125	64	64
$-r_A$	50	32	48

Solution

Guess that,

$$-r_A = K^* C_A^p C_B^q$$

In this Equation, There are three unknown k,p and q

From question we can make three equations

$$32 = K (2)^p (64)^q \quad \dots \dots \dots \quad (2)$$

$$48 = K (3)^p (64)^q \quad \dots \dots \dots \quad (3)$$

Now Equation (3) divided by Equation (2),

$$\frac{48}{32} = \frac{K(3)^p(64)^q}{K(2)^p(64)^q}$$

$$3/2 = (3/2)^p$$

$$\text{So, } p = 1$$

$$p = 1$$

Now Equation (1) divided by Equation (2),

$$\frac{50}{32} = \frac{K(2)^p (125)^q}{K(2)^p (64)^q}$$

$$(5/4)^2 = (5/4)^{3q}$$

$$\text{So, } 3q = 2$$

$$q = 2/3$$

Put the values of p, q in Equation (1),

$$50 = K(2)^1 (125)^{2/3}$$

$$50 = K(2)(5)^2$$

$$K = 1$$

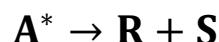
So, from value of p, q, and K we get rate equation,

$$-r_A = C_A C_B^{2/3}$$

EXAMPLE 2.18:-

The decomposition of reactant A at 400^0C for pressure between 1 and 10 atm follows a first order rate law.

A) Show that a mechanism similar to azo-methane decomposition

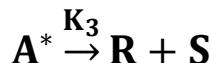
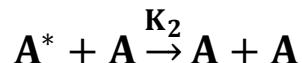
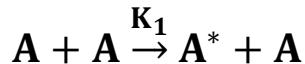


Is consistent with observed kinetics

Different mechanisms can be proposed to explain first order kinetics. To claim that this method is correct in the face of other alternatives requires additional evidence.

B) For this purpose, what further experiments would you suggest we run and what results we expect to find?

Solution



Rate of disappearance of A,

$$-r_A = K_1[A]^2 - K_2[A][A^*]$$

And rate of formation of A,

$$r_A^* = K_1[A]^2 - K_2[A][A^*] + K_3[A^*]$$

Also the rate of formation of intermediate is zero therefore,

$$r_A^* = 0$$

$$K_1[A]^2 = [A^*](K_2[A] + K_3)$$

$$[A^*] = \frac{K_1[A]^2}{K_2[A] + K_3}$$

So,

$$-r_A = K_1[A]^2 - K_2 \left[\frac{K_1[A]^2}{K_2[A] + K_3} \right]$$

$$-r_A = \frac{K_3 K_1[A]}{K_2}$$

Hence it is a first order reaction

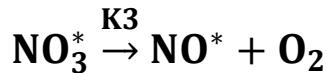
Now at low enough concentration of C_A the rate of decomposition of A will reduce to

$$-r_A = K_1[A]^2$$

That is it would be a second order reaction.

EXAMPLE 2.19

Show that the following scheme



Proposed by R.Ogg J.Chem.Phys., 15,337(1947) is consistent with and can explain the first order decomposition of $[N_2O_5]$.

Solution

Rate of formation of NO_2 ,

$$r_{NO_2} = K_1[N_2O_5] - K_2[NO_2][NO_3^*] - \frac{K_4}{2}[NO^*][NO_3^*]$$

Rate of disappearance of N_2O_5 ,

$$-r_{N_2O_5} = -K_1[N_2O_5] + K_2[NO_2][NO_3^*] \quad \text{--- (1)}$$

Rate of intermediate,

$$r_{NO_3^*}^* = K_1[N_2O_5] - K_2[NO_2][NO_3^*] - K_3[NO_3^*] - K_4[NO_3^*][NO^*]$$

Also,

$$r_{NO_3^*}^* = 0$$

Therefore;

$$K_1[N_2O_5] = K_2[NO_2][NO_3^*] + K_3[NO_3^*] + K_4[NO_3^*][NO^*]$$

$$K_1[N_2O_5] = [NO_3^*] (K_2[NO_2] + K_3 + K_4[NO^*])$$

$$[\mathbf{NO}_3^*] = \frac{K_1[N_2O_5]}{K_2[\mathbf{NO}_2] + K_3 + K_4[\mathbf{NO}^*]}$$

Rate of intermediate,

Also

$$\mathbf{r}_{\mathbf{NO}}^* = \mathbf{0}$$

And,

$$r_{\mathbf{NO}}^* = K_3[\mathbf{NO}_3^*] - K_4[\mathbf{NO}_3^*][\mathbf{NO}^*]$$

$$[\mathbf{NO}^*] = \frac{K_3[\mathbf{NO}_3^*]}{K_4[\mathbf{NO}_3^*]}$$

$$[\mathbf{NO}^*] = \frac{K_3}{K_4}$$

Therefore,

$$\mathbf{NO}_3^* = \frac{K_1[N_2O_5]}{K_2[\mathbf{NO}_2] + K_3 + K_4[\frac{K_3}{K_4}]}$$

$$\mathbf{NO}_3^* = \frac{K_1[N_2O_5]}{K_2[\mathbf{NO}_2] + 2K_3}$$

So, now put value in equation (1),

$$-r_{\mathbf{N}_2\mathbf{O}_5} = -K_1[N_2O_5] + K_2[\mathbf{NO}_2][\mathbf{NO}_3^*]$$

$$-r_{\mathbf{N}_2\mathbf{O}_5} = -K_1[N_2O_5] + K_2[\mathbf{NO}_2]\left(\frac{K_1[N_2O_5]}{K_2[\mathbf{NO}_2] + 2K_3}\right)$$

$$-r_{\mathbf{N}_2\mathbf{O}_5} = [N_2O_5]\left(K_2[\mathbf{NO}_2]\left(\frac{K_1}{K_2[\mathbf{NO}_2] + 2K_3}\right) - K_1\right)$$

$$-r_{\mathbf{N}_2\mathbf{O}_5} = [N_2O_5]\left(\left(\frac{K_1K_2[\mathbf{NO}_2]}{K_2[\mathbf{NO}_2] + 2K_3}\right) - K_1\right)$$

$$-r_{N_2O_5} = K_1[N_2O_5] \left(\left(\frac{K_2[NO_2]}{K_2[NO_2] + 2K_3} \right) - 1 \right)$$

$$-r_{N_2O_5} = K_1[N_2O_5] \left(\frac{K_2[NO_2] - K_2[NO_2] - 2K_3}{K_2[NO_2] + 2K_3} \right)$$

Assume $K_3 \gg K_2, K_2 \approx 0$

$$-r_{N_2O_5} = -K_1[N_2O_5]$$

Therefore this is a first order reaction

EXAMPLE-2.20

Experimental analysis shows that the homogeneous decomposition of ozone proceeds with a rate

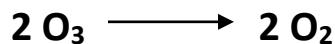
$$-r_{O_3} = k [O_3]^2 [O_2]^{-1}$$

[1] What is the overall order of reaction?

[2] Suggest a two-step mechanism to explain this rate.

Solution:-

The homogeneous decomposition of ozone proceeds as,

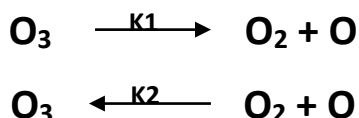


And follows the rate law

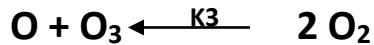
$$-r_{O_3} = K [O_3]^2 [O_2]^{-1}$$

The two step mechanism, consistent with the rate suggested is,

Step 1:- Fast, at equilibrium



STEP 2:- Slow



The step 2 is the slower, rate determining step and accordingly, the reaction rate is

$$-r_{\text{O}_3} = \frac{-d[\text{O}_3]}{dt} = K_3 [\text{O}_3] [\text{O}]$$

Thus step 1 is fast and reversible, for this equilibrium step, we have

$$K = \frac{K_1}{K_2} = \frac{[\text{O}_2] [\text{O}]}{[\text{O}_3]}$$

$$[\text{O}] = \frac{K [\text{O}_3]}{[\text{O}_2]}$$

Putting value of [O] from equation (2) into equation (1), we get

$$-r_{\text{O}_3} = \frac{d[\text{O}_3]}{dt} = K_3 * K \frac{[\text{O}_3]^2}{[\text{O}_2]}$$

Let, $K = K_3 * K$

$$-r_{\text{O}_3} = k [\text{O}_3]^2 [\text{O}_2]^{-1}$$

Overall order of reaction is $2 - 1 = 1$

EXAMPLE 2.21:-

Under the influence of oxidizing agents hypo phosphorus acid is transformed into phosphorus acid



The kinetics of this transformation present the following features. At a low concentration of oxidizing agent.

$$r_{\text{H}_3\text{PO}_3} = K [\text{oxidizing agent}] [\text{H}_3\text{PO}_2]$$

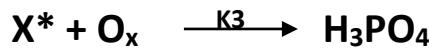
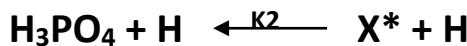
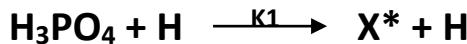
At a high concentration of oxidizing agent

$$r_{\text{H}_3\text{PO}_3} = k [\text{H}^*] [\text{H}_3\text{PO}_2]$$

To explain the observed kinetics it has been postulated that, with hydrogen ions as catalyst normal unreactive H_3PO_2 is transformed reversibly into an active form the nature of which is unknown, this intermediate then react with the oxidizing agent to give H_3PO_3 show that this scheme does explain the observed kinetics.

Solution :-

Hypothesize



[where X^* is an unstable intermediate]

$$r_{\text{H}_3\text{PO}_3} = k_3 [\text{X}^*] [\text{O}_x] - k_4 [\text{H}_3\text{PO}_3] \quad \dots \dots \dots (1)$$

$$r[\text{X}^*] = k_1 [\text{H}_3\text{PO}_2] [\text{H}^+] - k_2 [\text{X}^*] [\text{H}^+] - k_3 [\text{X}^*] [\text{O}_x] + k_4 [\text{H}_3\text{PO}_3] = 0$$

(steady state assumption)

Thus,

$$[\text{X}^*] = \frac{k_1 [\text{H}_3\text{PO}_2] [\text{H}^+] + k_4 [\text{H}_3\text{PO}_3]}{k_2 [\text{H}^+] + k_3 [\text{O}_x]} \quad \dots \dots \dots (2)$$

Assuming $k_4 = 0$, replacing (2) in (1) then gives,

$$r_{\text{H}_3\text{PO}_3} = \frac{k_1 k_3 [\text{H}_3\text{PO}_2] [\text{H}^+] [\text{O}_x]}{k_2 [\text{H}^+] + k_3 [\text{O}_x]} \quad \dots \dots \dots (3)$$

now when $k_3 [\text{O}_x] \gg k_2 [\text{H}^+]$...i.e. high oxidized concentration equations (3) gives

$$r_{\text{H}_3\text{PO}_4} = k_1 [\text{H}_3\text{PO}_2] [\text{H}^+] \quad \dots \dots \dots (4)$$

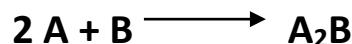
on the other hand when $k_2 [\text{H}^+] \gg k_3 [\text{O}_x]$...i.e. low oxidized concentration equation (3) gives,

$$r_{\text{H}_3\text{PO}_3} = \frac{k_1 k_3}{k_2} [\text{H}_3\text{PO}_2] [\text{O}_x] \quad \dots \dots \dots (5)$$

Equation (4) & (5) is fit in the hypothesized model is accepted.

EXAMPLE 2.22:-

Come up with (guess and then verify) a mechanism that is consist with the experimentally found rate equation for the following reaction

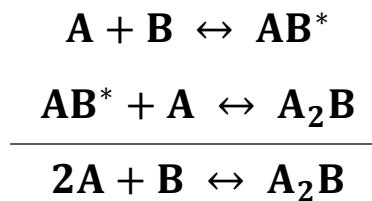


With

$$r [A_2B] = K [A] [B]$$

Solution

It is the non-elementary reaction. So, assume reaction mechanism,



From reaction (3) & (4) rate of formation of $r [A_2B]$,

$$r [A_2B] = K_3 [A_2^*] [B] - K_4 [A_2B] \quad \dots \dots \dots (5)$$

In reaction (4) A_2B is dispersed.

Rate of disappearance,

$$r_A = K_1 [A]^2$$

Rate of formation of A,

$$r_A = \frac{K_1[A]^2}{2}$$

(2 moles of A consume give 1 mole of A* so $\frac{1}{2}$)

$$r[A_2^*] = \frac{K_1[A]^2}{2} - K_2[A_2^*] - K_3[A_2^*][B] + K_4[A_2B]$$

$$r[A_2^*] = 0$$

$$0 = \frac{K_1[A]^2}{2} - K_2[A_2^*] - K_3[A_2^*][B] + K_4[A_2B]$$

$$K_3[A_2^*][B] + K_2[A_2^*] = K_4[A_2B] + \frac{K_1[A]^2}{2}$$

$$[A_2^*] [K_3[B] + K_2] = K_4[A_2B] + \frac{K_1[A]^2}{2}$$

$$[A_2^*] = \frac{K_4[A_2B] + \frac{K_1[A]^2}{2}}{[K_3[B] + K_2]}$$

Put value of $[A_2^*]$ in equation (5),

$$r_{A2B} = K_3 \left(\frac{K_4[A_2B] + \frac{K_1[A]^2}{2}}{[K_3[B] + K_2]} \right) [B] - K_4[A_2B]$$

$$r_{A2B} = K_3 \frac{K_1[A]^2}{2} [B] + K_3 K_4[A_2B] [B] - \frac{K_4[A_2B] K_3[B]}{[K_3[B] + K_2]} - K_4 K_2[A_2B]$$

$$r_{A2B} = \frac{K_3 \frac{K_1[A]^2}{2} [B] + K_2 K_4[A_2B]}{[K_3[B] + K_2]}$$

If K_4 is very small, $K_4 \approx 0$

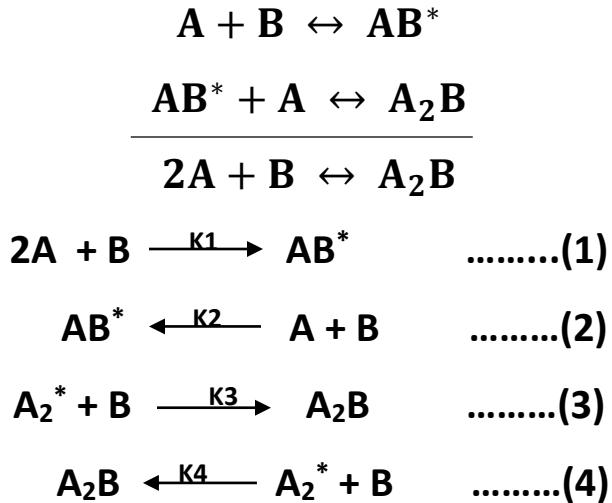
$$r_{A2B} = \frac{K_3 \frac{K_1[A]^2}{2}[B]}{[K_3[B] + K_2]}$$

If K_2 is very small, $K_2 \approx 0$

$$r_{A2B} = \frac{K_1 K_3 [A]^2 [B]}{K_3 [B]}$$

So, from above equation we can conclude that our first assumption is wrong so, mechanism also wrong.

Now, we can assume for second order reaction



From reaction (3) and (4) rate of formation of $r[A_2B]$,

$$r_{AB^*} = K_1[A][B] - K_2[AB^*] - K_3[AB^*][B] + K_4[A_2B] \quad \dots \dots \dots (5)$$

$$r[AB^*] = 0$$

$$0 = K_1[A][B] - K_2[AB^*] - K_3[AB^*][B] + K_4[A_2B]$$

$$[AB^*] = \frac{K_1[A][B] + K_4[A_2B]}{[K_3[A] + K_2]}$$

Put $[AB^*]$ value in equation (5),

$$r_{A2B} = K_3 \left(\frac{K_1[A][B] + K_4[A_2B]}{[K_3[A] + K_2]} \right) [A] - K_4[A_2B]$$

$$r_{A2B} = K_3 K_1 [A]^2 [B] + K_3 K_4 [A_2B] [A] - \frac{K_4 K_3 [A][A_2B]}{[K_3[A] + K_2]} - K_4 K_2 [A_2B]$$

If K_4 is very small, $K_4 \approx 0$

$$r_{A2B} = \frac{K_3 K_1 [A]^2 [B]}{[K_3[A] + K_2]}$$

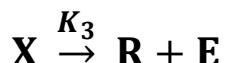
If K_2 is very small, $K_2 \approx 0$

$$r_{A2B} = \frac{K_1 K_3 [A]^2 [B]}{K_3[A]}$$

$$r_{A2B} = K_1 [A][B]$$

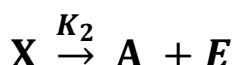
EXAMPLE 2.23:-

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



And where $[E_0]$ represents the total enzyme and $[E]$ represents the free unattached enzyme.

G.E. Briggs and J.B.S Haldane, Bochem.J. 19,338 (1925), on the other hand employed a steady state assumption in place of the equilibrium assumption

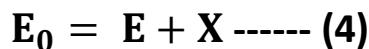
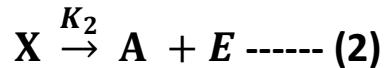
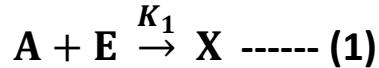


What final rate from $-r_a$ in terms of $[A]$, $[E_0]$, K_1 , K_2 and K_3 does

1) The Michaelis and Menten mechanism gives?

2) The Briggs-Haldane mechanism give?

Solution



M-M assume that the reverse reaction of (1) approach equilibrium quickly, or

$$K = \frac{X}{AE} = \frac{K_1}{K_2}$$

B-H assume that quickly $\frac{dy}{dt} = 0$ $\dots \quad (5)$

for Michaeli's – Menten

From equation (3)

$$r_R = K_3 X$$

From equation (5)

$$X = \frac{K_1}{K_2} AE \quad \dots \quad (6)$$

Eliminate E with (4)

$$X = \frac{K_1}{K_2} A(E_0 - X) \quad \dots \quad (7)$$

Or

$$X = \frac{K_1}{K_2} AE_0 / 1 + \frac{K_1}{K_2} A \quad \dots \quad (8)$$

Equation (8) in (7) gives

$$r_R = \frac{K_3 A E_0}{\frac{K_2}{K_1} + A}$$

These equation gives essentially the same result.

(a) For the Briggs - Haldane Mechanisms

From equation (3),

$$r_R = K_3 X \text{ ----- (9)}$$

From equation (6)

$$\frac{dy}{dt} = 0 = K_1 A E - (K_2 + K_3) X$$

Eliminate E with (A)

$$K_1 A (E_0 - X) - (K_2 + K_3) X = 0$$

Or

$$X = \frac{K_1 A E_0}{K_1 A + K_2 + K_3}$$

Equation (10) in (9) gives

$$r_R = \frac{K_3 A E_0}{\frac{K_2 + K_3}{K_1} + A} \text{ ----- (10)}$$

These equation give essentially the same result. $\frac{K_2 + K_3}{K_1}$ (Michaels const.)

CRE-1 Term Paper

Example 3.1-3.11

Submitted By:

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3.1. If $-r_A = -(dC_A/dt) = 0.2 \text{ mol/liter}\cdot\text{sec}$ when $C_A = 1 \text{ mol/liter}$, what is the rate of reaction when $C_A = 10 \text{ mol/liter}$?

Note: the order of reaction is not known.

Since the reaction order, hence concentration dependency is not known we are not given enough information to find the rate of reaction at higher concentration.

$$-r_a = kC_a$$

$$0.2 = k * 1$$

$$K = 0.2 \text{ sec}^{-1}$$

$$-r_a = kC_a = 0.2 * 10 = 2 \text{ mol/l.s}$$

3.2. 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?

For given first order reaction by equation,

$$\ln\left(\frac{1}{1-X_a}\right) = Kt$$

For $X_a = 0.5$ then $t = 5 \text{ min}$.

$$\text{So, } K = 0.1386 \text{ min}^{-1}$$

Now for 75% conversion $X_a = 0.75$ & $K = 0.1386 \text{ min}^{-1}$

$$\ln\left(\frac{1}{1-0.75}\right) = 0.1386 * t$$

$$t = 10 \text{ min}$$

So, for 75% conversion time required is 10min

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

For the second order disappearance of single reactant gives,

$$kt = \frac{1}{Ca_0} * \left(\frac{xa}{1-xa} \right)$$

Now, for 50% conversion

$$T_{50} = \frac{1}{KCa_0} * \left(\frac{\left(\frac{1}{2}\right)}{1 - \left(\frac{1}{2}\right)} \right) = 5 \text{ min.}$$

Now, for 75% conversion

$$T_{75} = \frac{1}{KCa_0} * \left(\frac{\left(\frac{3}{4}\right)}{1 - \left(\frac{3}{4}\right)} \right) = 15 \text{ min.}$$

So, extra time needed is 10 minutes.

3.4. A 10-minute experimental run shows that 75% of liquid reactant is converted to product by a $\frac{1}{2}$ -order rate. What would be the fraction converted in a half-hour run?

$$-r_a = kC_a^{0.5}$$

$$C_{ao} \frac{dXa}{dt} = k C_a^{0.5} (1 - xa)^{0.5}$$

$$\int_0^{xa} \frac{dXa}{(1-Xa)^{0.5}} = k C_a^{0.5} dt$$

$$2[-(1 - Xa)^{0.5} + 1] = k't$$

Case I : Xa= 0.75 when t = 10 min

$$2[-(1 - 0.75)^{0.5} + 1] = k' * 10$$

$$k' = 0.1$$

Case II : Xa= ? when t = 30 min

$$2[-(1 - Xa)^{0.5} + 1] = 0.1 * 30$$

$$Xa = 0.75$$

3.5. 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?

Since the fractional disappearance is independent of initial concentration we have first order rate equation,

$$\ln\left(\frac{C_{a0}}{Ca}\right) = Kt$$

Where, Ca = Monomer concentration

We also can find the rate constant, thus replacing values.

Case I: $C_{a0} = 0.04 \text{ mol/l}$

$$\ln\left(\frac{0.04}{0.8*0.04}\right) = k*34$$

$$\text{So, } k = 0.00657 \text{ min}^{-1}.$$

Case II: $C_{a0} = 0.8 \text{ mol/l}$

$$\ln\left(\frac{0.8}{0.8*0.8}\right) = k*34$$

$$k = 0.00657 \text{ min}^{-1}.$$

Hence the rate of disappearance of monomer is given by,

$$-r_a = (0.00657 \text{ min}^{-1}) * C$$

3.6. After 8 minutes in a batch reactor, reactant ($C_{A0} = 1 \text{ mol/liter}$) is 80% converted; after 18 minutes, conversion is 90%. Find a rate equation to represent this reaction.

$$C_{a0} = 1 \frac{\text{mol}}{\text{lit}}$$

$t = 8 \text{ min}$ then conversion 80%

$t = 18 \text{ mins}$ then conversion 90%

Assume the reaction is second order

$$-r_a = k * C_a^2$$

$$\frac{xa}{(1-xa)} = k C_{a0} t$$

$$\frac{0.8}{(1-0.8)} = k * 1 * 8$$

$$k = 0.5 \text{ (mol/l)}^{-1} \text{(min)}^{-1}$$

$$\frac{0.9}{(1-0.9)} = k * 1 * 18$$

$$k = 0.5 \text{ (mol/l)}^{-1} \text{(min)}^{-1}$$

From the same value of k in both case, the reaction is second order

$$-r_a = k * C_a^2$$

$$-r_a = 0.5 * C_a^2$$

3.7. Snake-Eyes Magoo is a man of habit. For instance, his Friday evenings are all alike—into the joint with his week's salary of \$180, steady gambling at "2-up" for two hours, then home to his family leaving \$45 behind. Snake Eyes's betting pattern is predictable. He always bets in amounts proportional to his cash at hand, and his losses are also predictable—at a rate proportional to his cash at hand. This week Snake-Eyes received a raise in salary, so he played for three hours, but as usual went home with \$135. How much was his raise?

Magoos batting habits and his losses can be described by,

$$-\left(\frac{dA}{dt}\right) = kA$$

Where, A = money in hand

Now, t=0 then A₀ = 180

t=2hrs then A= 135

$$K = \frac{1}{t} * \ln\left(\frac{A_0}{A}\right) = \frac{1}{2} * \ln\left(\frac{180}{135}\right) = 0.144 \text{ hr}^{-1}$$

After raise we have,

$t=0$ then $A_0=?$

$t=3\text{hrs}$ then $A=135$

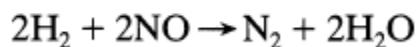
For unchanged habits,

$$\ln\left(\frac{A_0}{135}\right) = 0.144*3$$

$$A_0 = 208$$

Hence his raise is $208-180 = 28$

3.8. Find the overall order of the irreversible reaction



from the following constant-volume data using equimolar amounts of hydrogen and nitric oxide:

Total pressure, mm Hg	200	240	280	320	360
Half-life, sec	265	186	115	104	67

Equimolar quantities of H_2 and NO are used...

$$C_{ao} = C_{bo}$$

$$C_o = C_{ao} + C_{bo}$$

$$C_o = 2C_{ao}$$

$$C_a \propto P_a$$

$$P_{ao} = P_o/2$$

$$C_{ao} = \frac{P_{ao}}{RT}$$

$$C_{ao} = \frac{P_o}{2RT}$$

$$P_o = 200 \text{ mmHg} = 0.263 \text{ atm}$$

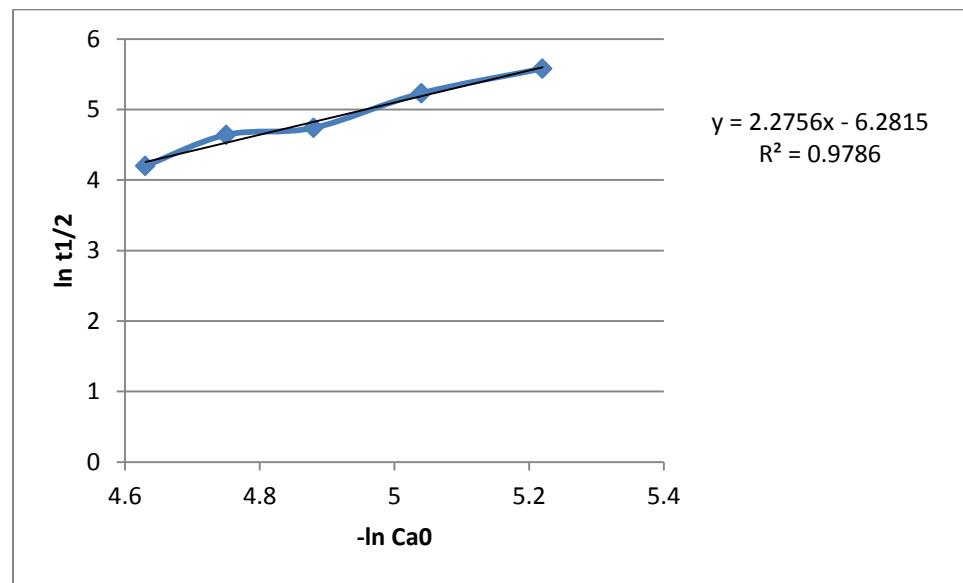
$$C_{ao} = \frac{0.263}{2 * 0.08206 * 296} = 5.414 * 10^{-3}$$

$$\ln C_{ao} = -5.22$$

$$t_{1/2} = 265 \text{ sec}$$

$$\ln t_{1/2} = 5.58$$

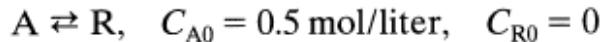
P(mm Hg)	200	240	280	320	360
P(atm)	0.263	0.316	0.368	0.421	0.474
Cao* 10^-3	5.414	6.5	7.57	8.67	9.76
ln Cao	-5.22	-5.04	-4.88	-4.75	-4.63
t1/2	265	186	115	104	67
ln t1/2	5.58	5.23	4.74	4.64	4.2



$$\text{Slope} = (n-1) = 2.275$$

$$n = 3.275$$

3.9. The first-order reversible liquid reaction



takes place in a batch reactor. After 8 minutes, conversion of A is 33.3% while equilibrium conversion is 66.7%. Find the rate equation for this reaction.

For a first order reversible reaction,



Where, \rightleftharpoons = Reversible reaction

K_1 = Forward reaction rate const.

K_2 = Backward reaction rate const.

$$C_{A0} = 0.05 \frac{\text{mol}}{\text{lit}}$$

$$C_{R0} = 0$$

$$M = 0/0.5 = 0$$

$$X_{Ae} = 0.67$$

The integral conversion in a batch reactor is given by,

$$-\ln\left(1 - \frac{X_a}{X_{Ae}}\right) = k_1 * t * \frac{M+1}{M+X_{Ae}}$$

Replacing values we then find,

$$-\ln\left(1 - \frac{\frac{1}{3}}{\frac{2}{3}}\right) = k_1 * t * \frac{M+1}{M+X_{Ae}} \dots \dots (1)$$

$$k_1 = 0.0577 \text{ min}^{-1}$$

Now from thermodynamics we know that,

$$K = \frac{K_1}{K_2} = \frac{M+X_{Ae}}{1-X_{Ae}} = \frac{C_{Re}}{C_{Ae}}$$

$$\text{So, } K_1 = (0.667/0.332) K_2 \dots \dots (2)$$

From equation (1) & (2)

$$K_1 = 0.057750$$

$$K_2 = 0.028875$$

Thus, rate expression for the disappearance of A.

$$-r_a = 0.057750 C_a - 0.028875 C_r$$

3.10. Aqueous A reacts to form R ($A \rightarrow R$) and in the first minute in a batch reactor its concentration drops from $C_{A0} = 2.03$ mol/liter to $C_{Af} = 1.97$ mol/liter. Find the rate equation for the reaction if the kinetics are second-order with respect to A.

For the second order disappearance of single reactant gives,

$$k*t = \frac{1}{C_a} * \left(\frac{X_a}{1-X_a} \right) \dots \dots (1)$$

Here it is given that $C_{A0} = 2.03 \frac{mol}{lit}$ & $C_a = 1.97 \frac{mol}{lit}$

So, $X_a = \frac{C_{A0} - C_a}{C_{A0}}$ by putting values of C_a & C_{A0} , X_a will be 0.029

So, putting value of X_a and C_{A0} in equation (1)

$$K(1) = \frac{1}{2.03} * \left(\frac{0.029}{1-0.029} \right)$$

$$K = 0.0147 \text{ min}^{-1}$$

So, for second order rate expression is $-r_a = 0.0147(\text{min}^{-1})C_a^2$

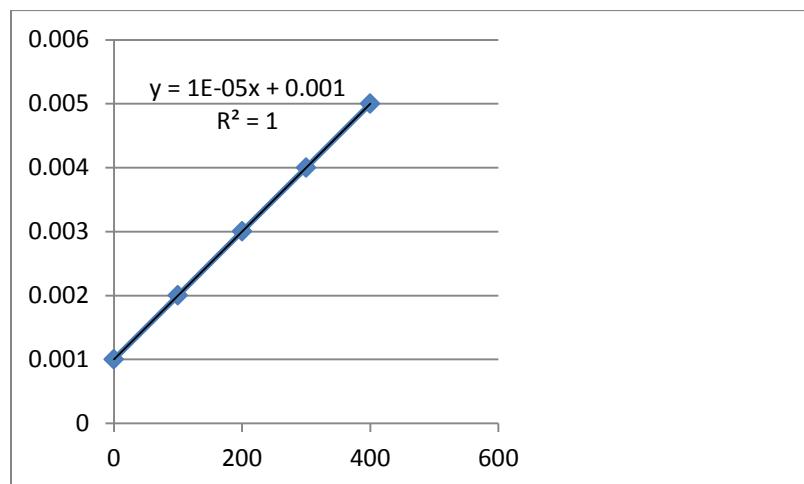
- 3.11.** Aqueous A at a concentration $C_{A0} = 1 \text{ mol/liter}$ is introduced into a batch reactor where it reacts away to form product R according to stoichiometry $A \rightarrow R$. The concentration of A in the reactor is monitored at various times, as shown below:

$t, \text{ min}$	0	100	200	300	400
$C_A, \text{ mol/m}^3$	1000	500	333	250	200

For $C_{A0} = 500 \text{ mol/m}^3$ find the conversion of reactant after 5 hours in the batch reactor.

From the table of data,

$\frac{1}{C_A} \rightarrow t$ is straight line, Reaction is second order.



C_A	t	$1/C_A$
1000	0	0.001
500	100	0.002
333	200	0.003003
250	300	0.004
200	400	0.005

$$k = 1 * 10^{-5} \text{ (mol/l)}^{-1}(\text{min})^{-1}$$

$$\frac{1}{C_A} = \frac{1}{C_{A0}} + kt$$

$$t = 5 * 60 = 300 \text{ min}$$

$$C_{A0} = 500 \text{ mol/m}^3$$

$$\frac{1}{C_A} = 0.003 + \frac{1}{500}$$

$$C_A = 200 \text{ mol/m}^3$$

$$X_A = \frac{C_{A0} - C_A}{C_{A0}} = \frac{500 - 200}{500} = 0.6$$

Ex - 3.12

Aqueous A at a concentration $C_{ao} = 1 \text{ mol/liter}$ is introduced into a batch reactor where it reacts away to form product R according to stoichiometry $A \rightarrow R$. The concentration of A in the reactor is monitored at various times, as shown below:

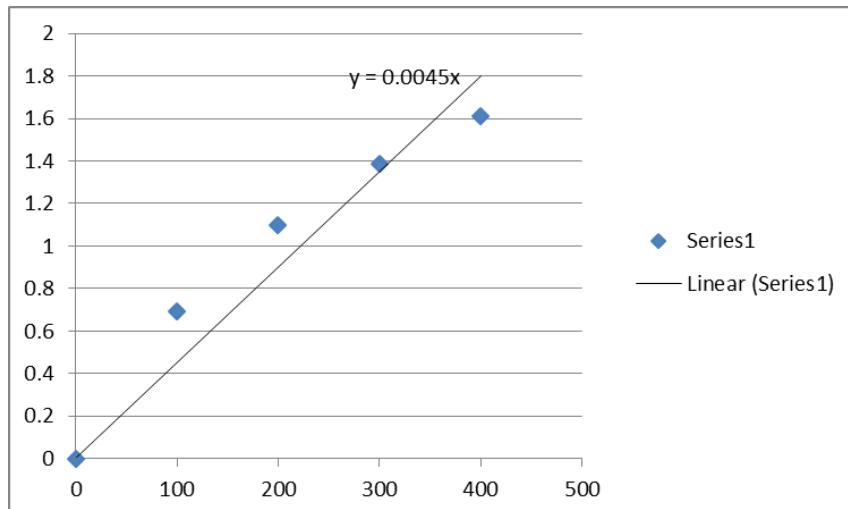
T (min)	0	100	200	300	400
Ca mol/m ³	1000	500	333	250	200

Find the rate for the reaction

Ans: For batch reactor $t = -C_{ao} \int_{Ca}^{C_{ao}} \frac{dCa}{KCa}$, $C_{ao} = 100 \text{ mol/m}^3$

$$\frac{kt}{C_{ao}} = \ln \frac{C_{ao}}{Ca}$$

$\ln(C_{ao}/Ca)$	t
0	0
.693	100
1.099	200
1.386	300
1.609	400



$$\text{slope} = \frac{k}{C_{ao}}$$

$$0.0045 = \frac{k}{C_{ao}}$$

$$0.0045 = \frac{k}{1000}$$

$$K = 4.5 \text{ min}^{-1}$$

Ex – 3.13

Betahundert Bash by likes to play the gaming tables for relaxation. He does not expect to win, and he doesn't, so he picks games in which losses area given small fraction of the money bet. He plays steadily without a break, and the sizes of his bets are proportional to the money he has. If at "galloping dominoes" it takes him 4 hours to lose half of his money and it takes him 2 hours to lose half of his money at "chuk-a-luck," how long can he play both games simultaneously if he starts with \$1000 and quits when he has \$10 left, which is just enough for a quick nip and carfare home?

Ans:

$$\text{Money} \xrightarrow{K_1} \text{Game 1}$$

Game 1:

$$K_1 = 0.693 / (t_{1/2})_1$$

$$= 0.693 / 4$$

$$= 0.17325 \text{ hour}^{-1}$$

$$\text{Money} \xrightarrow{K_2} \text{Game 2}$$

Game 2:

$$K_2 = 0.693 / (t_{1/2})_2$$

$$= 0.693 / 2$$

$$= 0.3465 \text{ hour}^{-1}$$

$$(-\text{rate of reaction}) = (K_1 + K_2) \cdot C_A$$

$$\frac{-dm}{dt} = M e^{-(k_1+k_2)t}$$

$$M = M_0 e^{-(k_1+k_2)t}$$

$$10 = 1000 e^{-(0.3465 + 0.17325)t}$$

$$0.01 = e^{-(0.5197t)}$$

$$t = 8.82 \text{ hour}$$

Ex - 3.14

For the elementary reactions in series



$$C_{A0} = C_A, C_{R0} = C_{S0} = 0$$

find the maximum concentration of R and when it is reached.

Ans :

$$-r_a = K_1 C_a \quad +r_a = K_1 C_a - K_2 C_R \quad +r_S = \\ K_2 C_R$$

$$\frac{-dC_a}{dt} = K_1 C_a \quad \frac{dC_R}{dt} = K_1 C_{a0} e^{-K_1 t} - K_2 C_R$$

$$C_a = C_{a0} e^{-K_1 t} \quad \frac{dC_R}{dt} + K_2 C_R = K_1 C_{a0} e^{-K_1 t}$$

$$C_R = \int K_1 C_{a0} e^{-K_1 t} e^{-K_2 t} dt + C$$

$$C_R e^{-K_2 t} = K_1 C_{a0} t + C$$

$$\text{at } t = 0,$$

$$C_R = K_1 C_{a0} t \cdot e^{-kt} \quad C_R = 0,$$

$$C = 0,$$

$$\frac{dC_R}{dt} = 0$$

$$k_1 C_{a0} e^{-kt} + k_1 C_{a0} e^{-kt} \cdot t \cdot (-k) = 0$$

$$k_1 - k_1^2 \cdot t = 0$$

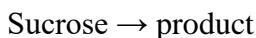
$$t = 1/k_1$$

$$(c_r)_{\max} = k_1 c_{A0} \cdot \frac{1}{k_1} \cdot e^{(-1/k_1) \cdot k_1 t}$$

$$C_r = \frac{C_{A0}}{e}$$

Ex – 3.15

At room temperature sucrose is hydrolyzed by the catalytic action of the enzyme sucrase as follows:



Starting with a sucrose concentration $C_{A0} = 1.0$ millimol/liter and an enzyme concentration $C_{E0} = 0.01$ millimol/liter, the following kinetic data are obtained in a batch reactor (concentrations calculated from optical rotation measurements):

C_A	.84	.68	.53	.38	.27	.16	.09	.04	.018	.006	.0025
t	1	2	3	4	5	6	7	8	9	10	11

Determine whether these data can be reasonably fitted by a kinetic equation of the Michaelis-Menten type, or

$$-r_A = \frac{K_3 C_A C_{E0}}{C_A + C_m}$$

If the fit is reasonable, evaluate the constants K_3 and C_m . Solve by the integral method.

Ans:

$$-r_A = \frac{-dC_A}{dt}$$

$$= \frac{K_3 C_A C_{E0}}{C_A + C_m}$$

$$\int_{C_{A0}}^{C_A} \frac{-dC_A (C_A + C_m)}{K_3 C_A C_{E0}} = \int_0^t dt$$

$$-(C_A - C_{A0}) - C_m \ln \frac{C_A}{C_{A0}} = K_3 \cdot t \cdot C_{E0}$$

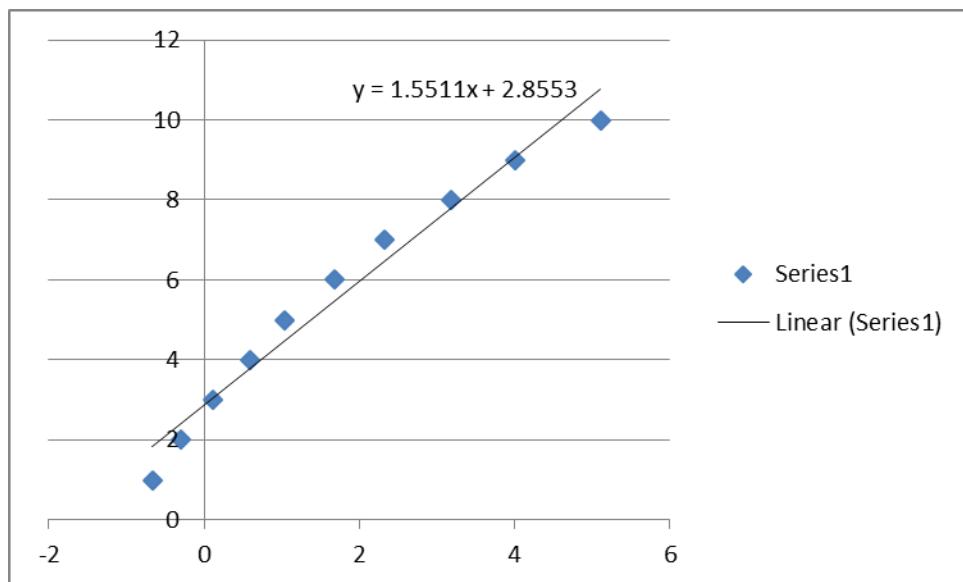
$$T = \frac{C_m}{K_3 C_{E0}} \cdot \left(\frac{\ln C_{A0}}{C_{A0}} - C_A \right) + \frac{C_{A0}}{K_3 C_{E0}}$$

Compare with , $Y = mx + c$

$$m = \frac{C_m}{K_3 C_{eo}}$$

$$c = \frac{C_{ao}}{K_3 C_{eo}}$$

$x = \ln \left[\frac{C_{ao}}{C_a} - C_A \right]$	Y=time
-.665	1
-.294	2
0.104	3
0.587	4
1.039	5
1.672	6
2.317	7
3.178	8
3.999	9
5.109	10



$$\text{Slope} = 1.5511$$

$$\text{Intercept} = 2.885$$

$$C = 2.885 = \frac{C_{ao}}{K_3 C_{eo}}$$

$$K_3 = \frac{1}{.01*2.885}$$

$$K_3 = 35.02$$

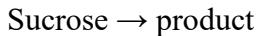
$$M = \text{slope} = 1.5511 = \frac{C_m}{K_3 C_{eo}}$$

$$C_m = 1.5511 * 35.02 * 0.01$$

$$C_m = 0.5431 \frac{\text{m mol}}{\text{liter}}$$

Ex - 16.

At room temperature sucrose is hydrolyzed by the catalytic action of the enzyme sucrase as follows:



Starting with a sucrose concentration $C_{ao} = 1.0$ millimol/liter and an enzyme concentration $C_{eo} = 0.01$ millimol/liter, the following kinetic data are obtained in a batch reactor (concentrations calculated from optical rotation measurements):

C_A	.84	.68	.53	.38	.27	.16	.09	.04	.018	.006	.0025
t	1	2	3	4	5	6	7	8	9	10	11

Determine whether these data can be reasonably fitted by a kinetic equation of the Michaelis-Menten type, or

$$-r_A = \frac{K_3 C_a C_{eo}}{C_a + C_m}$$

If the fit is reasonable, evaluate the constants K_3 and C_m . Solve by the differential method.

Ans:

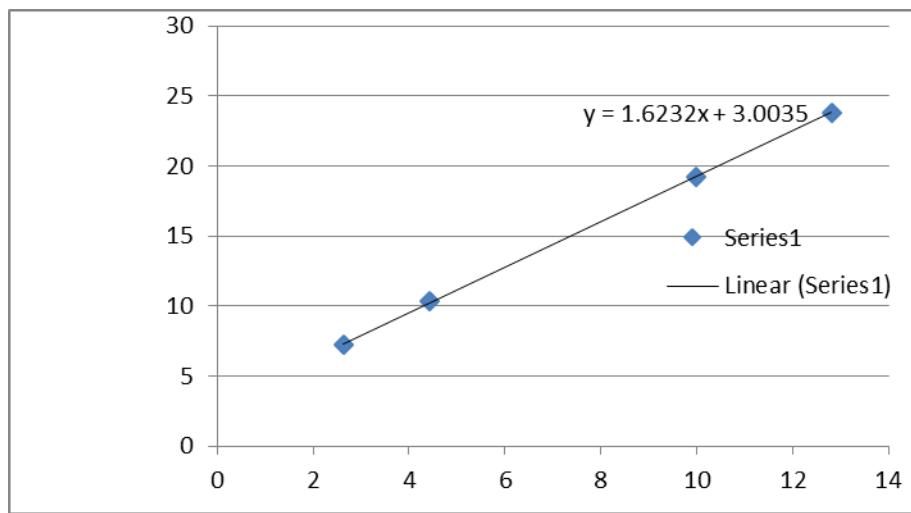
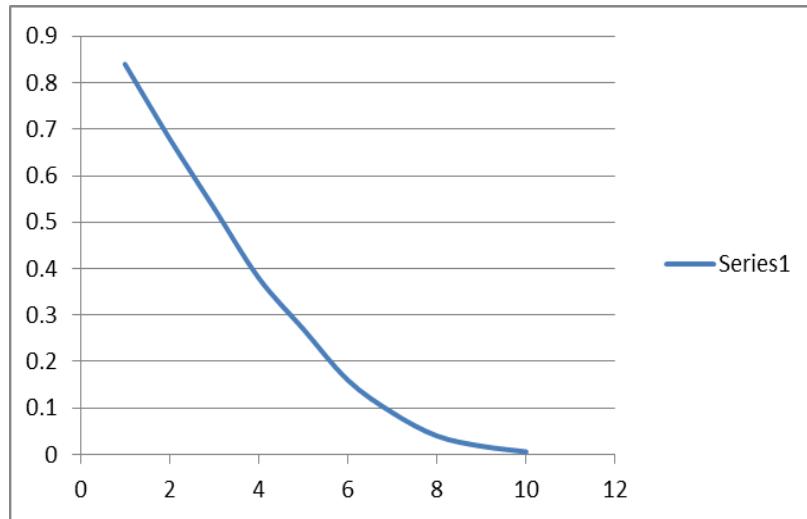
$$-r_A = \frac{k C_a C_{eo}}{C_a + m}$$

$$\frac{1}{-r_A} = \frac{m + ca}{k C_a C_{eo}}$$

$$\frac{1}{-r_A} = \frac{m}{K C_{eo} C_a} + \frac{1}{k C_{eo}}$$

Plot C_A v/s t & take slope at different C_A

C _A	$\frac{-dC_A}{dt}$	$\frac{1}{C_A}$	$\frac{1}{-r_A}$
0.38	0.139	2.63	7.2
0.225	0.097	4.44	10.3
0.1	0.052	10	19.23
0.075	0.042	12.82	23.8



Slope = 1.623

Intercept = 3.0035

$$= \frac{1}{K_{CeO}}$$

$$= \frac{1}{3.0025*01}$$

$K = 33.33$

$$\text{Slope} = 1.623 = \frac{m}{k_{\text{Ceo}}}$$

$$M = 1.623 * 33.33 * 0.01$$

$M = 0.54 \frac{\text{m mol}}{\text{liter}}$

Ex - 17

Enzyme E catalyzes the transformation of reactant A to product R as follows:



$$-r_A = \frac{200 C_E O \cdot C_A}{2 + C_A}$$

If we introduce enzyme ($C_{EO} = 0.001 \text{ mol/liter}$) and reactant ($C_{AO} = 10 \text{ mol/liter}$) into a batch reactor and let the reaction proceed, find the time needed for the concentration of reactant to drop to 0.025 mol/liter . Note that the concentration of enzyme remains unchanged during the reaction.

Ans :

$$C_{EO} = 0.001 \text{ M}$$

$$C_{AO} = 10 \text{ M}$$

$$\text{For batch reactor, } t = -C_{AO} \int_{-r_A}^{\frac{dca}{-r_A}}$$

$$= -C_{AO} \int_{C_{AO}}^{C_A} \frac{dca}{200 C_A \cdot C_{EO}} = .001M$$

$$= -C_{AO} \int_{10}^{0.025} \frac{dca}{100 C_A \cdot C_{EO}} + \frac{dca}{100 \cdot C_{EO}}$$

$$= -C_{AO} \left[\frac{1}{100 \cdot C_{EO}} * \ln C_A + \frac{1}{200 \cdot C_{EO}} 8 C_A \right]$$

$$= -10 [-3.678 - 7.305]$$

$t = 109.87 \text{ min.}$

Ex - 18

An ampoule of radioactive Kr-89 (half life = 76 minutes) is set aside for a day. What does this do to the activity of the ampoule? Note that radioactive decay is a first-order process.

Ans :

$$t_{1/2} = 76 \text{ min.}$$

$$k = \frac{0.693}{76} = 9.1184 * 10^{-3}$$

$$t = 1440 \text{ min}^{-1}$$

$$C_A = C_{AO} e^{-(0.00911 * 1440)}$$

$$= C_{AO} \cdot 1.98 * 10^{-6}$$

$$\% \text{ concentration} = (C_{AO} - \frac{C_A}{C_{AO}}) * 100$$

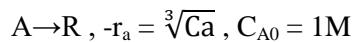
$$= \left(\frac{1 - (1.98 * 0.000001)}{1} \right) * 100$$

$$= 99.99 \%$$

Activity reduced to 99.99 %

Ex - 19

Find the conversion after 1 hour in a batch reactor for



Ans: For batch reactor,

$$t = -C_{AO} \int \frac{dc_A}{-r_a} \quad C_{AO} = 1M$$

$$1 = -1 \int_1^{C_A} \frac{dC_A}{3 C_A^2}$$

$$-1 = 2 [\sqrt[2]{C_A}]$$

$$-0.5 = \sqrt{C_A} - 1$$

$$C_A = 0.25$$

$$X_A = 1 - \frac{C_A}{C_{A0}}$$

$$= 1 - 0.25/1$$

$$X_A = 0.75$$

Ex - 20.

M. Hellin and J. C. Jungers, Bull. soc. chim. France, 386 (1957), present the data in Table P3.20 on the reaction of sulfuric acid with diethylsulfate in aqueous solution at 22.9 degree Celsius:



Initial concentrations of H_2SO_4 and $(C_2H_5)_2SO_4$ are each 5.5 mollliter. Find a rate equation for this reaction.

t, (min.)	$C_2H_5SO_4H, (M)$	t, (min.)	$C_2H_5SO_4H, (M)$
0	0	180	4.11
41	1.18	194	4.31
48	1.38	212	4.45
55	.63	267	4.86
75	2.2	318	5.15
96	2.75	368	5.32
127	3.31	379	5.35
146	3.76	410	5.42
162	3.81	∞	5.8

Ans:



$$C_{AO} = C_{BO} = 5.5 \text{ M}$$

$$-r_a = K C_A C_B$$

$$= K C_{AO} \cdot C_{BO} \cdot (1-X_A) \cdot (1-X_B) \quad (C_{AO} \cdot X_A = C_{BO} \cdot X_B)$$

$$= K C_{AO} \cdot (1-X_A) \cdot (1-MX_A)$$

$$= K \cdot (1-X_A)^2$$

$$\frac{-dca}{dt} = K \cdot (1-X_A)^2$$

$$\frac{-dCao(1-Xa)}{dt} = (1-Xa)^2 \cdot K$$

$$\int \frac{dx_a}{(1-x_a)^2} = K \int_0^t \frac{dt}{Cao}$$

$$\frac{Xa}{1-Xa} = \frac{kt}{Cao}$$

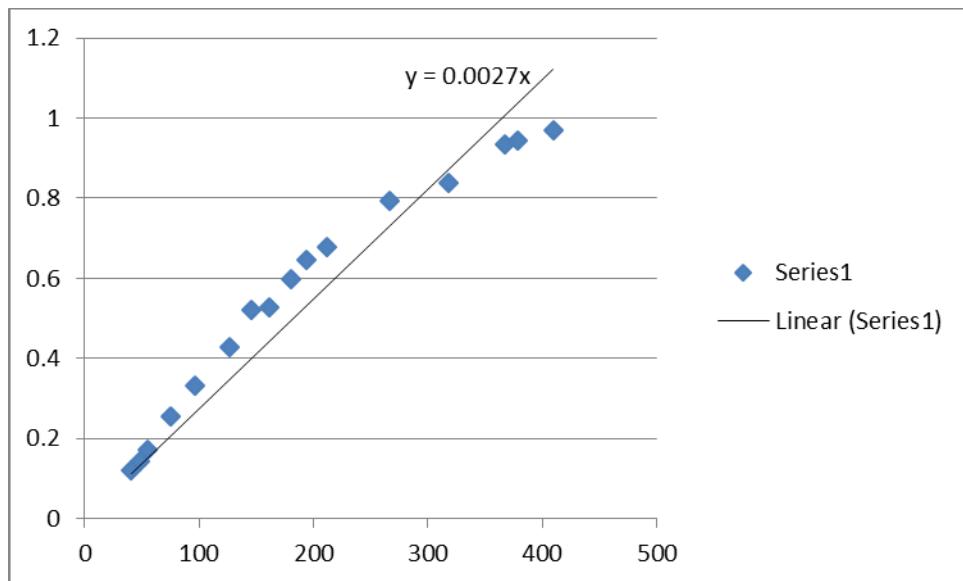
Xa	$\frac{Xa}{(1-Xa)}$
0.107	0.119
0.125	0.142
0.148	0.173
0.204	0.256
0.25	0.33
0.346	0.529
0.392	0.644

$$\text{Slope} = .0027$$

$$\frac{k}{Cao} = .0027$$

$$K = 5.5 * 0.0027$$

$K = 0.01485 \text{ min}$
$-r_a = 0.01485 C_A C_B$



Ex – 21

A small reaction bomb fitted with a sensitive pressure-measuring device is flushed out and then filled with pure reactant A at 1-atm pressure. The operation is carried out at 25°C , a temperature low enough that the reaction does not proceed to any appreciable extent. The temperature is then raised as rapidly as possible to 100°C by plunging the bomb into boiling water, and the readings in Table are obtained. The stoichiometry of the reaction is $2\text{A} \rightarrow \text{B}$, and after leaving the bomb in the bath over the weekend the contents are analyzed for A; none can be found. Find a rate equation in units of moles, liters, and minutes which will satisfactorily fit the data.

T,(min)	Π (atm)	T,(min)	Π (atm)
1	1.14	7	0.85
2	1.04	8	0.832
3	0.982	9	0.815

4	0.94	10	0.8
5	0.905	15	0.754
6	0.87	20	0.728

Ans:

Constant volume reaction

$$V_1 = V_2$$

$$P_2 = (T_2/T_1) \cdot P_1$$

$$= (373/298) \cdot 1$$

$$= 1.25 \text{ atm}$$

$$P_A = P_{A0} - (a/\Delta n)(P - P_0)$$

$$= 1.25 - (2/-1) \cdot (1.14 - 1.25)$$

$$= 2P - 2P_0 + P_0$$

$$= 2P - P_0$$

$$C_{A1} = \frac{2(1.14) - 1.25}{0.08314 * 373}$$

$$= 0.041$$

t	0	1	2	3	4	5	6	7	8	9	10	15	20
C _A	0.041	0.034	0.027	0.023	0.021	0.018	0.016	0.015	0.013	0.012	0.0114	0.0089	0.0067

Assume 2nd order reaction

$$K = \{ [1/C_A] - [1/C_{A0}] \} * (1/t)$$

$$K_1 = [\frac{1}{.034} - \frac{1}{.041}] * \frac{1}{1} = 5.02 \text{ M}^{-1} \text{ min.}^{-1}$$

$$K_2 = \left[\frac{1}{.027} - \frac{1}{.041} \right] * \frac{1}{2} = 6.32 \text{ M}^{-1} \text{ min.}^{-1}$$

$$K_3 = \left[\frac{1}{.023} - \frac{1}{.041} \right] * \frac{1}{3} = 6.36 \text{ M}^{-1} \text{ min.}^{-1}$$

$$K_4 = \left[\frac{1}{.021} - \frac{1}{.041} \right] * \frac{1}{4} = 5.81 \text{ M}^{-1} \text{ min.}^{-1}$$

$$K_5 = \left[\frac{1}{.018} - \frac{1}{.041} \right] * \frac{1}{5} = 6.23 \text{ M}^{-1} \text{ min.}^{-1}$$

$$K_6 = \left[\frac{1}{.016} - \frac{1}{.041} \right] * \frac{1}{6} = 6.35 \text{ M}^{-1} \text{ min.}^{-1}$$

There is not much variation in the value of K.

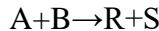
$$\text{Avg. K} = \frac{36.4}{6}$$

$$K = 6.067 \frac{\text{L}}{\text{mol}} \cdot \text{min}^{-1}$$

$$\boxed{\text{Rate equation} - r_A = 6.067 C_A^2 \frac{\text{mol}}{\text{l.min}}}$$

Ex. 4.1

Gaseous Feed,



$$CA_0 = 100, CB_0 = 200, X_A = 0.8$$

For $X_A = 0, V_I = 100A + 200B + 0R + 0S = 300$,

For $X_A = 1, V_F = 0A + 100B + 100R + 100S = 300, \text{ So } \varepsilon_a = 0$

$$CA = CA_0(1 - X_A) = 100(1 - 0.8) = \underline{\underline{20}} \text{ ...ans(1)}$$

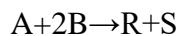
$$X_B CB_0 = b CA_0 X_A$$

$$X_B = CA_0 X_A / CB_0 = (100/200)(0.8) = \underline{\underline{0.4}} \text{ ...ans(2)}$$

$$CB = CB_0(1 - X_B) = 200(1 - 0.4) = \underline{\underline{120}} \text{ ...ans(3)}$$

Ex. 4.2

Dilute aqueous feed, So $\varepsilon_a = 0$



$$CA_0 = 100, CB_0 = 100, CA = 20$$

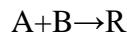
$$CA = CA_0(1 - X_A), \text{ So } X_A = 1 - (20/100) = \underline{\underline{0.8}} \text{ ...ans(1)}$$

$$X_B CB_0 = b CA_0 X_A,$$

$$X_B = CA_0 X_A / CB_0 = 2(100/100)(0.8) = \underline{\underline{1.6(\text{impossible})}} \text{ ...ans(2 & 3)}$$

Ex. 4.3

Gaseous Feed,



$$CA_0 = 200, CB_0 = 100, C_A = 50$$

For $X_A = 0, V_I = 200A + 100B + 0R = 300, \text{ So } \varepsilon_a = (V_F - V_I) / V_I = (100 - 300) / 300 = -0.667$

For $X_A = 1, V_F = 0A - 100B + 200R = 100$,

$$X_A = (CA_0 - CA) / (CA_0 + \varepsilon_a X_A) = (200 - 50) / (200 - 0.667 * 50) = \underline{\underline{0.9}}$$

$$X_B CB_0 = b CA_0 X_A$$

$$X_B = CA_0 X_A / CB_0 = (200/100)(0.9) = 1.8 \text{ (impossible)} \dots \text{ans(2)}$$

$$CB = CB_0(1 - X_B) = 200(1 - 1.8) = \text{impossible} \text{ ...ans(3)}$$

Ex. 4.4

Gaseous Feed,



$$CA_0 = 100, CB_0 = 100, C_A = 20$$

For $X_A = 0, V_I = 100A + 100B + 0R = 200, \text{ So } \varepsilon_a = (V_F - V_I) / V_I = (0 - 200) / 200 = -1$

For $X_A = 1, V_F = 0A + 100B + 100R = 0,$

$$X_A = (CA_0 - CA) / (CA_0 + \varepsilon_a X_A) = (100 - 20) / (100 - 2 * 50) = \underline{1}$$

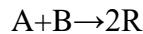
$$X_B CB_0 = b CA_0 X_A$$

$$X_B = CA_0 X_A / CB_0 = (100 / 100)(1) = 2 \text{ (impossible)} \dots \text{ans(2)}$$

$$CB = CB_0(1 - X_B) = 100(1 - 2) = \text{impossible} \dots \text{ans(3)}$$

Ex. 4.5

Gaseous Feed,



$$CA_0 = 100, CB_0 = 200, T_0 = 400 \text{ K}, T = 300 \text{ K}, \pi_0 = 4 \text{ atm}, \pi = 3 \text{ atm}, C_A = 20$$

For $X_A = 0, V_I = 100A + 200B + 0R = 300, \text{ So } \varepsilon_a = (V_F - V_I) / V_I = 0$

For $X_A = 1, V_F = 0A + 100B + 200R = 300,$

$$X_A = (CA_0 - CA) (T \pi_0 / T_0 \pi) / (CA_0 + \varepsilon_a X_A) (T \pi_0 / T_0 \pi)$$

$$= (100 - 20) (300 * 4 / 400 / 3) / (100 + 0 * 20) (300 * 4 / 400 / 3) = \underline{0.8}$$

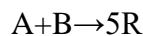
$$X_B CB_0 = b CA_0 X_A$$

$$X_B = CA_0 X_A / CB_0 = (100 / 200) = \underline{0.8} \dots \text{ans(2)}$$

$$CB = CB_0(1 - X_B) = 200(1 - 0.8) = \underline{120} \dots \text{ans(3)}$$

Ex. 4.6

Gaseous Feed,



$$CA_0 = 100, CB_0 = 200, T_0 = 1000 \text{ K}, T = 400 \text{ K}, \pi_0 = 5 \text{ atm}, \pi = 4 \text{ atm}, C_A = 20$$

For $X_A = 0, V_I = 100A + 200B + 0R = 300, \text{ So } \varepsilon_a = (V_F - V_I) / V_I = 2$

For $X_A = 1, V_F = 0A + 100B + 500R = 600,$

$$X_A = (CA_0 - CA) (T\pi_0 / T_0 \pi) / (CA_0 + \epsilon_a X_A) (T\pi_0 / T_0 \pi)$$

$$= (100-20)(400*5/1000/4) / (100+2*20)(400*5/1000/4) = 0.75 \dots \text{ans}(1)$$

$$X_B C B_0 = b C A_0 X_A$$

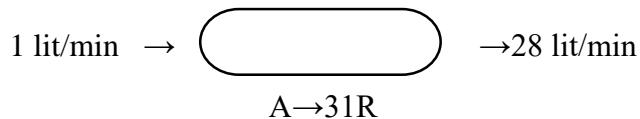
$$C B / C A_0 = ((C B_0 / C A_0) - b X_A / a) / (T\pi_0 / T_0 \pi) = ((200/100) - 0.75) / (400*5/1000/4),$$

$$\text{So } \underline{C B = 100} \dots \text{ans}(2)$$

$$X_B C B_0 = b C A_0 X_A$$

$$\underline{X_B = 0.75} \dots \text{ans}(3)$$

Ex. 4.7



X =Popcorn produced

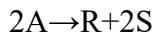
$(1-X)$ =disappearance of A

$$\text{So, outlet} = 31X + (1-X)1 = 28 \text{ lit/min}$$

$$X = 27/30 = 0.9$$

Ans : 90% popcorn popped.

Ex. 5.1



$$X_A = 0.9$$

$$\text{Space velocity (s)} = 1/\text{min}$$

$$\text{So, space time}(\tau) = 1/\text{s}$$

$$= \underline{\mathbf{1 \text{ min}}} \quad \dots \text{ans(1)}$$

$$\text{Here, } \varepsilon_a = (3-2)/2 = 0.5 \quad V_F = V_0(1 + \varepsilon_a X_A)$$

$$= V_0(1 + 0.5 * 0.9)$$

$$= 1.45 V_0$$

$$\text{So. Holding time, } t = V/V_F$$

$$= V/V_0 * 1.45$$

$$= 0.69 \text{ min}$$

But in the plug flow reactor since the gas reacts progressively as it passes through the reactor, expands correspondingly, therefore holding time = 1 min. ...ans (2)

Ex 5.2

Liquid phase reaction, $X_A = 0.7$, time = 13 min, first order reaction

$$\text{For first order reaction, } -r_A = k C_A$$

$$-\ln(1 - X_A) = kt, \text{ so, } k = 0.0926 / \text{min}$$

Case -1(for mixed flow reactor),

$$\text{Here } \tau_m = C_A_0 * X_A / (-r_A)$$

$$= C_A_0 * X_A / (k * C_A_0 (1 - X_A))$$

$$= (0.7 / (0.926 * 0.3))$$

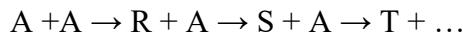
$$\underline{\mathbf{\tau_m = 25.2 \text{ min}}} \quad \dots \text{ans(1)}$$

Case -2(for plug flow reactor),

$$\text{Same as batch reactor, } \underline{\mathbf{\tau_p = \tau = 13 \text{ min}}} \quad \dots \text{ans(2)}$$

Ex. 5.3

Aqueous monomer A , $V = 2$ litre , $v = 4$ lit/min , $CA_0 = 1$ mol/lit , $CA = 0.01$ mol/lit



Here, $\tau = V/v = 2/4 = 0.5$ min

For reaction rate of A,

$$\begin{aligned}-r_A &= (CA_0 - CA) / \tau \\ &= (1-0.01)/0.5 = \underline{\underline{1.98 \text{ mol/(lit*min)}}} \quad \dots \text{ans(1)}$$

For W, $CW = 0.0002$ mol/lit

$$\begin{aligned}-r_W &= (-CW_0 + CW) / \tau \\ &= (0.0002-0)/0.5 = \underline{\underline{0.0004 \text{ mol/(lit*min)}}} \quad \dots \text{ans(2).}$$

Ex 5.4

$$-r_A = k CA^{1.5}$$

$$X_A = 0.7$$

For mixed flow reactor , $\tau = V/ V_0$

$$\begin{aligned}&= X_A / (-r_A) \\ &= X_A * CA_0 / (k * CA_0^{1.5} * (1 - X_A)^{1.5})\end{aligned}$$

From above equation , $k = X_A / ((CA_0^{0.5} * (1 - X_A)^{1.5}) * (V / V_0)) \quad \dots \text{equ (1)}$

Putting $X_A = 0.7$

$$\text{So, } k = 4.260 / (CA_0^{0.5} (V / V_0))$$

Now if volume is doubles so $V' = 2V$

$$\begin{aligned}\text{So , } \tau &= V' / V_0 \\ &= X_A * CA_0 / (k * CA_0^{1.5} * (1 - X_A)^{1.5}) \\ 8.52 &= X_A / (1 - X_A)^{1.5} \quad \dots \text{from equ (1)}$$

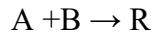
Take square both side ,

$$72.6 = X_A^2 / (1 - X_A)^3$$

$$\text{So, } 72.6 - 72.6 X_A^3 + 216 X_A^2 - 217 X_A = 0$$

Solving by numerical method we get $\underline{\underline{X_A=0.7947}}$ $\dots \text{ans}$

Ex. 5.5



$$-r_A = 200 CA * CB$$

$$CA_0 = 100, CB_0 = 200, v = 400 \text{ lit/min}, X_A = 0.999$$

For second order reaction, (different reactants)

$$k \tau * CA_0 * (M-1) = \ln((M-X_A)/(M * (1-X_A)))$$

here $M=2$, so substituting values,

$$\begin{aligned} V/v &= \ln((2-0.999)/2(1-0.999)) / (200 * 0.10 * 1) \\ &= 0.31 \end{aligned}$$

$$\text{So } \underline{V=0.31 * 400 = 124 \text{ litre}} \quad \dots \text{ans.}$$

Ex. 5.6



$$-r_A = 0.04 CA * 0.01 CB$$

$$\text{so } k_1 = 0.04, k_2 = 0.01, M = CR_0/CA_0 = 0$$

$$k_1/k_2 = X_{Ae}/(1-X_{Ae}) \text{ from there } X_{Ae} = 0.8 \quad \dots \text{ans (1)}$$

For first order plug flow reactor (reversible reaction),

$$\begin{aligned} V/(v * CA_0) &= \int_0^{X_A f} dX_A / (-r_A) \\ -r_A &= 0.04 CA_0(1-X_A) - 0.01 CA_0(M + X_A) \end{aligned}$$

So by integrating term we get,

$$\begin{aligned} -\ln(1 - X_A/X_{Ae}) &= k_1 * V/v * (M + 1) / (M + X_{Ae}) \end{aligned}$$

Substituting all values, we get

$$-\ln(1 - X_A/X_{Ae}) = 0.64$$

$$X_A/X_{Ae} = 0.48$$

$$\underline{X_A = 0.38} \quad \dots \text{ans}$$

Ex 5.7

Half time for this reaction ($\tau_{1/2}$) = 5.2 days

Mean resident time (τ) = 30 days

$$\text{So } k = 0.693 / \tau_{1/2} = 0.693 / 5.2 = 0.1333 \text{ /day}$$

For mixed flow reactor, $CA / CA_0 = 1 / (1 + k \tau) = 0.2$

So fraction of activity = $1 - CA / CA_0 = 0.8$

Ans = 80%

Ex. 5.8

$A \leftrightarrow R$ (reversible reaction)

$$-r_A = 0.04 CA * 0.01 CB$$

$$\text{so } k_1 = 0.04, k_2 = 0.01, M = CR_0 / CA_0 = 0$$

$$k_1 / k_2 = X_{Ae} / (1 - X_{Ae}) \text{ from there } X_{Ae} = 0.8 \quad \dots \text{ans (1)}$$

For first order mixed flow reactor (reversible reaction),

$$V / (v^* CA_0) = X_A / (-r_A)$$

$$-r_A = 0.04 CA_0 (1 - X_A) - 0.01 CA_0 (M + X_A)$$

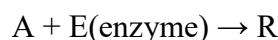
$$V/v = 0.10 X_A / (0.04 CA_0 (1 - X_A) - 0.01 CA_0 (M + X_A))$$

Substituting all values, we get

$$X_A = 0.8 - 0.8 X_A - 0.01 X_A$$

$$\underline{\underline{X_A = 0.40}} \quad \dots \text{ans}$$

Ex. 5.9



$$-r_A = 0.1 CA / (1 + 0.5 CA)$$

Here, $v = 25 \text{ lit/min}$, $CA_0 = 2 \text{ mol/litr}$, $X_A = 0.95$

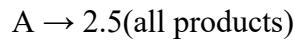
$$\text{Now, } V/v = \int_{CA_0}^{CAF} dCA / (-r_A)$$

Substituting $-r_A = 0.1 CA / (1 + 0.5 CA)$ and $CA = CA_0 (1 - X_A)$

$$\text{So, } V/v = [-10(\ln(0.10/2) - 5(0.10-2))] = 39.452$$

$$\text{So, } \underline{\underline{V = 986.25 \text{ lit}}} \quad \dots \text{ans.}$$

Ex 5.10



$-r_A = 10 CA$, plug flow reactor

Here, $v = 100 \text{ lit/min}$, $CA_0 = 2 \text{ mol/litr}$, $V = 22 \text{ L}$

From the stoichiometry $\varepsilon_a = (2.5-1)/1 = 1.5$

If we write equation for plug flow reaction,

$$(V/v) * CA_0 = \int_0^{X_A f} dX_A / (-r_A)$$

$$CA = CA_0(1 - X_A) / (1 + \varepsilon_a X_A)$$

$$\text{So } (V/v) * CA_0 * k = - (1 + \varepsilon_a) \ln(1 - X_A) - 1.5 X_A$$

$$4.4 = -2.5 \ln(1 - X_A) - 1.5 X_A$$

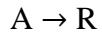
$$\underline{X_A = 0.733} \quad \dots \text{ans.}$$

Group 12

13bch024, 13bch033, 13bch048, 13bch059

Solution 5.11:

Solution-



$$-r_A = 0.1C_A / (1 + 0.5C_A)$$

According to the performance equation of mixed flow reactor,

$$\frac{\tau_m}{C_{A0}} = \frac{X_A}{-r_A} \quad - (1)$$

Now substituting the value of X_A from the equation,

$$C_A = C_{A0}(1 - X_A) \quad - (2)$$

We get,

$$\tau_m = \frac{C_{A0} - C_A}{\frac{0.1C_A}{(1 + 0.5C_A)}} \quad - (3)$$

Now, conversion is 95 % so, $X_A = 0.95$

Therefore, substituting the values in the equation, we get

$$\tau_m = \frac{(2 - 0.1)(1 + 0.5(0.1))}{0.1(0.1)} = 199.5 \text{ min}$$

Therefore,

$$V = \tau_m V_0 = 199.5(25) \text{ L} = 4987.5 \text{ L} = 5 \text{ m}^3$$

$$\mathbf{V = 5 m^3}$$

Problem 5.12:**Solution-**

$$-r_A = 200C_A C_B \text{ (mol)/(litre).(min)}$$

Now,

$$C_A = 0.1 \text{ mol/L}$$

$$C_B = 0.4 \text{ mol/L}$$

$$v_o = 400 \text{ L/min}$$

Hence, from the equation: $C_A = C_{A0}(1 - X_A)$, we get $X_A = 0.99$

$$\tau_m = \frac{X_A \cdot C_{A0}}{-r_A},$$

$$C_A = C_{A0}(1 - X_A)$$

$$C_B = C_{A0}(M_B - (b/a)X_A) \quad \text{Here, } M_B = 200/100 = 2$$

Now, $b = a = 1$

$$-r_A = 200(0.1)^2(1 - X_A)(2 - X_A)$$

$$= 0.0202$$

$$\tau_m = \frac{X_A \cdot C_{A0}}{-r_A} = \tau_m = \frac{(0.99)(0.1)}{0.0202} = 49.9 \text{ min}$$

Therefore,

$$V = \tau_m v_o = 49.9(400) \text{ L} = 19960 \text{ L} = 19.96 \text{ m}^3$$

$$\mathbf{V = 19.96 \text{ m}^3}$$

Problem 5.13

Solution-



$$X_A = 0.75$$

$$P = 11.4 \text{ atm}$$

$$F_{AO} = 10 \text{ mol/hr}$$

$$\text{PH}_3 = (2/3) \text{ of feed} \quad \text{Inerts} = (1/3) \text{ of feed}$$

As it is a gaseous reaction we need to find ε_A Hence,

$$\varepsilon_A = (1 + 6 - 4)(2) / 4(3) = 0.5$$

The reaction is of a first order hence, the integral law can be written as

$$\tau_p = \frac{1}{10}[(1 + \varepsilon_A)(-\ln(1-X_A) - \varepsilon_A X_A)]$$

$$\tau_p = 0.17$$

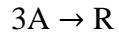
$$C_{AO} = \frac{P_{AO}}{RT_o} = \frac{11.4(2/3)}{0.082(649+273)} = 0.1 \text{ mol/L}$$

$$v_0 = \frac{F_{AO}}{C_{AO}} = 10/0.1 = 100 \text{ L/h}$$

Therefore,

$$V = \tau_p v_0 = 0.17(100) \text{ L} = 17 \text{ L}$$

$$\mathbf{V = 17 \text{ L}}$$

Problem 5.14**Solution-**

$$-r_A = 54 \text{ mmol/L} \cdot \text{min} = 0.054 \text{ mmol/L} \cdot \text{min}$$

$$C_{A0} = 0.6 \text{ mol/L}$$

$$C_A = 0.33 \text{ mol/L}$$

$$F_{AO} = 0.54 \text{ mol/min}$$

Now,

$$\varepsilon_A = 2/3$$

Hence,

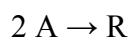
$$C_A = \frac{C_{A0}(1-X_A)}{(1+\varepsilon_A X_A)}$$

$$330 = 660 \frac{(1-X_A)}{(1+\left(\frac{2}{3}\right)X_A)} \text{ therefore, } X_A = 0.75$$

Therefore,

$$\tau_p = \int_0^{0.75} \frac{dX_A}{-r_A} = \frac{C_{A0} X_A}{-r_A} = 9.17 \text{ min}$$

$$V = \tau_p V_o = \tau_p \frac{F_{AO}}{C_{AO}} = 9.17(540/660) = 7.5 \text{ L}$$

Problem 5.15**Solution-**

$$-r_A = 0.05 C_A^2 \text{ mol/L s}$$

Now,

$$\tau_m = \frac{X_A \cdot C_{A0}}{-r_A}$$

$$\varepsilon_A = 0.5$$

From the equation,

$$C_A = \frac{C_{A0}(1 - X_A)}{(1 + \varepsilon_A X_A)}$$

$$330 = 660 \frac{(1 - X_A)}{(1 - 0.5X_A)}, \text{ therefore on solving we get } X_A = 0.66$$

Now on expanding the rate expression we get,

$$-r_A = 0.05 C_{A0}^2 \left(\frac{(1 - X_A)}{(1 - 0.5X_A)} \right)^2$$

Hence from,

$$\tau_m = \frac{X_A \cdot C_{A0}}{-r_A} = 54.442 \text{ min}$$

Therefore,

$$V_o = \frac{V}{\tau_m} = 2/54.442 = 0.036 \text{ L/min}$$

Problem 5.16**Solution-**

$$A \rightarrow 3 R \quad -r_A = 0.6 C_A \text{ min}^{-1}$$

The feed contains of 50% A and 50% inerts

$$v_0 = 180 \text{ litre/min}$$

$$C_{A0} = 0.3 \text{ mol/litre}$$

$$V = 1000 \text{ L} = m^3$$

Now,

$$\tau_m = \frac{X_A \cdot C_{A0}}{-r_A} = \frac{V}{v_0}$$

$$\varepsilon_A = 2(0.5) = 1,$$

Hence the rate expression can be expanded as,

$$-r_A = 0.6 C_A \frac{(1-X_A)}{(1+\varepsilon_A X_A)} = 0.6 C_A \frac{(1-X_A)}{(1+X_A)},$$

$$\tau_m = \frac{X_A \cdot C_{A0}}{-r_A} = \frac{V}{v_0} = \frac{X_A(1+X_A)}{C_{A0}(1-X_A)}$$

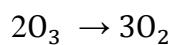
we obtain,

$$3X_A^2 + 13X_A - 10 = 0$$

$$X_A = \frac{-13 \pm \sqrt{169+40(3)}}{2(3)} = 0.67$$

Problem 5.17

Solution-



$$-r_{ozone} = kC_{ozone}^2, k = 0.05 \text{ litre/ (mol.s)}$$

The rate expression shows that it is a second order reaction so, the integral expression is defined as,

$$k\tau_p C_{A0} = 2\varepsilon_A(1 + \varepsilon_A) \ln(1 - X_A) + \varepsilon_A^2 X_A + (\varepsilon_A + 1)^2 \frac{X_A}{1 - X_A}$$

Now,

$$C_{A0} = \frac{P_{A0}}{RT_0} = 1.5(0.2)/(0.082)(95 + 273) = 0.01 \text{ mol/L}$$

$$\varepsilon_A = (3-2)/2 \times (0.2) = 0.1$$

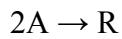
Hence, putting in the equation we get

$$\tau_p = \frac{V}{v_0} = \frac{1}{0.05(0.01)} \{2[0.1(1.1)\ln 0.5 + 0.1^2(0.5) + 1.1^2(1)]\}$$

$$\tau_p = 2125.02 \text{ s}$$

$$V = 2125.02 \text{ (1 L/s)} = 2125 \text{ L} = 2.125 \text{ m}^3$$

$$\mathbf{V = 2.125 \text{ m}^3}$$

Problem 5.18**Solution-**

$$-r_A = 0.05C_A^2, \text{ mol/litre.s}$$

$$F_{A0} = 1 \text{ mol/litre}$$

$$V = 2 \text{ L}$$

$$v_0 = 0.5 \text{ litre/min}$$

Therefore,

$$\tau_p = \frac{V}{v_0} = \frac{2 L}{0.5 L/min} = 4(60) \text{ s} = 240 \text{ s}$$

The integral rate expression for the 2nd order reaction is given by,

$$k\tau_p C_{A0} = 2\varepsilon_A(1 + \varepsilon_A) \ln(1 - X_A) + \varepsilon_A^2 X_A + (\varepsilon_A + 1)^2 \frac{X_A}{1 - X_A}$$

Now,

$$\varepsilon_A = 0$$

Therefore, the equation will reduce to

$$k\tau_p C_{A0} = \frac{X_A}{1 - X_A}$$

So, substituting the values we get,

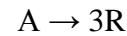
$$k\tau_p C_{A0} = \frac{X_A}{1 - X_A}$$

$$X_A = \frac{k\tau_p C_{A0}}{1 + k\tau_p C_{A0}} = \frac{0.05(240)(1)}{1 + (0.05)(240)(1)} = 0.92$$

Problem 5.19

Solution

$$P = 3 \text{ atm}$$



$$T = 30^\circ C$$

$$C_{AO} = 0.12 \text{ mol/litre}$$

V_0	C_A
0.06	30
0.48	60
1.5	80
8.1	105

Now,

$$\tau_m = \frac{X_A \cdot C_{AO}}{-r_A} = \frac{v}{v_0} - (1)$$

Similarly,

$$\varepsilon_A = \frac{(3-1)1}{1} = 2$$

Now, from the equation

$$C_A = \frac{C_{AO}(1-X_A)}{(1+\varepsilon_A X_A)}$$

We get different values of X_A and from that we calculate different values of $-r_A$

Hence, we obtain the following data

X_A	$-r_A$
0.5	3.6

0.25	14.4
0.143	25.74
0.045	44.18

Hence, from the rate expression

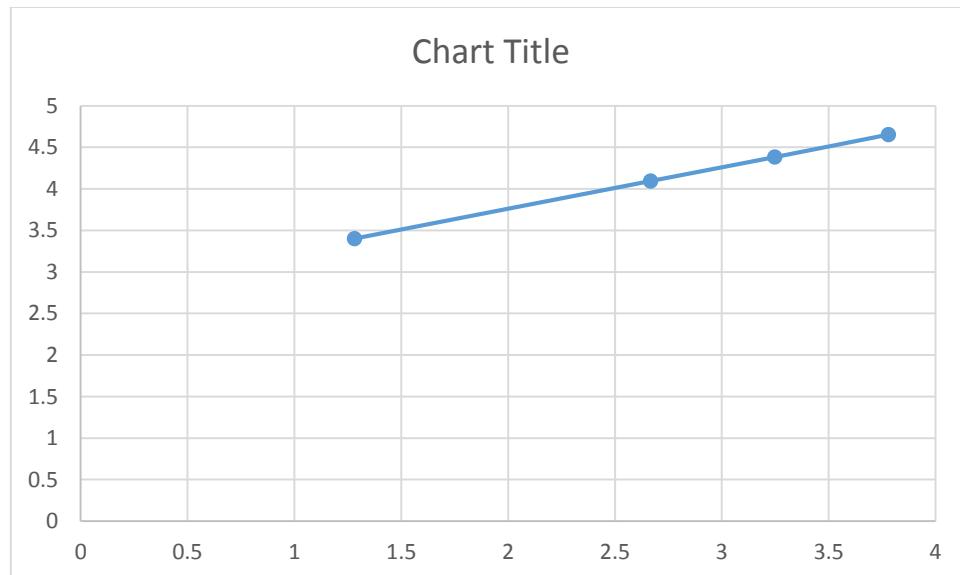
$$-r_A = k C_A^n$$

Taking log on both sides

$$\ln(-r_A) = \ln k + \ln C_A$$

Now plotting $\ln(-r_A)$ on Y-axis and $\ln C_A$ on X-axis

We get,

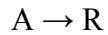


$$\text{Hence, slope } n = (3.78 - 1.2809) / (4.653 - 3.4011) = 2$$

$$\text{Similarly, } k = 250$$

Hence, final rate expression will be

$$-r_A = 250 C_A^2$$

Problem 5.20**Solution-**

$$C_{A0} = 0.1 \text{ mol/litre}$$

$$V = 1 \text{ m}^3$$

v	C_A
1	4
16	20
24	50

For mixed flow reactor, performance equation is written as

$$\tau_m = \frac{C_{A0} - C_A}{-r_A}$$

Therefore,

$$-r_A = \frac{C_{A0} - C_A}{\tau_m}$$

$$-r_A = \frac{(100 - C_A)v_0}{V}$$

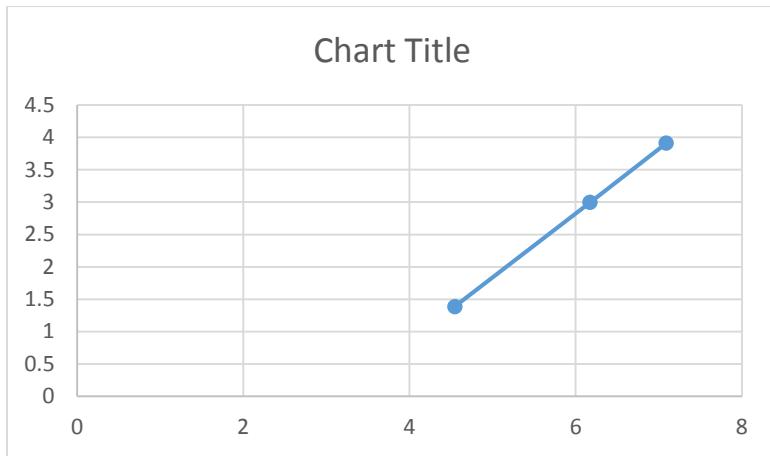
So,

$-r_A$	C_A	$\ln(-r_A)$	$\ln(C_A)$
96	4	4.5643	1.386
480	20	6.173	2.995
1200	50	7.09007	3.91

$$-r_A = k C_A^n$$

Now taking log on both sides,

$$\ln(-r_A) = \ln k + \ln C_A$$

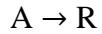


Therefore, slope = $n = 1$

Similarly the value of k can be evaluated by $k = \frac{C_A}{-r_A} = \frac{50}{1200} = 0.0417 \text{ min}^{-1}$

So,

$$-r_A = 0.0417 C_A \text{ mmol/L.min}$$

Problem 5.21**Solution-**

$$C_{A0} = 1.3 \text{ mol/litre}$$

$$C_A = 0.3 \text{ mol/litre}$$

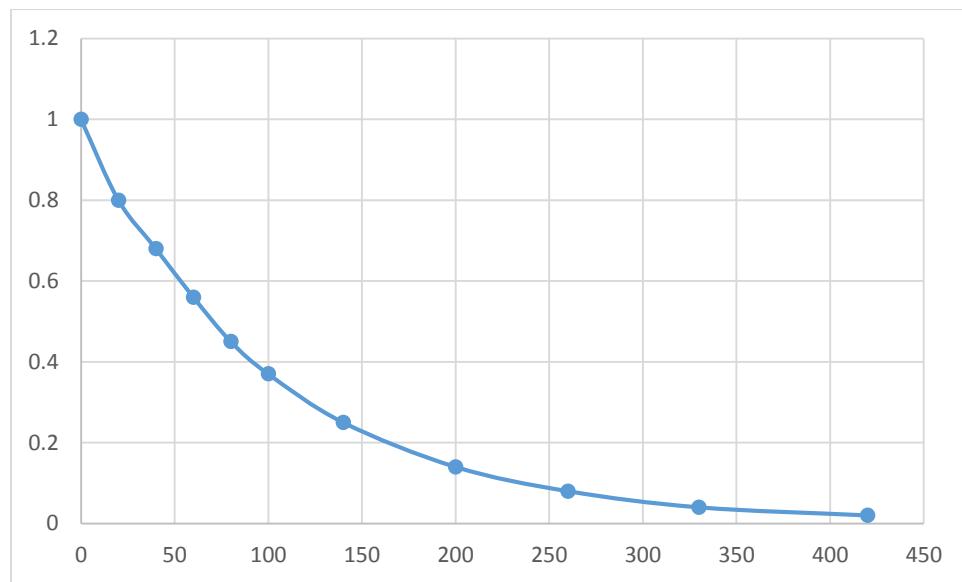
C_A	$-r_A$
0.1	0.1
0.2	0.3
0.3	0.5
0.4	0.6
0.5	0.5
0.6	0.25
0.7	0.1
0.8	0.06
1.0	0.05
1.3	0.045
2.0	0.042

It is a batch reactor so, the performance equation of the reactor is,

$$\int_{C_A}^{C_{A0}} \frac{dC_A}{-r_A} = \int_{0.3}^{1.3} \frac{dC_A}{-r_A} =$$

Therefore, we need to find the area under the curve of $-r_A$ and C_A from 0.3 to 1.3

Hence, in this plot the area under the curve from 0.3 to 1.3 we can calculate the residence time



$$t = \int_{0.3}^{1.3} \frac{dC_A}{-r_A} = 12.6 \text{ min}$$

Problem 5.22

Solution-

Given,

$$X_A = 0.8$$

$$F_{A0} = 1000 \text{ mol/hr}$$

$$C_{A0} = 1.5 \text{ mol/litre}$$

From, $C_A = C_{A0}(1 - X_A)$ we get $C_A = 0.3 \text{ mol/litre}$

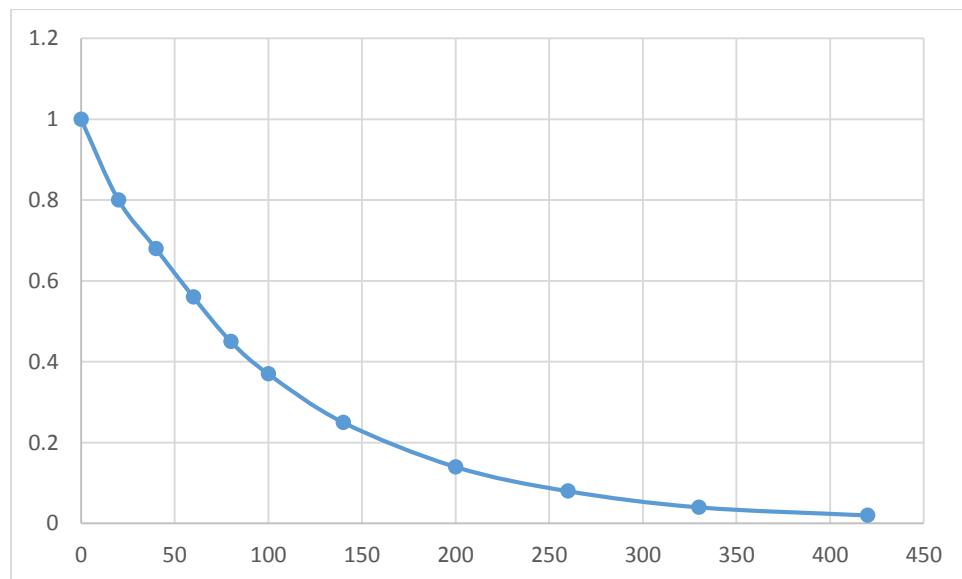
Now, the performance equation of the plug flow reactor is

$$\tau_p = \int_{C_A}^{C_{A0}} \frac{dC_A}{-r_A}$$

Similarly from the example 5.21 we obtain

$$\int_{0.3}^{1.3} \frac{dC_A}{-r_A} = 12.8 \text{ min}$$

Now, the time can be found by finding out the area between 1.3 to 1.5



So, the area between 1.3 to 1.5 we obtain the area = 4.5 min

Therefore,

$$\text{The total area} = 12.8 + 4.5 \text{ min}$$

$$= 17.3 \text{ min}$$

Problem 5.23

Solution-

$$X_A = 0.75$$

$$F_{A0} = 1000 \text{ mol/hr}$$

$$C_{A0} = 1.2 \text{ mol/litre}$$

(a) The performance equation of mixed flow reactor is

$$\tau_m = \frac{X_A \cdot C_{A0}}{-r_A}$$

Now from the equation, $C_A = C_{A0}(1 - X_A)$ so, substituting the values we get $C_A = 0.3 \text{ mol/L}$ and $-r_A = 0.5 \text{ mol/L}$

Therefore,

$$\frac{V}{F_{A0}} = \frac{(C_{A0} - C_A)}{-r_A}$$

$$V = 1000(1.2 - 0.3) / 1.2(0.5) (60) = 1500 \text{ L}$$

(b)

$$F_{A0} = 2000 \text{ mol/hr}$$

Hence, when the feed rate is doubled the volume also doubles.

Therefore, **V = 50 ltr**

(c)

$$C_{A0} = 2.4 \text{ mol/litre}$$

$$C_A = 0.3 \text{ mol/litre}$$

Therefore putting it in the performance equation we get,

$$\frac{V}{F_{A0}} = \frac{(C_{A0} - C_A)}{-r_A}$$

$$V = 1000(2.4 - 0.3) / (2.4)(0.5)(60) = \mathbf{29.167 \text{ ltr}}$$

Problem 5.24

Solution-

$$A \rightarrow 5 R$$

$$V = 0.1 \text{ litre}$$

$$C_{A0} = 100 \text{ mmol/litre} = 0.1 \text{ mol/litre}$$

F_{A0} mmol/ltr	C_A mmol/ltr
300	16
1000	30
3000	50
5000	60

$$\varepsilon_A = 4$$

$$\tau_m = \frac{X_A \cdot C_{A0}}{-r_A} = \frac{V}{v_0}$$

$$-r_A = \frac{v_0 X_A \cdot C_{A0}}{V} = 10 F_{A0} X_A$$

Therefore,

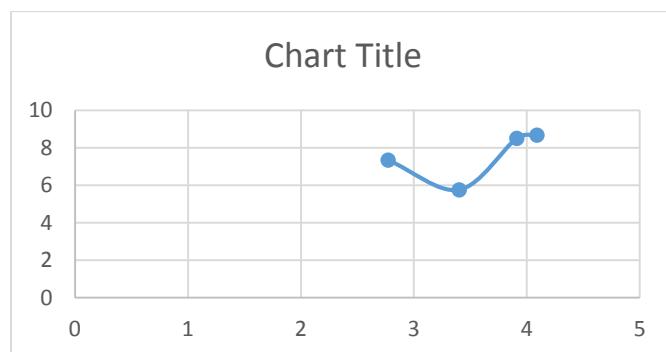
$$X_A = \frac{1 - \frac{C_A}{C_{A0}}}{1 + \varepsilon_A \frac{C_A}{C_{A0}}}, \text{ from this we generate the following data}$$

F_{A0}	C_A	X_A	$-r_A$
300	16	0.512	1536.6
1000	30	0.318	318.8
3000	50	0.167	5000
5000	60	0.118	5882.4

$$-r_A = k C_A^n$$

Now taking log on both sides,

$$\ln(-r_A) = \ln k + n \ln C_A$$



$$\text{Slope} = 1; k = 0.01$$

$$-r_A = 0.01 C_A$$

Problem 5.25

Solution-

$X_A = 0.75$; It is a batch reactor

$C_{A0} = 0.8 \text{ mol/litre}$

C_A in feed stream	C_A in exit stream	Holding time
2	0.65	300
2	0.92	240
2	1	250
1	0.56	110
1	0.37	360
0.48	0.42	24
0.48	0.28	200
0.48	0.20	560

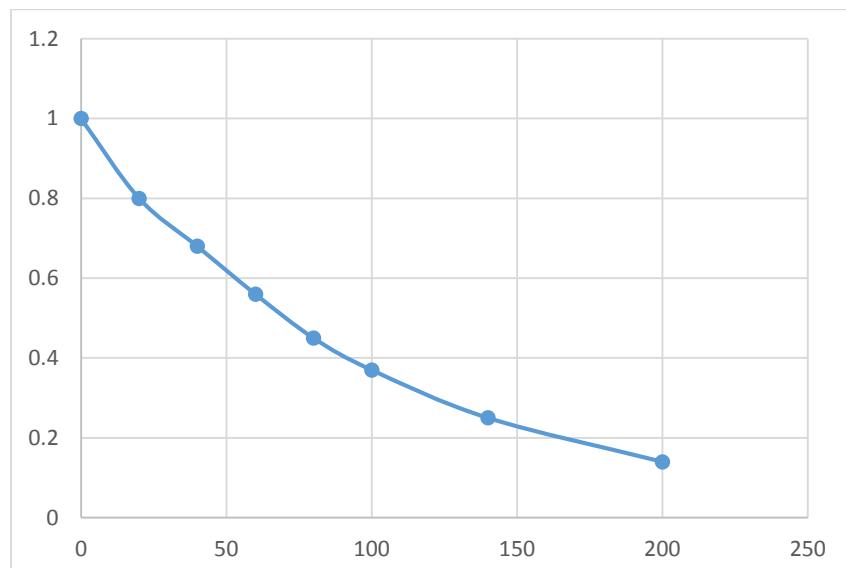
Hence, holding time = residence time = τ

$$\tau = - \int_{C_{A0}}^{C_A} \frac{dC_A}{-r_A};$$

So, we generate the following data, by using the correlation of $\tau = \frac{C_{A0} - C_A}{-r_A}$

C_A	$1/(-r_A)$
0.65	222
0.92	222
1	250
0.56	250
0.37	572
0.42	400
0.28	1000
0.2	2000

On plotting the graph of $1/(-r_A)$ vs C_A



Therefore, area under the curve will give the residence time

$$\tau = 300 \text{ s}$$

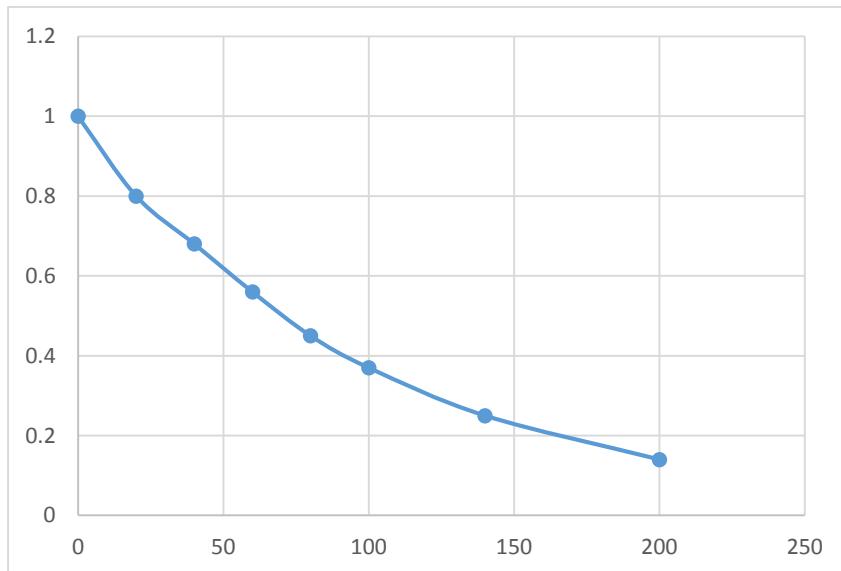
Problem 5.26

Solution-

If it is a mixed flow reactor

$$\tau_m = \frac{X_A \cdot C_{A0}}{-r_A} = \frac{V}{v_0}$$

Following the same procedure and plotting the same graph of $1/(-r_A)$ vs C_A we find the area of the complete rectangle because it is a MFR so,

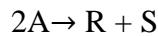


$$\tau = 900 \text{ s}$$

Problem 5.27**Solution-**

(a) The conversion drops from 80 to 75 % so, it is quite possible that Imbibit fell into the vat containing alcohol. The reason for the drop in conversion is due to decrease in the volume of liquid available for the reaction.

(b) The revelation couldn't be made because Watson asked for some dill (for smoking) but he didn't have any idea that smoking near a vat of ethanol isn't a very good idea.

Problem 5.28**Solution-**

The PFR is operating at 100°C and 1 atm

$$F_{A0} = 100 \text{ mol/hr}$$

$$X_A = 0.95$$

The feed contains 20% inerts and 80% A

So,

$$-r_A = kC_A^n$$

The reaction is of 1st order

So, the integral form of equation in terms of conversion is obtained which is

$$kt = -\ln(1 - X_A), \text{ which can be also written as } X_A = 1 - \frac{C_A}{C_{A0}} \quad (1)$$

Now,

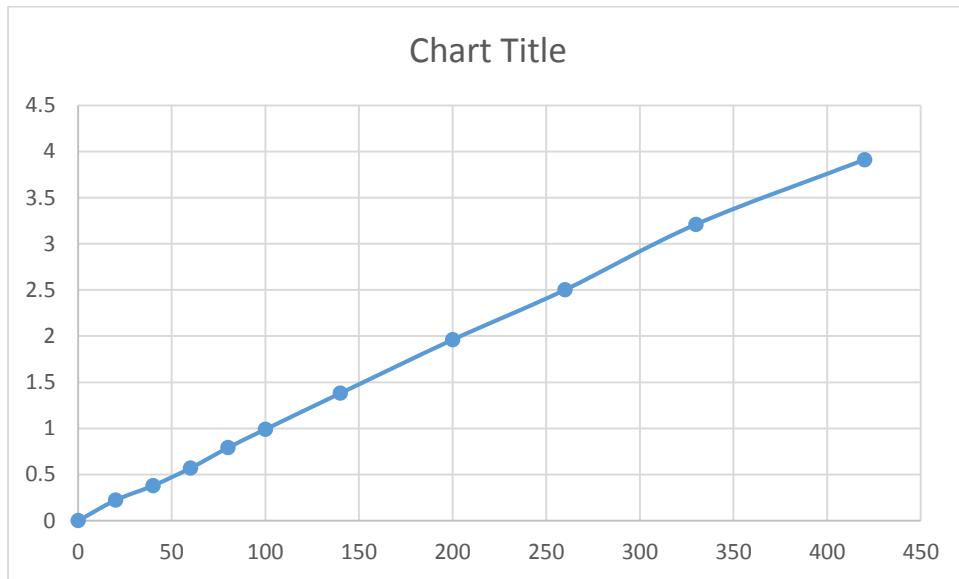
$$C_A = \frac{p_A}{RT}$$

So, replacing the term in the equation (1) we get,

$$kt = \ln \frac{p_{A0}}{p_A}$$

Hence, we now generate a data

T	$\ln(p_{A0}/p_A)$
0	1
20	1.25
40	1.47
60	1.78
80	2.22
100	2.702
140	4
200	7.14
260	12.5
330	25
420	50



Therefore, slope = $k = 0.01116 \text{ s}^{-1}$

The reaction is 1st order reaction hence, the rate expression is given by

$$-r_A = 0.01116 C_A$$

We can also write the equation like

$$k\tau_p = k \frac{V}{v_0} = -\ln(1 - X_A)$$

$$\text{Therefore, } V = -\frac{v_0}{k} \ln(1 - X_A)$$

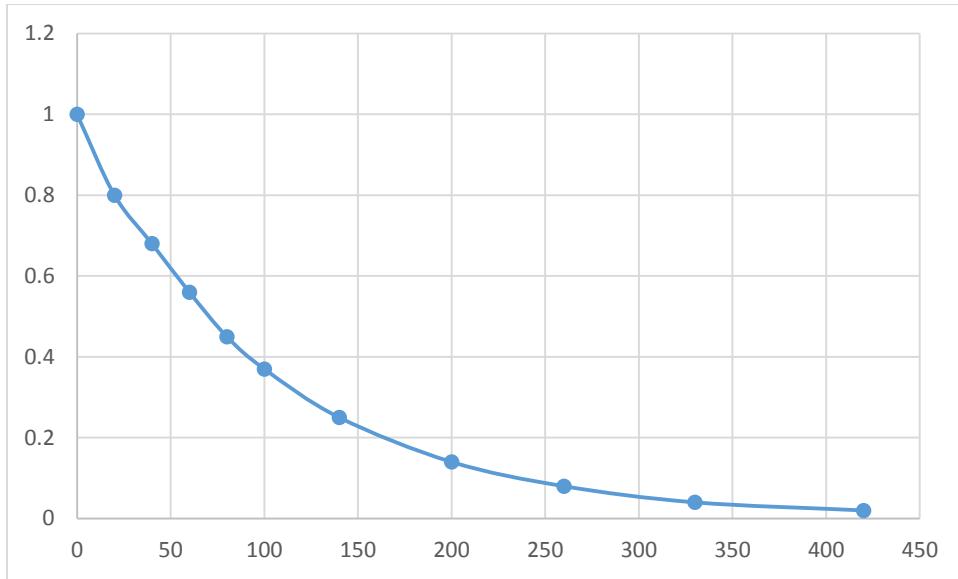
$$v_0 = \frac{F_{A0}}{C_{A0}} = \frac{F_{A0} T_0 R}{p_{A0}} = \frac{100(373)(0.082)}{0.8} = 3823.25 \frac{L}{h} = \frac{1.06L}{s}$$

$$V = 1.06 \ln(1 - 0.95) / 0.01116 = 284.54 \text{ L} = 2.84 \text{ m}^3$$

Problem 5.29**Solution-**

Now, for the same problem if we take a MFR then, the performance equation is written as

Plotting P_A v τ



$$\text{Slope} = \text{rate} = 0.000375$$

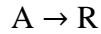
$$\tau_m = \frac{(p_{A0} - p_A)}{-r_A} = (0.8 - 0.04) / (0.000375) = 2026.67 \text{ s}$$

$$v_o = \frac{F_{A0}}{C_{A0}} = \frac{F_{A0}T_0R}{p_{A0}} = \frac{100(373)(0.082)}{0.8} = 3823.25 \frac{L}{h} = \frac{1.06L}{s}$$

$$V = 2026.67(1.06) = 2.148 \text{ L} = 2.15 \text{ m}^3$$

Problem 5.30

Solution-



$$C_{A0} = 0.8 \text{ mol/litre}$$

$$F_{A0} = C_{A0}(V) = 0.8 \text{ mol/s}$$

$$0.8 \text{ mol/litre}$$

$$X_A = 0.75$$

$$V = 1 \text{ litre/s}$$

(a) The reactor is a plug flow reactor

The performance equation is

$$\frac{V}{F_{A0}} = \frac{\tau}{C_{A0}} = \int_0^{X_A} \frac{dX_A}{-r_A}$$

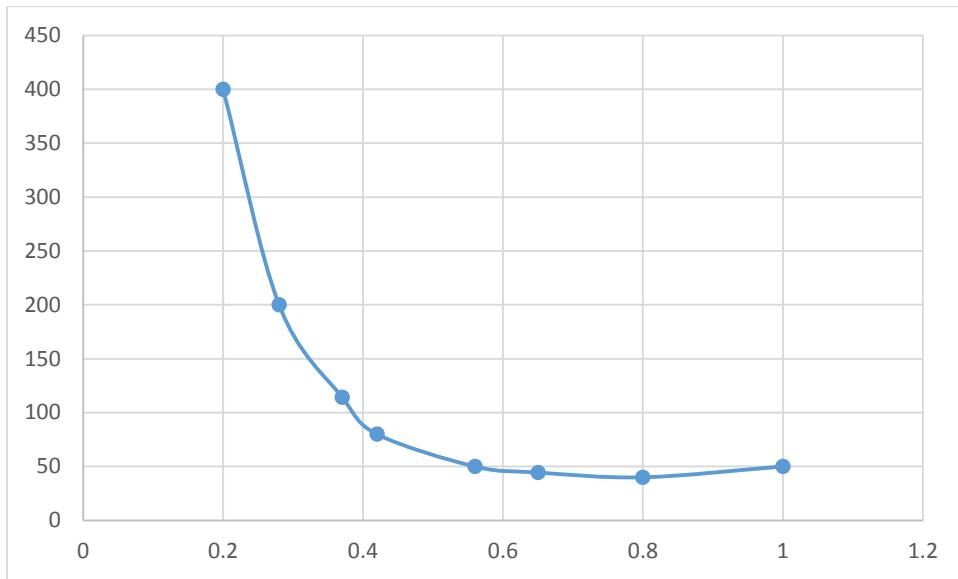
It can be modified as

$$\frac{V}{F_{A0}} = \tau = - \int_{C_{A0}}^{C_A} \frac{dC_A}{-r_A}$$

Hence, now from the equation, $\tau = \frac{C_{A0} - C_A}{-r_A}$ we can generate the following table

τ	C_{A0}	C_A	$-r_A$
50	2	1	0.02
16	1.2	0.8	0.025
60	2	0.65	0.0225
22	1	0.56	0.02
4.8	0.48	0.42	0.0125
72	1	0.37	0.00875
40	0.48	0.28	0.005
1122	0.48	0.2	0.0025

Hence, on plotting the graph of $1/(-r_A)$ vs C_A



So, for PFR we need to find the area under the curve.

Therefore, Area = $\tau = 70$ s

So, putting in the performance equation we get,

$$V = (70)0.8/0.8 = 70 \text{ ltr}$$

(2) The reactor is MFR

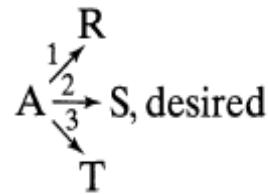
For MFR, we need to find the rectangular area which is

$$\text{Area} = \tau = 320 \text{ s}$$

$$V = 320(0.8)/ (0.8) = 320$$

Therefore, volume required = 320 ltr

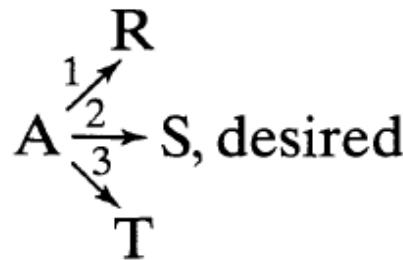
7.1. For a given feed stream having C_{A0} should we use a PFR or a MFR and should we use a high or low or some intermediate conversion level for the exit stream if we wish to maximize $\varphi(S/A)$? The reaction system is



where n_1 , n_2 , and n_3 are the reaction orders of reactions 1, 2, and 3.

- (a) $n_1 = 1, n_2 = 2, n_3 = 3$
- (b) $n_1 = 2, n_2 = 3, n_3 = 1$
- (c) $n_1 = 3, n_2 = 1, n_3 = 2$

Solution:-



Case 1:- $n_1=1, n_2=2, n_3=3$

Use MFR with some particular concentration of A.

Case 2) $n_1=2, n_2=3, n_3=1$

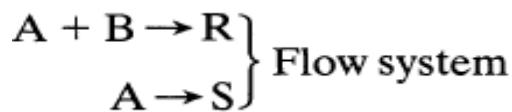
Use PFR with low X_A

Case 3) $n_1=3, n_2=1, n_3=2$

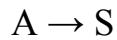
Use MFR with high X_A

7.2

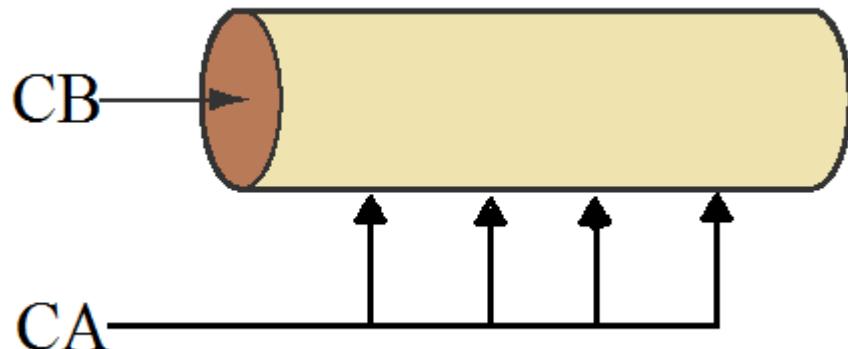
Using separate feeds of A and B sketch the contacting pattern and reactor conditions which would best promote the formation of product R for the following systems of elementary reactions.



Solution:-

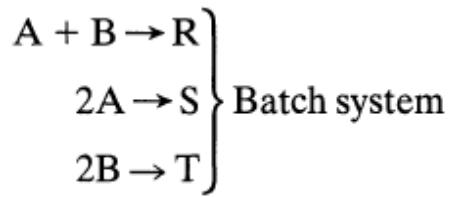


Low C_A , high C_B

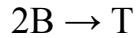


7.3

Using separate feeds of A and B sketch the contacting pattern and reactor conditions which would best promote the formation of product R for the following systems of elementary reactions.



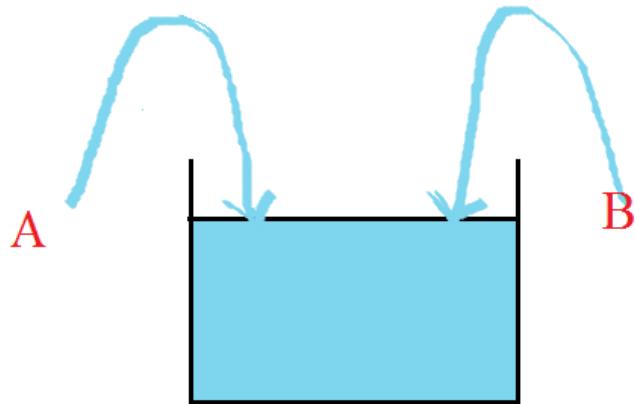
Solution:-



Use low C_A and low C_B

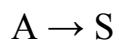
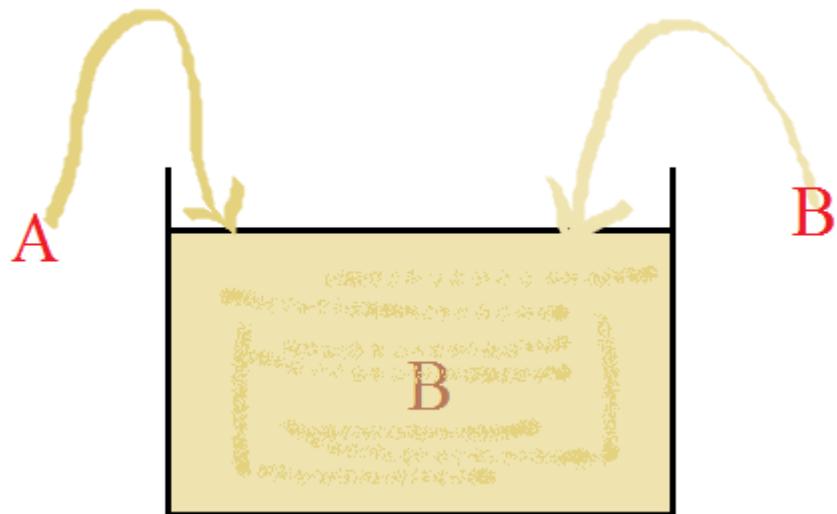
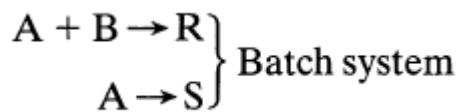
Slowly add A & B

Don't add excess of A or B.



7.4

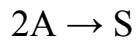
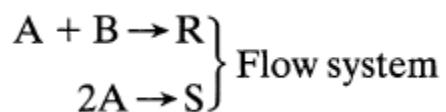
Using separate feeds of A and B sketch the contacting pattern and reactor conditions which would best promote the formation of product R for the following systems of elementary reactions.



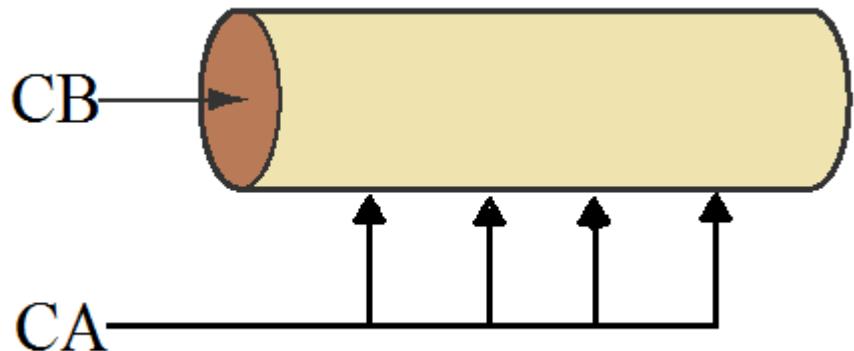
First add B completely then add A slowly & steadily.

7.5

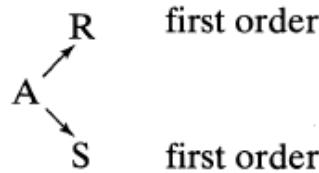
Using separate feeds of A and B sketch the contacting pattern and reactor conditions which would best promote the formation of product R for the following systems of elementary reactions.



Keep C_A low, C_B high.

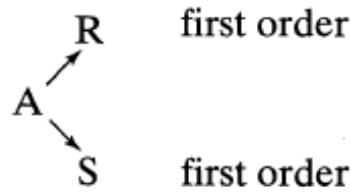


7.6. Substance A in a liquid reacts to produce R and S as follows:



A feed ($C_{A0} = 1$, $C_{R0} = 0$, $C_{S0} = 0$) enters two mixed flow reactors in series, ($\tau_1 = 2.5$ min, $\tau_2 = 5$ min). Knowing the composition in the first reactor ($C_{A1} = 0.4$, $C_{R1} = 0.4$, $C_{S1} = 0.2$), find the composition leaving the second reactor.

Solution:-



FOR TANK-1

$$\psi_{R/A} = \frac{0.4 - 0}{1 - 0.4} = \frac{0.4}{0.6} = 0.67$$

$$\tau_1 = \frac{C_R - C_{R0}}{k_1 * C_A}$$

$$2.5 = \frac{0.4}{k_1 * 0.4}$$

$$K_1 = 0.4$$

$$\tau_1 = \frac{C_S - C_{S0}}{k_2 * C_A}$$

$$2.5 = \frac{0.2}{k_1 * 0.4}$$

$$K_2 = 0.2$$

For tank – 2

$$\tau_2 = \frac{C_{A1} - C_{A2}}{-r_A}$$

$$5 = \frac{0.4 - C_{A2}}{(K_1 + K_2)C_{A2}}$$

$$3 C_{A2} = 0.4 - C_{A2}$$

$$C_{A2} = 0.1 \frac{mol}{hr}$$

$$C_{R2} = C_{R1} + \psi_{\frac{R}{A}}(C_{A1} - C_{A2})$$

$$= 0.4 + \frac{K_1}{K_1 + K_2}(0.4 - 0.1)$$

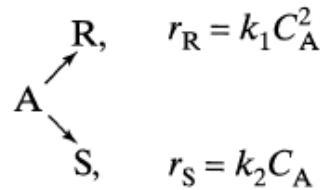
$$= 0.6 mol/hr$$

$$C_{S2} = C_{S1} + \varphi_{\frac{S}{A}}(C_{A1} - C_{A2})$$

$$= 0.2 + \frac{K_1}{K_1 + K_2}(0.3)$$

$$= 0.3 \text{ mol/hr}$$

7.7. Substance A in the liquid phase produces R and S by the following reactions:



The feed ($C_{A0} = 1.0$, $C_{R0} = 0$, $C_{S0} = 0.3$) enters two mixed flow reactors in series ($\tau_1 = 2.5$ min, $\tau_2 = 10$ min). Knowing the composition in the first reactor ($C_{A1} = 0.4$, $C_{R1} = 0.2$, $C_{S1} = 0.7$), find the composition leaving the second reactor.

Solution:-

FOR TANK-1

$$\psi_{\frac{R}{A}} = \frac{N_{R1} - N_{R0}}{N_{A0} - N_{A1}}$$

$$= \frac{0.2 - 0}{1 - 0.7}$$

$$= 0.2857$$

$$\tau = \frac{C_{A0} * X_A}{-r_R}$$

$$= \frac{C_R - C_{R0}}{k_1 * C_A^2}$$

$$2.5 = \frac{0.2 - 0}{K_1 * 0.4^2}$$

$$K_1 = 0.5$$

$$\tau = \frac{C_S - C_{S0}}{k_2 * C_A}$$

$$2.5 = \frac{0.7 - 0.3}{K_2 * 0.4}$$

$$K_2 = 0.4$$

FOR TANK -2

$$\tau_2 = \frac{C_{A1} - C_{A2}}{-r_A}$$

$$10 = \frac{0.4 - C_{A2}}{K_1 C_{A2}^2 + K_2 C_{A2}}$$

$$5C_{A2}^2 + 4C_{A2} = 0.4 - C_{A2}$$

$$5C_{A2}^2 + 5C_{A2} - 0.4 = 0$$

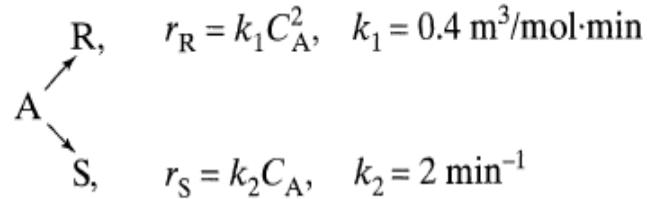
$$C_{A2} = 0.074$$

$$\begin{aligned} C_{R2} &= C_{R1} + \psi_{\frac{R}{A}} (C_{A1} - C_{A2}) \\ &= 0.2 + \frac{K_1 C_{A2}}{K_1 C_{A2}} (0.4 - 0.074) \\ &= 0.2 + \frac{0.5 * 0.074 (0.0326)}{0.5 * 0.074 + 0.4} = 0.227 \end{aligned}$$

$$\begin{aligned} C_{S2} &= C_{S1} + \psi_{\frac{S}{A}} (C_{A1} - C_{A2}) \\ &= 0.7 + \frac{K_2}{K_1 C_{A2} + K_2} (0.4 - 0.074) \\ C_{S2} &= 0.998 \end{aligned}$$

7.8. Find C_R , and C_S and τ for $X_A = 0.9$ in a mixed flow reactor.

Liquid reactant A decomposes as follows:



A feed of aqueous A ($C_{A0} = 40 \text{ mol/m}^3$) enters a reactor, decomposes, and a mixture of A, R, and S leaves.

Solution:---

$$C_R = C_{R0} + \psi_{R/A} (C_{A0} - C_A)$$

$$= 0 + \frac{0.4*4}{0.4*4+2} (40 - 4)$$

$$= 1.6*36/3.6$$

$$= 16 \text{ mol/L}$$

$$C_S = 36 - 16 = 20 \text{ mol/L}$$

$$\tau = \frac{C_{A0} - C_A}{-r_A}$$

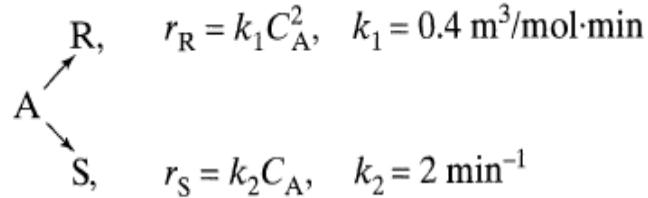
$$\tau = \frac{40 - 4}{0.4(4)^2 + 2(4)}$$

$$\tau = 36/14.4$$

$$\tau = 2.5 \text{ sec}$$

7.9. Find C_R , and C_S and τ for $X_A = 0.9$ in a plug flow reactor.

Liquid reactant A decomposes as follows:



A feed of aqueous A ($C_{A0} = 40 \text{ mol/m}^3$) enters a reactor, decomposes, and a mixture of A, R, and S leaves.

Solution::---

$$\frac{dC_R}{dt} = r_R = k_1 C_A^2 = 0.4 C_A^2$$

$$\frac{dC_S}{dt} = r_S = k_2 C_A = 0.4 C_A$$

$$\psi_{R/A} = \frac{r_R}{-r_A}$$

$$= \frac{K_1 C_A^2}{K_1 C_A^2 + K_2 C_A}$$

$$= \frac{0.4 C_A}{0.4 C_A + 2}$$

$$C_R = \int_{C_A}^{C_{A0}} \psi \, dC_A$$

$$= \int_4^{40} \left(\frac{0.4 C_A}{0.4 C_A + 2} \right) dC_A$$

$$= \int\limits_4^{40} \left(1 - \frac{2}{0.4C_A + 2}\right) dC_A$$

$$= (40-4) - [\frac{2}{0.4}\ln(0.4C_A+2)]_4^{40}$$

$$= 36 - 5\ln\frac{18}{3.6}$$

$$C_R=27.953$$

$$C_S=36-C_R=8.047$$

$$\tau = \int\limits_4^{40} \frac{dC_A}{-r_A}$$

$$= \int\limits_4^{40} \frac{dC_A}{4{C_A}^2 + 2C_A}$$

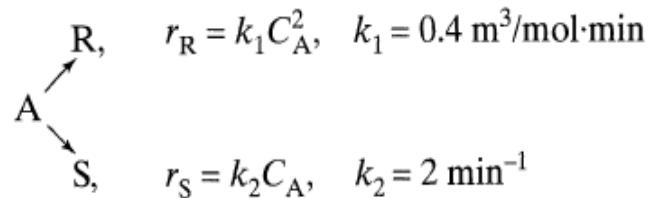
$$= 2.5 \int\limits_4^{40} \frac{dC_A}{{C_A}^2 + 5C_A + (\frac{5}{2})^2 - (\frac{5}{2})^2}$$

$$= 2.5 \int\limits_4^{40} \frac{dC_A}{(C_A + \frac{\pi}{2})^2 - \left(\frac{5}{2}\right)^2}$$

$$= 0.346\;\mathrm{sec}$$

- 7.10.** Find the operating condition (X_A , τ , and C_S) which maximizes C_S in a mixed flow reactor.

Liquid reactant A decomposes as follows:



A feed of aqueous A ($C_{A0} = 40 \text{ mol/m}^3$) enters a reactor, decomposes, and a mixture of A, R, and S leaves.

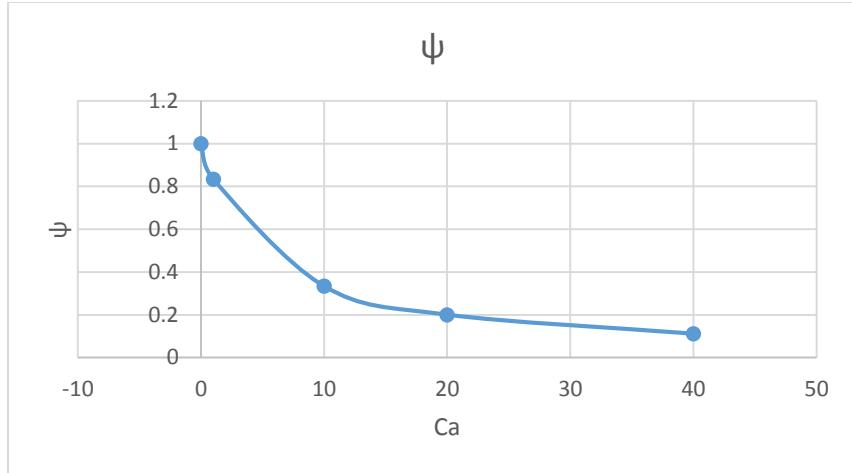
Solution:---

$$r_R = 0.4 * C_A^2$$

$$r_S = 2 * C_A$$

$$\psi_{S/A} = \frac{dC_S}{-dC_A} = \frac{2C_A}{2C_A + 0.4C_A^2} = \frac{1}{1 + 0.2C_A} = \frac{10}{10 + 2C_A}$$

Ca	ψ
0	1
1	0.833333
10	0.333333
20	0.2
40	0.111111



$$A = \left(\frac{10}{10 + 2c_{Af}} \right) (40 - c_{Af}) = \frac{400 - 10c_{Af}}{10 + 2c_{Af}}$$

$$\frac{d_A}{dC_A} = 10 + 2C_{Af}(-10) - (400 - 10C_{Af})(2)$$

$$0 = -100 - 20C_{Af} - 800 + 20C_{Af}$$

$$-100 - 20C_{Af} = 800 - 20C_{Af}$$

$$C_{Af} = 0$$

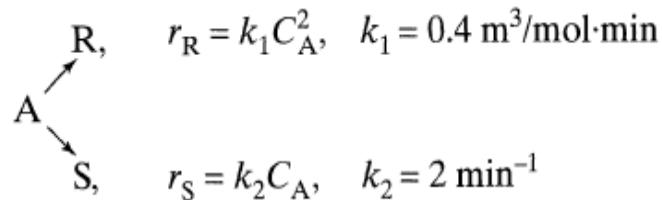
$$XA = 100\%$$

$$\frac{\tau}{40} = \frac{1}{2(0) + 0.4(0)}$$

$$\tau = \infty$$

- 7.11. Find the operating condition (X_A , τ , and C_R) which maximizes C_R in a mixed flow reactor.

Liquid reactant A decomposes as follows:



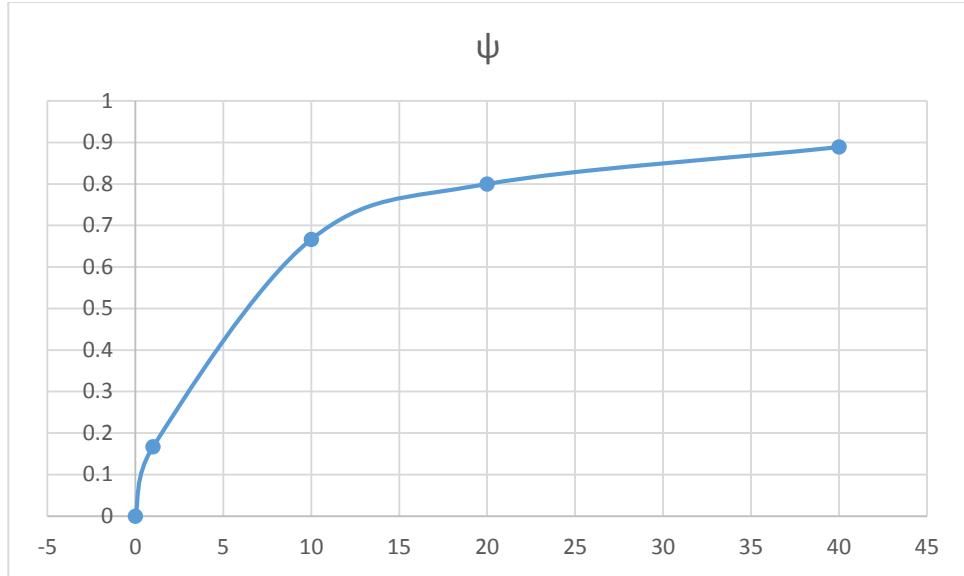
A feed of aqueous A ($C_{A0} = 40 \text{ mol/m}^3$) enters a reactor, decomposes, and a mixture of A, R, and S leaves.

SOLUTION:---

$$\psi_{R/A} = \frac{K_1 C_A^2}{K_1 C_A^2 + K_2 C_A} = \frac{0.4 C_A}{0.4 C_A + 2} = \frac{C_A}{C_A + 5}$$

$$\frac{d\psi_{R/A}}{dC_A} = (C_A + 5) * 1 - C_A * 1$$

Ca	ψ
0	0
1	0.166667
10	0.666667
20	0.8
40	0.888889



$$A = \frac{40C_{Af} - C_{Af}^2}{C_{Af} + 5}$$

$$\frac{dA}{dC_{Af}} = (C_{Af} + 5)(40 - 2C_{Af}) - \left(\frac{40C_{Af} - C_{Af}^2}{(C_{Af} + 5)^2}\right)$$

$$40C_{Af} - 2C_{Af}^2 + 200 - 10C_{Af} - 40C_{Af} + C_{Af}^2 = 0$$

$$C_{Af}^2 + 10C_{Af} - 200 = 0$$

$$C_{Af} = \frac{-10 + 30}{2} = 10$$

$$XA = 1 - \left(\frac{10}{40}\right)$$

$$\frac{\tau}{40} = \frac{0.75}{0.4C_A^2 + 2C_A}$$

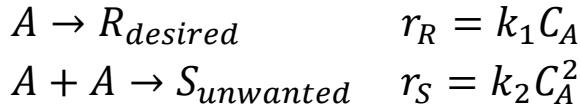
$$\tau = \frac{30}{0.4 * (10)^2 + 2 * (10)}$$

$$\tau = \frac{30}{40+20} = 0.5$$

CRE-I SPECIAL ASSIGNMENT

QUESTION: [7.12.]

Reactant A in a liquid either isomerizes or dimerizes as follows:



(a) Write $\varphi \left(\frac{R}{A} \right)$ and $\varphi \left[\frac{R}{(R+S)} \right]$.

With a feed stream of concentration C_{A0} , find $C_{R,\max}$ which can be formed:

- (b) In a plug flow reactor.
(c) In a mixed flow reactor.

A quantity of A of initial concentration $C_{A0} = 1$ mol/liter is dumped into a batch reactor and is reacted to completion.

(d) If $C_s = 0.18$ mol/liter in the resultant mixture, what does this tell of the kinetics of the reaction?

ANSWER:

$$(a) \varphi \left[\frac{R}{(R+S)} \right] = \frac{r_R}{r_R + r_S} = \frac{k_1 C_A}{k_1 C_A + k_2 C_A^2}$$

$$\varphi \left(\frac{R}{A} \right) = \frac{r_R}{-r_A} = \frac{k_1 C_A}{k_1 C_A + 2k_2 C_A^2}$$

(b)

We get $C_{R,\max}$ when we have $C_{AF} = 0$.

$$\text{So, } C_{R,\max} = \int_0^{C_{A0}} \varphi dC_A = \int_0^{C_{A0}} \frac{1}{1 + \frac{2k_2}{k_1} C_A} dC_A = \frac{k_1}{2k_2} \left\{ \ln \left(1 + \frac{2k_2}{k_1} C_A \right) \right\} \Big|_0^{C_{A0}}$$

$$C_{R,\max} = \frac{k_1}{2k_2} \left\{ \ln \left(1 + \frac{2k_2}{k_1} C_{A0} \right) - \ln 1 \right\} = \frac{k_1}{2k_2} \left\{ \ln \left(1 + \frac{2k_2}{k_1} C_{A0} \right) \right\}$$

(c)

$$C_{Rm} = \varphi_f (C_{A0} - C_A)$$

$$C_{Rm, \max} = 1(C_{A0} - 0) = C_{A0}$$

(d)

$$C_S = 0.18 \text{ gives } C_R = C_{A0} - C_A - C_S = 1 - 0 - 0.18 = 0.82$$

Also,

C_R can be calculated from the following equation:

$$C_{R, \max} = \frac{k_1}{2k_2} \left\{ \ln \left(1 + \frac{2k_2}{k_1} C_{A0} \right) \right\}$$

Let's say, $K = k_1/k_2$ and assume $K = 4$ and $K = 5$.

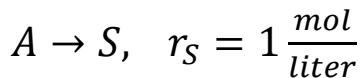
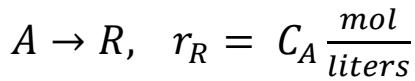
So, C_R calculated from the above equation is 0.84 and 0.81 respectively.

K	4	5
C_R calculated	0.84	0.81

Hence, for different values of k_1 and k_2 , $C_{R, \max}$ is different. It may be more or less than the C_R value.

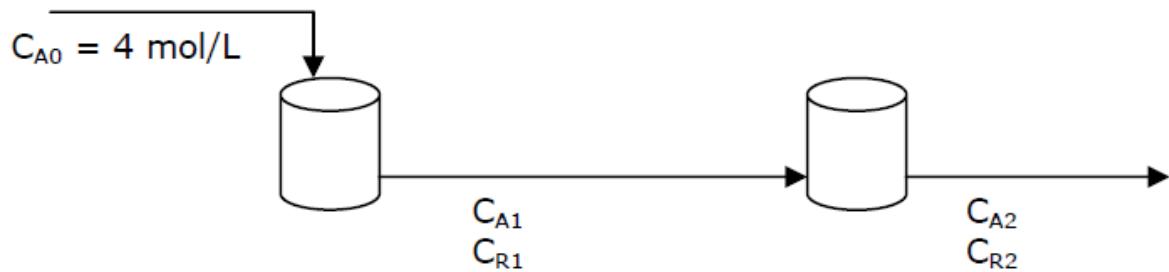
QUESTION: [7.13.]

In a reactive environment, chemical A decomposes as follows:



For a feed stream $C_{A0} = 4 \frac{\text{mol}}{\text{liters}}$ what size ratio of two mixed flow reactors will maximize the production rate of R? Also give the composition of A and R leaving these two reactors.

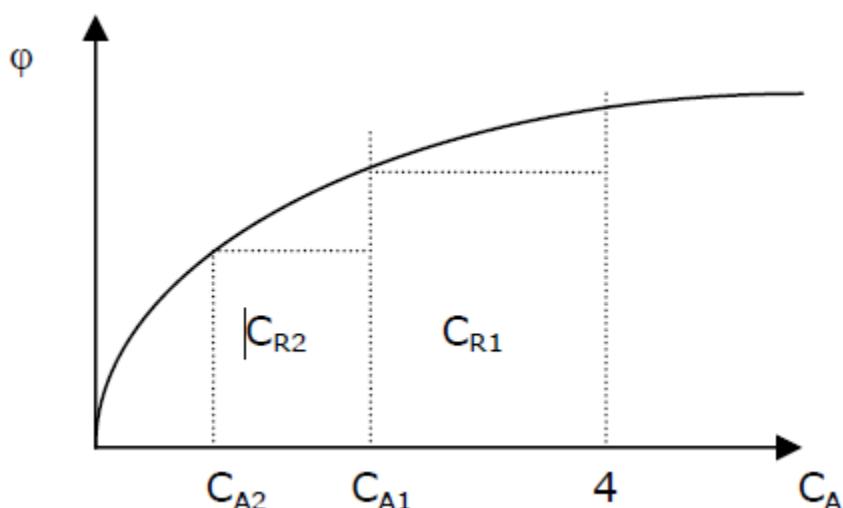
ANSWER:



$$\varphi = \frac{r_r}{-r_A} = \frac{C_A}{1 + C_A}$$

$$C_A \rightarrow 0, \quad \varphi \rightarrow 0 \quad \text{and} \quad C_A \rightarrow \infty, \quad \varphi \rightarrow 1$$

$$C_R = \varphi \Delta C_A = \left(\frac{C_{A1}}{1 + C_{A1}} \right) (4 - C_{A1}) + = \left(\frac{C_{A2}}{1 + C_{A2}} \right) (C_{A1} - C_{A2})$$



C_{A1} and C_{A2} are not known, but there is a fixed C_{A1} and C_{A2} value that maximizes C_R and is what makes $dC_R/dC_{A1} = 0$

$$\begin{aligned} \frac{dC_R}{dC_{A1}} = 0 = & \frac{(1 + C_{A1})(4 - 2C_{A1}) - (4C_{A1} - C_{A1}^2)(1)}{(1 + C_{A1})^2} \\ & + \frac{C_{A2}}{1 + C_{A2}}(1) \end{aligned}$$

So,

$$\frac{4 - 2C_{A1} - C_{A1}^2}{(1 + C_{A1})^2} = -\frac{C_{A2}}{1 + C_{A2}}$$

If $C_{A2} = 0.5 \text{ mol}$,

$$\frac{4 - 2C_{A1} - C_{A1}^2}{(1 + C_{A1})^2} = -\frac{0.5}{1 + 0.5}$$

$$13 - 4C_{A1} - 2C_{A1}^2 = 0$$

$$C_{A1} = \frac{4 \pm \sqrt{4^2 - 4(13)(-2)}}{2(-2)} = 1.7386 \frac{\text{mol}}{\text{liter}}$$

$$\begin{aligned} C_{R2} &= \frac{1.7386}{1 + 1.7386} (4 - 1.7386) + \frac{0.5}{1 + 0.5} (1.7386 - 0.5) \\ &= 1.8485 \end{aligned}$$

QUESTION:

Consider the parallel decomposition of A of different orders as follows:

$$A \rightarrow R, \quad r_R = 1$$

$$A \rightarrow S, \quad r_S = 2C_A$$

$$A \rightarrow T, \quad r_T = C_A^2$$

Determine the maximum concentration of desired product obtainable in (a) plug flow, (b) mixed flow.

[7.14.]: R is the desired product and $C_{A0} = 2$.

ANS:

$$\varphi_R = \frac{1}{1 + 2C_A + C_A^2}$$

(a)

$$\begin{aligned} C_{R,max} &= \int_0^2 \frac{dC_A}{1 + 2C_A + C_A^2} = \int_0^2 \frac{dC_A}{(C_A + 1)^2} = \left(\frac{(C_A + 1)^{-1}}{-1} \right)_0^2 \\ &= -\frac{1}{1+2} + \frac{1}{1} = \frac{2}{3} \end{aligned}$$

(b)

$$\varphi_R = \frac{1}{1 + 2C_A + C_A^2}$$

When, $C_A = 0$; $C_R = C_{R,max}$

So, $C_{Rm, max} = \varphi_{CA=0} (2 - 0) = 1(2) = 2 \text{ mol/liter}$

[7.15.]: S is the desired product and $C_{A0} = 4$.

ANS:

$$\varphi_R = \frac{2C_A}{1 + 2C_A + C_A^2} =$$

(a)

When, $C_A = 0$; $C_S = C_{SP, \ max}$

$$C_{SP, \ max} = \int_0^4 \frac{dC_A}{\frac{1}{2C_A} + 1 + \frac{C_A}{2}} = 2 \int_0^4 \frac{C_A dC_A}{(C_A + 1)^2}$$

$$\int \frac{xdx}{(a + bx)^2} = \frac{1}{b^2} \left[\ln(a + bx) + \frac{a}{a + bx} \right]$$

So,

$$C_{SP, \ max} = 2 \left\{ \frac{1}{1} \left[\ln(1 + C_A) + \frac{1}{1 + C_A} \right] \right\}_0^4$$

$$C_{SP, \ max} = 2 \left\{ \frac{1}{1} \left[\ln(1 + 4) + \frac{1}{5} - \ln(1 + 0) - 1 \right] \right\} = 1.6188 \frac{mol}{liter}$$

(b)

$$C_{SP, \ max} = \varphi_{C_{Af}} (C_{A0} - C_{Af})$$

$$C_{Sm} = \frac{2C_A}{2C_A + 1 + C_A^2} (4 - C_A) = 2 \left\{ \frac{C_A (4 - C_A)}{2C_A + 1 + C_A^2} \right\}$$

$$\begin{aligned} & \frac{dC_{Sm}}{dC_A} \\ &= 2 \left\{ \frac{(2C_A + 1 + C_A^2)[C_A(-1) + 4 - C_A] - (4C_A - C_A^2)(2 + 2C_A)}{(2C_A + 1 + C_A^2)^2} \right\} \\ &= 0 \end{aligned}$$

So,

$$2\{(2C_A + 1 + C_A^2)(2 - C_A) - (4C_A - C_A^2)(1 + C_A)\} = 0$$

$$3C_A^2 + C_A - 2 = 0$$

Therefore,

$$C_A = \frac{-1 \pm \sqrt{1 - 4(3)(-2)}}{2(3)} = \frac{2}{3}$$

$$C_{sm, \ max} = \frac{2 \left(\frac{2}{3} \right)}{2 \left(\frac{2}{3} \right) + \left(\frac{2}{3} \right)^2 + 1} \left(4 - \frac{2}{3} \right) = 1.6 \frac{mol}{liter}$$

[7.16.]: T is the desired product and $C_{A0} = 5$.

ANS:

$$\varphi_T = \frac{C_A^2}{1 + 2C_A + C_A^2} = \frac{1}{1 + \frac{2}{C_A} + \frac{1}{C_A^2}}$$

(a)

C_{TP} is maximum when $C_{Af} = 0$.

$$C_{TP, \ max} = \int_0^5 \frac{dC_A}{\frac{2}{C_A} + 1 + \frac{1}{C_A^2}} = \int_0^5 \frac{C_A^2 dC_A}{(C_A + 1)^2}$$

$$\int \frac{x^2 dx}{(a + bx)^2} = \frac{1}{b^3} \left[a + bx - 2a \ln(a + bx) - \frac{a^2}{a + bx} \right]$$

So,

$$\begin{aligned} C_{TP, \ max} &= \left\{ 1 + C_A - 2 \ln(1 + C_A) - \frac{1}{1 + C_A} \right\}_0^5 \\ &= 6 - 2 \ln 6 - \frac{1}{6} - [1 - 2 \ln 1 - 1] = 2.2498 \frac{mol}{liter} \end{aligned}$$

(b)

$$C_{Tm} = \frac{C_A^2}{1 + 2C_A + C_A^2} (5 - C_A)$$

So,

$$\begin{aligned} & \frac{dC_{Tm}}{dC_A} \\ &= \frac{(1 + 2C_A + C_A^2)[(5 - C_A)(2C_A) + C_A^2(-1)] - C_A^2(5 - C_A)(2C_A + 2)}{(1 + 2C_A + C_A^2)^2} \\ &= 0 \end{aligned}$$

So,

$$C_A\{(C_A + 1)^2[-C_A + 2(5 - C_A)] - C_A(5 - C_A)(2C_A + 2)\} = 0$$

$$(C_A + 1)\{(C_A + 1)(-C_A + 10 - 2C_A) - (5C_A - C_A^2)(2)\} = 0$$

$$(C_A + 1)(10 - 3C_A) - 2(5C_A - C_A^2) = 0$$

$$C_A^2 + 3C_A - 10 = 0$$

$$C_A = \frac{-3 \pm \sqrt{9 - 4(1)(-10)}}{2} = 2 \text{ mol/liter}$$

$$C_{Tm, \ max} = \frac{2^2}{2^2 + 2(2) + 1} = \frac{8}{9} = 0.89 \text{ mol/liter}$$

QUESTION:

Under ultraviolet radiation, reactant A of $C_{A0} = 10 \text{ kmol/m}^3$ in a process stream ($\vartheta = 1 \text{ m}^3/\text{min}$) decomposes as follows:

$$A \rightarrow R, \quad r_R = 16C_A^{0.5}$$

$$A \rightarrow S, \quad r_S = 12C_A$$

$$A \rightarrow T, \quad r_T = C_A^2$$

We wish to design a reactor setup for a specific duty. Sketch the scheme selected, and calculate the fraction of feed transformed into desired product as well as the volume of reactor needed.

[7.17.]: Product R is the desired material.

ANS:

The reaction of the desired product is the lowest order, so it is better to use a mixed reactor with high conversion.

$C_{Rm, \max}$ is obtained when $C_{Af} = 0$.

$$C_{Rm, \max} = \varphi(C_{A0} - C_{Af}) = 1(10 - 0) = 10 \text{ mol/liter}$$

$$\varphi_R = \frac{16C_A^{0.5}}{16C_A^{0.5} + 12C_A + C_A^2}$$

$$C_{Rm} = \varphi_R(C_{A0} - C_A)$$

$$\tau_m = \frac{C_{A0} - C_A}{16C_A^{0.5} + 12C_A + C_A^2}$$

$$V = \tau_m(\vartheta_0)$$

Select a high conversion and make the calculations for each of them.

X_A	C_A	τ	V	φ	C_R
0.98	0.2	1.0130	1.0130	0.7370	5.8960

0.99	0.1	1.5790	1.5790	0.8070	7.9894
0.995	0.05	2.3803	2.3803	0.8558	8.5159

As we can see above, going from $X_A = 0.99$ to 0.995 , $\Delta C_R = 0.5265$ mol / L and to achieve this, $\Delta V = 0.8013$ m³ (almost 1 m³) is required, then $X_A = 0.995$ could be selected.

[7.18.]: Product S is the desired material.

ANS:

The desired reaction is the middle order, so there corresponds an intermediate concentration, which makes maximum performance.

$$\varphi_S = \frac{12C_A}{16C_A^{0.5} + 12C_A + C_A^2}$$

(A)

If you cannot recirculate unreacted A, then use a mixed reactor until the concentration giving $\varphi_{\text{máx}}$ and thereafter a piston.

(B)

If the A can be recirculated unreacted economically, then use a mixed reactor with concentration giving $\varphi_{\text{máx}}$.

(A)

$$\frac{d\varphi_S}{dC_A} = \frac{12(16C_A^{0.5} + 12C_A + C_A^2) - 12C_A(12 + 8C_A^{-0.5} + 2C_A)}{(16C_A^{0.5} + 12C_A + C_A^2)^2} = 0$$

So,

$$18C_A^{0.5} - C_A^2 = 0$$

$$C_A = 4 \frac{\text{kmol}}{\text{m}^3}$$

$$C_{Sm} = 0.5(10 - 4) = 3 \frac{\text{kmol}}{\text{m}^3}$$

$$\tau_m = \frac{10 - 4}{16(4)^{0.5} + 12(4) + 4^2} = 0.0625 \text{ m}^3 = 62.5 \text{ liter}$$

C_A	4	3	2	1	0.6	0.4	0.11	0.02
φ_S	0.5	0.4951	0.4740	0.4138	0.3608	0.2501	0.1988	0.0959

Suppose, $X_A = 0.998$, implies $C_A = 0.02$

$$\begin{aligned}
 C_{SP} &= \int_{0.02}^4 \varphi dC_A = \frac{\Delta C_A}{2} \left[\varphi_0 + \varphi_f + 2 \sum_{i=1}^{f-1} \varphi_i \right] \\
 C_{SP} &= \frac{1}{2} [0.4138 + 0.5 + 2(0.4740 + 0.4951)] \\
 &\quad + \frac{0.4}{2} [0.4138 + 0.2501 + 2(0.3608)] \\
 &\quad + \frac{0.09}{2} [0.2501 + 0.0959 + 2(0.1988)]
 \end{aligned}$$

$$C_{SP} = 1.7367 \text{ mol/m}^3$$

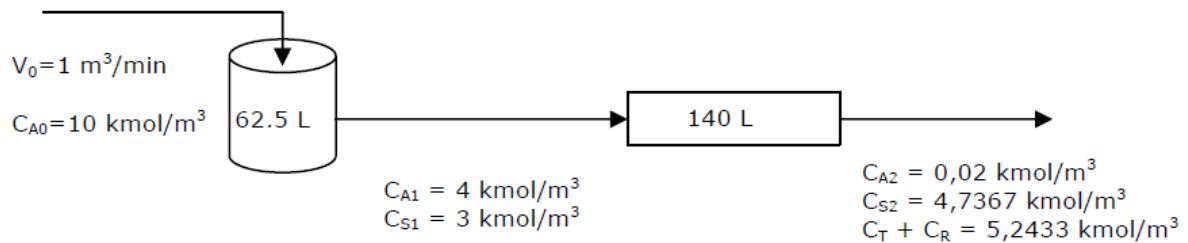
$$C_{S, \text{ total}} = 3 + 1.7367 = 4.7367 \text{ mol/m}^3$$

$$\tau_P = \int_{C_{A0}}^{C_{Af}} \frac{dC_A}{-r_A} \approx \frac{\Delta C_A}{2} \left\{ (-r_A)_0^{-1} + (-r_A)_f^{-1} + 2 \sum_{i=1}^{f-1} (-r_A)_i^{-1} \right\}$$

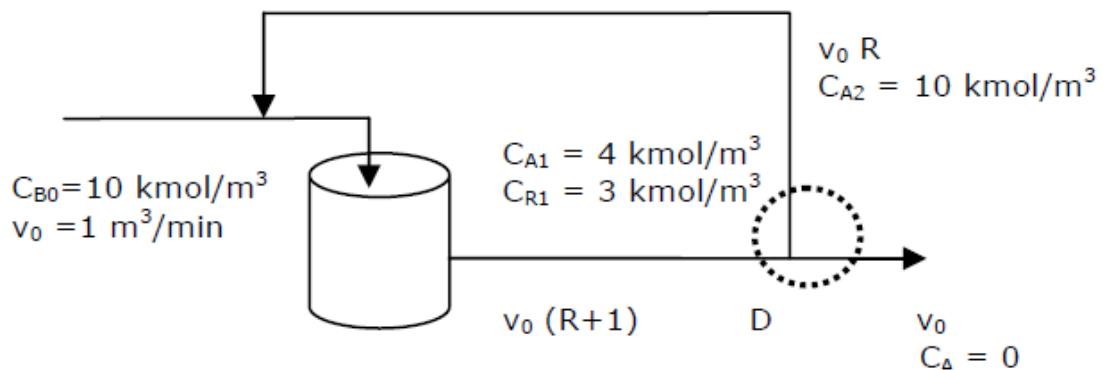
C_A	4	3	2	1	0.6	0.2	0.11	0.02
$-r_A$	96	72.71	50.62	29	19.95	9.60	6.64	2.50

So,

$$\begin{aligned}
\tau_P = & \frac{1}{2} \left[\frac{1}{29} + \frac{1}{96} + 2 \left(\frac{1}{72.71} + \frac{1}{50.62} \right) \right] \\
& + \frac{0.4}{2} \left[\frac{1}{29} + \frac{1}{9.60} + 2 \left(\frac{1}{19.95} \right) \right] \\
& + \frac{0.09}{2} \left[\frac{1}{9.6} + \frac{1}{2.5} + 2 \left(\frac{1}{6.64} \right) \right] = 0.1399 \text{ min}
\end{aligned}$$



(B)



At point D, balance the flow:

$$\vartheta_0(R+1)(4) = 0 + \vartheta_0 R(10) \text{ which gives } R = 2/3.$$

Now,

$$\frac{V_m}{\vartheta_0(R+1)} = \frac{10-4}{96} \text{ which gives } V_m = 0.104 \text{ m}^3 = 104 \text{ liters}$$

[7.19.]: Product T is the desired material.

ANS:

The reaction occurs where T is of the highest order. So we should use a flow reactor.

$$\varphi_s = \frac{C_A^2}{16C_A^{0.5} + 12C_A + C_A^2}$$

$$C_{TP} = \int_{C_{A0}}^{C_{Af}} \varphi dC_A \approx \frac{\Delta C_A}{2} \left[\varphi_0 + \varphi_f + 2 \sum_{i=1}^{f-1} \varphi_i \right]$$

$$\tau_P = \int_{C_{A0}}^{C_{Af}} \frac{dC_A}{-r_A} \approx \frac{\Delta C_A}{2} \left\{ (-r_A)_0^{-1} + (-r_A)_f^{-1} + 2 \sum_{i=1}^{f-1} (-r_A)_i^{-1} \right\}$$

Most T is formed when $C_{Af} = 0$, but that requires $\tau = \infty$, so let's choose $X_A = 0.998$.

C_A	φ	$-r_A$
0.02	0.0959	2.5031
0.11	0.1988	6.6387
0.2	0.2501	9.5954
0.6	0.3601	0.3608
1	0.0345	29.0000
2	0.0790	50.6274
3	0.1238	72.7128
4	0.1667	96.0000
5	0.2070	120.7771
6	0.2446	147.1918
7	0.2795	175.3320
8	0.3118	205.2548
9	0.3418	237.0000
10	0.3696	270.5964

So,

$$C_{TP} = \frac{1}{2} \{ [0.0345 + 0.3696 \\ + 2(0.079 + 0.1238 + \dots + 0.3118 + 0.3418)] \\ + (1 - 0.05)[0.0345 + 0.0598] \}$$

$$C_{TP} = 1.9729 \frac{kmol}{m^3}$$

$$\tau_P = \int_4^{10} \frac{dC_A}{-r_A} + \int_{0.02}^{4_f} \frac{dC_A}{-r_A}$$

$$\tau_P = \frac{1}{2} \{ [270.6^{-1} + 96^{-1} \\ + 2(120.8^{-1} + 147.2^{-1} + 175.3^{-1} + 205.3^{-1} \\ + 237^{-1}) + 0.1399] \} = 0.0369 + 0.1399$$

$$\tau_P = 0.1768 \text{ min}$$

This gives, $V = 177 \text{ litres}$

$$V_0 = 1 \text{ m}^3/\text{min}$$

$$C_{A0} = 10 \text{ kmol/m}^3 \rightarrow \boxed{177 \text{ L}} \rightarrow C_A = 0.02 \text{ kmol/m}^3$$

$$C_T = 1,9715 \text{ kmol/m}^3$$

$$C_R + C_S = 8,008 \text{ kmol/m}^3$$

SOLUTION 7.20

Since we know that fractional yield is defined by,

$$\Phi_m = \frac{CR}{CA_0 - CA} = \frac{CR}{100 - CA}$$

C _A	C _R	Φ _m
90	7	0.7
80	13	0.65
70	18	0.6
60	22	0.55
50	25	0.5
40	27	0.45
30	28	0.4
20	28	0.35
10	27	0.3
0	25	0.25

Given,

$$C_{A0} = 100$$

$$C_{Af} = 20$$

$$\begin{aligned}
 C_{Rp} &= \int_{CAf}^{CA0} \Phi_m dC_A \\
 &= \frac{\Delta CA}{2} (\Phi_0 + \Phi_f) \\
 &= \frac{(100 - 20)}{2} * (0.75 + 0.25) \\
 &= 40 \text{ mol/ lit}
 \end{aligned}$$

SOLUTION 7.21

$$C_{Rm} = \Phi_m (\Delta C_A) = 0.35 (100 - 20) = \mathbf{28 \text{ mol/lit}}$$

SOLUTION 7.22

$$y = mx + b$$

$$\Phi_m = 0.25 + (0.4/80) C_A$$

$$C_R = \Phi_m (100 - C_A)$$

$$= (0.25 + 0.005 C_A)(100 - C_A)$$

$$C_R = 25 + 0.25 C_A - 0.005 C_A^2$$

$$\frac{dC_R}{dC_A} = 0 \text{ (for maximum } C_R \text{)}$$

$$= 0.25 - 0.005(2)C_A$$

Therefore, **$C_A = 25 \text{ mol/lit}$**

Now putting this value in equation, we get

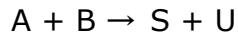
$$C_R = \mathbf{28.125 \text{ mol/lit}}$$

SOLUTION 7.23

Given,



$$r_R = 50 C_A$$



$$r_S = 100 C_B$$

Given that $C_{A0} + C_{B0} = 60 \text{ mol/m}^3$

And they both are equimolar, therefore $C_{A0} = 30 \text{ mol/m}^3 = C_{B0}$

Also given, $F_{A0} = F_{B0} = 300 \text{ mol/hr}$

and, $X_A = 0.9$

Now we know,

$$C_{A0} = \frac{F_{A0}}{v_0}$$

$$\text{or, } v_0 = \frac{F_{A0}}{C_{A0}} = \frac{300}{30} = 10 \text{ m}^3/\text{hr}$$

Now, rate of disappearance of A = rate of formation of R and S

Therefore, $-r_A = r_R + r_S$

$$= 50C_A + 100C_B$$

$$= 150C_A \rightarrow (1)$$

Now,

Performance equation curve for MFR is given by:

$$\frac{\tau}{C_{A0}} = \frac{X_A}{-r_A} = \frac{V}{F_{A0}}$$

Therefore,

$$\tau = \frac{X_A * C_{A0}}{150C_A} = \frac{X_A * C_{A0}}{150C_{A0}(1-X_A)} = \frac{0.9}{150 * 0.1} = 0.06 \text{ hr}$$

$$\text{Now, } \tau = \frac{V}{v_0}$$

or, $V = \text{Volume of reactor}$

$$= 0.06 * 10 = 0.6 \text{ m}^3 = \mathbf{600 \text{ litres.}}$$

SOLUTION 7.24

Performance equation for a PFR or Plug Flow Reactor is given by:

$$\frac{\tau}{CA_0} = \frac{V}{FA_0} = \frac{\int dXA}{-rA}$$

Here, we know

$$-r_A = 150C_A$$

$$= 150 * C_{A0} * (1 - X_A)$$

Therefore,

$$\frac{\tau}{CA_0} = \frac{\int dXA}{150 * CA_0 * (1 - XA)}$$

$$\text{or, } \tau = -\frac{\ln(1-XA)}{150}$$

$$= -\frac{\ln 0.1}{150} = 0.0153 \text{ hr}$$

Therefore, $V = \tau * (v_0)$

$$= 0.0153 * 10 = 0.15 \text{ m}^3 = \mathbf{150 \text{ litres.}}$$

SOLUTION 7.25

Given,

$$C_B \text{ everywhere} = 3 \text{ mol/m}^3$$

$$\Phi_{(R/A)} = \frac{50CA}{50CA + 100CB}$$

Therefore,

$$\begin{aligned} C_{RF} &= \int_{CAF}^{CA_0} \Phi(R/A) dCA \\ &= \int_3^{30} \frac{CA}{CA + 2CB} dCA \end{aligned}$$

$$\text{Given } C_B = 3$$

$$C_{RF} = 18.68$$

$$\begin{aligned} \text{Similarly, } C_{SF} &= \int_{CAF}^{CA_0} \Phi\left(\frac{S}{A}\right) dCA \\ &= \int_3^{30} \frac{2CB}{CA + 2CB} dCA \end{aligned}$$

$$\text{or, } C_{SF} = 8.32$$

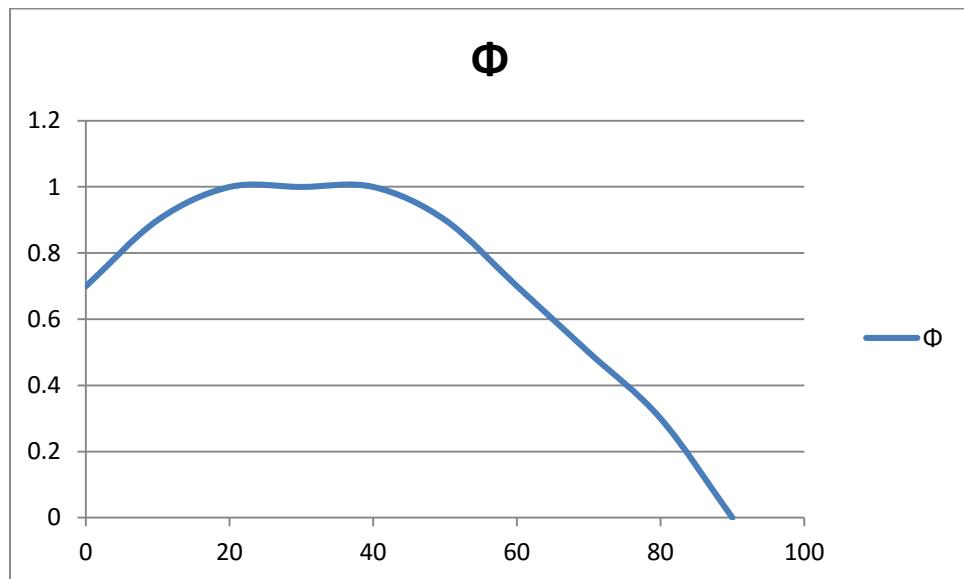
Finally,

$$\begin{aligned} V &= (F_{A0}/C_{A0}) \int_{CA_0}^{CAF} \frac{dCA}{-rA} = \frac{300}{30} * \int_{30}^{300} \frac{dCA}{50CA + 100(3)} \\ &= 0.2773 \text{ m}^3 = \mathbf{277.3 \text{ litres.}} \end{aligned}$$

SOLUTION 7.26

$$\Phi = \frac{dCR}{-dCA}$$

CA	CR	dCA	Φ
90	1	10	0
80	4	10	0.3
70	9	10	0.5
60	16	10	0.7
50	25	10	0.9
40	35	10	1
30	45	10	1
20	55	10	1
10	64	10	0.9
0	71	10	0.7



a) For MFR,

$$\begin{aligned} CR &= \varphi_{10}(C_{A0} - C_{Af}) \\ &= 0.9(100 - 10) \\ &= 0.9 * 90 \\ &= \mathbf{81 \text{ mol/lit}} \end{aligned}$$

b) For PFR,

$$\begin{aligned} \Phi_{\text{Nmixed}} &= \frac{\varphi_1(C_{A0} - C_{A1}) + \varphi_2(C_{A1} - C_{A2}) + \dots}{(C_{A0} - C_{AN})} \\ &= \frac{10}{100}(0.3 + 0.7 + 0.9 + 0.5 + 3 + 0.7 + 0.9) \\ &= 0.1 * 7 = 0.7 \end{aligned}$$

Therefore,

$$\begin{aligned} C_R &= \varphi(C_{A0} - C_{Af}) \\ &= 0.7 * (100 - 10) = 0.7 * 90 = \mathbf{63 \text{ mol/lit}} \end{aligned}$$

c) Given,

$$C_{A0} = 70$$

Therefore,

For MFR,

$$\begin{aligned} C_R &= \varphi_{10}(C_{A0} - C_{Af}) \\ &= 0.9(70 - 10) \\ &= 0.9 * 60 \\ &= \mathbf{54 \text{ mol/lit}} \end{aligned}$$

d) For PFR,

$$\begin{aligned} \Phi_{\text{Nmixed}} &= \frac{\varphi_1(C_{A0} - C_{A1}) + \varphi_2(C_{A1} - C_{A2}) + \dots}{(C_{A0} - C_{AN})} \\ &= \frac{10}{70}(0.7 + 0.9 + 3 + 0.7 + 0.9 + 0.5) \\ &= 0.142 * 6.7 = 0.9571 \end{aligned}$$

$$CR = \Phi_{\text{Nmixed}}(C_{A0} - C_{Af})$$

$$= 0.9571 * (70 - 10) = \mathbf{57.426 \text{ mol/lit}}$$

SOLUTION 7.28

Given,



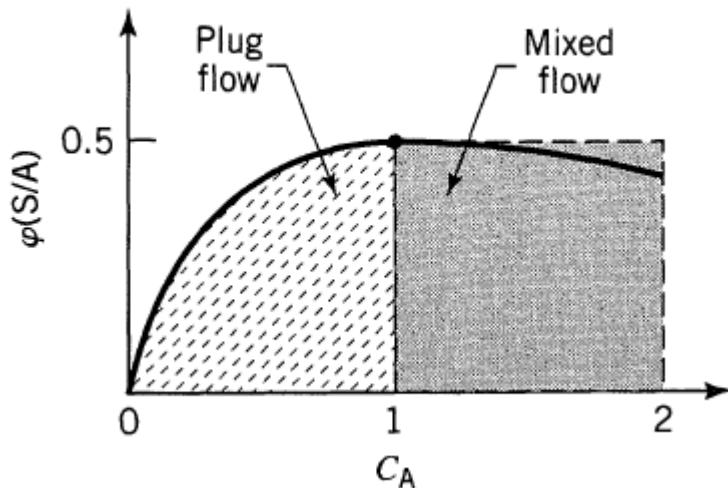
$$r_R = 1$$



$$r_S = 2C_A$$



$$r_T = C_A^2$$



Now, given flow rate of the reactor = 100 lit/sec

$$\text{i.e. } v_0 = 100$$

$$\text{Now } -r_A = r_R + r_S + r_T$$

$$= 1 + 2C_A + C_A^2$$

$$= (1 + C_A)^2$$

Now, taking the first case i.e. MFR from 2-1

Therefore, here, $C_{A0}=2$; $C_{Af}=1$

For MFR,

$$\tau_m = \frac{CA_0 - CA_f}{-rA} = \frac{2-1}{4} = 0.25$$

therefore, $V_1 = \tau * (v_0)$

$$= 0.25 * 100 = \mathbf{25 \text{ litres}}$$

Now taking the second case for PFR,

Here $C_{A1}=1$; $C_{A2}=0$

Therefore,

$$\tau_p = \int_1^0 \frac{dCA}{-rA} = \int_1^0 \frac{dCA}{(1+CA)^2}$$

$$= -\left[\frac{1}{1+CA} \right] = 1 - \frac{1}{2} = 0.5$$

Therefore,

We get, $V_2 = 0.5 * (100)$

$$= \mathbf{50 \text{ litres}}$$

Hence, total volume required = $V_1 + V_2$

$$= 25 + 50 = \mathbf{75 \text{ litres}}$$

SOLUTION 7.27

Let B be the no of british ships and F be the no of French Ships and if French wins

$$dF/dt = -KF \dots\dots (1)$$

$$dB/dt = -KB \dots\dots (2)$$

Div 1 by 2

$$dF/dB = F/B$$

Integrating we get,

$$\int_{F_0}^F F dF = \int_{B_0}^B B dB$$

$$F^2 - F_0^2 = B^2 - B_0^2$$

Since british is losing $B=0$

$$F^2 = 33^2 - 27^2 = 360$$

$$F = 19 \text{ ships(approx)}$$

$$8.1 \text{ (a)} \quad r_1 = k_1 C_A C_B^2$$

$$r_2 = k_2 C_R C_B$$

$$\text{(b)} \quad r_1 = k_1 C_A C_B$$

$$r_2 = k_2 C_R^2 C_B$$

$$\text{(c)} \quad r_1 = k_1 C_A C_B$$

$$r_2 = k_2 C_R^2 C_B$$

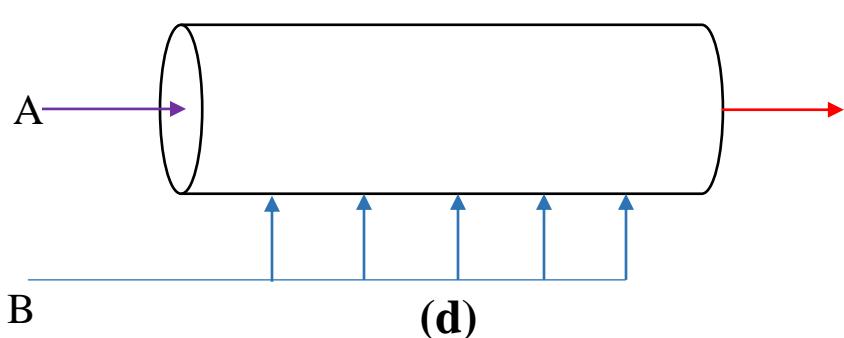
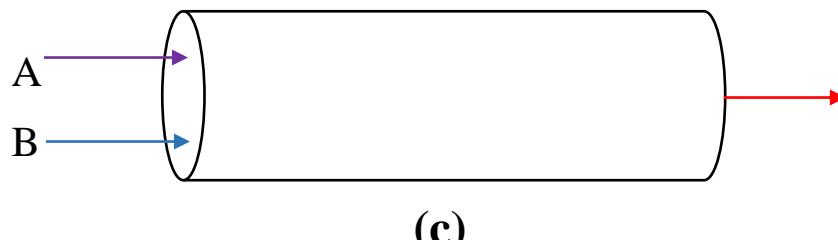
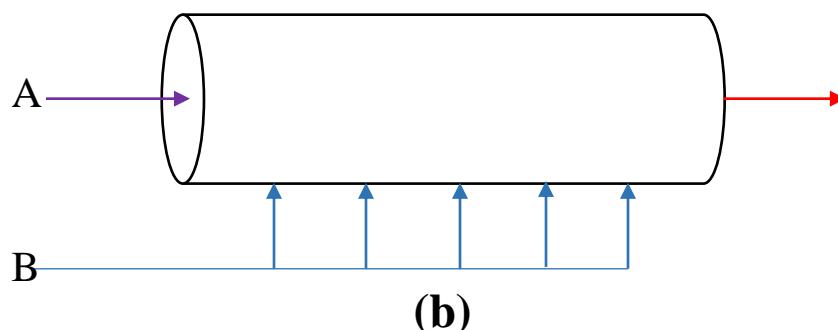
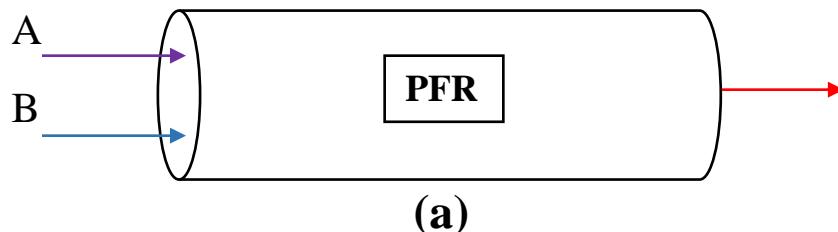
$$\text{(d)} \quad r_1 = k_1 C_A^2 C_B$$

$$r_2 = k_2 C_R C_B$$

Sketch the best contacting patterns for both continuous and non-continuous operations.

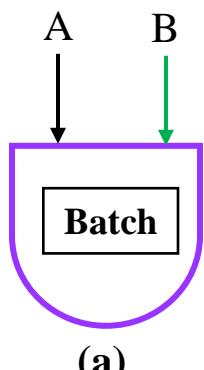
Solution 8.1

Continuous

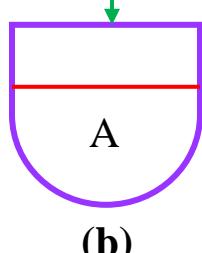


Non-Continuous

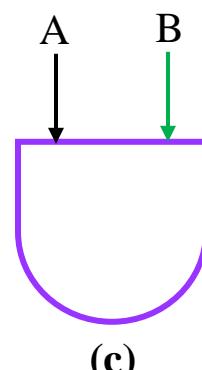
Instantaneously



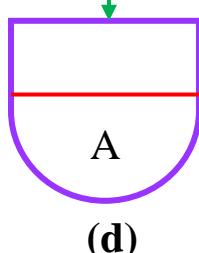
B
(Drop by drop)



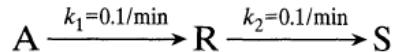
Instantaneously



B
(Slowly)



8.2. Under appropriate conditions A decomposes as follows:



R is to be produced from 1000 liter/hr of feed in which $C_{A0} = 1 \text{ mol/liter}$, $C_{R0} = C_{S0} = 0$.

- (a) What size of plug flow reactor will maximize the concentration of R, and what is that concentration in the effluent stream from this reactor?
- (b) What size of mixed flow reactor will maximize the concentration of R, and what is $C_{R,\text{max}}$ in the effluent stream from this reactor?

Solution 8.2

a) PFR

$$C_{A0} = 1 \text{ mol/L} \quad C_{R0} = C_{S0} = 0$$

$$\frac{C_{R,\text{max}}}{C_{A0}} = e^{-1}$$

$$C_{R,\text{max}} = \frac{1}{e} = 0.3679 \text{ mol/L}$$

$$t_{\text{max}} = k^{-1} = \frac{1}{0.1} = 10 \text{ min}$$

$$\text{residence time} = \frac{\text{volume of reactor}}{\text{volumetric flowrate}}$$

$$10 = \frac{\text{volume of reactor}}{\frac{1000}{60}}$$

$$\text{Volume of reactor} = 166.67 \text{ L}$$

b) MFR

$$\frac{C_{R,\text{max}}}{C_{A0}} = \frac{1}{\left[\left(\frac{k_2}{k_1}\right)^{1/2} + 1\right]^2}$$

$$C_{R,\text{max}} = \frac{1}{\left[\left(0.1/0.1\right)^{1/2} + 1\right]^2}$$

$$C_{R,\text{max}} = 0.25 \text{ mol/L}$$

$$t_{\text{max}} = \frac{1}{\sqrt{k_1 k_2}}$$

$$t_{\text{max}} = 10 \text{ min}$$

$$\text{Volume of reactor} = 166.67 \text{ L}$$

Here the volume to get maximum of R is 166.67 L but the maximum concentration of R in PFR is 0.3679 mol/L and in MFR 0.25 mol/L. So maximum concentration of R can be obtained from PFR.

Pure A ($C_{A0} = 100$) is fed to a mixed flow reactor, R and S are formed, and the following outlet concentrations are recorded. Find a kinetic scheme to fit this data.

8.3. Run	C_A	C_R	C_S
1	75	15	10
2	25	45	30

8.4. Run	C_A	C_R	C_S
1	50	$33\frac{1}{3}$	$16\frac{2}{3}$
2	25	30	45

8.5. Run	C_A	C_R	C_S	$t, \text{ min}$
1	50	40	10	5
2	20	40	40	20

Solution 8.3

Assuming parallel reaction A

$$C_{A0} = 100 \text{ mol/L} \quad C_{R0} = C_{S0} = 0$$

Run	C_A	C_R	C_S	$\frac{C_R}{C_S} = \frac{k_1}{k_2}$
1	75	15	10	1.5
2	25	45	30	1.5

$$\tau = \frac{C_R - C_{R0}}{k_1 C_A} \quad \dots (1)$$

$$\tau = \frac{C_S - C_{S0}}{k_2 C_A} \quad \dots (2)$$

Residence time will be equal from both equations

From eq. (1) and (2)

$$\frac{C_R}{k_1} = \frac{C_S}{k_2} \quad \& \quad \frac{C_R}{C_S} = \frac{k_1}{k_2}$$

For both the runs the value of $\frac{k_1}{k_2}$ is same which is 1.5

Therefore, the assumption of parallel reaction is correct.

Solution 8.4

$$C_{A0} = 100 \text{ mol/L} \quad C_{R0} = C_{S0} = 0$$

Assuming parallel reaction taking place

Run	C_A	C_R	C_S	$\frac{C_R}{C_S} = \frac{k_1}{k_2}$
1	75	15	10	1.976
2	25	45	30	0.666

$$\tau = \frac{C_R - C_{R0}}{k_1 C_A} \quad \dots (1)$$

$$\tau = \frac{C_S - C_{S0}}{k_2 C_A} \quad \dots (2)$$

Residence time will be equal from both equations

From eq. (1) and (2)

$$\frac{C_R}{k_1} = \frac{C_S}{k_2}$$

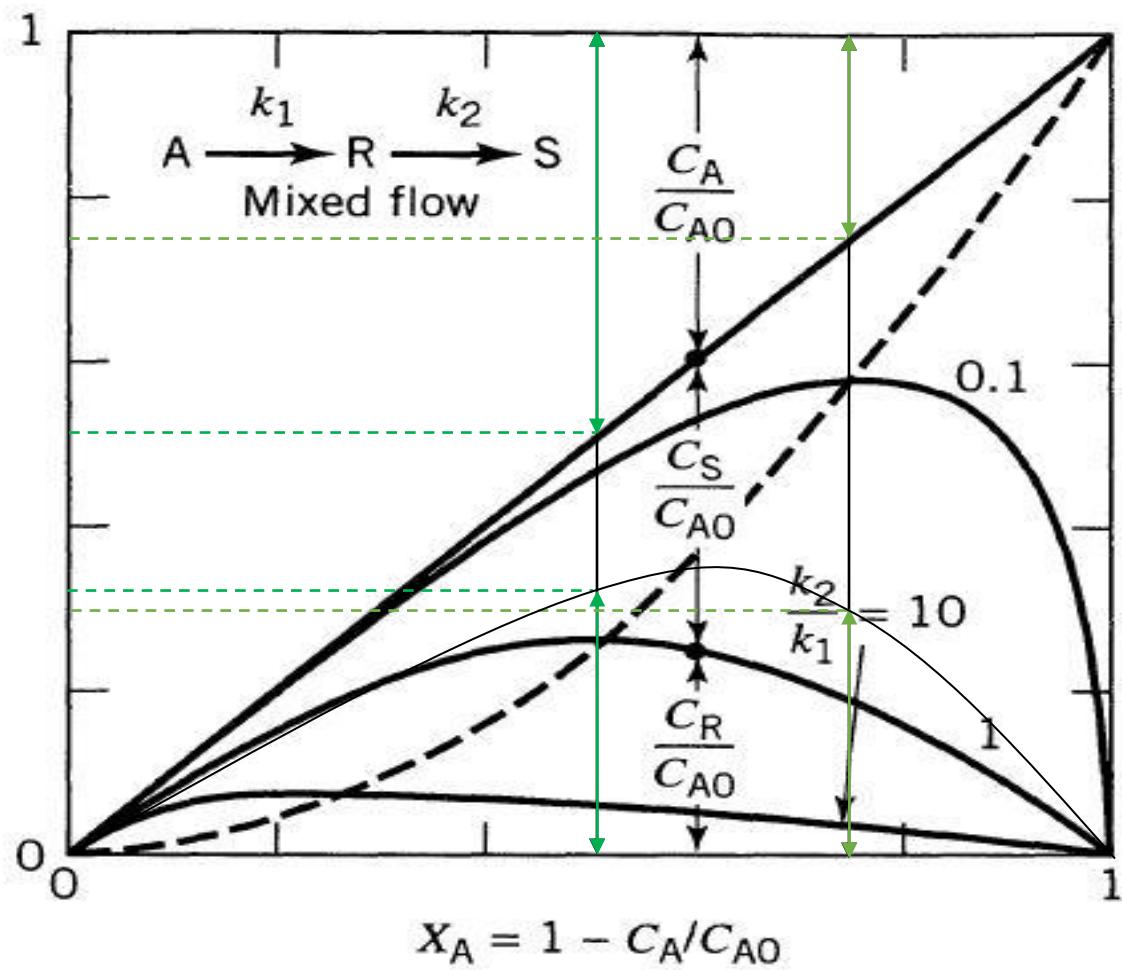
$$\frac{C_R}{C_S} = \frac{k_1}{k_2}$$

For both the runs the value of $\frac{k_1}{k_2}$ is coming different

Therefore, the assumption of parallel reaction is not correct.

Now, assuming series reaction taking place

Run	C_A	C_R	C_S	$\frac{C_R}{C_S} = \frac{k_1}{k_2}$	C_A/C_{A0}	C_R/C_{A0}	C_S/C_{A0}	$\frac{k_2}{k_1}$
1	50	33.3	16.7	1.976	0.5	0.33	0.167	0.8
2	25	30	45	0.666	0.25	0.3	0.45	0.8



Solution 8.5

Assuming parallel reaction

Run	C_A	C_R	C_S	$\frac{C_R}{C_S} = \frac{k_1}{k_2}$
1	50	40	10	4
2	20	40	40	1

$$\tau = \frac{C_R - C_{R0}}{k_1 C_A} \quad \text{---(1)}$$

$$\tau = \frac{C_S - C_{S0}}{k_2 C_A} \quad \text{---(2)}$$

Residence time will be equal from both equations

From eq. (1) and (2)

$$\frac{C_R}{k_1} = \frac{C_S}{k_2}$$

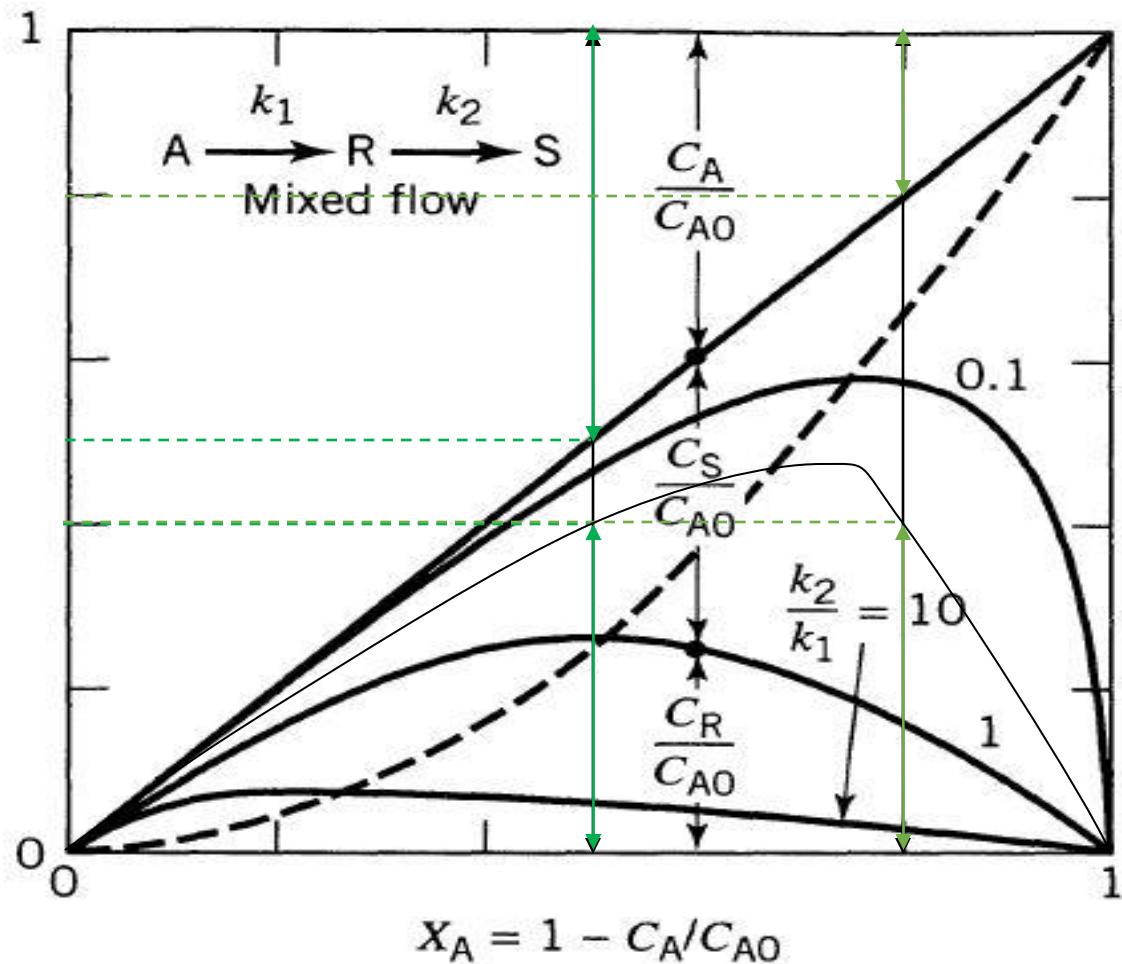
$$\frac{C_R}{C_S} = \frac{k_1}{k_2}$$

For both the runs the value of $\frac{k_1}{k_2}$ is coming different

Therefore, the assumption of parallel reaction is not correct.

Now, assuming series reaction

Run	C_A	C_R	C_S	$\frac{C_R}{C_S} = \frac{k_1}{k_2}$	C_A/C_{A0}	C_R/C_{A0}	C_S/C_{A0}	$\frac{k_2}{k_1}$
1	50	40	10	4	0.5	0.4	0.1	0.3
2	20	40	40	1	0.2	0.4	0.4	0.3



- 8.6. In grinding a continuous flow of pigments for paint, our company finds that too many too-small and too many too-large particles exit from our well-mixed grinder. A multistage grinder, approximating plug flow, could also have been used, but wasn't. Anyway, in either type of grinder the pigments are progressively ground into smaller and smaller particles.

At present, the exit stream from our well-mixed grinder contains 10% too-large ($d_p > 147 \mu\text{m}$); 32% just-right ($d_p = 38 - 147 \mu\text{m}$); and 58% too-small ($d_p < 38 \mu\text{m}$) particles.

- (a) Can you suggest a better grinding scheme for our present unit, and what would it give?
 (b) How about the multistage grinder? How would it do?

By “better” we mean giving more just right-sized pigment in the product stream. Also, separation and recycle of the size cuts is not practical.

Solution 8.6

As grinding will progress as,

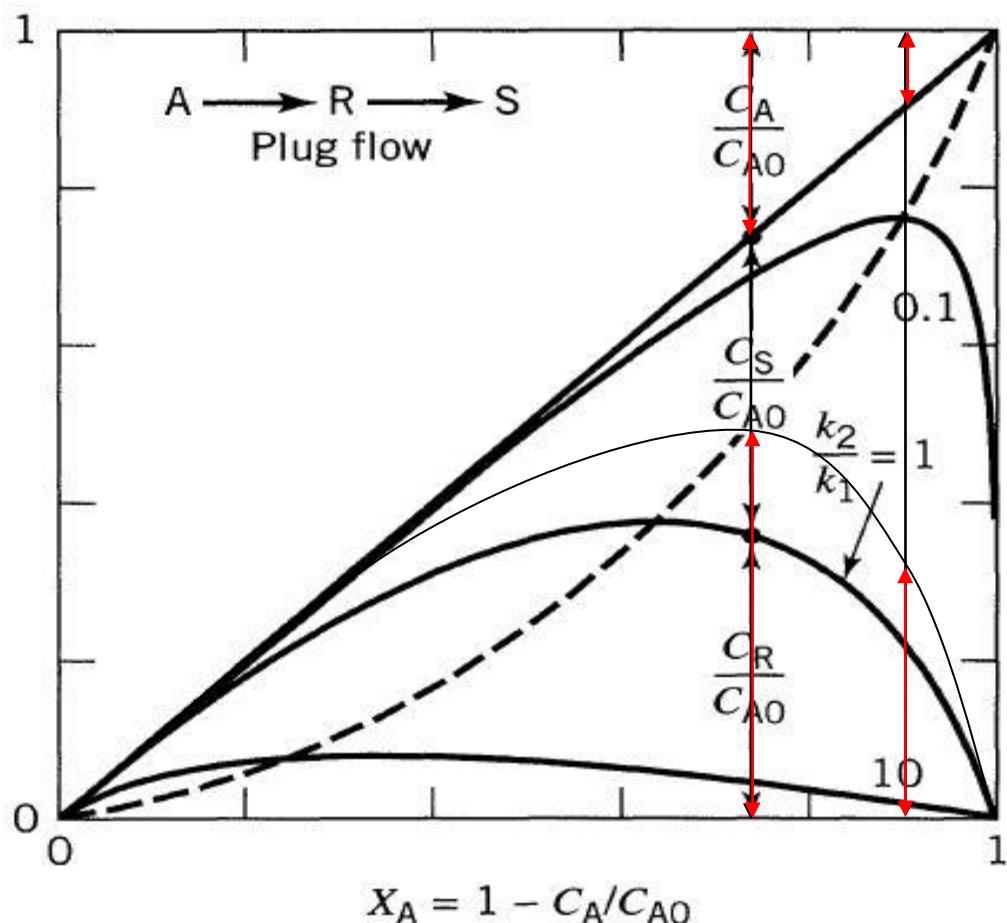
large particles \rightarrow appropriate particles \rightarrow small particles
denoting this process as,



a) Basis: 100 particles (10 A, 32 R and 58 S)

Too small particles so you have to reduce the residence time, increasing the feed flow to make an estimate, assume that a series of first reaction order may represent milling process.

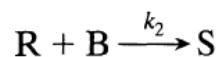
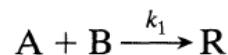
$X_A = 0.9$ and $C_R/C_{A0} = 0.32$ is that $k_2/k_1 \approx 0.7$



If $\frac{k_2}{k_1} \approx 0.7 \Rightarrow C_{R\max} / C_{A0} = 0.5$ and $X_A = 0.75$ and will get 25% of very large particles, 50% of particles of appropriate size and 25% of very small particles.

b) Multi-stage is better, as single stage grinder will act as single MFR and multi-stage grinder will act as MFR in series which will act as PFR and in PFR we get more uniform product. So using multistage grinder is best option.

8.7. Consider the following elementary reactions:



- (a)** One mole A and 3 moles B are rapidly mixed together. The reaction is very slow, allowing analysis of compositions at various times. When 2.2 moles B remain unreacted, 0.2 mole S is present in the mixture. What should be the composition of the mixture (A, B, R, and S) when the amount of S present is 0.6 mole?
- (b)** One mole A is added bit by bit with constant stirring to 1 mole B. Left overnight and then analyzed, 0.5 mole S is found. What can we say about k_2/k_1 ?
- (c)** One mole A and 1 mole B are thrown together and mixed in a flask. The reaction is very rapid and goes to completion before any rate measurements can be made. On analysis of the products of reaction 0.25 mole S is found to be present. What can we say about k_2/k_1 ?

Solution 8.7

a) $A_0 = 1 \quad B_0 = 3$

B consumed is 2.2 so $\Delta B = 0.8$

$S = 0.2$

$$\frac{k_2}{k_1} = 0.85$$

For $S = 0.6$ and $\frac{k_2}{k_1} = 0.85$ from graph $R = 0.3$



To produce 0.6 mol of S, B required is 0.6 and R required is 0.6

The final mol of R is 0.3 so total mol of R must be produced is 0.9 and to produce it 0.9 mole of A and B required

Therefore $\Delta B = 0.6 + 0.9 = 1.5$

The final concentration of A, B, R and S is 0.1, 1.5, 0.3 and 0.9 respectively.

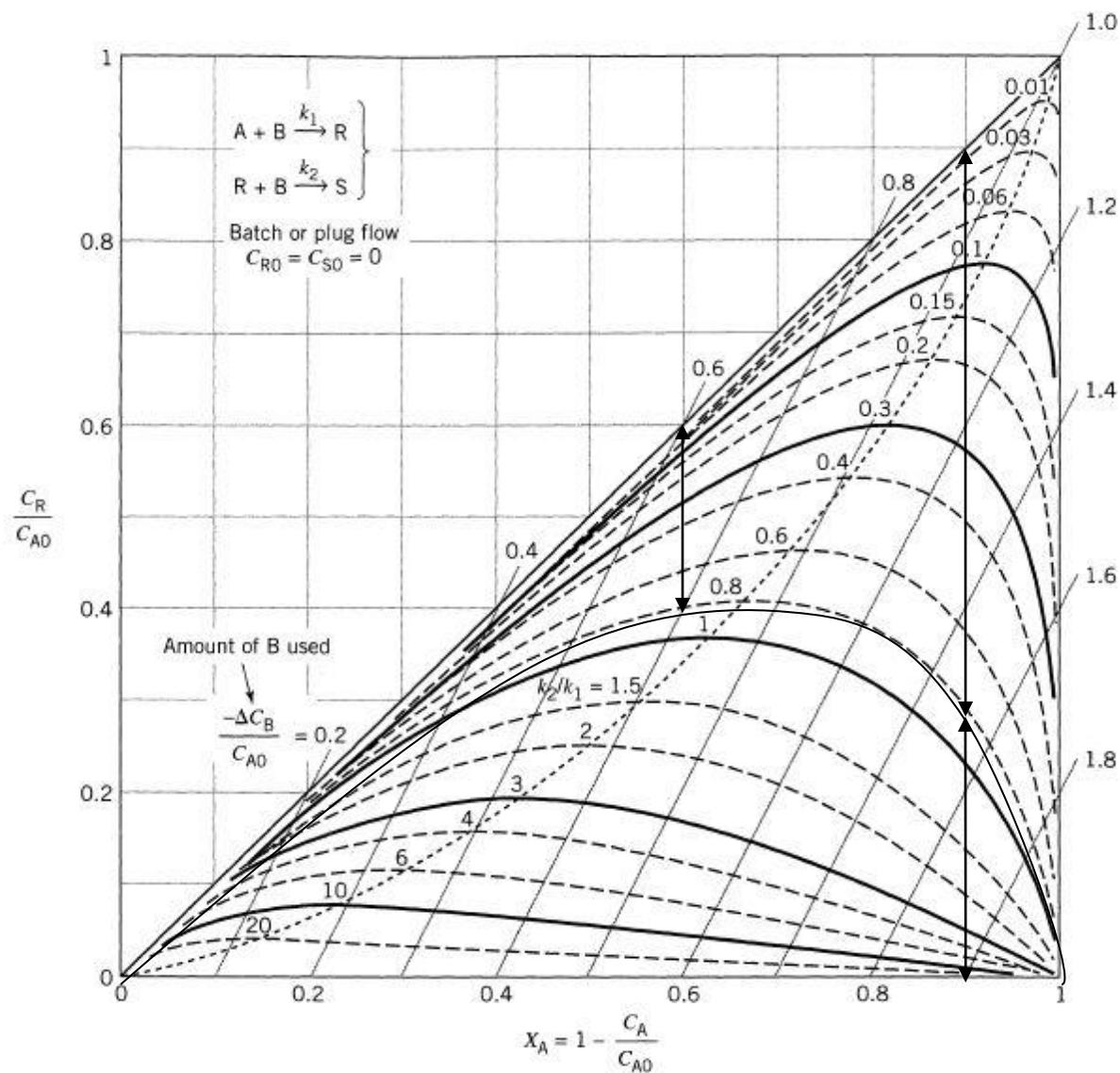


Figure 8.13 Distribution of materials in a batch or plug flow reactor for the elementary series-parallel reactions

b)

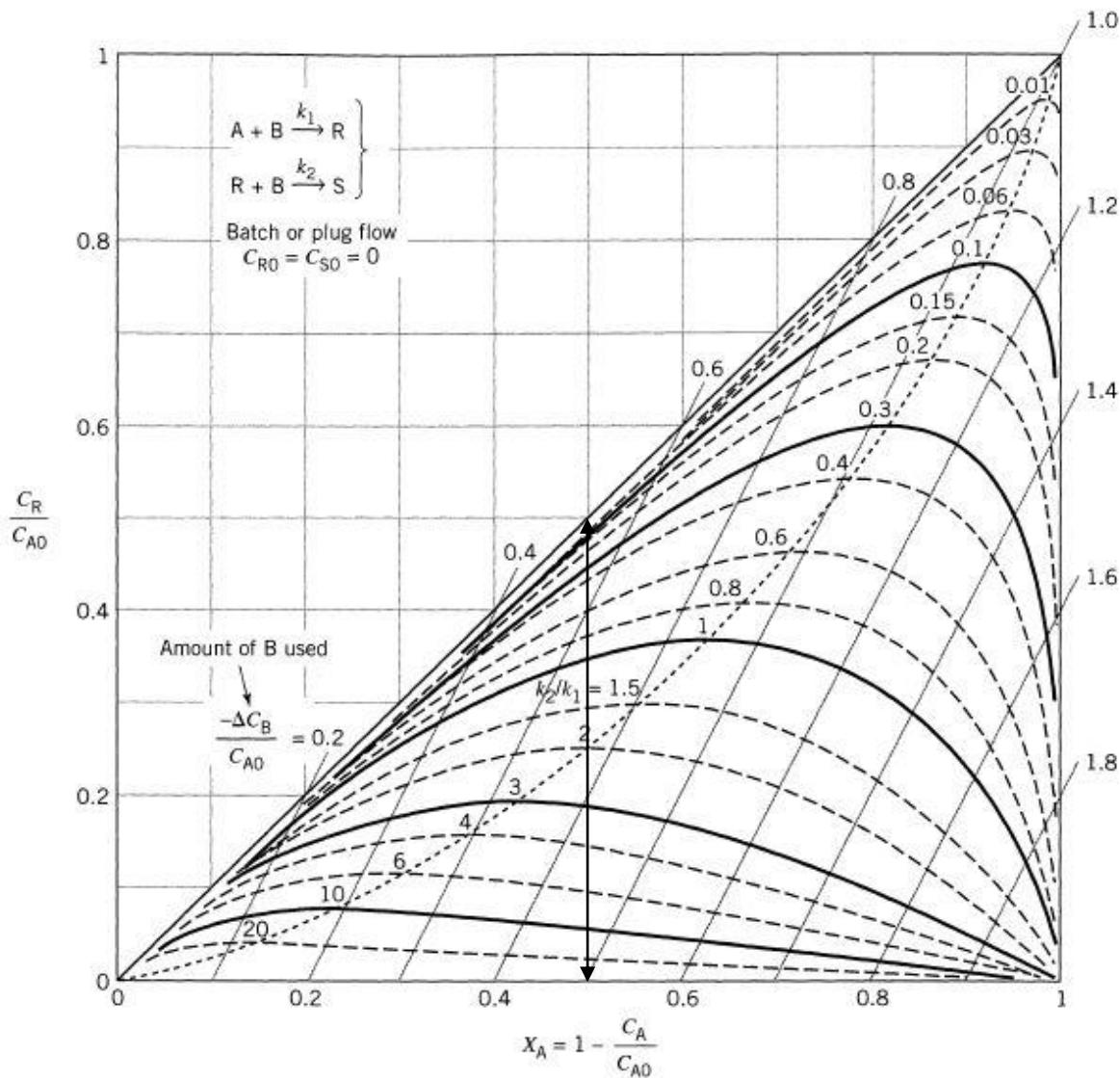


Figure 8.13 Distribution of materials in a batch or plug flow reactor for the elementary series-parallel reactions

Only S is found so as the R is formed it is directly converted to S and it indicates that $k_2 \gg k_1$ which cannot be determined from the graph shown above.

c)

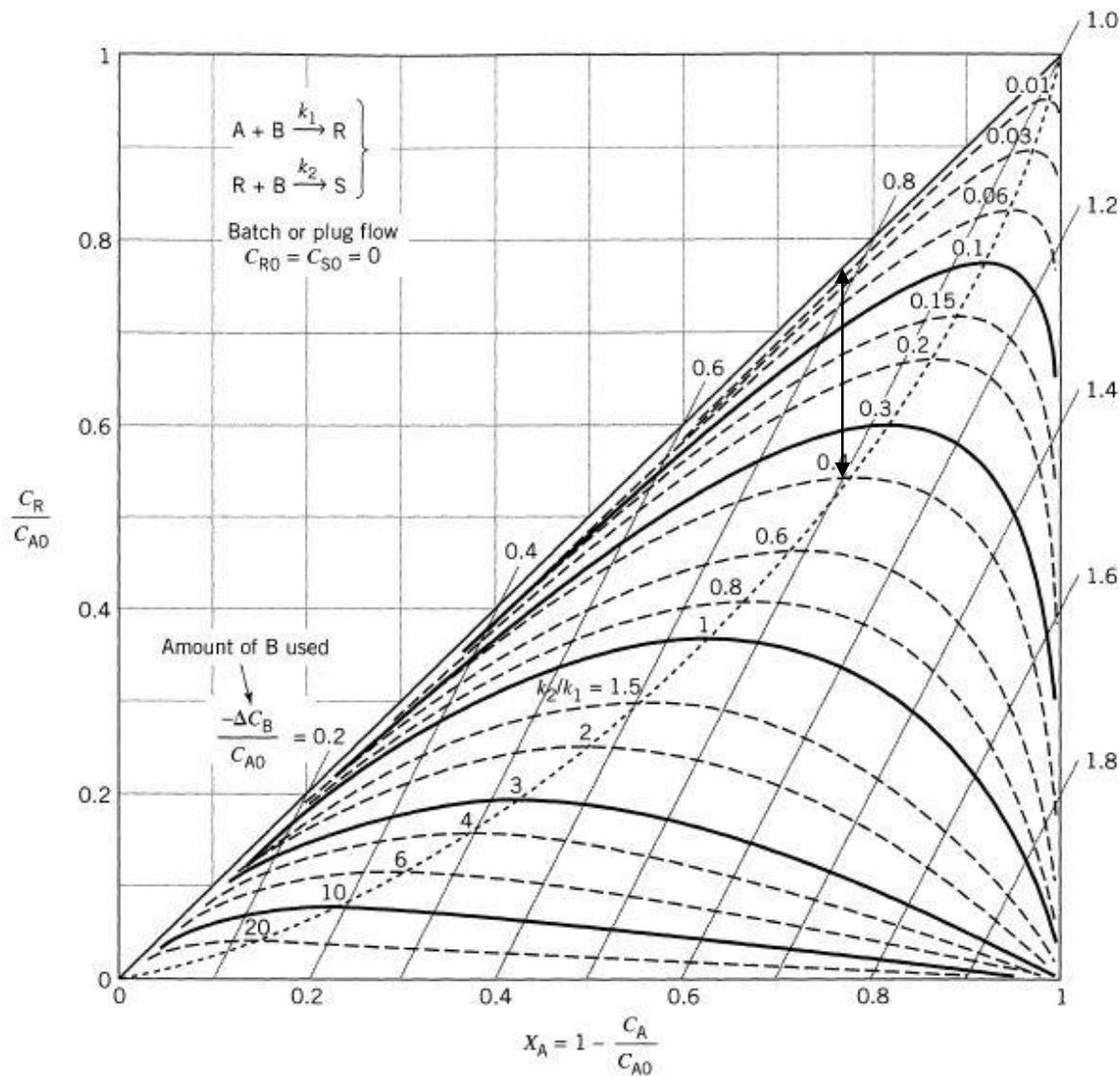
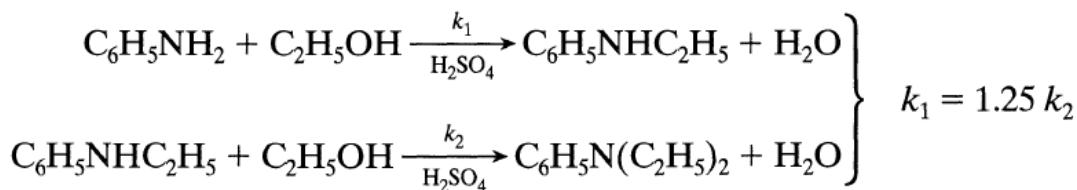


Figure 8.13 Distribution of materials in a batch or plug flow reactor for the elementary series-parallel reactions

$$\frac{\Delta B}{A} = 1 \text{ and } S = 0.25 \text{ from graph } \frac{k_2}{k_1} = 0.4$$

8.8. The liquid phase reaction of aniline with ethanol produces wanted mono-ethylaniline and unwanted diethylaniline



- (a) An equimolar feed is introduced into a batch reactor, and reaction is allowed to proceed to completion. Find the concentration of reactants and products at the end of the run.
- (b) Find the ratio of mono- to diethylaniline produced in a mixed flow reactor for an alcohol-to-aniline feed ratio of 2 to 1 for 70% conversion of alcohol.
- (c) For an equimolar feed to a plug flow reactor, what will be the conversion of the two reactants when the concentration of monoethylaniline is at its highest?

Solution 8.8

a) Here, $\frac{k_2}{k_1} = 0.8$

From graph concentration of diethyl-aniline is 0.2mol and mono-ethyl-aniline is 0.4mol

Water will be formed in second reaction is 0.2mol

For producing 0.2 mol of di-ethyl-aniline 0.2 mol of mono-ethyl-aniline will be consumed so total mono-ethyl-aniline produced in first reaction is 0.6 mol and 0.6 mol of water will be formed

Total mol of water formed is 0.8

0.6 mol of ethanol in first and 0.2 mol ethanol in second reaction will be consumed so total ethanol consumed is 0.8 mol

0.6 mol of aniline will be consumed in first reaction

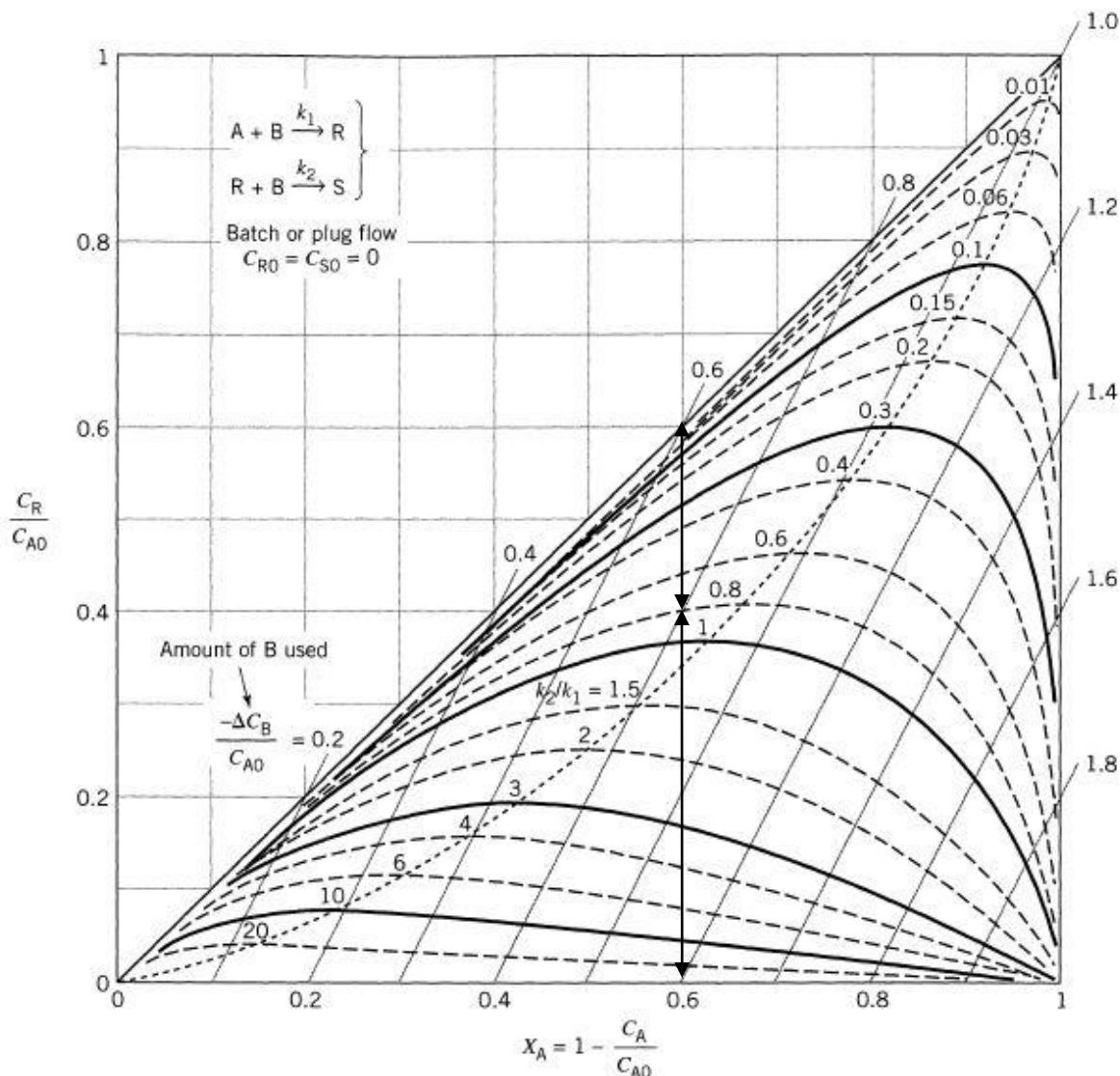


Figure 8.13 Distribution of materials in a batch or plug flow reactor for the elementary series-parallel reactions

Final composition of mixture from batch reactor

Aniline	Ethanol	Mono-ethyl-aniline	Di-ethyl-aniline	Water
0.4	0.2	0.4	0.2	0.8

b)

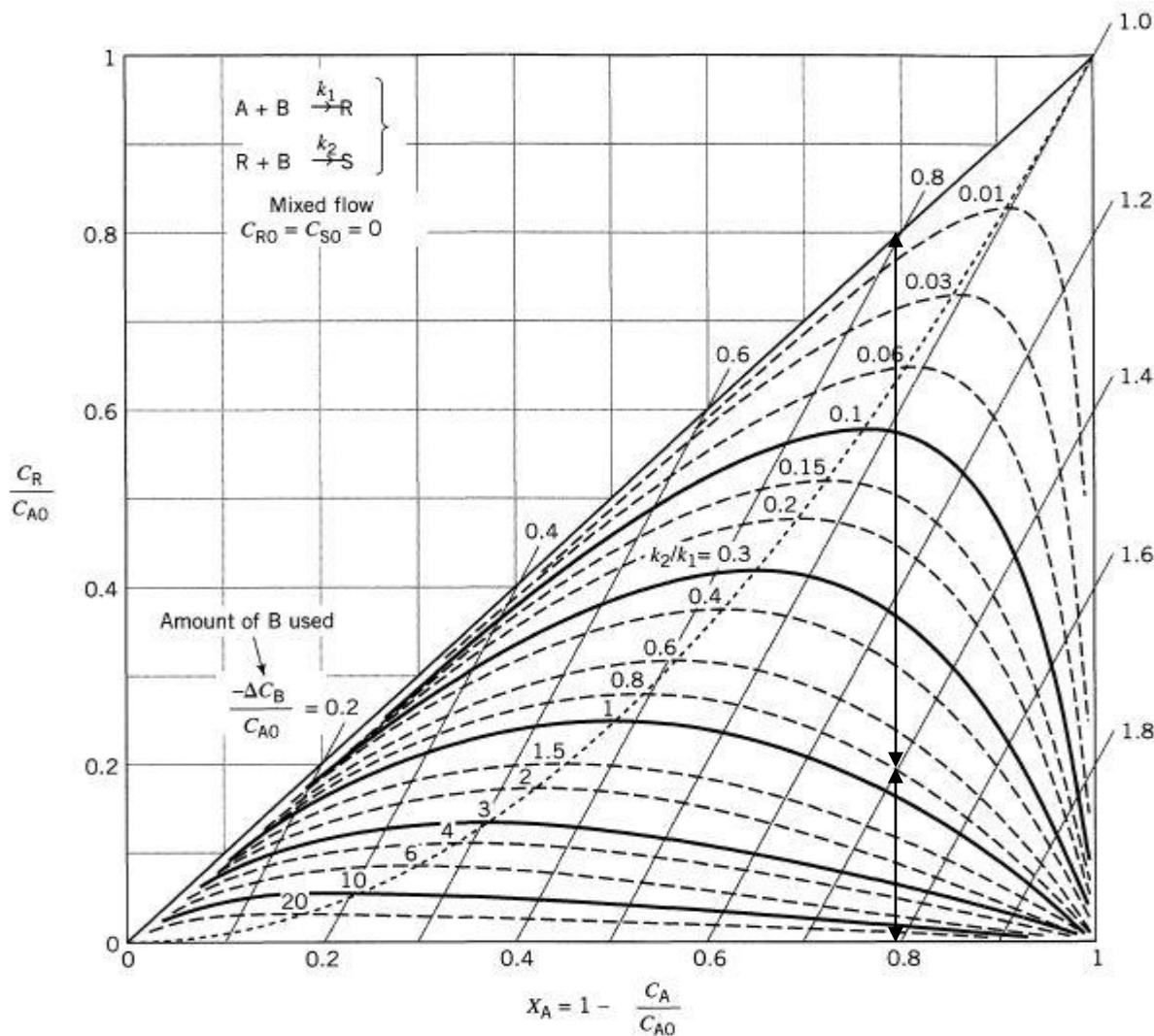


Figure 8.14 Distribution of materials in a mixed flow reactor for the elementary series-parallel reactions

For 70% conversion of ethanol value of $\Delta B = 1.4$

$$\frac{\Delta B}{A} = 1.4$$

For this data final moles of mono-ethyl-aniline and di-ethyl-aniline are 0.2 mol and 0.6 mol respectively.

Ratio of mono to di-ethyl-aniline is 0.333

c)

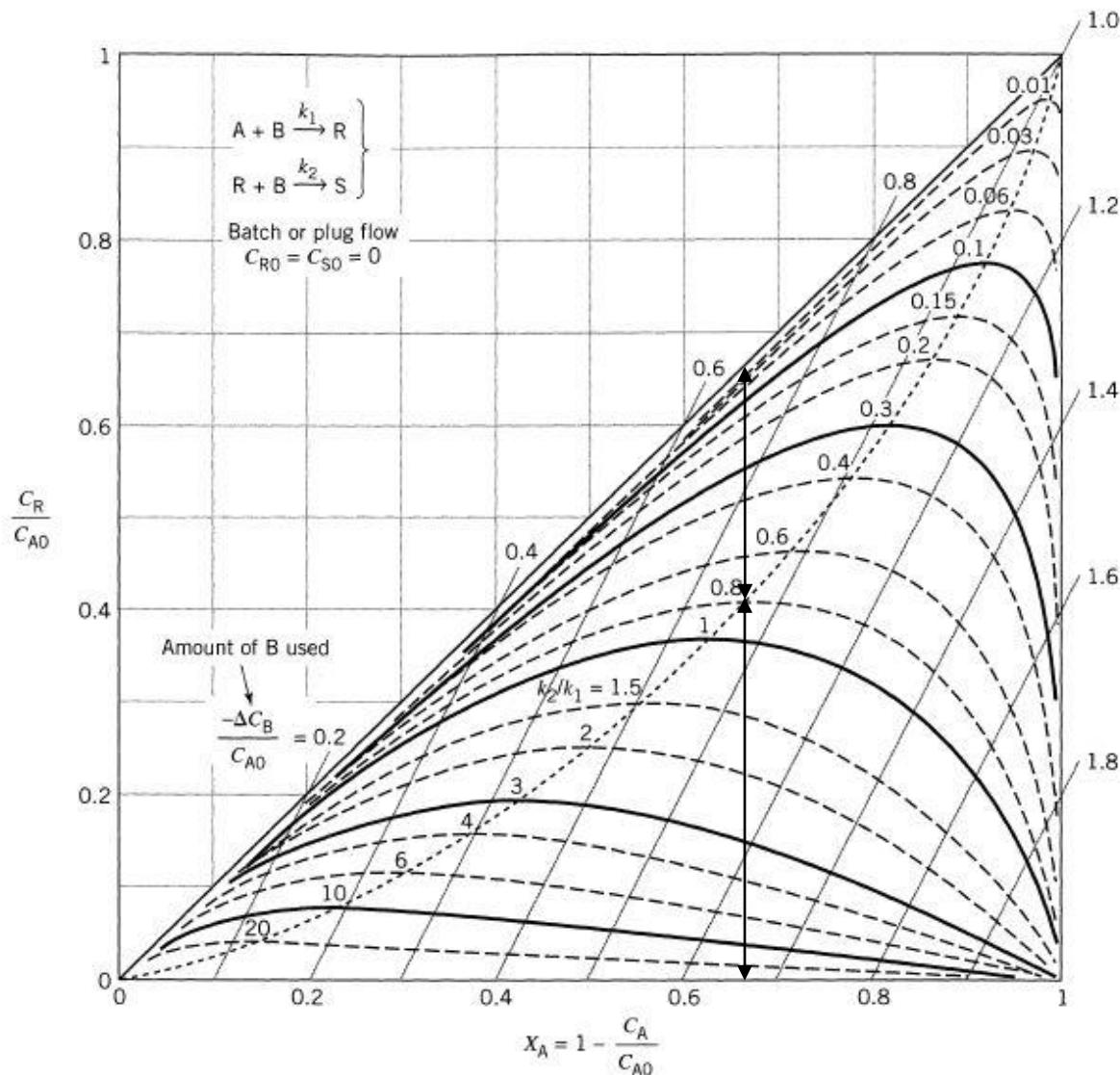


Figure 8.13 Distribution of materials in a batch or plug flow reactor for the elementary series-parallel reactions

From graph for equimolar feed in plug flow reactor for highest concentration of mono-ethyl-aniline the conversion of A is 67%

From graph $\Delta B = 0.92$

Therefore, overall conversion of B is 92% considering both reactions

- 8.9. Monoethylaniline can also be produced in the vapor phase in a fluidized bed using natural bauxite as the solid catalyst. The elementary reactions are shown in the previous problem. Using an equimolar feed of aniline and ethanol, the fluidized bed produces 3 parts monoethylaniline to 2 parts diethylaniline for a 40% conversion of aniline. Assuming mixed flow of gas in the fluidized bed, find k_2/k_1 and the concentration ratio of reactants and products at the exit of the reactor.

Solution 8.9

Considering aniline (A), ethanol (B), mono-ethyl-aniline (R) and di-ethyl-aniline (S)

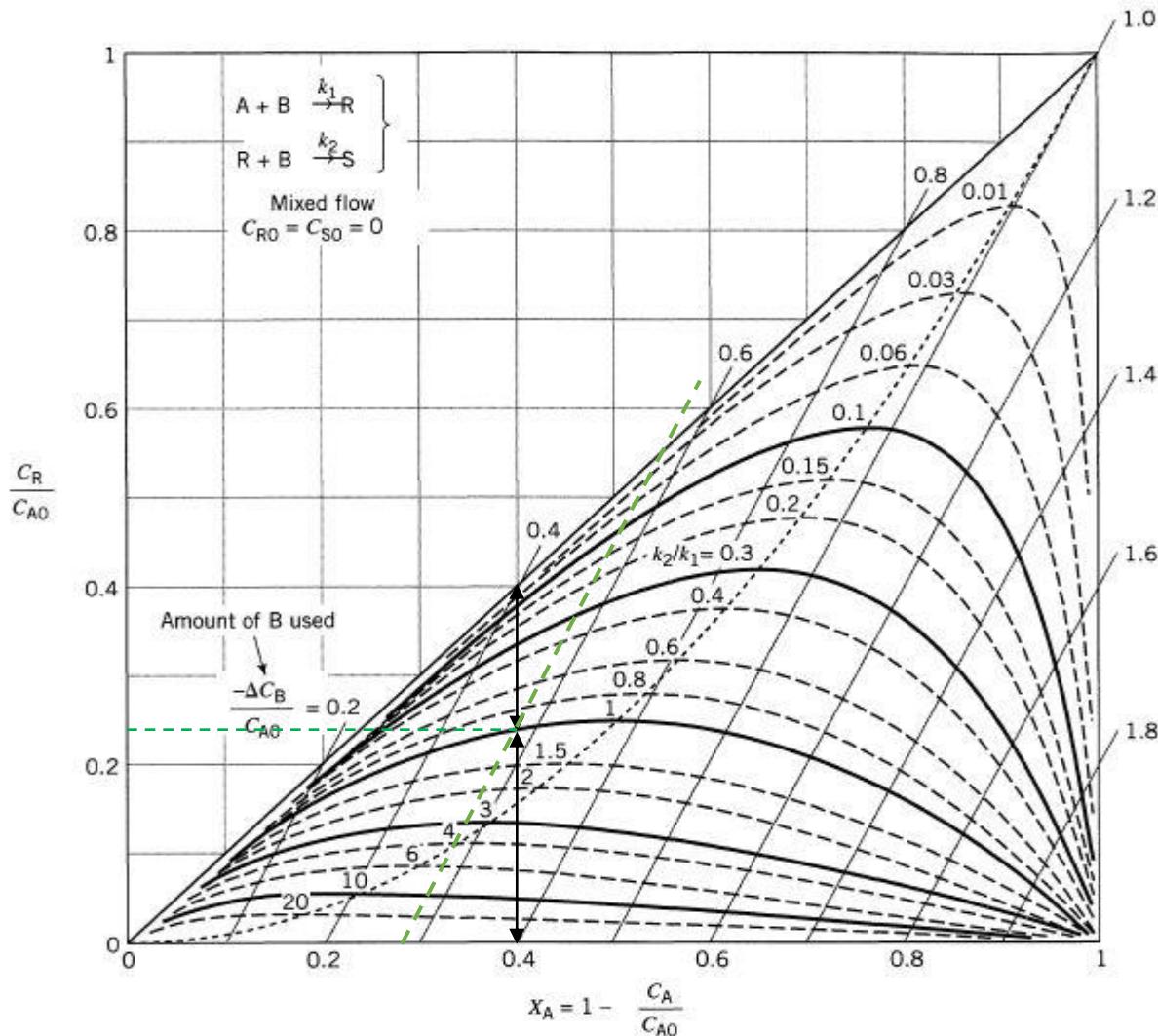


Figure 8.14 Distribution of materials in a mixed flow reactor for the elementary series-parallel reactions

$$A_0 = 1 \text{ mol}, B_0 = 2 \text{ mol}$$

$$\frac{\Delta B}{A} = 0.56$$

After reaction conversion of A is 40% so 60% will remain unconverted

$$A = 0.6$$

B reacted in first reaction is 0.4 mol

The remaining final mixture R is 3 parts and S is 2 parts to produce 2 parts of S, 2 parts of R must react in second reaction so total R formed in first reaction is 5 parts which is 0.4 mol.

$$2 \text{ parts reacted so remaining moles of R is } 0.4 - \left(\frac{2}{5} * 0.4\right) = 0.24$$

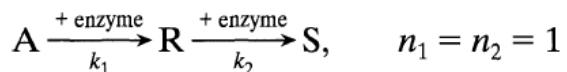
S formed is 0.16 mol

$$\text{The value from graph } \frac{k_2}{k_1} = 1$$

The final composition in outlet of MFR

Aniline	Ethanol	Mono-ethyl-aniline	Di-ethyl-aniline	Water
0.6	0.44	0.24	0.16	0.56

Under the action of mixed enzymes reactant A is converted to products as follows:



where the rate constants are dependent on the pH of the system.

- (a) What reactor set-up (plug flow, mixed flow, or staged mixed flow units) and what uniform pH level would you use?
- (b) If it were possible to change the pH level along the plug flow reactor, or from stage to stage in mixed flow units, in what direction would you change the pH level?

8.10. $k_1 = \text{pH}^2 - 8 \text{ pH} + 23$ with $2 < \text{pH} < 6$, and R the desired product
 $k_2 = \text{pH} + 1$

Solution 8.10

pH	k_1	k_2	k_1/k_2
2	11	3	3.666667
3	8	4	2
4	7	5	1.4
5	8	6	1.333333
6	11	7	1.571429

- a) Here, the value of $\frac{k_1}{k_2}$ is highest at $\text{pH}=2$ so the pH which should be maintained should be slightly higher than 2 and should be maintained throughout the reactor to get maximum of R as the k_1 will be higher compared to k_2 then R will be more formed. MFR should be used to maintain pH throughout the reactor as 100% mixing and uniform pH will be there in MFR.
- b) As, the pH required to be constant no PFR is used and in MFR no stages with different pH should be kept.

CRE-I Term paper

Sums 8.11-8.21

Group members: 13BCH012, 13BCH013, 13BCH037, 13BCH045, 13BCH055

Problem 8.11

As S is desired it requires both k_1 as high as k_2

pH	k_1	k_2
2	3	11
3	4	8
4	5	7
5	6	8
6	7	11

When pH=6, $k_1=7$ (maximum value) and $k_2=11$ (maximum value), so it is best to work with pH=6 and keep it constant.

Problem 8.12

(a) R is in series with A and S, so it is best to use the plug flow reactor.

(b) As in parallel reactions C_R is the area under the curve Φ vs C_A . So, let's take $\Phi = f(C_A)$

$$\Phi = -\frac{dC_A}{dC_R} = (k_1 * C_A - k_4 * C_R) / k_{12} * C_A \quad , \text{ where } k_{12} = k_1 + k_2$$

It is not possible to separate variables and integrate because Φ is also a function of C_R ; but it is a linear differential equation of first order with integral factor.

$$\frac{dC_R}{dC_A} - (k_4 * C_R) / (k_{12} * C_A) = -\frac{k_1}{k_{12}}$$

Comparing this equation with,

$$\frac{dy}{dx} + P(x) y = Q(x)$$

$$y = C_R, x = C_A, P(x) = -\frac{k_4}{k_{12} * C_A}, Q(x) = -\frac{k_1}{k_{12}}$$

$$y = e^{-\int P(x)dx} \left\{ \int Q(x) e^{\int P(x)dx} dx \right\}$$

$$\int P(x)dx = -\int \left(\frac{k_4}{k_{12} * C_A} \right) dC_A = \ln C_A^{k_4/k_{12}}$$

$$e^{-\int P(x)dx} = C_A$$

$$e^{\int P(x)dx} = C_A^{-k_4/k_{12}}$$

$$\int Q(x) e^{\int P(x)dx} dx = -\frac{k_1}{k_{12}} \int C_A^{k_4/k_{12}} dC_A = \left(\frac{-k_1}{k_{12}} \right) * \frac{C_A^{(1-\frac{k_4}{k_{12}})}}{(1-\frac{k_4}{k_{12}})}$$

Put all these values in main equation,

$$C_R = C_A^{-k_4/k_{12}} \left\{ \left(\frac{-k_1}{k_{12}} \right) * \left(C_A^{(1-\frac{k_4}{k_{12}})} / (1 - \frac{k_4}{k_{12}}) \right) + \text{constant} \right\}$$

$$\text{When } C_A = C_{A0} \text{ then } C_R = 0 \text{ and constant} = \left(\frac{k_1}{k_{12}} \right) * \frac{C_{A0}^{(1-\frac{k_4}{k_{12}})}}{(1-\frac{k_4}{k_{12}})}$$

$$C_R = C_A^{k_4/k_{12}} \left\{ \left(\frac{-k_1}{k_{12}} \right) * \frac{C_A^{(1-\frac{k_4}{k_{12}})}}{(1-\frac{k_4}{k_{12}})} + \left(\frac{k_1}{k_{12}} \right) * \frac{C_{A0}^{(1-\frac{k_4}{k_{12}})}}{(1-\frac{k_4}{k_{12}})} \right\}$$

Dividing the whole equation for C_{A0} and removing the common factor constant ratio within the key and performing the indicated multiplication,

$$\frac{C_R}{C_{A0}} = \frac{\frac{k_1}{k_{12}}}{1 - \frac{k_4}{k_{12}}} \left\{ \frac{C_{A0} C_{A0}^{-\frac{k_4}{k_{12}}} C_A^{\frac{k_4}{k_{12}}}}{C_{A0}} - \frac{C_A^{(1-\frac{k_4}{k_{12}} + \frac{k_4}{k_{12}})}}{C_{A0}} \right\}$$

$$\frac{C_R}{C_{A0}} = \frac{k_1}{k_{12} - k_4} \left\{ \left(\frac{C_A}{C_{A0}} \right)^{\frac{k_4}{k_{12}}} - \frac{C_A}{C_{A0}} \right\}$$

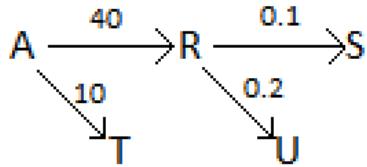
Note that you could have obtained from the equation 8.48 (p. 195) by $k_{34} = k_3 + k_4 = k_4$ (because $k_3 = 0$)

$$\frac{C_R}{C_{A0}} = \frac{k_1}{k_{12}} \left\{ \left(\frac{k_{12}}{k_4} \right)^{\frac{k_4}{k_{12} - k_4}} \right\} = \frac{3}{4} \left\{ \left(\frac{4}{0.2} \right)^{\frac{0.2}{0.2 - 4}} \right\} = 0.865$$

$$C_R = 2(0.865) = 1.73 \text{ mol}$$

Problem no. 8.13

(a)



$$k_1 = 40, k_2 = 10, k_3 = 0.1, k_4 = 0.2$$

$$C_S = 0.2C_{A0}$$

$$k_{12} = k_1 + k_2 = 50; k_{34} = k_3 + k_4 = 0.1 + 0.2 = 0.3$$

$$\frac{C_S}{C_{A0}} = \frac{k_1 k_3}{k_{34} - k_{12}} \left(\frac{e^{1-k_{34}t}}{k_{34}} - \frac{e^{-k_{12}t}}{k_{12}} \right) + \frac{k_1 k_3}{k_{34} - k_{12}} + \frac{C_{R0} k_3}{C_{A0} k_{34}} (1 - e^{-k_{34}t}) + \frac{C_{S0}}{C_{A0}}$$

$$\text{We have, } C_{A0} + C_{R0} + C_{T0} + C_{U0} = C_A + C_R + C_T + C_U$$

$$\text{Or } C_{A0} = C_A + C_R + C_T + C_U$$

Therefore,

$$\frac{0.2C_{A0}}{C_{A0}} = \frac{(40)(0.1)}{0.3 - 50} \left(\frac{e^{-0.3t}}{0.3} - \frac{e^{-50t}}{50} \right) + \frac{40 * 0.1}{50 * 0.3} + 0 + 0$$

$$\rightarrow 0.2 = \frac{-0.0804}{15} (50e^{-0.3t} - 0.3e^{-50t}) + 0.2667$$

$$\text{Or } 12.44 = 50e^{-0.3t} - 0.3e^{-50t}$$

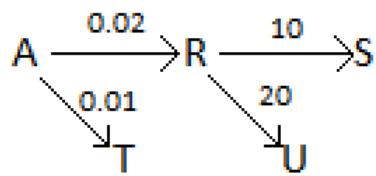
$$\rightarrow \ln 12044 = \ln 50 - 0.3t - \ln 0.3 + 50t$$

$$\rightarrow 2.52 = 3.91 + 49.7t + 1.2$$

So, $t = -0.0521$ minutes.

Negative value of time is not possible. Thus there is some error in the data.

(b)



The above rate constants show that the first reaction is a slow reaction and the second reaction is a fast reaction.

$$C_{A0} + C_{R0} + C_{T0} + C_{U0} = C_A + C_R + C_T + C_U$$

$$\frac{C_S}{C_{A0}} = \frac{k_1 k_3}{k_{34} - k_{12}} \left(\frac{e^{1-k_{34}t}}{k_{34}} - \frac{e^{-k_{12}t}}{k_{12}} \right) + \frac{k_1 k_3}{k_{34} * k_{12}}$$

$$\text{Let } C_{A0} = 100 \text{ mol/lit}$$

$$\text{So, } C_S = 0.2 * 100 = 20 \text{ mol/lit}$$

$$\rightarrow \frac{0.2 C_{A0}}{C_{A0}} = \frac{(0.2)(10)}{30 - 0.03} \left(\frac{e^{-30t}}{30} - \frac{e^{-0.03t}}{0.03} \right) + \frac{0.02 * 10}{0.03 * 30}$$

$$\text{Or } 0.02 = 6.67 \times 10^{-3} \left(\frac{0.03 e^{-30t} - 30 e^{-0.03t}}{30 * 0.03} \right) + 0.222$$

$$\text{Therefore, } 0.2 - 0.222 = 7.414 * 0.03 * 10^{-3} e^{-30t} - 70417 * 30 * e^{-0.03t} * 10^{-3}$$

$$0.0222 = -2.224 \times 10^{-4} e^{-30t} + 0.2224 x e^{-0.03t}$$

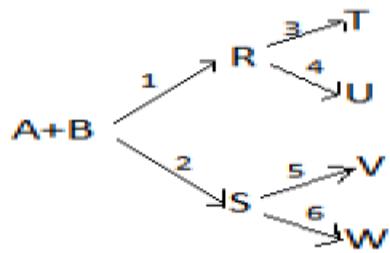
$$-8.411 - 30t - 1.4961 + 0.03t = -3.867$$

$$-8.417 - 1.4961 + 3.8167 = 29.97t$$

$$\text{Thus } t = \frac{-6.0904}{29.97} = -0.2032 \text{ minutes}$$

Which is negative so the data given is incorrect.

Problem 8.14



(a) Arguably $k_3 > k_4$ and $k_5 > k_6$. we cannot conclude anything about k_1 and k_2 because although the branch of R there are fewer moles than by the branch of S may be that $k_1 > k_2$ and k_3 and k_4 to be small and has accumulation of R may also be that $k_1 < k_2$ and $k_1 < k_3$ and k_4 so that all R formed pass T and U.

(b) If the reaction was now complete and is T, U, V and W only by the branch above 5 moles of T and 1 mole of U formed, so it was 6 moles of R transformed to U and T, whereas below the branch 9 mol of V and 3 mol of W were formed, meaning that there were 12 mol of S. In this case can be concluded that,

$$k_1 < k_2$$

$$\text{Formation rate of R} = \frac{dC_R}{dt} = k_1 C_A C_B$$

$$\text{Formation rate of S} = \frac{dC_S}{dt} = k_2 C_A C_B$$

$$dC_R = \frac{k_1}{k_2} dC_S \Rightarrow \frac{k_1}{k_2} = \frac{C_R}{C_S} = \frac{6}{12} \Rightarrow k_2 = 2k_1$$

$$\text{Formation rate of } T = \frac{dC_T}{dt} = k_3 C_A C_B$$

$$\text{Formation rate of } U = \frac{dC_U}{dt} = k_4 C_A C_B$$

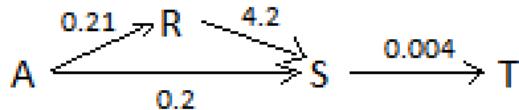
$$dC_T = \frac{k_3}{k_4} dC_U \Rightarrow \frac{k_3}{k_4} = \frac{C_T}{C_U} = \frac{5}{1} \Rightarrow k_2 = 5k_1 \quad \text{valid for (a)}$$

$$\text{Formation rate of } V = \frac{dC_V}{dt} = k_5 C_A C_B$$

$$\text{Formation rate of } W = \frac{dC_W}{dt} = k_6 C_A C_B$$

$$dC_V = \frac{k_5}{k_6} dC_W \Rightarrow \frac{k_5}{k_6} = \frac{C_V}{C_W} = \frac{9}{3} \Rightarrow k_2 = 3k_1 \quad \text{valid for (a)}$$

Problem 8.15



For series reaction, the overall rate constant is given by,

$$\frac{1}{k_{13}} = \frac{1}{k_1} + \frac{1}{k_3} = \frac{1}{0.21} + \frac{1}{4.2} = 5$$

$$\text{So, } k_{13} = 0.2$$

$$\text{Overall rate constant is given by, } K = k_{13} + k_2 = 0.2 + 0.2 = 0.4$$

Since S is desired product, if we use mixed flow reactor, there will be more mixing and hence intermediate formation will be less. So we can use plug flow reactor.

By using equation,

$$\frac{C_{Smax}}{C_{A0}} = \frac{k_{123}}{k_4} \frac{k_4}{k_4 - k_{123}} = \frac{0.4}{0.004} \frac{0.004}{0.004 - 0.4} = 0.9545$$

$$C_{Smax} = 0.9545 C_{A0}$$

$$\tau = \frac{\ln(\frac{k_2}{k_1})}{k_2 - k_1} = \frac{\ln(\frac{0.004}{0.4})}{0.004 - 0.4} = 8.128 \quad [\text{therefore } k_1 = k_{123} = 0.4]$$

As we know equation,

$$C_A = C_{A0} e^{-k_1 t}$$

$$\text{But } C_{A0} = 100 e^{-(0.4*8.128)}$$

$$= 100 * 0.03872$$

$$= 3.872 \text{ mol/L}$$

$$X_A = \frac{C_{A0} - C_A}{C_{A0}} = \frac{100 - 3.872}{100} = 96.12\%$$

Problem no. 8.16

The initial gravel handling rate of shovel is 10 ton/min. It is also mentioned that the shovel's gravel handling rate is directly proportional to the size of the pile still to be moved. So it shows that the removal of the sand using shovel can be compared to the first order reaction.

The conveyor on the other hand works at the uniform rate of 5 ton/min. This shows that the working of the conveyor is independent of the amount of sand in the hopper. So it can be considered as the zero order reaction.

So for shovel,

$$10 \text{ ton/min} = k_1 * 20000 \dots \dots \dots (1)$$

$$k_1 = 10/20000 = 5 * 10^{-4}$$

For Conveyor,

$$5 \text{ ton/min} = k_2$$

(a) $\frac{C_{bin}}{C_{A0}} = 1 - K(1 - \ln K)$

$$K = \frac{k_2}{C_{A0} k_1} = \frac{5}{20000 * 5 * 10^{-4}} = 0.5$$

$$C_{bin} = 20000 * (1 - 0.5(1 - \ln 0.5)) = 3068.52 \text{ tonnes}$$

(b) $t_{Rmax} = \ln(1/K)/k_1 = \ln(1/0.5)/(5 * 10^{-4}) = 1386.29 \text{ min}$

(c) Input = Output

$$k_1 * C_{A0} = k_2$$

$$5 * 10^{-4} * C_{A0} = 5$$

$$C_{A0} = 10000 \text{ tonne}$$

(d) When $C_{\text{bin}} = 0$,

$$\frac{k_2 t}{C_{A0}} + e^{-k_1 t} = 1$$

By using trial and error method,

$$t = 0.0132 \text{ min}$$

Problem no. 8.17



Where, A = Garbage still to be collected

$$A_0 = 1140 \text{ tonnes (initial garbage load)}$$

R = Garbage in bin

S = Garbage in incinerator

Since the rate of collection is proportional; to amount of garbage still to be collected –

Therefore, $A \rightarrow R$ is a First order reaction.

Since the conveyor is operated at uniform rate to the incinerator –

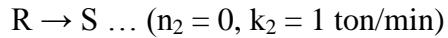
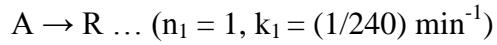
$R \rightarrow S$ is a zero order reaction.

$$\text{Therefore, } \frac{-dA}{dt} = k_1 A$$

At $t = 0$,

$$\frac{-dA_0}{dt} = 6 \text{ tons/min}$$

$$k_1 = \frac{\frac{-dA}{dt}}{A} = \frac{6}{1140} = \frac{1}{240} \text{ min}^{-1}$$



(a) For 95% of A collected –

$$\frac{dR}{dt} = k_1 A - k_2$$

From the given equation:

$$\frac{C_A}{C_{A0}} = e^{-k_1 t}$$

$$A_0 = 1140 \text{ tonnes}$$

$$A \text{ (at 95\%)} = 0.05 * 1440 = 72 \text{ tonnes}$$

$$k_1 = \frac{1}{240}$$

$$\frac{A}{A_0} = \frac{72}{1140} = e^{-t/240}$$

$$\text{Therefore, } \frac{1}{20} = e^{-t/240}$$

$$\text{Or, } \ln\left(\frac{1}{20}\right) = \frac{-t}{240}$$

$$\text{So, } t = 718 \text{ min} = 12 \text{ hrs.}$$

(b) For maximum collection in bin,

$$\frac{R_{max}}{A_0} = 1 - k (1 - \ln k)$$

$$\text{Thus, } k = \frac{(k_2/A_0)}{k_1} = \frac{(1/1440)}{(1/240)} = 0.1667$$

$$\text{Therefore, } R_{max} = 1140[1 - (0.1667)(1 - \ln(0.1667))] = 769.9 \text{ ton}$$

$$(c) t_{max} = \frac{1}{k_1} \ln\left(\frac{1}{k}\right) = 240 \ln\left(\frac{1}{0.1667}\right) = 430 \text{ min}$$

(d) Bin empties when R = 0

Therefore, $R = 0 = A_0 (1 - e^{-k_1 t}) - k_2 t$

Implies, $0 = 1440(1 - e^{-t/240}) - t$

Or, $e^{-t/240} + \frac{t}{1440} = 1$

By using Goal Seek method,

$t = 1436$ min

Problem no. 8.18

Suppose Upper Slobbovians = U and Lower Slobbovians = L

Here it is given that,

$$\frac{-dU}{dt} = L \text{ and } \frac{-dL}{dt} = U$$

Last week, after the encounter of 10U and 3L, 8 U survived

It means that 2 U died in this encounter and all the 3 L died.

So, when 1U dies 1.5 L die

(a) Upper Slobbovians are better fighters. And one Upper Slobbovian is as good as 1.5 Lower Slobbovians.

(b) When 10 U and 10 L encountered

$$1.5L \rightarrow 1U$$

$$10L \rightarrow \frac{1*10}{1.5} = 6.6 \approx 7U$$

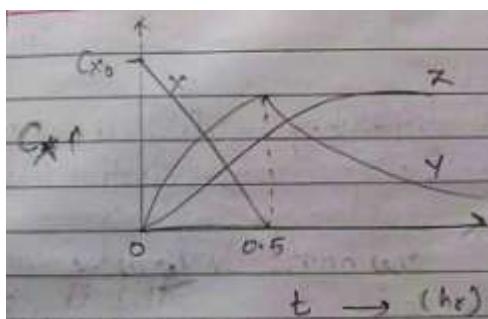
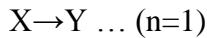
So here we can conclude that, after this encounter 3 U lived and 7 U died. Whereas all the 10 L were killed.

Problem no. 8.19-

Since chemical X is added slowly and it dissolves quickly, this shows that it is a zero order reaction.

Since Y decomposes slowly it shows that it is a 1st order reaction.

Thus it can be said that, the overall reaction is zero order followed by 1st order.



$$C_{X0} = 100 \text{ mol/m}^3$$

Now,

$$\frac{-dC_X}{dt} = k_1 = \frac{100}{0.5} = 200 \text{ mol/ (m}^3 \cdot \text{hr}) \dots \text{ as } n=0$$

$$\frac{-dC_Y}{dt} = k_2 C_Y$$

Overall rate constant can be given by 'k' where –

$$K = \frac{k_2 * C_0}{k_1} = \frac{1.5 * 100}{200} = 0.75$$

(a) At half hour Y_{max}

$$\frac{C_{Y_{max}}}{C_{X0}} = \frac{1}{k} (1 - e^{-k}) = \frac{1}{0.75} (1 - e^{-0.75}) = 0.7035$$

$$\text{Or, } C_{Y_{max}} = 100(0.7035) = 70.35 \text{ mol/m}^3$$

$$\text{Thus, } t_{max} = \frac{C_{X0}}{k_1} = \frac{100}{200} = 0.5 \text{ hours}$$

(b) After 1 hour, $C_{X0} = 0$

$$\frac{C_Y}{C_{X0}} = \frac{1}{k} (e^{k_1 - k_1 t} - e^{-k_2 t}) = \frac{1}{0.75} (e^{-0.75 \cdot 1.5} - e^{-1.5}) = 0.3323$$

$$C_Y = 100(0.3323) = 33.23 \text{ mol/m}^3$$

$$C_Z = C_{X0} - C_X - C_Y = 100 - 0 - 33.23 = 66.7 \text{ mol/m}^3$$

Problem no. 8.20

$$(1) \frac{dC_X}{dt} \neq 0 \text{ and } \frac{dC_R}{dt} \neq 0$$

$$C_A = C_{A0} - kt$$

$$C_A - C_{A0} = kt$$

From initial slope of C_X Vs t and C_R Vs t , which is not zero we can say that A gives X and R in a Parallel reaction.



(2) But when A is completely exhausted, still C_X decreases and C_R and thus X decomposes to give the final product R.



Therefore $A \rightarrow X$, $A \rightarrow R$, and $X \rightarrow R$



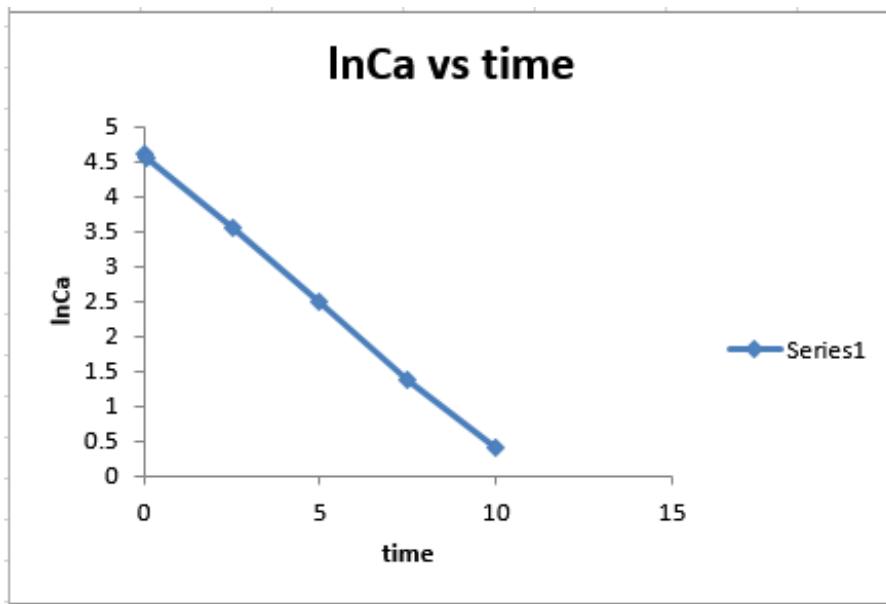
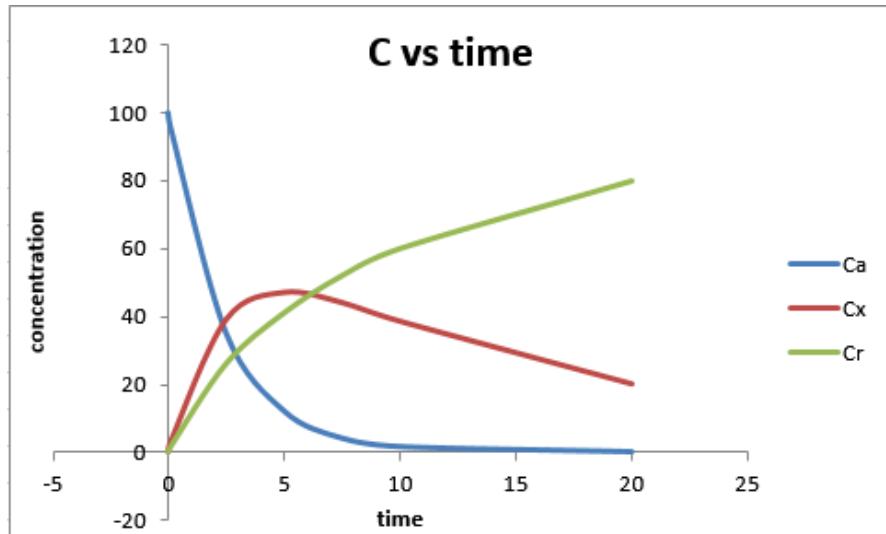
We know, $C_{A0} = C_X + C_A + C_R$

Therefore $C_X = 100 - C_A - C_R$

$t(\text{min})$	0	0.1	2.5	5	7.5	10	20	∞
$C_A(\text{mol/m}^3)$	100	95.8	35	12	4	1.5	-	0
$C_R(\text{mol/m}^3)$	0	1.4	26	41	52	60	80	100
$C_X(\text{mol/m}^3)$	0	2.8	39	47	44	38.5	20	0

$$C_A = C_{A0} e^{-kt}$$

$$\text{Or } \ln C_A = \ln C_{A0} - kt$$



Thus from the graph of $\ln C_A$ vs t we get a straight line with intercept $\ln C_{A0}$. Thus it follows 1st order kinetics.

$$\text{We know, } \ln \frac{C_{A0}}{C_A} = (k_1 + k_2) * t$$

$$\text{And } k_1 + k_2 = k_{12}$$

$$\text{Therefore, } k_{12} = \frac{\ln(95.8) - \ln(12)}{0.1 - 5}$$

$$\text{Or } k_{12} = 0.42 \text{ min}^{-1}$$

$$\left(\frac{dC_R}{dt}\right)_{t=0} = \frac{1.4}{0.1} = k_2 C_{A0}$$

$$\text{Thus } k_2 = \frac{1.4}{(0.1) * (100)} = 0.14 \text{ min}^{-1}$$

$$\left(\frac{dC_X}{dt}\right)_{t=0} = \frac{2.8}{0.1} = k_1 C_{A0}$$

$$\text{So } k_1 = \frac{2.8}{(0.1) * (100)} = 0.28 \text{ min}^{-1}$$

Therefore, X is the intermediate product and has a maximum at 5 minutes.

→ for $C_{R0} = C_{X0} = 0$,

$$\frac{C_{Xmax}}{C_{A0}} = \frac{k_1 * k_{12}}{k_2 * k_{34}} \frac{k_{34}}{k_{34} - k_{12}}$$

Here $K_{34} = k_3$

$$\text{Thus } \frac{C_{Xmax}}{C_{A0}} = \frac{47}{100} = 0.47$$

$$\text{Or } 0.47 = \frac{0.28}{0.42} * \frac{0.42}{k_3 - 0.42} \frac{k_3}{k_3}$$

By using seek method we get, $k_3 = 0.067$

To verify whether the method is correct,

Recalculating C_R ,

$$\begin{aligned} \frac{C_R}{C_{A0}} &= \frac{k_1 k_3}{k_3 - k_{12}} \left(\frac{e^{-k_3 t}}{k_3} - \frac{e^{-k_{12} t}}{k_{12}} \right) + \frac{k_1}{k_2} + \frac{k_2}{k_{12}} (1 - e^{-k_{12} t}) \\ &= \frac{0.28(0.067)}{0.067 - 0.42} \left(\frac{e^{-0.067 * 5}}{0.067} - \frac{e^{-0.42 * 5}}{0.42} \right) + \frac{0.28}{0.42} + \frac{0.14}{0.42} (1 - e^{-0.42 * 5}) \end{aligned}$$

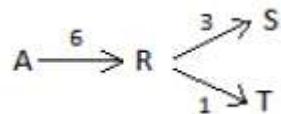
$$\rightarrow \frac{C_R}{C_{A0}} = 0.4087$$

Therefore $C_R = 0.4087 \times 100 = 40.87 \text{ or } 41 \text{ mol/m}^3$

At $C_{X_{\max}}$, i.e. $t = 5$ minutes

$$C_R = 41 \text{ mol/m}^3$$

Problem no. 8.21



$$k_1 = 6 \text{ hr}^{-1}$$

$$k_2 = 3 \text{ hr}^{-1}$$

$$k_3 = 1 \text{ hr}^{-1}$$

$$C_{A0} = 1 \text{ mol/litre}$$

$$\frac{C_{R_{\max}}}{C_{A0}} = \frac{k_1}{k_{12}} * \frac{k_{12}^{k_{34} - k_{12}}}{k_{34}}$$

Since $k_1 = k_{12}$ for one case,

$$\frac{C_{R_{\max}}}{C_{A0}} = \frac{6}{6} \left(\frac{6}{4}\right)^{(4/6)}$$

$$= \frac{3^2}{2}$$

$$\text{Therefore, } C_{R_{\max}} = \frac{4}{9} = 0.44 \text{ mol/litre}$$

$$t_{\max} = \frac{\ln(4/6)}{4-6} = 0.202 \text{ hours.}$$

Cre Term Paper
Submitted by – 13bch005, 13bch023,13bch041,13bch042

Problem 9.1

For the reacting system of example 9.4

- A) What τ is required for the 60 % conversion of reagent using the optimal progression of temperature in a flow reactor in piston?
 B) Find the outlet temperature of the reactor. Use $k_{10}=33*10^6$, $k_{20}= 1.8*10^{18}$

Use any information you need from the example 9.4

Solution

A)

The treaty system in the example 9.4 $A \leftrightarrow R$ with $-r_A = k_1 C_A - K_2 C_R$, where $k_1 = \exp(17,34 - 48900/RT)$ and $k_2 = \exp(42,04 - 124200/RT)$ and $C_0 = 4 \text{ mol/L}$. The chart shown in the example, to not be squared, makes the collection of data from it is very vague and that is why we are going to develop the necessary data, without using the chart.

If you want to find the optimal profile is considered that in the same

$$\left[\frac{d(-r_A)}{dT} \right] = 0$$

$$-r_A = k_1 C_{A0} (1 - X_A) - k_2 C_{A0} X_A$$

$$\frac{K_1}{K_2} = \frac{K_{01} \exp(\frac{E_1}{RT})}{K_{02} \exp(\frac{E_2}{RT})} = \frac{E_2 C_{A0} X_A}{E_1 C_{A0} (1 - X_A)} = \frac{E_2 X_A}{E_1 (1 - X_A)}$$

$$\exp \frac{E_2 - E_1}{RT} = \frac{K_{02} E_2 X_A}{K_{01} E_1 (1 - X_A)}$$

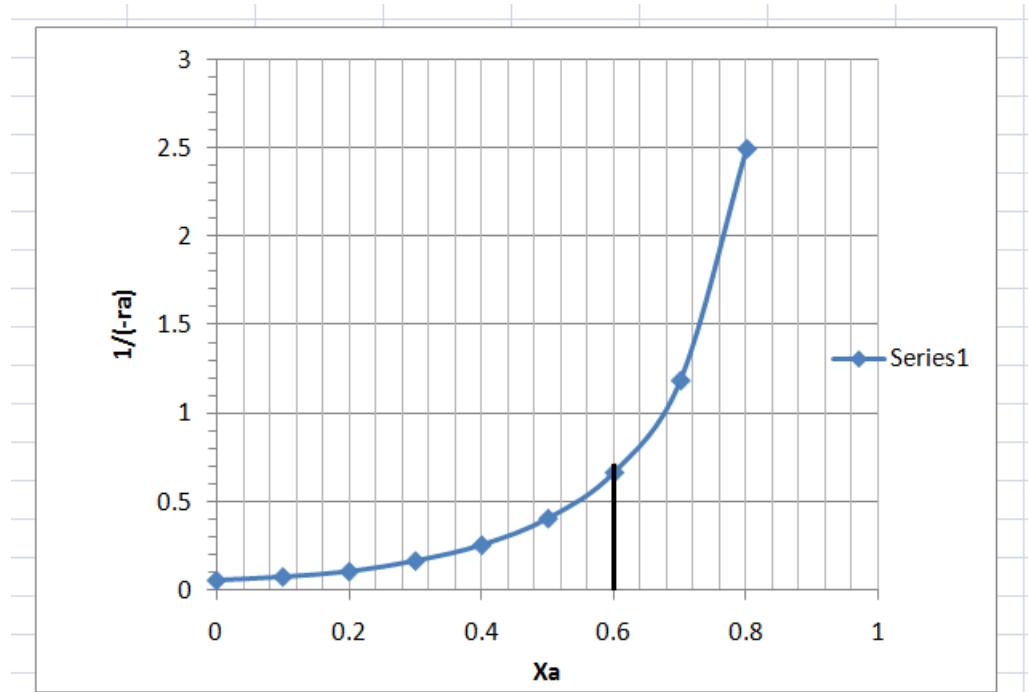
$$T_{opt} = \frac{\frac{E_2 - E_1}{R}}{\ln \frac{K_{02} E_2}{K_{01} E_1} + \ln \frac{X_A}{1 - X_A}}$$

With the previous equations and data taken from the example you can assess the temperature of the optimal profile for each X_A and then see how varies $-r$ with X_A along the optimal profile

X_{T0}	0	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8
$T_{opt} (\text{K})$	368	386,47	373,54	365,43	359,02	353,35	347,84	342,04	335,22
$-r_{to}$	15.54	12.29	9.04	5.89	3.79	2.43	1.49	0.84	0.40
$1/-R_{T0}$	0.06	0.08	0.11	0.17	0.26	0.41	0.67	1.19	2.5

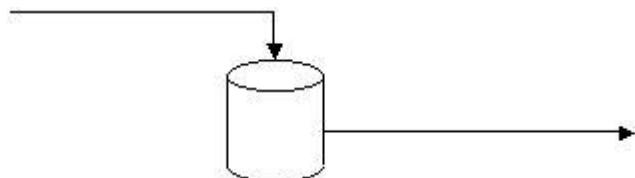
With these values are estimated the volume of flow reactor in piston, using area under the curve

$$\tau = C_{A0} \int_0^{X_a} \frac{dX_A}{-r_A} = 4 \int_0^{0.6} \frac{dX_A}{-r_A} = 0.558 \text{ min}$$



B)

In the table above we see that if X = 0.6 The temperature in the optimal profile is 347,84 K = 74,84°C



Problem 9.2 (p. 238)

You want to convert the concentrated aqueous solution of previous example ($C_0 = 4 \text{ mol/L}$; $F_0 = 1000 \text{ mol/min}$) up to 70 % with the smaller size of reactor for thorough mixing. Make an outline of recommended system, indicating the temperature of the input and output current and the required space weather

Solution

In the table that appears in the problem 9.1 we take the temperature and the speed of the optimal profile $X = 0.7$

$$T = 342.04 - 273 = 69^\circ\text{C}, -r_A = 0.84 \text{ mol/l min}$$

$$\tau_m = C_{A0} X_A / -r_A = 4(0.7) / 0.84 = 3.33 \text{ min}$$

$$X_A = C_p'(T - T_0) / -\Delta H_r, \quad T_0 = T + (X_A \Delta H_r) / C_p = 20^\circ C$$

Problem 9.3 (p. 238)

With regard to the flow reactor in piston which operates on the optimal profile The example 9.4 ($C_0 = 4 \text{ mol/L}$; $F_0 = 1000 \text{ mol/min}$; $X = 0.8$; $T_{\min} = 5^\circ C$; $T_{\max} = 95^\circ C$) and power and current product to $25^\circ C$, much heat or Cooling will be required
 (A)to the supply current
 (B)In the reactor itself
 (C)For the output current

Solution

In the table that appears in the problem 9.1 The temperature of the optimal profile for $X_A = 0.8$ is $335,22 \text{ K} = 62,22^\circ C$

$25^\circ C \quad 95^\circ C \quad \boxed{62.2^\circ C} \quad 25^\circ C$

$Q_1 \quad \quad \quad Q_3$

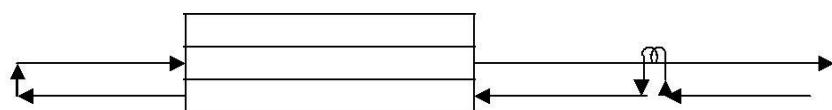
Q_2

$$Q_1 = c_p'(T_{\text{sat}} - T_{\text{exit}}) = 250 * 4187 * 70^\circ C = 73272,5 \text{ J/mol} \quad A = 73272,5 * 1000 = 73272,5 \text{ kJ/min}$$

$$Q_3 = c_p'(T_{\text{sat}} - T_{\text{exit}}) = 250 * 4187 * (25 - 62,2) * 1000 = -38939,1 \text{ kJ/min}$$

$$Q_2 = c_p'(T_{\text{sat}} - T_{\text{exit}}) = 250 * 4180 * (62,2 - 95) * 1000 = 34333,4 \text{ kJ/min}$$

There is that to provide the power $73272,5 \text{ kJ/min}$, while the output current there is that extract $38939,1 \text{ J/min}$. There are also removed from the reactor $34333,4 \text{ kJ/min}$. In total there are that remove $73272,5 \text{ kJ/min}$. I suggest the following



Problem 9.4 (p. 238)

It plans to carry out the reaction of the example 9.4 ($C_0 = 4 \text{ mol/L}$; $F_0 = 1000 \text{ mol/min}$) in a flow reactor in piston which is maintained at $40^\circ C$ to $X_{TO} = 90\%$. Find the required volume

Solution

Constant density system

$$k_I \tau / X_A = \ln(X_A/(X^* - X_A))$$

From example 9.4

$$k_I = \exp(17.34 - 48900/RT) \text{ min}^{-1}$$

$$K = \exp(75300/RT - 24.7) \quad R = 8.314 \text{ J/mol K}$$

$$T = 40 + 273 = 313$$

$$k_{313} = 0.2343 \text{ min}^{-1}$$

$$K_{313} = 69.1405$$

$$X_{AE} = K/(K+1) = 0.98$$

$$\tau_p = \frac{0.98}{0.2343} \ln \frac{0.98}{0.98 - 0.9} = 10.48 \text{ min}$$

Problem 9.5 (p. 238)

Rework the example 9.4 replacing C₀ with 1 mol/L/h.

Example 9.4. Using the optimal progression of temperature in a flow reactor in piston to the reaction of the previous examples. T_{max} = 95 °C

(a) Calculate the time space and the volume required for the 80 % conversion of 1000 mol to/min with C₀ = 4 mol/L

B) Plot the temperature and conversion profile along the reactor

Solution

Constant density system because it is Liquid

$$-r_A = k_1 C_{A0} (1 - X) - k_2 C_{A0} X_A = C_{A0} [k_1 (1 - X_A) - k_2 X_A]$$

$$(-r_A)_1 = [k_1 (1 - X_A) - k_2 X_A]$$

$$(-r_A)_4 = 4 [k_1 (1 - X_A) - k_2 X_A] = 4 (-r_A)_1$$

$$\int_0^{0.8} \frac{dX_A}{(-r_A)_1} = \int_0^{0.8} \frac{dX_A}{(-r_A)_4} = 4 \int_0^{0.8} \frac{dX_A}{(-r_A)_4}$$

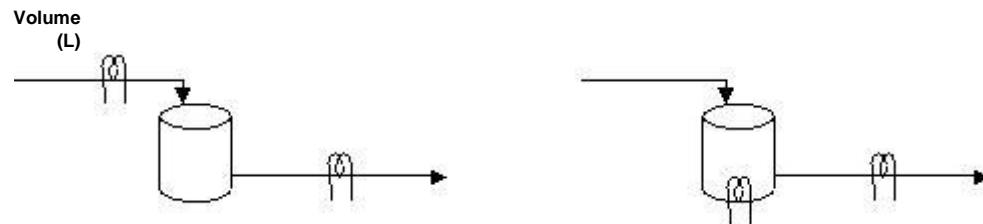
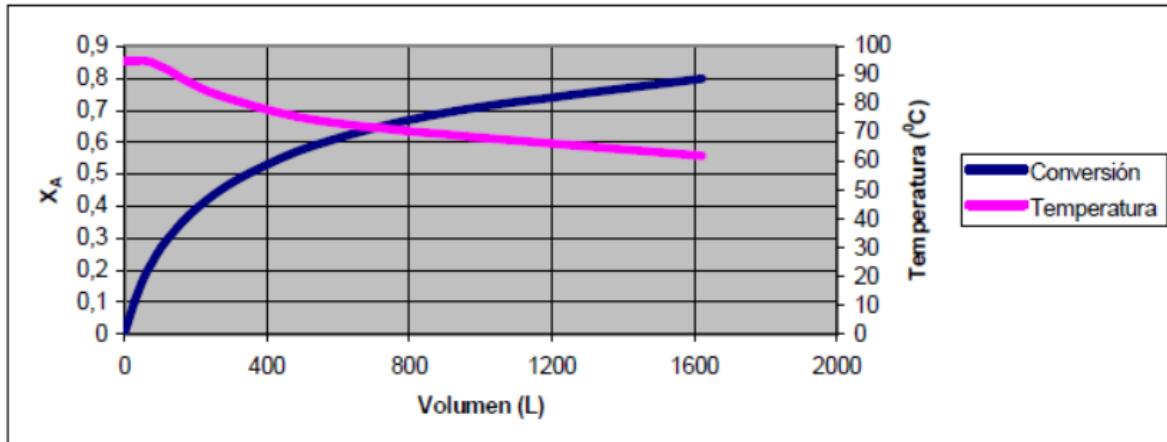
$$\int_0^{0.8} \frac{dX_A}{(-r_A)_4} = 0.405 \text{ taken from the example 9.4 (p. 230)}$$

$$\int_0^{0.8} \frac{dX_A}{(-r_A)_1} = 4(0.405)$$

$$\tau_p = \frac{1}{C_{A0}} \int_0^{0.8} \frac{dX_A}{(-r_A)_1} = 1 \int_0^{0.8} \frac{dX_A}{(-r_A)_4} = (1)(4)(0.405) = 1.63 \text{ min}$$

$$v_0 = F_{A0}/C_{A0} \\ = 1000 \text{ L/min} \\ V = \tau v_0 = 1620 \text{ L}$$

As they are reactions of first order the change in the value of C_0 did not affect the value of τ . The volume if it is affected because F_0 remained constant and therefore v_0 increased 4 times, causing the volume is 4 times more.



Problem 9.6 (p. 238)

Rework the example 9.5 replacing C_{A0} with 1 mol/L

Example 9.5. The concentrated solution of the previous examples ($C_0 = 4 \text{ mol/L}$; $F_0 = 1000 \text{ mol/min}$) is going to be 80% converted into a complete mix reactor

(A) What size reactor is required?

(B) What should be the transfer of heat if the power is at 25°C and the output current must be at the same temperature?

Solution

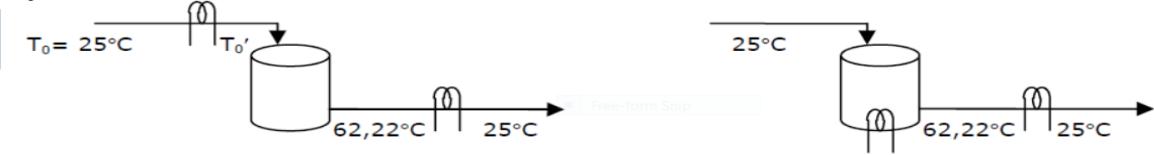
A) in the table of the problem 9.1 appears which the speed in reported the optimal profile $X = 0.8$ is 0.4 mol/l min; but for $C_{A0} = 4 \text{ mol/l}$ and that is needed is the corresponding to $C_0 = 1 \text{ mol/L}$

$$-r_{A1} = -r_{A4}/4 = 0.4/4 = 0.1 \text{ mol/Lmin}$$

$$\tau = C_{A0} X_A / -r_A = 1(0.8) / 0.1 = 8 \text{ min}, v_0 = 1000 \text{ L/min}$$

$$V = \tau v_0 = 8(1000) = 8000 \text{ L}$$

b)



Case 1

$$Q = c_p(T - T_0) + H X_A$$

$$0 = 250 * 4187 * (62.22 - T_0) + (-18000)(4187)(0.8)$$

$$T_0 = 4.62^\circ\text{C}$$

$$Q_1 = 250(4187)(4.62 - 25) = 21332.765 \text{ J/mol A}$$

$$Q_2 = 250(4187)(25 - 62.22) = -38960.035 \text{ J/mol A}$$

Case 2

$$Q_1' = 250(4187)(62.22 - 25) + (18000)(4187)(0.8) = -21332.765 \text{ J/mol A}$$

It can be seen that both forms of exchange of heat are equivalent

Problem 9.7 (p. 238)

Rework the example 9.6; but with $C_0 = 1 \text{ mol/l}$ instead of $C_0 = 4 \text{ mol/L}$ and recital $F_A0 = 1000 \text{ mol to/min}$

Example 9.6. Find the size of the flow reactor in piston required to convert up to 80 % the 1000 mol to/min with $C_0 = 4 \text{ mol/L}$, which is used in the example 9.5

Solution

In the example 9.6 appears that

$$T_{4\text{mol/L}} = 4 \int_{0}^{0.8} \frac{dX_A}{(-r_A)_{4\text{mol/L}}} = 8.66 \text{ min}$$

$$T_{1\text{mol/L}} = (1) \int_{0}^{0.8} \frac{dX_A}{(-r_A)_{1\text{mol/L}}} \\ (-r_A)_{4\text{mol/L}} = 4 (-r_A)_{1\text{mol/L}} \quad (-r_A)_{1\text{mol/L}} = (-r_A)_{4\text{mol/L}} / 4$$

$$T_{1\text{mol/L}} = (1) \int_{0}^{0.8} \frac{dX_A}{(-r_A)_{1\text{mol/L}}}$$

$$(-r_A)_{4\text{mol/L}} = 4 (-r_A)_{1\text{mol/L}} \quad (-r_A)_{1\text{mol/L}} = \frac{(-r_A)_{4\text{mol/L}}}{4}$$

$$T_{1\text{mol/L}} = (1) \int_0^{0.8} \frac{dX_A}{(-r_A)_{4\text{mol/L}}} = 4 \int_0^{0.8} \frac{dX_A}{(-r_A)_{1\text{mol/L}}} = 8.66 \text{ min}$$

$$V_{1\text{mol/L}} = \tau_{1\text{mol/L}}(v_0) = 8.66(1000/1) = 8660 \text{ L} = 8.66 \text{ m}^3$$

As is noted for a reaction of the first order, the τ is not dependent on C_{A0} ; but the volume yes because F_{A0} remains constant, that is to say that v_0 varied.

Problem 9.8 (p. 238)

Solution

$$(-r_A)_{4\text{mol/L}} = 4 (-r_A)_{1\text{mol/L}}$$

$$\frac{1}{(-r_A)_{4\text{mol/L}}} = \frac{1}{4} \frac{1}{(-r_A)_{1\text{mol/L}}}$$

$$\frac{1}{(-r_A)_{1\text{mol/L}}} = 4 \frac{1}{(-r_A)_{4\text{mol/L}}}$$

The scale of the fig. E9.7 (p. 234) is multiplied by 4 if it reduces the C_0 from 4 to 1 mol/L

Area under the curve of $1/-R_{t0}$ vs X to the example 9.7 with 4 mol/L $C_{A0} = 1.2$ Area under the curve of $1/-R_{t0}$ vs X with 1 mol/L $C_{A0} = 1.2 (4) = 4.8 = \tau/C_0$

$$T = 4.8 (1) = 4.8 \text{ min} \text{ (the same } \tau \text{ the example)}$$

$$V = \tau v_0 = 4.8 (1000) = 4800 \text{ L} \text{ (4 times larger than that of the example)}$$

Space weather is not affected by the variation of the concentration; but if F_0 remains constant volume v_0 varies

Problem 9.9 (p. 238)

You want to carry out the reaction of the example 9.4 in a reactor complete mix up to 95 % conversion of a power supply with $C_{A0} = 10 \text{ mol/L}$ and a volumetric flow of 100 L/min What size reactor is required?

Solution

$$T = \frac{\frac{E_2 - E_1}{R}}{\ln \frac{k_0 E_2}{k_0 E_1} + \ln \frac{X_A}{1-X_A}} = \frac{\frac{124200 - 48900}{8.314}}{\frac{e^{42.04}(124200)}{e^{17.34}(48900)} + \ln \frac{.95}{1-0.95}} = 316.94 \text{ K}$$

$$-r_A = 10 \left\{ \left[\exp \left(17.34 - \frac{48900}{RT} \right) \right] (1 - Xa) - \left[\exp \left(42.04 - \frac{124200}{RT} \right) (Xa) \right] \right\}$$

$$-r_A = 0.0897 \text{ L/mol min}$$

$$T_m = C_{A_0} X_A / -r_A = 10(0.95) / 0.0897 = 105.91 \text{ min}$$

$$V = \tau_m v_0 = 10590,85 \text{ L} \approx 10.6 \text{ m}^3$$

Problem 9.10 (p. 239)

As $E_1 < E_2$, low temperature at the beginning of the reaction is good to produce more of R

As $E_3 > E_4$, increasing the temperature when the reaction has already advanced induces to produce S which is the desired product. As $E_3 < E_5$ also $E_3 < E_6$, lowering the temperature in the final stages of the reaction while deduce the disintegration of S hence we can maximize concentration of S.

Problem 9.11 (p. 239)

If we analyze the E / R is concluded that in the first stage reaction (decomposition of A) the temperature should be in the high and then in low end. Let the values of the kinetic constants in the 2 extreme temperatures

T (° C)	K1	K2	K1/K2	K3	K4	K3/K4
10	0.62	7.27	0.085	$1.51 \cdot 10^{-6}$	$3.84 \cdot 10^{-7}$	4.00
90	66.31	163.82	.4	$1.71 \cdot 10^{-3}$	$4.40 \cdot 10^{-3}$	0.39

An analysis of the values of the constants is concluded what we already knew and more;

We know that the profile should be decreasing because the first reaction must occur in the decomposition of A and R is favored with high temperatures ($k_1 / k_2 = 0.4$ at 90 ° C), after lowering the temperature must

because the formation of S is favored by low temperatures ($k_3 / k_4 = 4.00$ at 10 ° C). Add to this, we did not know that k_1 and $k_2 \gg K_3$ and K_4 , then A is exhausted practically without R being reacted yet. It can therefore assumed that in the first tank only decomposition of A occurs and in the second of R. Thus the first tank is kept at 90 ° C and second at 10 ° C

$$\varphi_r = \frac{r_r}{-r_a} = \frac{k_1}{k_1 + k_2} = \frac{66.31}{163.82 + 66.31} = 0.288$$

$$\varphi_s = \frac{r_s}{-r_r} = \frac{k3}{k3 + k4} = \frac{1.51 * 10^{-6}}{1.51 * 10^{-6} + 3.84 * 10^{-7}} = 0.8$$

$$\varphi\left(\frac{S}{A}\right) = \varphi_R * \varphi_S = 0.288 * 0.8 = 0.2304$$

Problem 9.12 (p. 239)

The reversible reaction in the gaseous phase to $\leftrightarrow R$ is going to be carried out in a reactor of thorough mixing. If operated at 300 K the required volume of the reactor is 100 L for a 60 % conversion. What should be the volume of the reactor for the same power and the same conversion; but operating at 400 K.

Data: To Pure $K_1 = 10^3 \exp(-2416/T)$ $C_p' = 0$
 $K = 10$ to 300 K $H_r = -8000 \text{ cal/mol}$ to 300 K

Solution

With the data to 300 K you can calculate v_0 and v_0 the required volume to 400 K. It should be noted that v_0 varies by varying the temperature and that H_r is constant because $C_p' = 0$

$$t_m = \frac{V_m}{v_0} = \frac{C_{A0}X_A}{-r_A} = \frac{C_{A0}X_A}{K_1 C_{A0}(1-X_A) - K_2 C_{40}X_A} = \frac{X_A}{K_1(1-X_A) - K_2 X_A}$$

$$V_0 = V_m \left(\frac{K_1(1-X_A) - K_2 X_A}{X_A} \right)$$

$$K_{1(300k)} = 0.318 \text{ min}^{-1}$$

$$K_{2(300k)} = \frac{K_1}{K} = \frac{0.318}{10} = 0.0318 \text{ min}^{-1}$$

$$V_0 = \frac{100[0.318(1-0.6) - 0.0318(0.6)]}{0.6} = 18.2 \text{ L/min}$$

$$K_{400k} = K_{300k} \exp\left[-\frac{H_r}{R}\left(\frac{1}{400} - \frac{1}{300}\right)\right] = 10 \exp\left[-\frac{8000}{8314}\left(\frac{1}{400} - \frac{1}{300}\right)\right] = 4.485$$

$$K_{1(400k)} = 2.382 \text{ min}^{-1}$$

$$K_{2(400k)} = \frac{2.382}{4.485} = 0.531 \text{ min}^{-1}$$

$$V_{0(400k)} = V_{0(300k)}\left(\frac{400}{300}\right) = 18.02\left(\frac{400}{300}\right) = 24.03 \text{ L/min}$$

$$V = V_0 \left(\frac{X_A}{K_1(1-X_A) - K_2 X_A} \right) = 24.03 \left[\frac{0.6}{2.382(1-0.6) - 0.531(0.6)} \right] = 22.73 \text{ L}$$

Example 10.1

Given the two reaction



Where R is the desired product and is to be maximized. Rate the four schemes shown in Fig.P10.1-either “good” or “not so good.” Please, no complicated calculations, just reason it out.

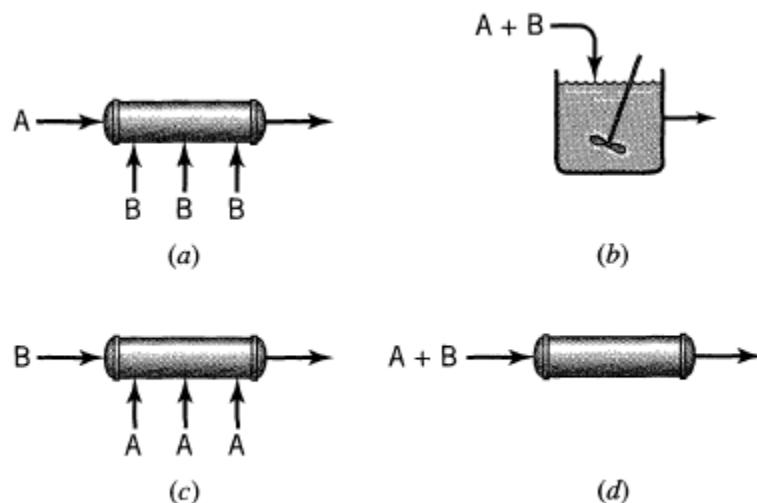


Figure P10.1

Answer:

$$\varphi = \frac{dC_R}{dC_A} = \frac{r_R}{-r_A} = \frac{k_1 C_A C_B - k_2 C_A C_B}{k_1 C_A C_B} = \frac{k_1 - k_2}{k_1}$$

The distribution of products (R / S) is determined by the ratio of k_1 / k_2 because reactions are of the same order with respect to A and B, so if I want more R, as in a simple reaction, which X_A require is greater. This is achieved by working with maximum speeds. Assuming isothermal operation, $-r_A$ grows when the concentration is high, so considering all of the above

(D) The C_A and C_B better because high (Very good)

- (A) is equally good because here C_A is in excess quantity. so formation of R is really high compare to formation of S.
- (C) Not so good. because C_B is in excess quantity. So rate of formation is S is very high compare to rate of formation of R.
- (B) The worse because both concentrations are low.

Example 10.2

Repeat Problem 1 with just one change

$$-r_2 = k_2 C_R C_B^2$$

Answer:

$$\varphi = \frac{\frac{dC_R}{dC_A}}{\frac{r_R}{-r_A}} = \frac{\frac{k_1 C_A C_B - k_2 C_R C_B^2}{k_1 C_A C_B}}{1} = 1 - \frac{k_2 C_R C_B}{k_1 C_A}$$

It is a typical reaction series and parallel performance tells us that precisely. We must analyze separately the components in series and components in parallel.

$A \rightarrow R \rightarrow S$ are in series so it should not be high.

The reagent parallel, B, has a lower order than the desired reaction unwanted, so B should be maintained at low concentrations and also we take difference is high so A has as high as possible.

- (A) The best Design because high C_A and low C_B .
- (B) and (D) Intermediate because in (B) C_A and C_B and lower (D) C_A and C_B high, only meet one requirement both

(C) The worse Design because C_A low and C_B high means difference is less so Desired quantity is R which is less form because Formation R it instantaneously react with B (It is in excess quantity) and form S. Which is undesired for us.

Example: 10.3

Repeat Problem 1 with just one change

$$-r_2 = k_2 C_R^2 C_B$$

Answer:

$$\varphi = \frac{dC_R}{dC_A} = \frac{r_R}{-r_A} = \frac{k_1 C_A C_B - k_2 C_R^2 C_B}{k_1 C_A C_B} = 1 - \frac{k_2 C_R^2}{k_1 C_A}$$

It is a parallel reaction and performance series tells us just that. We must analyze separately the components in series and components in parallel.

$A \rightarrow R \rightarrow S$ are in series so C_A should be high

The reagent parallel, B, has the same order that the desired reaction the unwanted, so B does not influence the distribution of products.

(A) and (d) are the best because high

(B) and (C) worse (not so good) design because rate is mainly dependent on C_R and also C_A is in denominator so A is low necessary but after it decreases concentration of R. and formation of S is high in (C).

Example: 10.4

For the reaction





Where R is the desired product, which of the following ways of running a batch reactor is favourable, which is not ? See Fig. P10.4

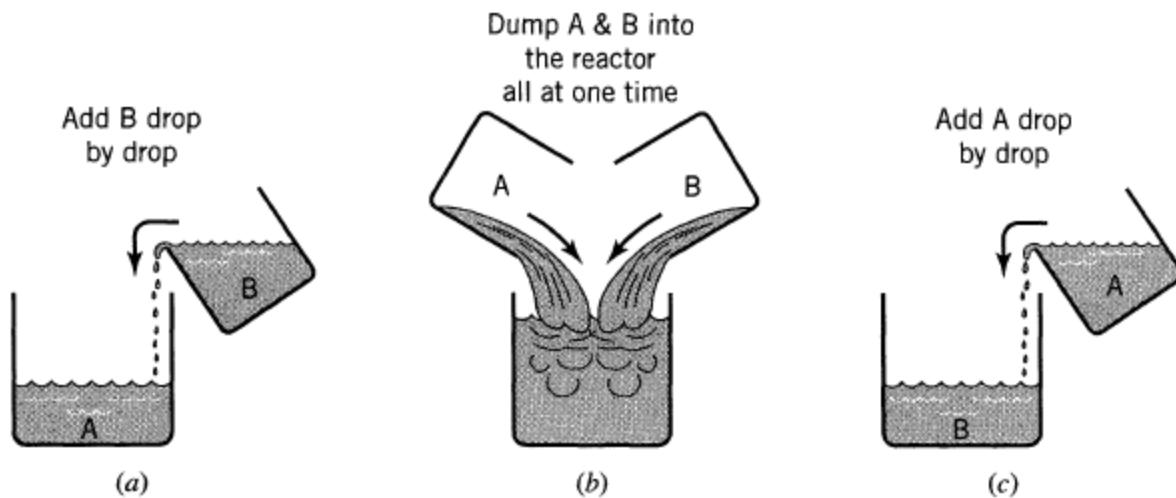


Figure P10.4

Answer:

(A) better because high CA and CB low

(B) Intermediate because CA = CB low. considering the third alternative where the contents of the two beakers are rapidly mixed together, the reaction being slow enough so that it does not proceed to any appreciable extent before the mixture becomes uniform. During the first few reaction increments R finds itself competing with a large excess of A for B and hence it is at a disadvantage. Carrying through this line of reasoning, we find the same type of distribution curve as for the mixture in which B is added slowly to A.

(C) The CA worse because low CA and high CB, is not suitable. For the first alternative pour A a little at a time into the beaker containing B, stirring thoroughly and making sure that all the A is used up and that the reaction stops before the next bit is added. With each addition a bit of R is produced in the beaker. But this R finds itself in an excess of B so it will react further to form S.

The result is that at no time during the slow addition will A and R be present in any appreciable amount. The mixture becomes progressively richer in S and poorer in B. This continues until the beaker contains only S.

Example: 10.5

The Oxydation of Xylene. The violent oxidation of xylene simply produces CO_2 and H_2O ; however, when oxidation is gentle and carefully controlled, it can also produce useful quantities of valuable phthalic anhydride as shown in Fig.P10.5. Also, because of the danger of explosion, the fraction of xylene in the reacting mixture must be kept below 1%. Naturally, the problem in this process is to obtain a favourable product distribution.

- (a) In a plug flow reactor what values of the three activation energies would require that we operate at the maximum allowable temperature?
- (b) Under what circumstances should the plug flow reactor have a falling temperature progression?

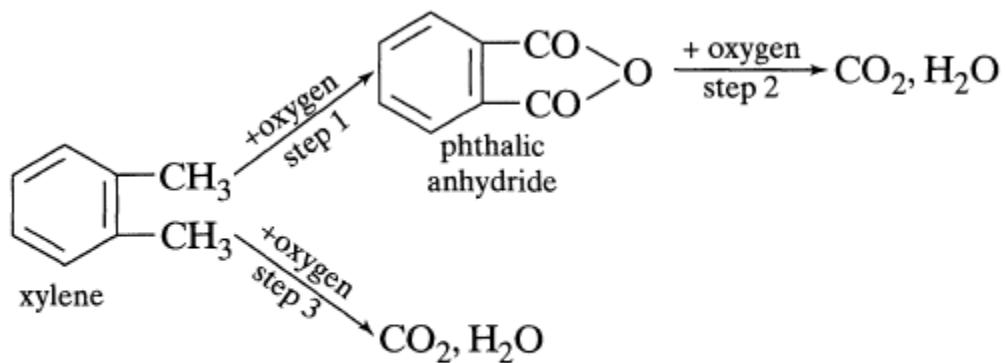


Figure P10.5

Answer:

- a) If $E_1 > E_2$ and $E_1 > E_3$

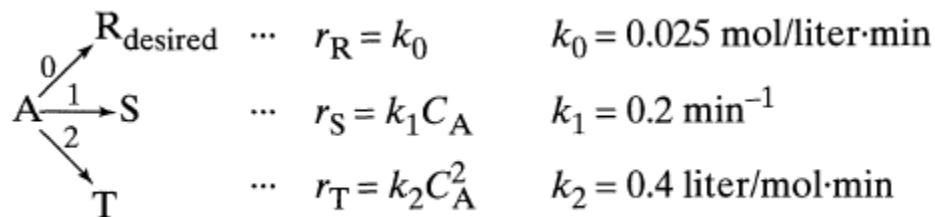
The most desired is the activation energy and will be favored by high temperatures, so it must work to the maximum allowable temperature.

- b) If $E_1 > E_3$ and $E_1 < E_2$

At first you must work with high temperatures to encourage 1 against the reaction 3 and then the temperature should drop to not favor the profile step 2. It is then to be used is decreasing.

Example 10.6

The Trambouze Reactions - Reactions in parallel. Given the set of elementary reactions with a feed of $C_{A0} = 1 \text{ mol/liter}$ and $V = 100 \text{ liters/min}$ we wish to maximize the fractional yield, not the production of S, in a reactor arrangement of your choice.



- Do you judge that arrangement of Fig.P10.6 is the best set up?
- If not, suggest a better scheme. Sketch your scheme and calculate the volume of the reactors you plan to use.

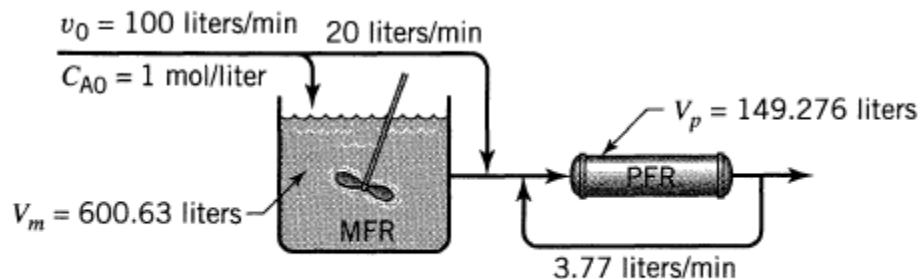


Figure P10.6

Answer:

$$\begin{array}{lll}
 \text{A} \rightarrow \text{R} & r_{\text{R}} = k_0 & k_0 = 0.025 \text{ mol/L min} \\
 \text{A} \rightarrow \text{S} & r_{\text{S}} = k_1 C_{\text{A}} & k_1 = 0.2 \text{ min}^{-1} \\
 \text{A} \rightarrow \text{T} & r_{\text{T}} = k_2 C_{\text{A}}^2 & k_2 = 0.4 \text{ L/mol min}
 \end{array}$$

The order of the desired reaction determines how they should be the concentrations, whether high or low. In this case

$$\text{Order A} \rightarrow \text{R} < \text{Order A} \rightarrow \text{S} < \text{Order A} \rightarrow \text{T}$$

The order of reaction is the desired intermediate. C_A favor high $A \rightarrow R$ and C_A low to $A \rightarrow T$. It is obvious that there must be an intermediate concentration $A \rightarrow S$. To find that C_A makes performance maximum must be raised that $d\phi(S/A) / dC_A = 0$

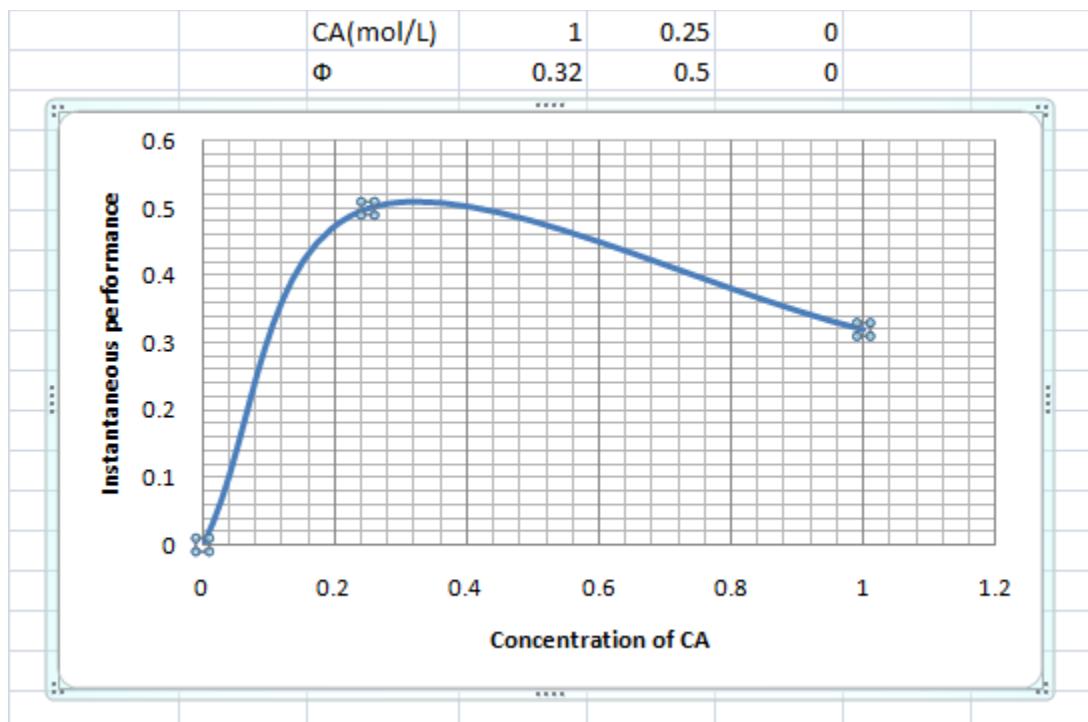
$$\Phi\left(\frac{S}{A}\right) = \frac{0.2 CA}{0.025 + 0.2 CA + 0.4 CA^2}$$

$$\frac{d\phi\left(\frac{S}{A}\right)}{dC_A} = \frac{(0.025 + 0.2 CA + 0.4 CA^2)0.2 - 0.2 CA(0.2 + 0.8 CA)}{(0.025 + 0.2 CA + 0.8 CA^2)^2} = 0$$

$$0.025 + 0.2 C_A + 0.4 C_A^2 + 0.2 C_A - 0.8 C_A^2 = 0$$

$$C_A = \pm \sqrt{\frac{0.025}{0.4}} = \pm 0.25$$

The only possible solution is $C_A = 0.25 \text{ mol / L}$ and the concentration value making the most appropriate performance



It is best to work with a mix Flow reactor that throughout the reactor instant performance equals 0.5 which is its maximum value.

b)

$$\tau = \frac{C_{A0} - C_A}{-r_A} = \frac{C_{A0} - C_A}{0.025 + 0.2C_A + 0.4C_A^2} = \frac{1 - 0.25}{0.025 + 0.2(0.25) + 0.4(0.25^2)} = 7.5 \text{ min}$$

$$V = \tau V_0 = 7.5(100) = 750 \text{ L}$$



$$C_S = \Phi \left(\frac{S}{A} \right) (C_{A0} - C_A) = 0.5(1 - 0.25) = 0.375$$

Example 10.7

For the set of elementary reaction of problem 10.6, with a feed of $C_{A0} = 1 \text{ mol/liter}$ and $v = 100 \text{ liters/min}$ we now wish to maximize the production rate of intermediate S (not the fractional yield) in a reactor arrangement of your choice. Sketch your chosen scheme and determine $C_{S \text{ max}}$ obtainable.

Answer:

Given the shape of the curve φ vs C_A there to work with a reactor will complete mixture $C_A = 1$ to 0.25 mol / L , which will have the maximum performance and with this a series of plug flow reactor that $C_A = 0.25$ go from to 0 mol / L , to take advantage as much as possible high yields. The final concentration is 0 because if $\Delta C_A \uparrow \Delta C_R \uparrow$ and C_R wants maximum

$$C_{S \text{ max}} = C_{S \text{ m}} + C_{S \text{ p}}$$

$$C_{S \text{ max}} = 0.5(1 - 0.25) = 0.375 \text{ mol/liter}$$

$$C_{S \text{ p}} = \int_0^{0.25} \varphi dC_A = \int_0^{0.25} \frac{0.2 C A dC_A}{0.025 + 0.2 C_A + 0.4 C_A^2}$$

Dividing numerator and denominator by 0.4

$$C_{sp} = 0.5 \int_0^{0.25} \frac{CA \, dCA}{0.0625 + 0.5CA + CA^2} = 0.5 \int_0^{0.25} \frac{CA \, dCA}{(0.25 + CA)^2}$$

$$\int \frac{xdx}{(a+bx)^2} = \frac{1}{b^2} \left[\ln(a+bx) + \frac{a}{a+bx} \right]$$

$$C_{sp} = 0.5 \left\{ \frac{1}{1^2} \left[\ln(0.25 + C_A) + \frac{0.25}{0.25 + CA} \right]^{0.25} \Big|_0 \right\}$$

$$= 0.5 \left[\ln(0.25 + 0.25) + \frac{0.25}{0.25 + 0.25} - \ln(0.25) - \frac{0.25}{0.25} \right]$$

$$C_{sp} = 0.5 \left[(\ln 2) - 0.5 \right] = 0.0966 \text{ mol/L}$$

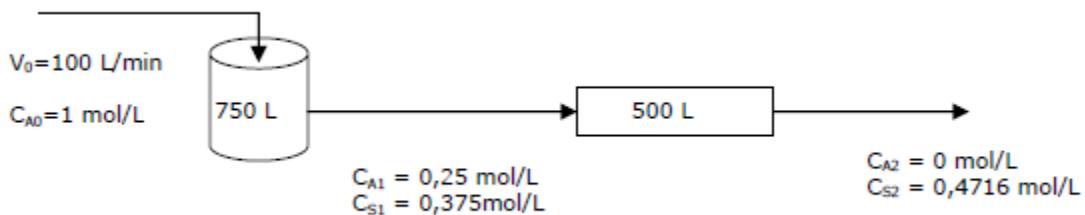
$$C_{smax} = 0.375 + 0.0966 = 0.4716 \text{ mol/L}$$

$$\tau_p = \int_0^{0.25} \frac{dC_A}{-r_A} = \int_0^{0.25} \frac{dC_A}{0.025 + 0.2C_A + 0.4C_A^2} = \frac{1}{0.4} \int_0^{0.25} \frac{dC_A}{(0.25 + C_A)^2}$$

$$\int \frac{dx}{(a+bx)^2} = -\frac{1}{b(a+bx)}$$

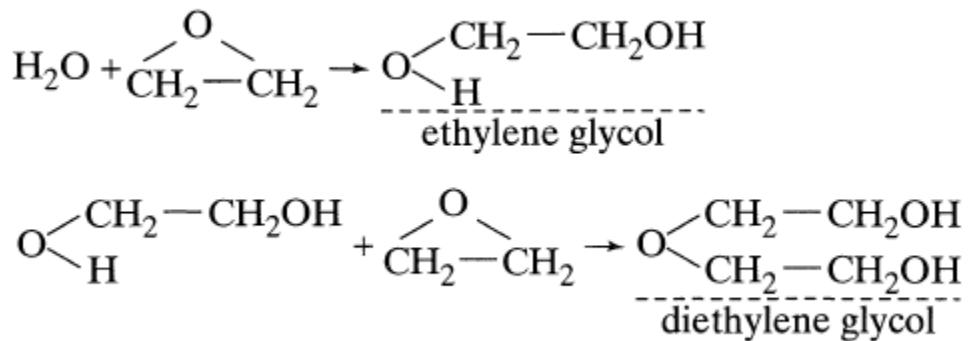
$$\tau_p = 2.5 \left\{ -\frac{1}{0.25 + C_A} \right\}^{0.25}_0 = 2.5 \left\{ -\frac{1}{0.5} + \frac{1}{0.25} \right\} = 5 \text{ min}$$

$$V_p = 5(100) = 500 \text{ L}$$



Example 10.8

Automobile Antifreeze Ethylene glycol and diethylene glycol are used as automobile antifreeze, and are produced by the reactions of ethylene oxide with water, as follows:



A mole of either glycol in water is as effective as the other in reducing the freezing point of water; however, on a molar basis the diethylene glycol is twice as expensive as the ethylene glycol. So we want to maximize ethylene glycol, and minimize the diethylene glycol in the mixture.

One of the country's largest suppliers produced millions of kilograms of antifreeze annually in reactors shown in Fig. P10.8a. One of the company's engineers suggested that they replace their reactors with one of the type shown in Fig. P10.8b. What do you think of this suggestion?

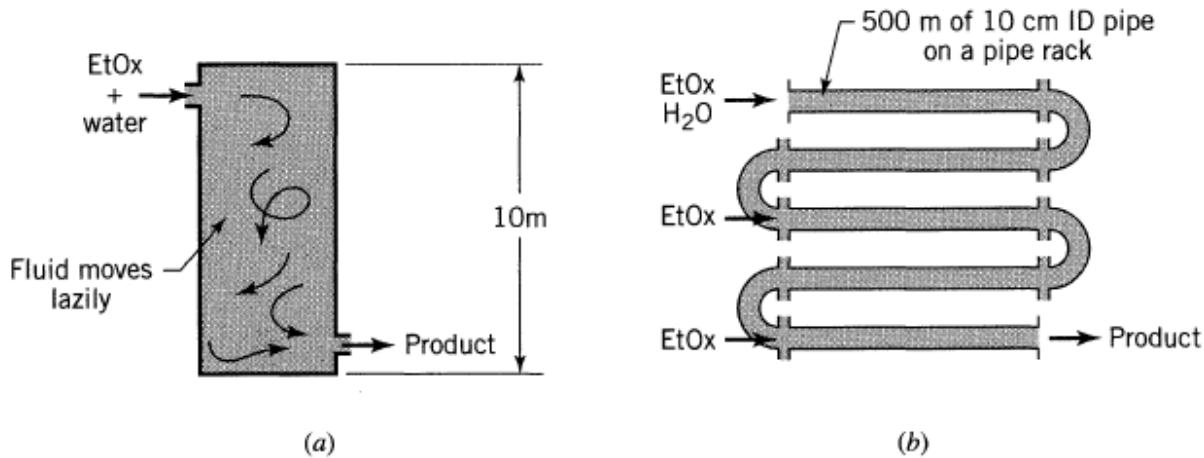
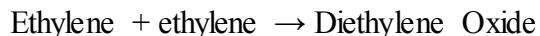
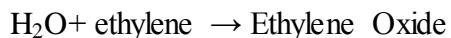


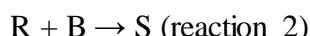
Figure P10.8a & P10.8b

Answer:



If $\text{H}_2\text{O} = \text{A}$, $\text{Y} = \text{ethylene oxide}$, $\text{ethylene glycol} = \text{R}$ and $\text{diethylene} = \text{S}$

The reaction can be expressed as



Analyzing the components in series $\text{A} \rightarrow \text{R} \rightarrow \text{S}$ is the most convenient plug flow reactor and the reactor of Figure (b) may be considered as diameter / length such by their relationship.

As for the addition of B, the component parallel can not conclude nothing because the reaction order of this component is not known in the desired and undesired reaction. If the desired out the higher order, then the addition of B, which raises the concentration of this component is appropriate.

We select PFR because length/diameter ratio is high in PFR and also undesired quantity (diaethylene glycol) is less.

Example 10.9

The Homogeneous catalytic Reaction. Consider the elementary reaction



For the following feed and reactor space time

$$\text{Flow rate} \quad v = 100 \text{ liters/min}$$

$$\text{Feed composition} \quad \begin{cases} C_{\text{A}0} = 0.45 \text{ mol/liter} \\ C_{\text{B}0} = 0.55 \text{ mol/liter} \end{cases}$$

$$\text{Space time} \quad \tau = 1 \text{ min}$$

We want to maximize the concentration of B in the product stream. Our clever computer [see problem 8, Chem. Eng. Sci., 45, 595-614 (1990)] gives the design of Fig. P10.9 as its best try.

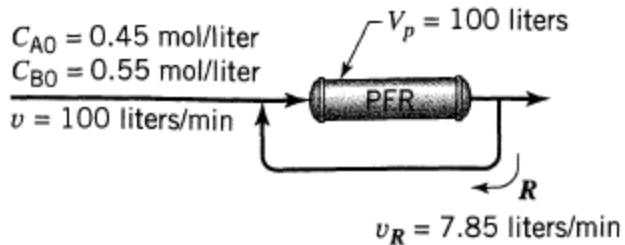


Figure P10.9

Do you think that this is the best way to run this reaction? If not, suggest a better scheme. Do not bother to calculate reactor size, recycle rate, etc. Just indicate a better scheme.

Answer:

As this is a simple reaction system criteria used is As the production efficiency, the more efficient is the system having higher speeds. So to know what is more suitable reactor is need to know how the conversion varies with $-r_A$

$$-r_A = kC_A C_B \text{ (Elementary system)}$$

$$C_A = C_{A0}(1-X_A)$$

$$C_B = C_{B0} - C_{A0}X_A + 2C_{A0}X_A \text{ (for stoichiometry)}$$

$$C_B = C_{A0}(M + X_A), \text{ where } M = \frac{C_{B0}}{C_{A0}} = \frac{0.55}{0.45} = 1.22$$

$$-r_A = k C_{A0}^2 (1-X_A)(M + X_A)$$

If $X_A \uparrow$, $(1-X_A) \downarrow$ so you can increase or decrease, according to the relative weight of the factors
 One way to know how varies $-r_A$ with X_A is to find the derivative of the function.

$$\frac{-dr_A}{dX_A} = k C_{A0}^2 [(1-X_A)(1) + (M + X_A)(-1)] = k C_{A0}^2 (1-M-2X_A) < 0$$

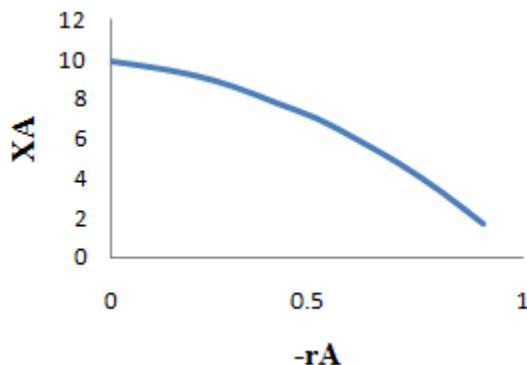
If we consider that $M = 1.22$ and analyze the derivative we see that it is negative over the entire range of conversions, indicating that the function is decreasing for any value of X_A , i.e., the speed decreases to increase conversion.

Another way to know how to vary the speed conversion, less accurate, it is to evaluate the function in the interval.

$$-r_A = 0.4 (0.45)^2 (1 - X_A) (1.22 + X_A)$$

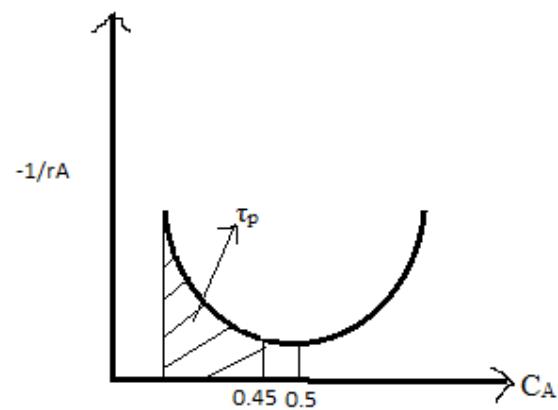
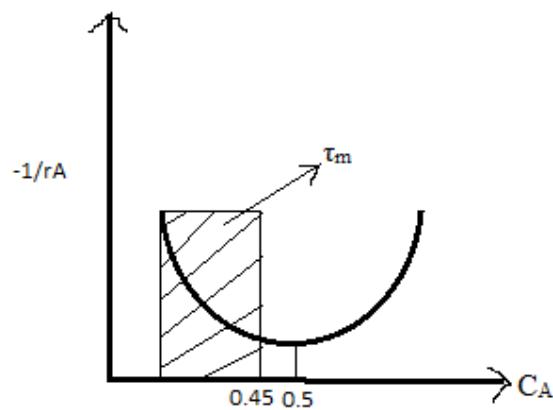
$$-r_A = 0.081 (1 - X_A) (1.22 + X_A)$$

X_A	0	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9
$-r_A \cdot 10^{-2}$	9.9	9.6	9.2	8.6	7.8	7.0	5.9	4.7	3.3	1.7



The higher speed is $X_A = 0$ (high concentrations) so that the reactor It is best piston without recycling, because the recycle low profile concentrations occurring in the reactor and thus lower the speed occurring in the reactor.

Compare both PFR and MFR



Here Plug flow is best design. but here recycling is not required if recycle then it is against the assumption of PFR.

Example 10.10

To Color Cola Drinks. When viscous corn syrup is heated it caramelizes (turns a deep dark brown). However, if it is heated a bit too long it transforms into carbon

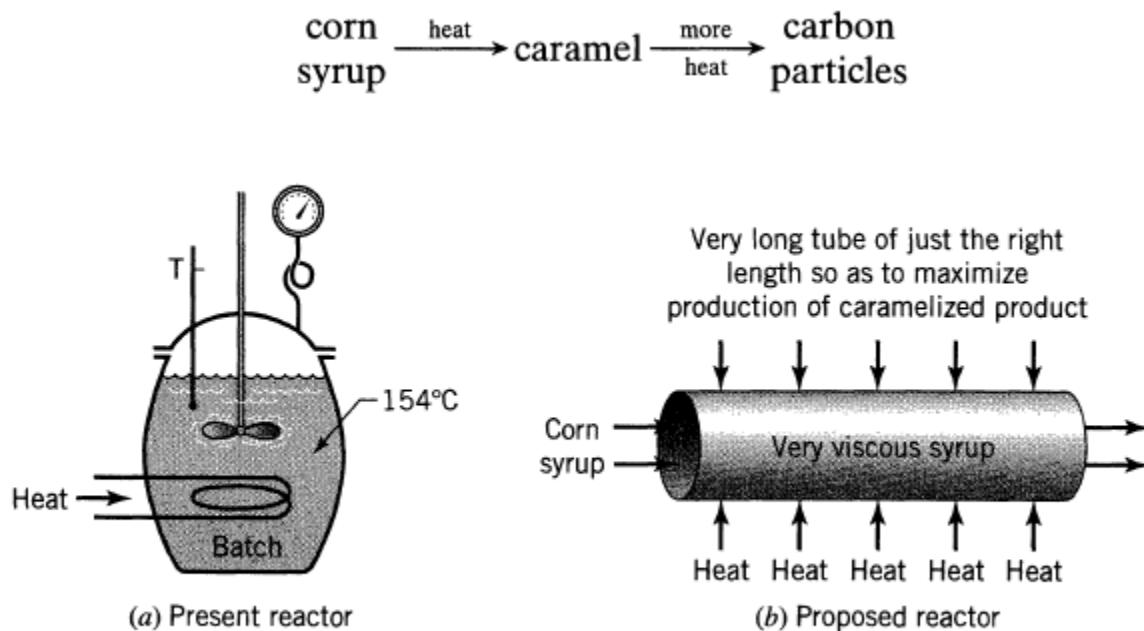


Figure P10.10 (a) Present reactor; (b) Proposed design.

The caramelized liquid is sent by railroad tank cars to the cola syrup formulators, who then test the solution for quality. If it is too light in color-penalty; if it has too many carbon particles per unit volume, then the whole tank car is rejected. There is thus a delicate balance between underreacting and overreacting.

At present a batch of corn syrup is heated at 154°C in a vat for a precise time. Then it is rapidly discharged and cooled, the vat is thoroughly cleaned (very labor intensive), and then is recharged.

The company wants to reduce costs and replace this costly labor intensive batch operation with a continuous flow system. Of course it will be a tubular reactor (rule 2). What do you think of their idea? Comment. please, as you sit and sip your Coke or Pepsi.

Answer:

The substitution is theoretically substantiated that over piston take place the same story of concentrations, and therefore speeds, which occur with time in the batch, and It was further added advantage of continuous operation.

However, in this system is formed inevitably solid, which adhere to the reactor wall to some extent (which is why the cleaning batch reactor was a daunting) task is that if the liquor is viscous and heated through the walls will create a temperature gradient and coal to be formed will adhere to the pipe walls preventing proper operation. or that think about stopping and clean the pipe.

10.11 A → R → S

$$C_{AO} = 6 \quad CR_O = 0.6 \quad CT_O = 0$$

The feed has $CR/CT = \infty$

- a) So to maximise CR/CT do not react at all, the design of figure is not good.
- b) To minimise CR/CT , run to completion. All the R will disappear.

Next reaction 1 is second order }
 Reaction 2 is first order } keep CA low
 So, use a large MFR you will end up with more CT

10.12 $C_{AO} = 90 \text{ mol/m}^3, C_{BO} = 10 \text{ mol/m}^3$ 

If we want minimum volume, which will be efficient in terms of production and with maximum speed, we have to know how rate varies with speed

$$-r_A = k C_A C_B$$

$$C_A = C_{AO} (1 - X_A) = C_{AO} (1 - X_A)$$

$$C_B = C_{BO} - C_{AO} X_A + 2 C_{AO} X_A = C_{AO} (M + X_A) \text{ where } M = C_{AO}/C_{BO}$$

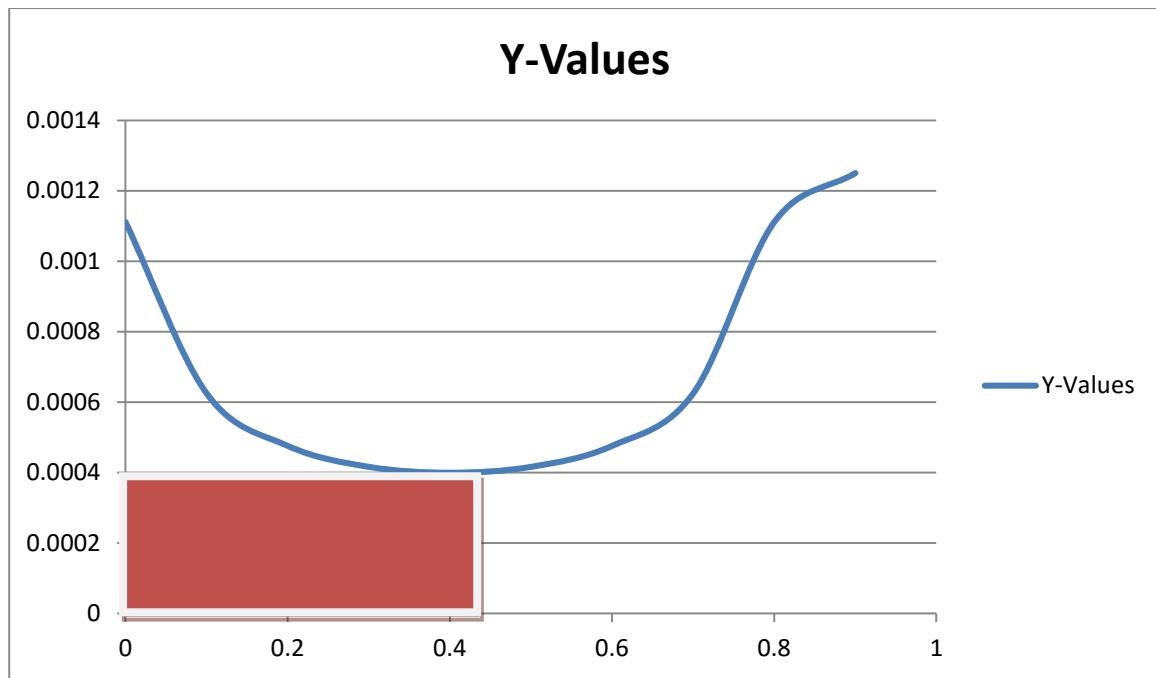
$$-r_A = k C_{AO}^2 (1 - X_A) (M + X_A)$$

$$\left(\frac{d(-r_A)}{dX_A} \right) = k C_{AO}^2 (1 - X_A) (M + X_A)$$

$M = 1/9 = 0.11$, so the derivative is positive for low values X_A and negative for high values and maximum $-r_A$ the derivative is 0, so
 $X_A = (1 - M)/2 = 0.44$

Speed will be : $(-r_A/k) = 8100 (1 - X_A) (1/9 + X_A)$

X_A	0	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9
$-r_A/k$	900	1600	2100	2400	2500	2400	2100	1600	900	810



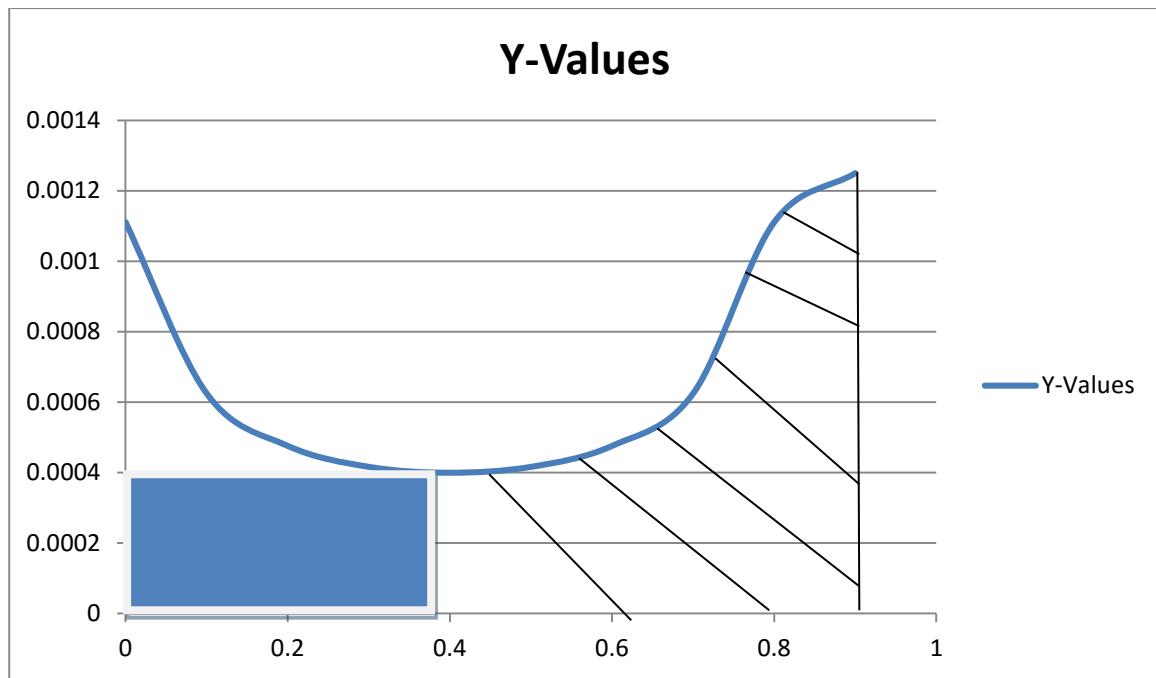
Use a MFR

10.13

$A \rightarrow B$ $B + B$

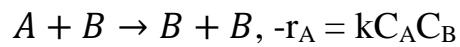
$$-r_A = KCACB \quad CA_f = 9 \quad CB_f = 91$$

$$CA_o = 90 \quad CB_o = 10$$



Use a MFR followed by a PFR

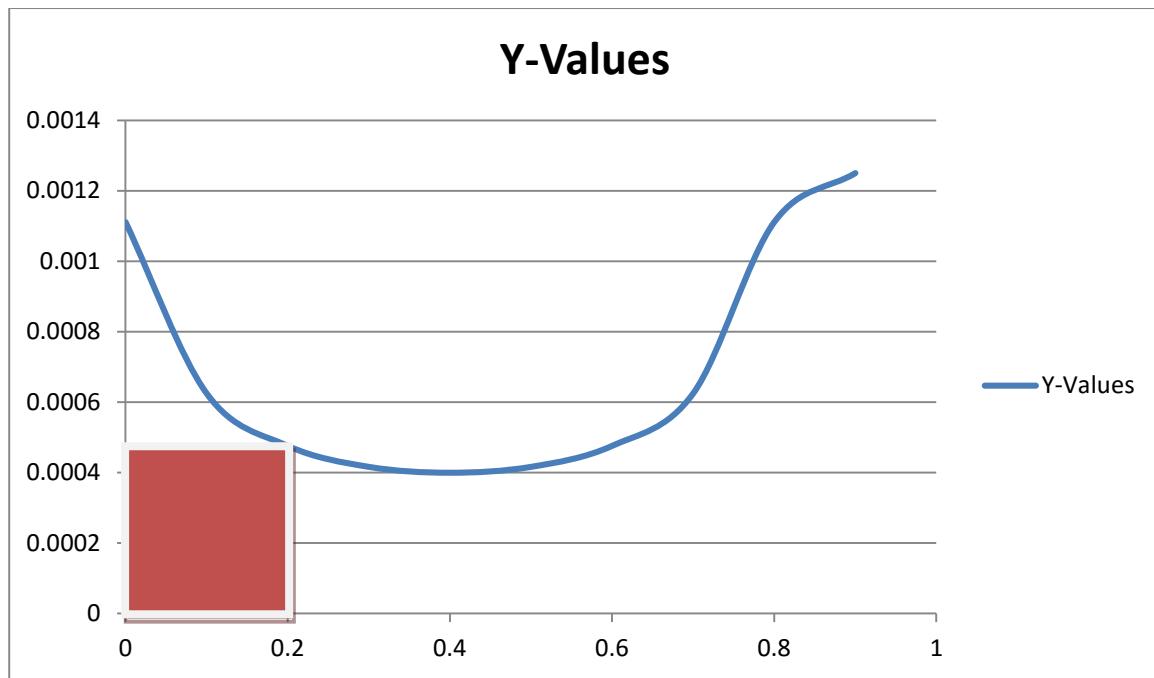
10.14



$$C_{A0} = 90 \text{ mol/m}^3 \quad C_{Af} = 72 \text{ mol/m}^3$$

$$C_{B0} = 10 \text{ mol/m}^3 \quad C_{Bf} = 28 \text{ mol/m}^3$$

X_A	0	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8
$-r_A/k$	900	1600	2100	2400	2500	2400	2100	1600	900



As curve $k/-r_A$ vs X_A downward slope in the range $X_A = 0$ to 0.2 , it is best to work with a mixing reactor complete, which will have the higher speed range and therefore will require the least τ . And for the 20% conversion it will give the lower volume as compared the other reactors.

10.15

Since $E_1 > E_2$ use a high temperature or $T = 90^\circ\text{C}$

At 90°C , $k_1 = 30e^{-20000/8.314(363)} = 0.0397 \text{ min}^{-1}$

$$k_2 = 1.9e^{-15000/8.314(363)} = 0.0132 \text{ min}^{-1}$$

Therefore, $k_2/k_1 = 0.3322$

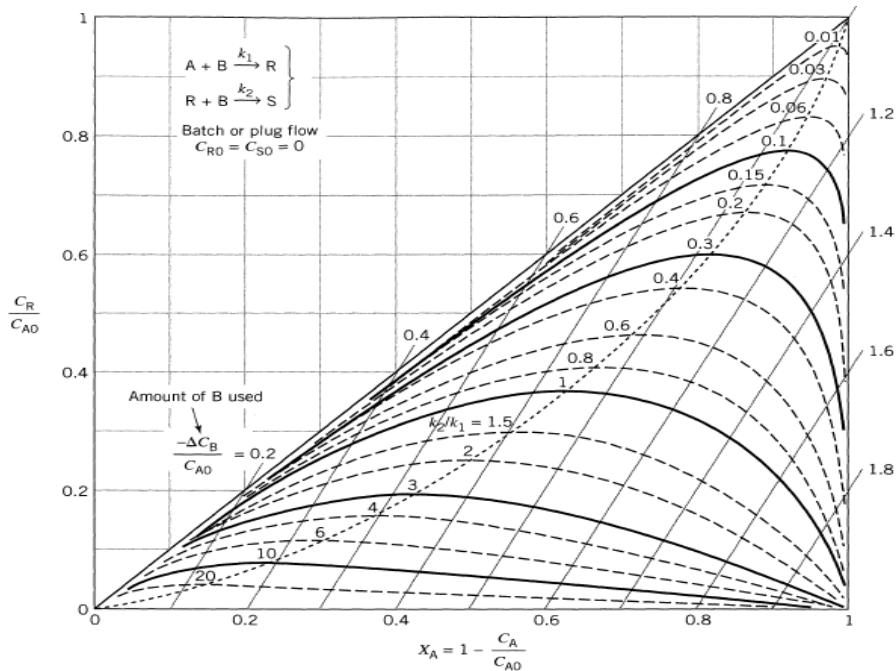


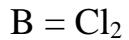
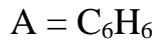
Figure 8.13 Distribution of materials in a batch or plug flow reactor for the elementary series-parallel reactions

Therefore, Form the above fig, $C_{R\max}/C_{A0} = 0.58$

$$t_{\text{opt}} = [\ln(k_2/k_1)]/[k_2 - k_1] = (\ln 0.3322)/(0.0132 - 0.0397) \\ = 4.16 \text{ min}^{-1}$$

10.16

The following system of elementary reactions have



It is best to use a plug flow reactor. You should not use the first recycle reactor. It should work at low conversions of benzene. For example,

$$X_A = 0.4,$$

with $k_2 / k_1 = 0.1335$, $C_R / C_{A0} = 0.3855$, $C_S / C_{A0} = 0.0145$ and $C_R / C_S = 26.68$.

10. 17- Let $A = C_3H_6$ $B = O_2$ $R = C_3H_4O$

Then $A + B \rightarrow R$ $K_2/K_1 = 0.1$

$A + 4.5B \rightarrow S$ $K_3/K_1 = 0.25$

$A \rightarrow R \rightarrow S$

From the Denbigh reaction

$$CR_{max}/CA_0 = K_1/K_2(K_{12}/K_3)^{(K_3/K_3 - K_{12})}$$

$$= 10/11 * (11/25)^{(2.5/2.5 - 11)}$$

$$= 0.588$$

10.18

It is a series parallel system, so selection is based on analyzing their series and parallel components as separate components. Parallel components are $A \rightarrow R$ and $A \rightarrow T$ and if we see the orders of the reactions, lower order is desired, therefore taking into account parallel components concentration must be kept low during the course of the reaction.

Series components are $A \rightarrow R \rightarrow S$ and R is the desired as having into account the components in series the concentration of A must remain as high as possible during the course of the reaction.

There is a contradiction and the final decision depends on the relative weight of reactions.

Considering the kinetic constants

T (K)	k_1	k_2	k_3	k_1/k_3	k_1/k_2
360	0.1306	0.0560	0.00006	2176	2.33
396	0.9700	0.1530	0.00120	808.3	6.3

Analysis of this table we see that between 360 and 396 K, $k_3 \ll k_1$ and k_1 and k_2 are almost similar.

The reaction $A \rightarrow T$ $\frac{1}{2}$ can be neglected because it occurs slowly compared to the other. if so then the plug flow reactor is the most convenient.

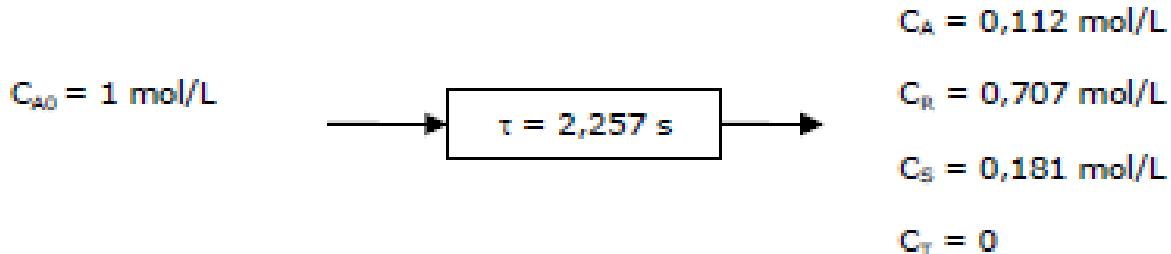
b) Working with a piston 396 K

$$\frac{Cr}{Cao} = \left(\frac{k1}{k2} \right)^{\frac{k2}{k2-k1}}$$

$$Cr = 0.707 \text{ mol/L}$$

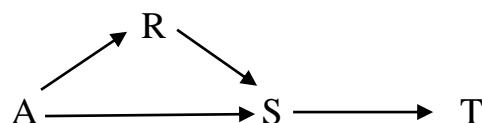
$$\tau = \left(\frac{\ln \frac{k2}{k1}}{k2 - k1} \right) = 2.252 \text{ s}$$

$$Xa = 1 - \exp(-k1\tau) = 0.888$$



QUES: 10.19 Phthalic Anhydride from Naphthalene.

The accepted mechanism for the highly exothermic solid catalysed oxidation of naphthalene to produce Phthalic anhydride is



Where

$$k_1 = k_2 = 2 * 10^{13} \exp(-159000/RT) [\text{hr}^{-1}]$$

$$k_3 = 8.15 * 10^{17} \exp(-209000/RT) [\text{hr}^{-1}]$$

$$k_4 = 2.1 * 10^5 \exp(-83600/RT) [\text{hr}^{-1}]$$

And where

A = naphthalene (reactant)

R = naphtha Quinone (postulated intermediate)

S = phthalic anhydride (desired product)

T = $\text{CO}_2 + \text{H}_2\text{O}$ (waste products)

and the Arrhenius activation energy is given in units of J/mol. This reaction is to be run somewhere between 900 K and 1200 K.

A local optimum reactor setup discovered by the computer [see example 1, *Chem. Eng. Sci.*, **49**, 1037-1051 (1994)] is shown in Fig. P10.19.

- Do you like this design? Could you do better? If so, how?
- If you could keep the whole of your reactors at whatever temperature and τ value desired, and if recycle is allowed, how much phthalic anhydride could be produced per mole of naphthalene reacted?

Suggestion: Why not determine the values of k_1 , k_2 , k_3 , and k_4 for both extremes of temperature, look at the values, and then proceed with the solution?

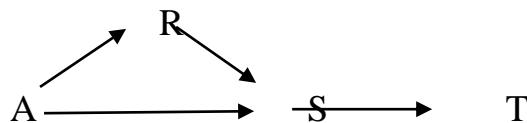
SOLUTION:

Given,

$$k_1 = k_2 = 2 * 10^{13} \exp(-159000/RT) [\text{hr}^{-1}]$$

$$k_3 = 8.15 * 10^{17} \exp(-209000/RT) [\text{hr}^{-1}]$$

$$k_4 = 2.1 * 10^5 \exp(-83600/RT) [\text{hr}^{-1}]$$



Since k_4 value is much smaller than the other values of k we use the highest allowable temperature of 1200K.

$$k_1 = 2.4 * 10^6 \text{ hr}^{-1}$$

$$k_2 = 2.4 * 10^6 \text{ hr}^{-1}$$

$$k_3 = 650 * 10^6 \text{ hr}^{-1}$$

$$k_4 = 48.2 \text{ hr}^{-1}$$

Now,

Since k_3 value is much bigger than k_2 value we can approximate the reaction as follows.



Now we find $C_{R\max}$

$$\frac{C_{R\max}}{C_{A0}} = \left(\frac{K_5}{K_6} \right)^{\frac{K_6}{K_6 - K_5}} = \left(\frac{4.8 \times 10^6}{48.2} \right)^{\frac{48.2}{48.2 - (4.8 \times 10^6)}} = 0.99988$$

$$t_{\text{plug}} = \frac{\ln\left(\frac{k_2}{k_1}\right)}{k_2 - k_1} = 2.4 \times 10^{-6} \text{ hr} = \mathbf{0.0086 \text{ sec} = \text{time of residence}}$$

With such a small time and high conversion practically we can use any type of reactor but we are using a straight plug flow reactor with no recycle which is the best.

Now we find C_R for this residence time

$$\frac{C_R}{C_{A0}} = \frac{k_5}{k_5 - k_6} [e^{-k_1 t} - e^{-k_2 t}] = (-1) [0 - 0.9762] = \mathbf{0.9762 = C_R}$$

10.20. Professor Turton dislikes using reactors in parallel, and he cringed when he saw my recommended "best" design for Example 10.1. He much prefers using reactors in series, and so for that example he suggests using the design of Figure E10.1a, but without any *recycle* of fluid. Determine the fractional yield of S, Φ (S/A), obtainable with Turton's design, and see if it matches that found in Example 10.1

SOLUTION:

Here,

$$\tau_1 = \frac{V}{25} = \frac{C_{A0} - C_{A1}}{(-rA)_1}$$

$$\tau_2 = \frac{V}{50} = \frac{C_{A1'} - C_{A2}}{(-rA)_2}$$

$$\text{where } C_{A1'} = \frac{1}{2} C_{A1} + \frac{1}{2}$$

$$\tau_3 = \frac{V}{75} = \frac{C_{A2'} - C_{A3}}{(-rA)_3}$$

$$\text{where } C_{A2'} = \frac{2}{3} C_{A2} + \frac{1}{3}$$

$$\tau_4 = \frac{V}{100} = \frac{CA3' - 0.25}{(-r_A)25}$$

$$\text{where } CA_3' = \frac{3}{4} CA_3 + \frac{1}{4}$$

It is a set of 4 equations and 4 unknowns, so it is determined; but must be solved by trial and error and once you know the C_R concentrations determine the output of each reactor. It is clear that the procedure is quite cumbersome and graphical method for solving the material balance of the reactor mixture can help to the solution. According to the method the operating point reactor located where the curve ($-r_A$) vs C_A is cut with balance materials in the plane ($-r_A$) - C_A is a straight line passing through the reactor inlet concentration and whose slope $-1 / \tau_1$.

$$(-r_A) = 0.025 + 0.2 C_A + 0.4 (C_A)^2$$

CA	0.6	0.55	0.5	0.45	0.4	0.35	0.3	0.25	0.2	0.15	0.1	0.05
(-r _A)	0.625	0.256	0.225	0.196	0.169	0.144	0.121	0.100	0.081	0.064	0.049	0.036

The steps followed in solving the problem are:

1. With these values the curve ($-r_A$) is obtained vs C_A
2. It is assumed C_{A1} and τ_1 is calculated by equation 1
3. τ_1 is calculated V
4. V is calculated τ_2 , and $\tau_1 \tau_3$
5. $C_A = \frac{1}{2} C_{A1} + \frac{1}{2}$, and τ_2 operating point is calculated reactor 2
6. $C_{A2} = \frac{2}{3} + \frac{1}{3} C_{A2}$ and τ_3 the operating point is calculated reactor 3
7. $C_{A3} = \frac{3}{4} C_{A3} + \frac{1}{4}$ and τ_4 operating point is calculated reactor 4
8. If $C_{A4} = 0.25$, the assumed value of C_{A1} is correct, if not return to Step 2

Suppose $C_{A1} = 0.3$

$$V = \frac{(1 - 0.3)(25)}{0.025 + 0.2(0.3) + 0.4(0.3^2)} = 144.6281 \text{ L}$$

$$T_2 = \frac{144.6281}{50} = 2.8925 \text{ min} \quad \Rightarrow \quad \frac{1}{T_2} = 0.3457$$

$$T_3 = \frac{144.6281}{75} = 1.9283 \text{ min} \quad \Rightarrow \quad \frac{1}{T_3} = 0.5186 \text{ min}^{-1}$$

$$T_2 = \frac{144.6281}{100} = 1.4462 \text{ min} \quad \Rightarrow \quad \frac{1}{T_2} = 0.6914 \text{ min}^{-1}$$

$$C'_{A1} = 0.2(3) + 12 = 0.65 \text{ mol/L}$$

$$C'_{A2} = 2(0.3, 3) + 13 = 0.5333 \text{ mol/L}$$

$$C'_{A3} = 3(0.4, 3) + 14 = 0.475 \text{ mol/L}$$

Suppose $C_{A1} = 0.25$

$$V = \frac{(1 - 0.25)(25)}{0.025 + 0.2(0.25) + 0.4(0.25^2)} = 187.5 \text{ L}$$

$$T_2 = \frac{187.5}{50} = 3.75 \text{ min} \quad \Rightarrow \quad \frac{1}{T_2} = 0.2667 \text{ min}^{-1}$$

$$T_3 = \frac{187.5}{75} = 2.5 \text{ min} \quad \Rightarrow \quad \frac{1}{T_3} = 0.4 \text{ min}^{-1}$$

$$T_2 = \frac{187.5}{100} = 1.875 \text{ min} \quad \Rightarrow \quad \frac{1}{T_2} = 0.5333 \text{ min}^{-1}$$

$$C'_{A1} = \frac{0.25}{2} + \frac{1}{2} = 0.625 \text{ mol/L}$$

$$C'_{A2} = \frac{2(0.25)}{3} + \frac{1}{3} = 0.5 \text{ mol/L}$$

$$C'_{A3} = \frac{3(0.25)}{4} + \frac{1}{4} = 0.4375 \text{ mol/L}$$

CRE 1 Unsolved examples chapter 11

11.1. A pulse input to a vessel gives the results shown in Fig. P11.1.

(a) Check the material balance with the tracer curve to see whether the results are consistent.

(b) If the result is consistent, determine t , V and sketch the E curve.

Ans. Area Under the curve = $C_{pulse} \times t = 0.05 \times 5 = 0.25$ mol min. / lit.

a. $M = 1$ mol at $t = 0$ (given); $v = 4$ lit. / min.

$$\text{Therefore, } \frac{M}{v} = \frac{1}{4} = 0.25 \text{ mol min. / lit.}$$

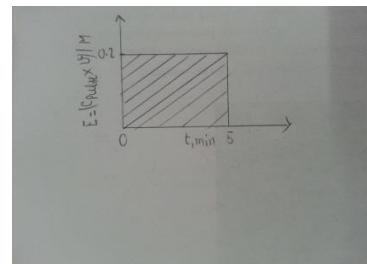
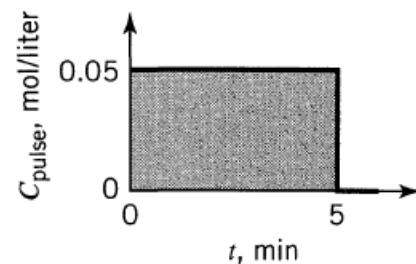
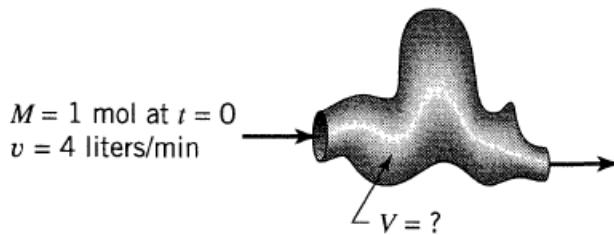
Since Area Under the curve equals $\frac{M}{v}$ the results are consistent.

b. $T_{\text{average}} = \frac{(\sum t_i C_i)}{\sum C_i} = \frac{(5 \times 0.05)}{0.05} = 5 \text{ min.}$

$$\text{Therefore, } T_{\text{average}} = \frac{V}{v}$$

$$V = T_{\text{average}} \times v = 5 \times 4 = 20 \text{ liters}$$

$$E = (C_{pulse} \times v) / M = (0.05 \times 4) / 1 = 0.2$$



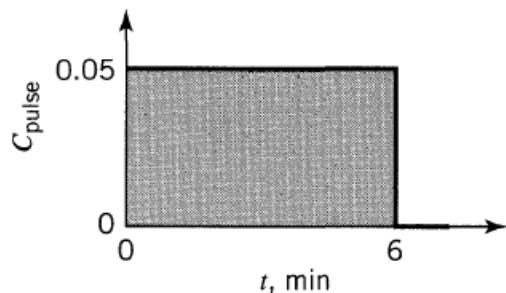
11.2. Repeat Problem P11.1 with one change: The tracer curve is now as shown in Fig. P11.2.

Ans. From the previous sum $\frac{M}{v} = \frac{1}{4} = 0.25 \text{ mol min. / lit.}$

Area Under the curve = $C_{\text{pulse}} \times t = 0.05 \times 6 = 0.3 \text{ mol min. / lit.}$

Therefore, $\frac{M}{v} \neq C_{\text{pulse}} \times t$

The tracer comes out late hence the experiment is not done correctly.



11.3. A pulse input to a vessel gives the results shown in Fig. P11.3.

- (a) Are the results consistent? (Check the material balance with the experimental tracer curve.)
 (b) If the results are consistent, determine the amount of tracer introduced M,

Ans. $v = 4 \text{ cm}^3/\text{s}$ $V = 60 \text{ cm}^3$

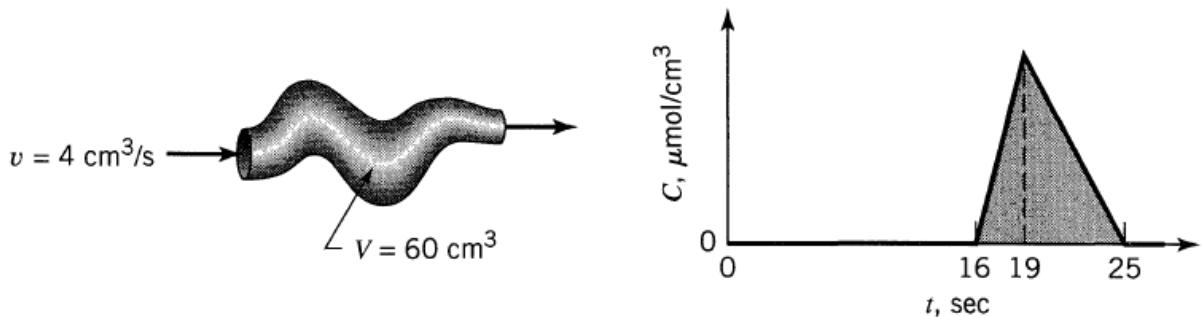
In Pulse Input $t_{\text{average}} = \frac{V}{v} = 60/4 = 15 \text{ s}$

From the graph (assuming the value of tip to be C)

$$\text{Area} = \frac{1}{2}[(3 \times C) + (6 \times C)] = 9 \times \frac{C}{2}$$

$$t_{\text{average}} = \frac{\sum t C \Delta t}{\text{Area}} = \frac{[(16 \times 0) + (19 \times C) + (25 \times 0)]}{\frac{9C}{2}} = \frac{38}{9}$$

Since t_{average} is not the same the result is not consistent



11.4. A step experiment is made on a reactor. The results are shown in Fig. P11.4.

(a) Is the material balance consistent with the tracer curve?

(b) If so, determine the vessel volume V , 7

Ans. Since Value of C_{\max} is not given this problem cannot be solved

11.6. A pipeline (10 cm I.D., 19.1 m long) simultaneously transports gas and liquid from here to there. The volumetric flow rate of gas and liquid are $60\ 000 \text{ cm}^3/\text{s}$ and $300 \text{ cm}^3/\text{s}$, respectively. Pulse tracer tests on the fluids flowing through the pipe give results as shown in Fig. P11.6. What fraction of the pipe is occupied by gas and what fraction by liquid?

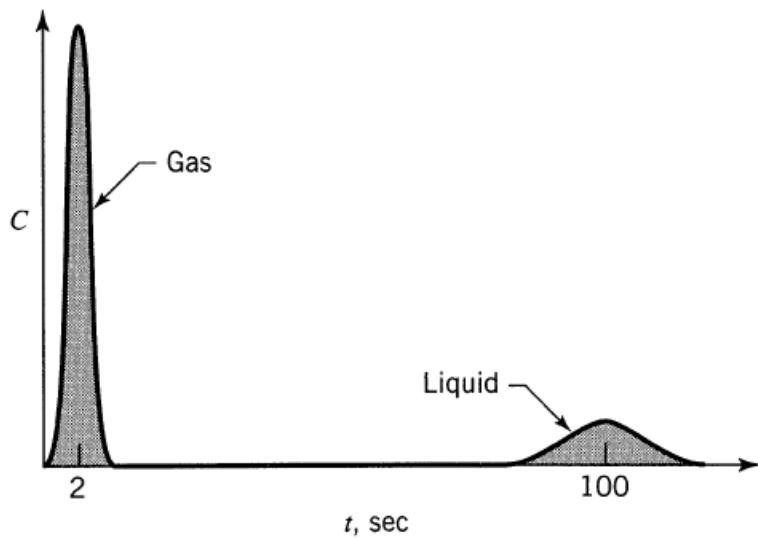


Figure P11.6

Ans. $V = \pi/4 \cdot D^2 \cdot H$

$$= \pi/4 \cdot 10^2 \cdot 10^{-4} \cdot 19.1 \text{ [Given } D=10\text{cm and } H= 19.1\text{m}]$$

$$\therefore V_T = 0.15$$

$$V_G = 60000 \text{ cm}^3/\text{s}$$

$$t_{RG} = 2\text{s}$$

$$V_G = 60000 \cdot 10^{-6} \cdot 2 \text{ m}^3$$

$$= 0.12 \text{ m}^3$$

$$V_L = 300 \text{ cm}^3/\text{s}$$

$$t_{RL} = 100\text{s}$$

$$\therefore V_L = 300 \cdot 10^{-6} \cdot 100 \text{ m}^3$$

$$= 0.03 \text{ m}^3$$

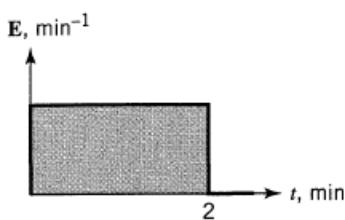
$$\therefore \% \text{ Volume occupied by gas} = 0.12/0.15 \cdot 100 = 80\%$$

$$\% \text{ Volume occupied by liquid} = 0.03/0.15 \cdot 100 = 20\%$$

A liquid macro fluid reacts according to $A + R$ as it flows through a vessel. Find the conversion of A for the flow patterns of Figs. P11.7 to P11.11 and kinetics as shown.

11.7)

$$\begin{aligned} C_{A0} &= 1 \text{ mol/liter} \\ -r_A &= kC_A^{0.5} \\ k &= 2 \text{ mol}^{0.5}/\text{liter}^{0.5} \cdot \text{min} \end{aligned}$$



Ans. $\int_0^{\infty} E \cdot dt = 1$

$$\therefore 2 \cdot E = 1$$

$$\therefore E = 0.5$$

$$= C/C_0 = \int_0^{\infty} \left(\frac{C}{C_0} \right) \cdot Edt$$

(C/C_0) for a batch material is given by Eqⁿ

Here $n = 0.5$ and $k = 2 \text{ mol}^{0.5}/\text{litre}^{0.5} * \text{min}$

$$(n-1) k C_{A0}^n t = (C_A/C_{A0})^{1-n} - 1$$

$$\therefore -1/2 * 2 * 1 * t = (C_A/C_{A0})^{1/2} - 1$$

$$\therefore (C_A/C_{A0}) = (1-t)^2$$

$$\therefore C/C_0 = \int_0^2 (1-t)^2 \cdot (1/2) dt$$

$$= -1/2 * [(1-t)^3/3]_0^2$$

$$= -1/2 * [-1/3 - 1/3]$$

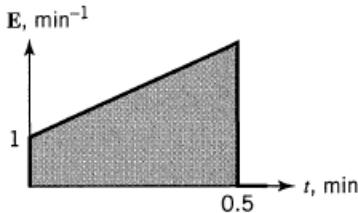
$$= -1/2 * -2/3$$

$$= 1/3$$

$$= X_A = 1 - 1/3 = 2/3$$

11.8)

$$\begin{aligned} C_{A0} &= 2 \text{ mol/liter} \\ -r_A &= k C_A^2 \\ k &= 2 \text{ liter/mol} \cdot \text{min} \end{aligned}$$



$$\text{Ans. } C/C_0 = \int_0^\infty (C/C_0) \cdot E dt$$

$$\int_0^\infty E dt = 1$$

$$\therefore 0.5 = 0.5 * 0.5 * E$$

$$\therefore E = 2$$

Here $n = 2$, $k = 2 \text{ litre/mol} * \text{min}$ and $C_{A0} = 2 \text{ mol/litre}$

$$(n-1) k C_{A0}^n t = (C_A/C_{A0})^{1-n} - 1$$

$$1 * 2 * 2^2 * t = (C_A/C_{A0})^{-1} - 1$$

$$1 + 8t = (C_A/C_{A0})^{-1}$$

$$= (C_A/C_{A0}) = 1/1+8t$$

$$= 2 \int_0^{0.5} 1/1 + 8t * dt$$

$$= 1/4 [\ln (1+8t)]_0^{0.5}$$

$$= 1/4 [\ln (5)]$$

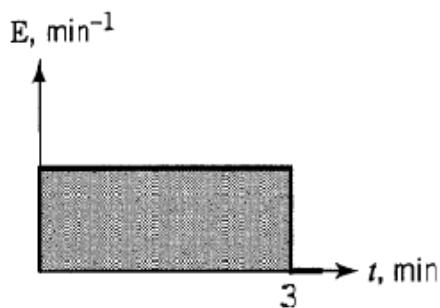
$$= X_A = 0.6$$

$$11.9$$

$$C_{A0} = 6 \text{ mol/Lit}$$

$$-r_A = k$$

$$k = 3 \text{ mol/lit min}$$



$$\text{Ans. The Performance Equation is } \frac{\overline{CA}}{CA_0} = \int_0^{\infty} \frac{CA}{CA_0} Edt$$

$$\text{For } t < C_{A0} / k = 6/3 = 2 \text{ min; we have } C_A / C_{A0} = 1 - (kt / C_{A0})$$

$$\text{For } t > 2 \text{ min; we have } C_A / C_{A0} = 0$$

Replacing it in the above equation,

$$\frac{\overline{CA}}{CA_0} = \int_0^2 \left(1 - \frac{kt}{CA_0}\right) Edt$$

$$\text{Putting } E = 1/3,$$

$$\frac{\overline{CA}}{CA_0} = \frac{1}{3} \int_0^2 \left(1 - 3 * \frac{t}{6}\right) dt$$

$$\frac{\overline{CA}}{CA_0} = \frac{1}{6} \int_0^2 (2-t) dt$$

$$\frac{\overline{CA}}{CA_0} = \frac{1}{3}$$

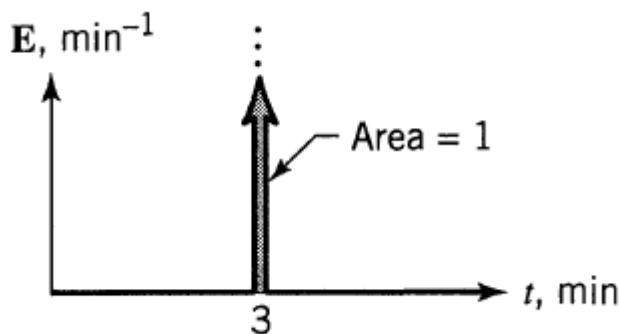
So the conversion is $X_A = 1 - \overline{CA} / CA_0 = 2/3 = 0.666 = 66.6\%$

11.10

$$CA_0 = 4 \text{ mol/lit}$$

$$-r_A = k$$

$$k = 1 \text{ mol/lit min}$$



Ans. Here Dirac Delta function is used. It is Zero everywhere except one point and that point is at Infinite value. The Equation to be used here is:

$$\frac{\overline{CA}}{CA_0} = \int_0^\infty f(t) \delta(t - t_0) dt$$

$$\text{We know that, } \int_0^\infty f(t) \delta(t - t_0) dt = f(t_0)$$

$$\text{For } t < CA_0 / k = 4/1 = 4 \text{ min; } CA / CA_0 = 1 - (kt / CA_0)$$

$$\text{For } t > 4 \text{ min; } CA / CA_0 = 0$$

$$\text{Here } f(t) = 1 - (kt / CA_0)$$

So putting it in the above equation and by Dirac Delta function,

$$\frac{\overline{CA}}{CA_0} = \int_0^4 \left(1 - \frac{kt}{CA_0}\right) \delta(t - 3) dt$$

$$\frac{\overline{CA}}{CA_0} = 1 - \frac{kt}{CA_0} \Big| \text{ at } t = 3$$

$$\frac{\overline{CA}}{CA_0} = 0.25$$

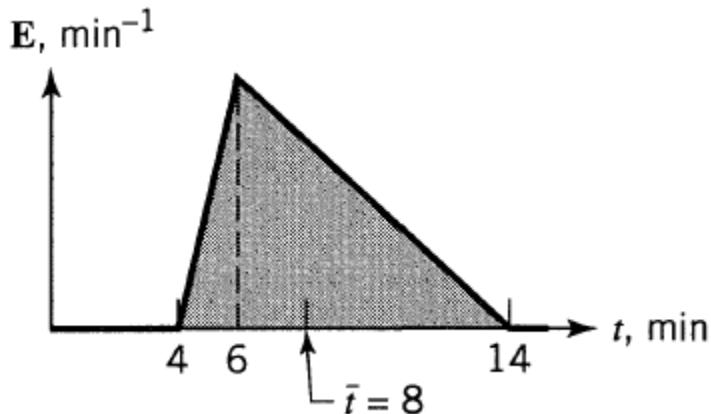
So $X_A = 0.75 = 75\%$

11.11

$$C_{A0} = 0.1 \text{ mol/lit}$$

$$-r_A = k$$

$$k = 0.03 \text{ mol/lit min}$$



Ans. The Performance Equation is :- $\frac{\overline{CA}}{CA_0} = \int_0^\infty \frac{CA}{CA_0} Edt$

For $t < C_{A0} / k = 0.1 / 0.03 = 3.33 \text{ min}$; $C_A / C_{A0} = 1 - (kt / C_{A0})$

For $t > 3.33 \text{ min}$; $C_A / C_{A0} = 0$

Here Nothing is leaving the Reactor after $t = 3.33$ min. so everything has been reacted .so $\frac{\overline{CA}}{CA_0} = 0$ and $X_A = 1$.

11.12-11.14. Hydrogen sulfide is removed from coal gas by contact with a moving bed of iron oxide particles which convert to the sulfide as follows:
 $\text{Fe}_2\text{O}_3 \rightarrow \text{FeS}$

In our reactor the fraction of oxide converted in any particle is determined by its residence time t and the time needed for complete conversion of

$$1 - X = \left(1 - \frac{t}{\tau}\right)^3 \quad \text{when } t < 1 \text{ hr, and with } \tau = 1 \text{ hr}$$

and

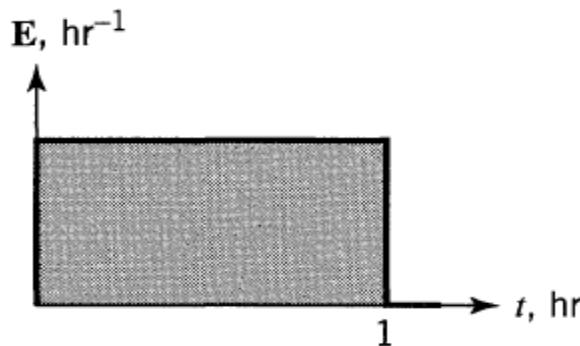
$$X = 1 \quad \text{when } t \geq 1 \text{ hr}$$

11.12

The reaction occurring here is $\text{Fe}_2\text{O}_3 \rightarrow \text{FeS}$.

$$1 - X = (1 - t/\tau)^3 \quad \text{where } t < 1 \text{ and } \tau = 1 \text{ hr}$$

$$X = 1 \quad \text{where } t \geq 1 \text{ hr}$$



$$\overline{1 - X} = \int_0^1 \left(1 - \frac{t}{\tau}\right)^3 Edt$$

$$\overline{1 - X} = \int_0^1 (1 - t)^3 Edt$$

Here $E=1$ [From figure Area = $E*t$ so we have $1=E*1$ which results to $E=1$]

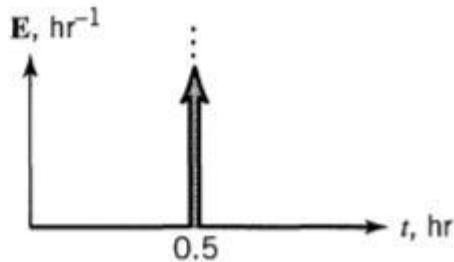
$$\overline{1 - X} = \int_0^1 (1 - t^3 - 3t + 3t^2) dt$$

$$\overline{1-X} = 0.25$$

$$\bar{X} = 0.75 = 75 \%$$

Find the conversion of iron oxide to sulfide if the RTD of solids in the contactor is approximated by the curve

11.13.



Ans.

For solid particles,

$$1 - X = \frac{\overline{CA}}{CA_0} = \int_0^{\infty} f(t) \delta(t - t_0) dt$$

$$\overline{1-X} = \int_0^1 \left(1 - \frac{t}{\tau}\right)^3 E dt, \quad \text{where } E = \delta(t - t_0)$$

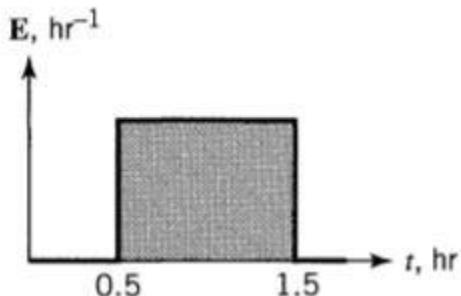
We know that, $\int_0^{\infty} f(t) \delta(t - t_0) dt = f(t_0)$

$$1 - X = (1 - t)^3 \text{ at } t = 0.5$$

$$1 - X = 0.125$$

Ans: X= 0.875

11.14.



Ans.

For solid particles,

$$1 - \bar{X} = \frac{\overline{CA}}{CA_0} = \int_0^{\infty} f(t) \delta(t - t_0) dt$$

$$\overline{1 - X} = \int_{0.5}^{1.5} \left(1 - \frac{t}{\tau}\right)^3 E dt$$

$$\overline{1 - X} = \int_{0.5}^{1.5} (1 - t)^3 E dt$$

Here $E=1$ [From figure Area = $E*t$ so we have $1=E*1$ which results to $E=1$]

$$\overline{1 - X} = \int_{0.5}^{1.5} (1 - t^3 - 3t + 3t^2) dt$$

$$\overline{1 - X} = 0$$

Ans: $\bar{X} = 1 = 100\%$

Q 11.15

Cold solids flow continuously into a fluidized bed where they disperse rapidly enough so that they can be taken as well mixed. They then heat up, they devolatilize slowly, and they leave. Devolatilization releases gaseous A which then decomposes by first-order kinetics as it passes through the bed. When the gas leaves the bed decomposition of gaseous A stops. From the following information determine the fraction of gaseous A which has decomposed. Data: Since this is a large-particle fluidized bed containing cloudless bubbles, assume plug flow of gas through the unit. Also assume that the volume of gases released by the solids is small compared to the volume of carrier gas passing through the bed.

Mean residence time in the bed: $6 = 15 \text{ min}$, $6 = 2 \text{ s}$ for carrier gas For the reaction:

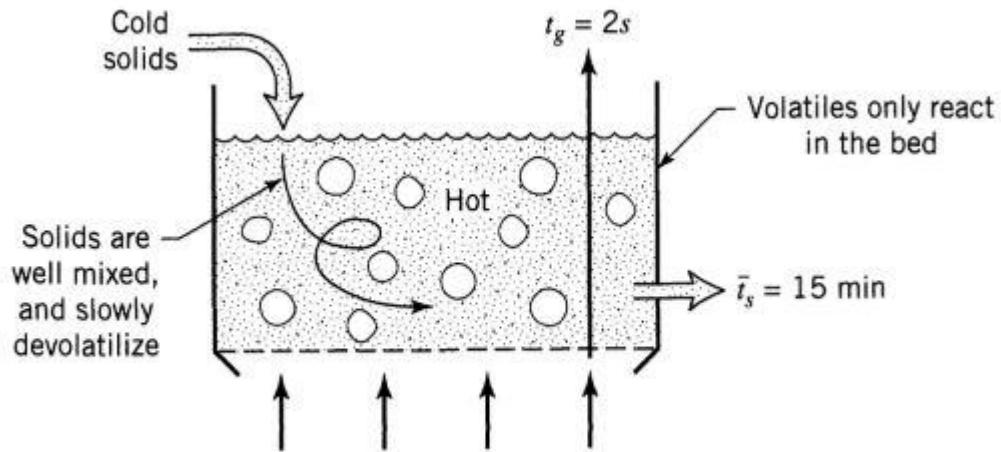
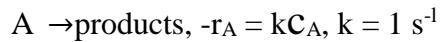
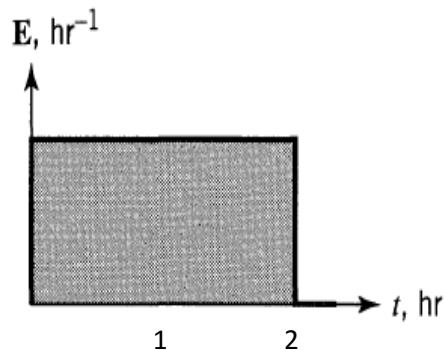


Figure P11.15

Ans.

Here A is released uniformly.



From the curve area under curve must be 1, therefore $E=0.5$

The Performance Equation is $\frac{\overline{CA}}{CA_0} = \int_0^{\infty} \frac{CA}{CA_0} E dt$

For first order reaction,

$$\frac{CA}{CA_0} = e^{-kt}$$

$$\frac{\overline{CA}}{CA_0} = \int_0^{\infty} e^{-kt} E dt$$

$$\frac{C_A}{C_{AO}} = [e^{-kt}]_0^2$$

$$\frac{C_A}{C_{AO}} = 0.4323$$

$$\text{Ans: } X = 1 - \frac{C_A}{C_{AO}} = 0.5677$$

Q 11.16

Reactant A ($C_{AO} = 64 \text{ mol/m}^3$) flows through a plug flow reactor ($r = 50 \text{ s}$), and reacts away as follows:

$$A \rightarrow R, \quad -r_A = 0.005 C_A^{1.5}, \text{ mol/m}^3 \cdot \text{s}$$

Determine the conversion of A if the stream is:

- (a) a microfluid,
- (b) a macrofluid.

A 11.16

(a) For Microfluid:

$$\frac{\tau}{C_{AO}} = \frac{\int_{C_{AO}}^{C_A} (dC_A)}{k C_A^{1.5} C_{AO}}$$

$$\tau = \frac{[C_A^{-1.5+1}]_{C_{AO}}^{C_A}}{-k[-1.5+1]}$$

$$50 * 0.005 * 0.5 = \frac{1}{C_A^{0.5}} - \frac{1}{C_{AO}^{0.5}}$$

$$C_A = 16,$$

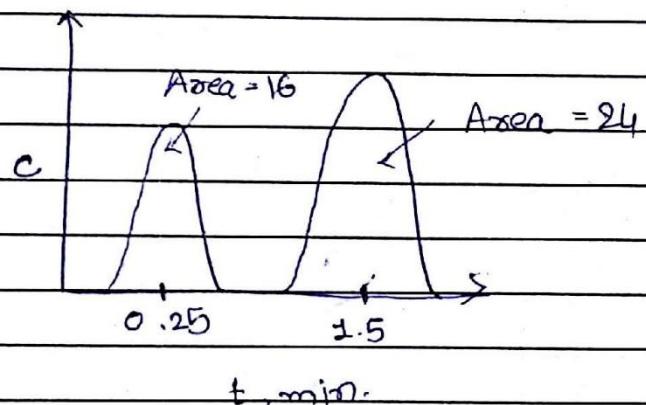
Since $C_{AO} = 64$

$$X = \frac{C_{AO} - C_A}{C_{AO}} = 0.75 \quad \text{Ans: } X = 0.75$$

CRE - II Term Papers.

- 12.1 to 12.6. A pulse of concentrated NaCl solution is introduced into the fluid entering a vessel ($V = 1 \text{ m}^3$, $\dot{V} = 1 \text{ m}^3/\text{min}$) and the concn of tracer is measured in the fluid leaving the vessel. Develop a flow model to represent the vessel from the tracer outlet data sketched in fig. 12.1 to 12.6

(4)



→ This figure is look like two PFR in parallel.

$$V_{\text{total}} = 1 \text{ m}^3 \quad \dot{V} = 1 \text{ m}^3/\text{s.}$$

$$\text{so, } \frac{V_1}{\dot{V}_1} = 0.25 \quad \text{&} \quad \frac{V_2}{\dot{V}_2} = 1.5$$

$$\rightarrow \text{now, } A_1 = 16 = \frac{V_1}{\dot{V}} \quad \therefore \dot{V}_1 = 16$$

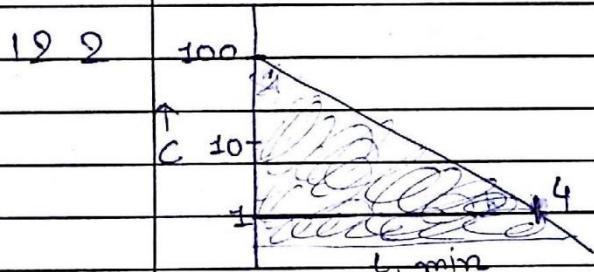
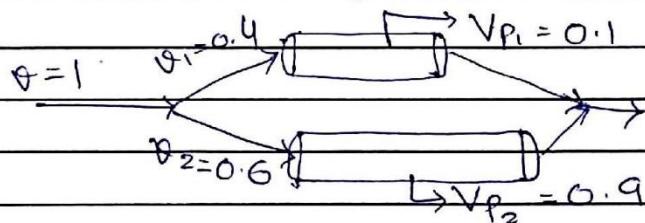
$$A_2 = 24 = \frac{V_2}{\dot{V}} \quad \therefore \dot{V}_2 = 24.$$

$$\therefore \dot{V} = \frac{16}{16+24} = 0.4 \text{ m}^3/\text{min}$$

$$\therefore \dot{V}_2 = \frac{24}{16+24} = 0.6 \text{ m}^3/\text{min}$$

$$\text{now, } V_{P_1} = F_1 \times \dot{V}_1 \\ = (0.25)(0.4) \\ = 0.1 \text{ m}^3$$

$$V_{P_2} = F_2 \times \dot{V}_2 \\ = (1.5)(0.6) \\ = 0.9 \text{ m}^3.$$



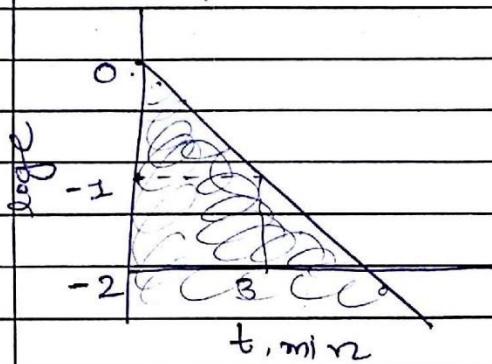
→ This figure is look like mixed flow reactor.

→ so, from the figure mean residence time is ~~less~~ less than 4 min and greater than 1 min.

→ But, $\bar{T}_{theoretical} = 3 \text{ min.}$

→ So, $\bar{t}_{\text{exp.}}$ is less than $\bar{t}_{\text{theoretical}}$. This clearly shows different non-idealities. Dead zone is present

Q. 3.



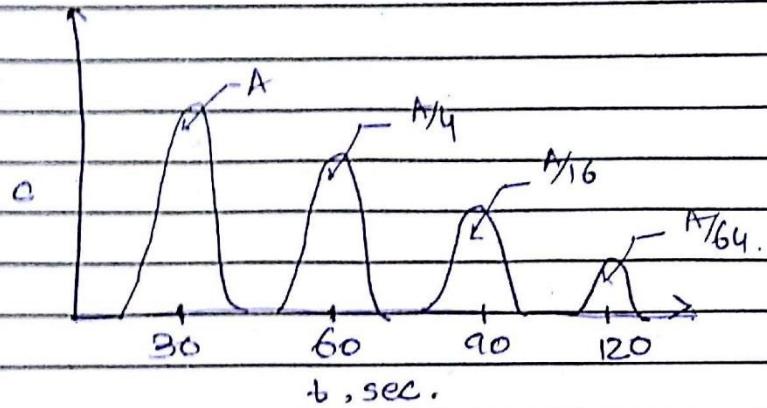
→ This also looks like a mixed slug unit.

→ From fig. $0.303\bar{t} = 3$
or $\bar{t} = 1.3 \text{ min}$
from experiment.

→ But we know that, $\bar{t} = \frac{V}{\dot{V}} = \frac{I}{f} = 1 \text{ min}$.

→ So, either tracer is used is not a proper tracer - denser than the fluid, absorbs on the wall of the vessel, etc. or something else is wrong

12.4



→ for this experiment,

$$\bar{t} = \frac{\int t + c + dt}{\int c dt}$$

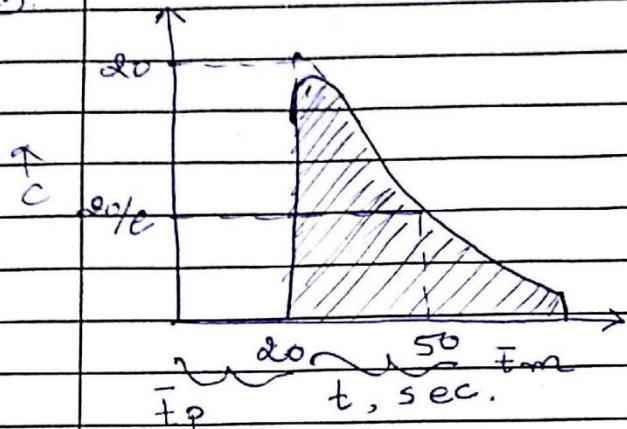
$$= \frac{A(30) + A(60/4) + A(90/16) + A(120/64)}{A + (A/4) + (A/16) + (A/64)}$$

$$t_{\text{exp}} = 37.175 \text{ sec}$$

But, $\bar{t}_{\text{then}} = 60 \text{ sec.}$

→ So, in this exp. traces is passed quickly through the reactor. It hasn't pass the enough time in the reactor. So, this is the indication of any non-ideality.

195.



→ This fig. is look like PFR & MFR in series.

from the figure,

$$\bar{t}_p = 20 \text{ sec}$$

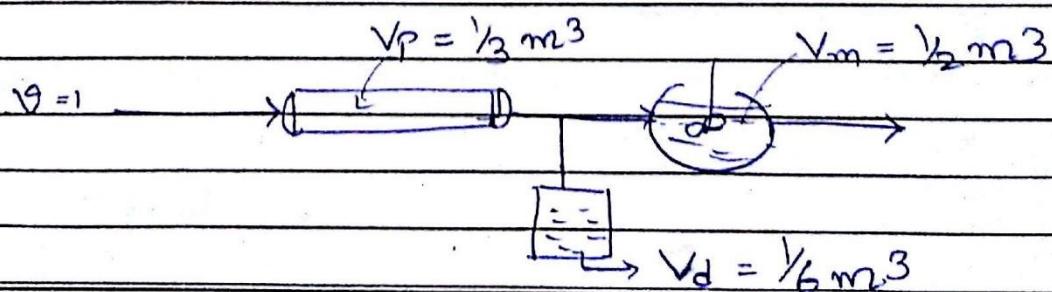
$$\bar{t}_m = 30 \text{ sec}$$

$$\therefore \bar{t}_{\text{active}} = 50 \text{ sec.}$$

But, $\bar{t}_{\text{total}} = \frac{V}{q} = 60 \text{ sec.}$

∴ $t_{\text{dead}} = 10 \text{ sec.}$

So, our model is,

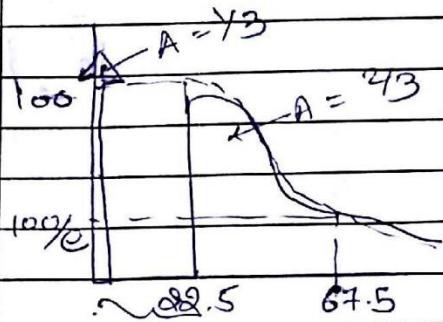


$$V_p = 20/60 = 1/3 \text{ m}^3$$

$$V_m = 30/60 = 1/2 \text{ m}^3$$

and rest is dead volume $V_d = 1/6 \text{ m}^3$

12.6



→ this fig is look like MFR-PFR in series with bypass.

$$\rightarrow \bar{t}_p = 22.5 \text{ sec} \text{ from the exp.}$$

$$\bar{t}_m = 45 \text{ sec}$$

$$\rightarrow \text{But, } \bar{t}_{\text{total}} = 60 \text{ sec}$$

$$\text{while } \bar{t}_{\text{exp}} = \bar{t}_p + \bar{t}_m \\ = 22.5 + 45 \\ = 67.5$$

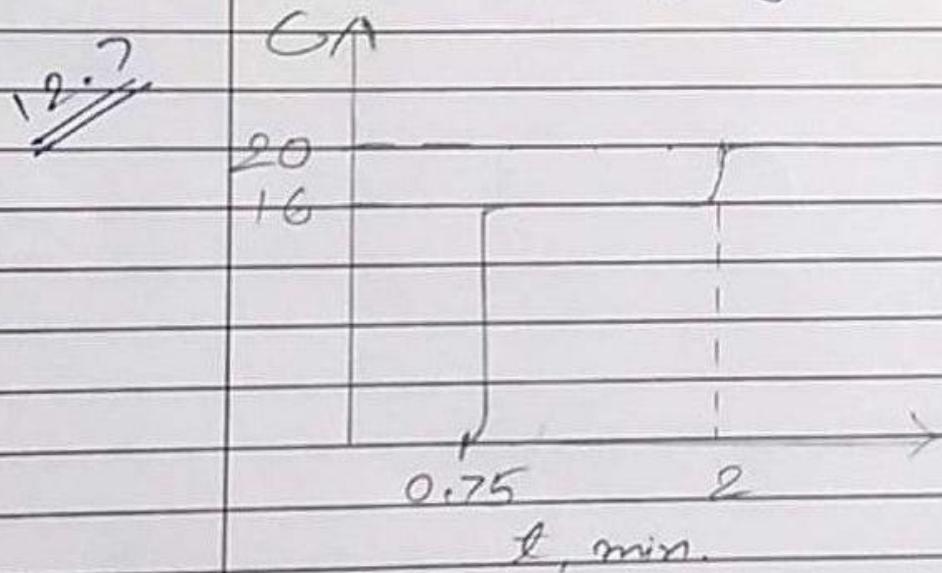
→ so, here $\bar{t}_{\text{exp}} > \bar{t}_{\text{theo}}$.

so, we can conclude that there will be traces accumulation & deadzone formation

$$\therefore \boxed{\bar{t}_{\text{dead}} = 7.5 \text{ sec.}}$$

12.7 to 12.10

A step input tracer test (switching from tap water to salt water), measuring the conductivity of fluid leaving the vessel, is used to explore the flow pattern of fluid through the vessel ($V = 1 \text{ m}^3$, $v = 1 \text{ m}^3/\text{min}$). Devise a flow model to represent the vessel from the data of Figs. 12.7 to 12.10.



$$v_1 = \frac{16}{20} v = (0.8)(1) = 0.8 \text{ m}^3/\text{min}$$

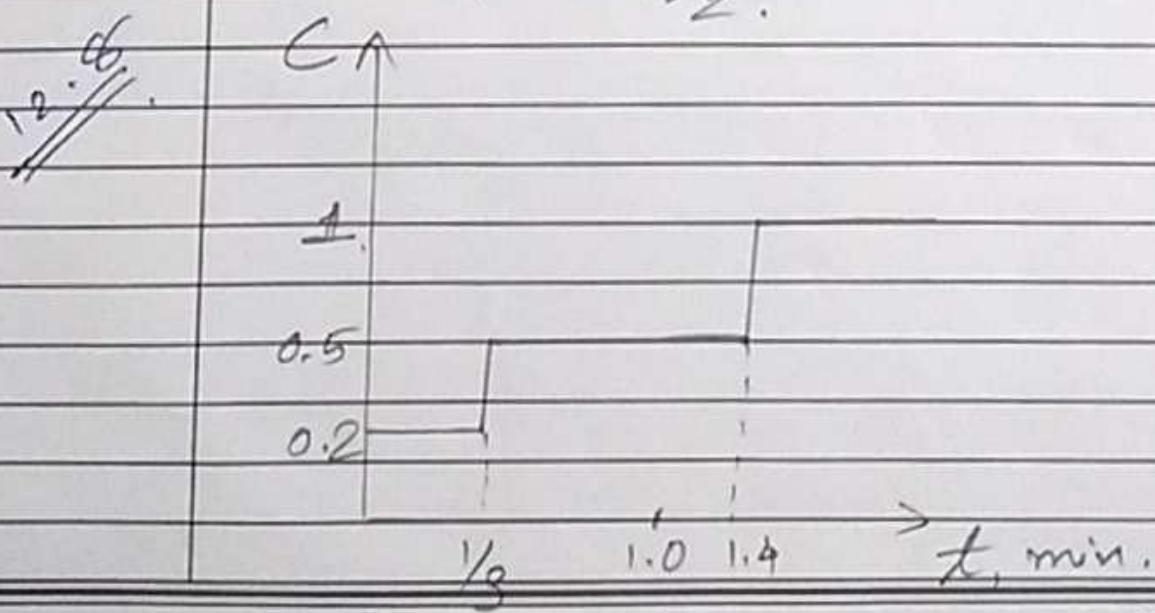
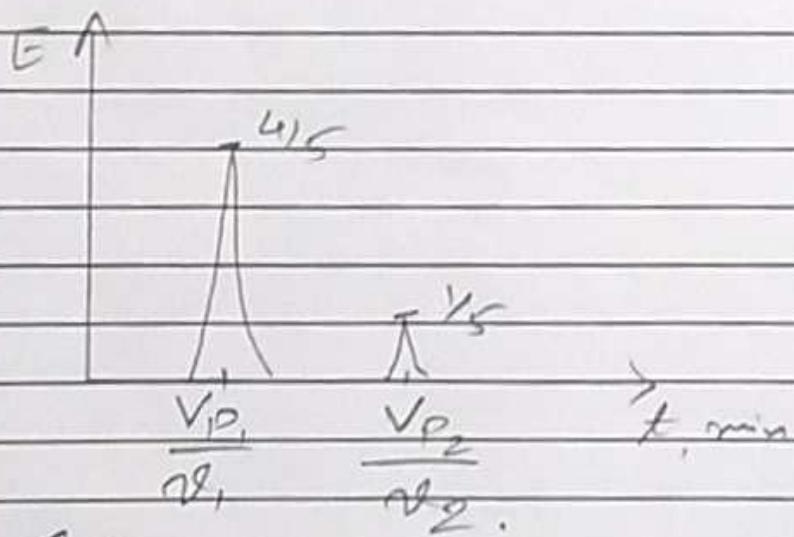
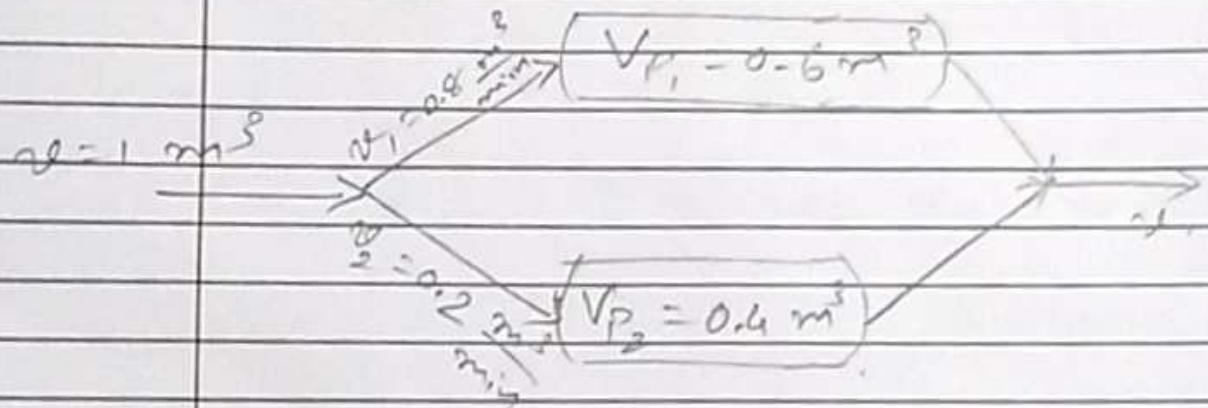
$$v_2 = \frac{4}{20} v = (0.2)(1) = 0.2 \text{ m}^3/\text{min.}$$

→ The 2 PFR are in parallel.

$$\therefore t_1 = 0.75 \text{ min}, t_2 = 2 \text{ min.}$$

$$V_{P_1} = (t_1) (v_1) = (0.75)(0.8) = 0.6$$

$$V_{P_2} = (t_2) (v_2) = (0.5)(0.2) = 0.4.$$



→ This graph indicates a PFR tank in parallel with bypassing.

$$\therefore V = V_{P_1} + V_{P_2} + V_{bypass} = 1 \text{ m}^3$$

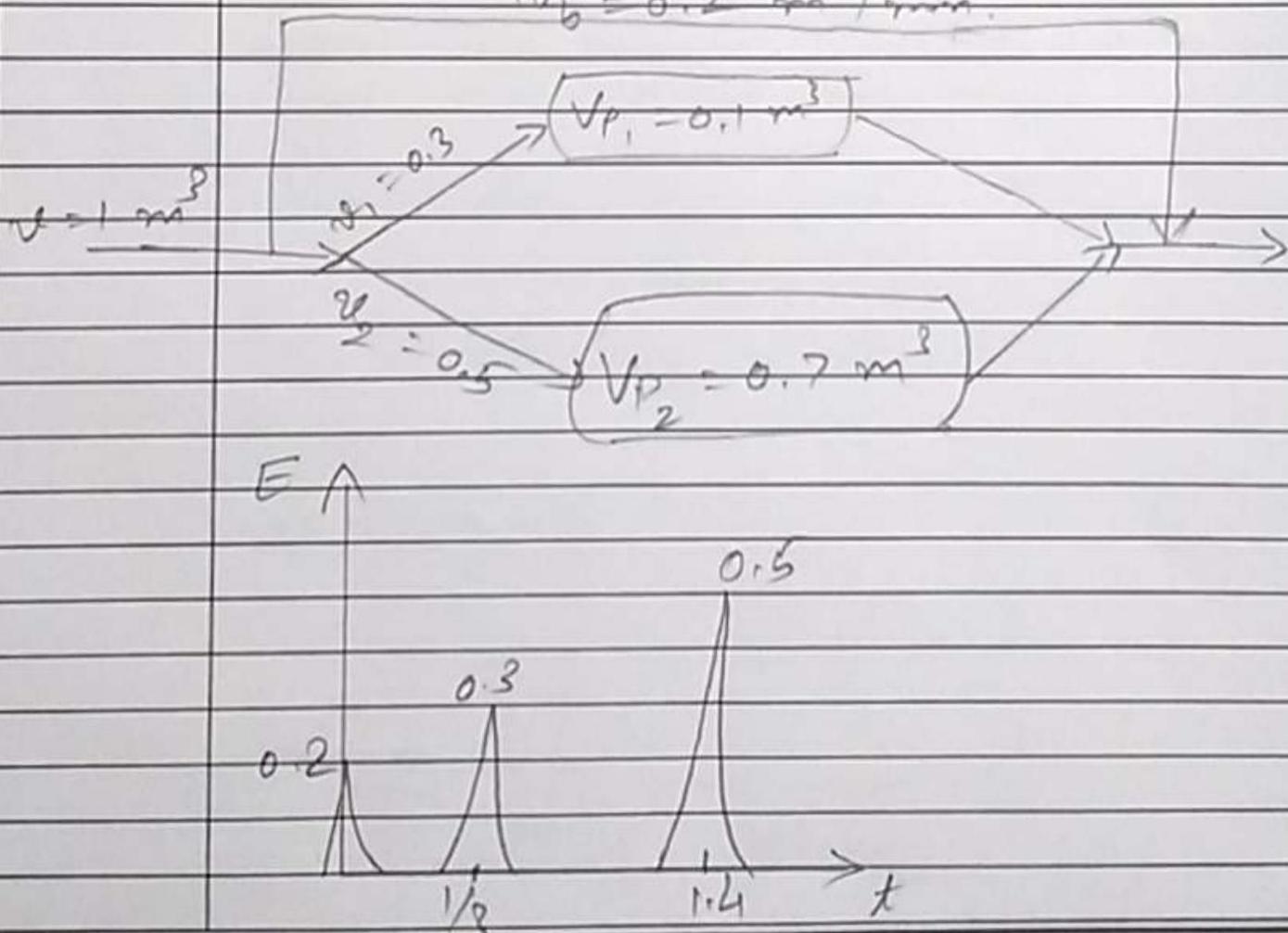
$$t_1 = \frac{1}{3}, \quad t_2 = 1.4.$$

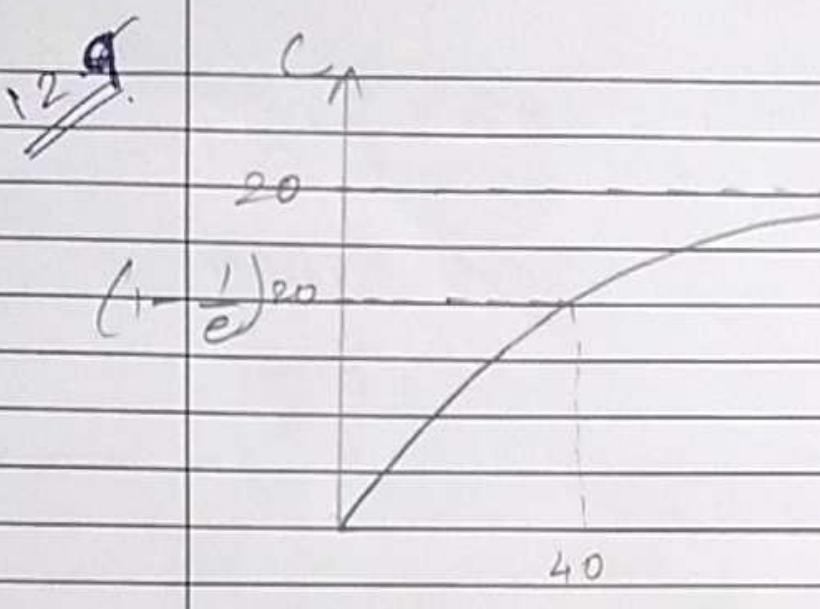
$$\therefore v_1 = 0.2, \quad v_2 = 0.3, \quad v_3 = 0.5 \quad (V = 1 \frac{\text{m}^3}{\text{min}})$$

$$V_{P_1} = (v_1)(t_1) = (0.2)(\frac{1}{3}) = 0.1 \text{ m}^3$$

$$V_{P_2} = (v_2)(t_2) = (0.3)(1.4) = 0.7 \text{ m}^3$$

$$V_{bypass} = 0.2 \text{ m}^3/\text{min.}$$



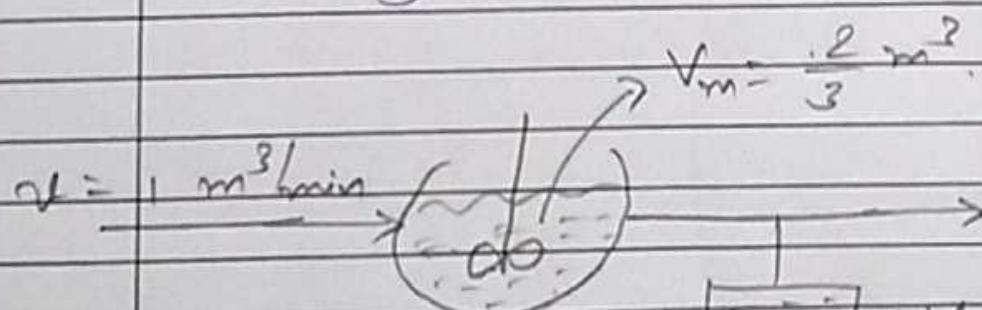


→ For mixed flow alone this should be 60 sec. However, this curve comes out early, meaning dead spaces are present. This tracer curve shows that $t = 40$ sec, thus.

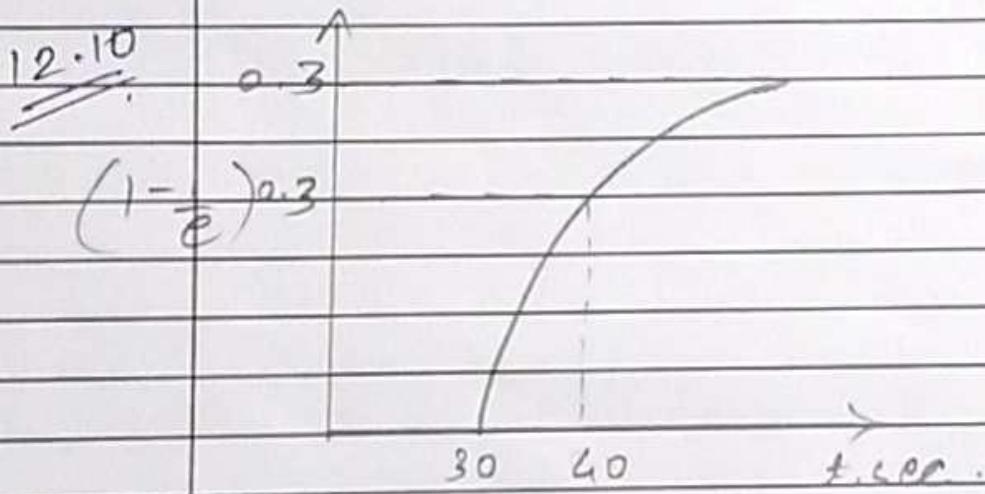
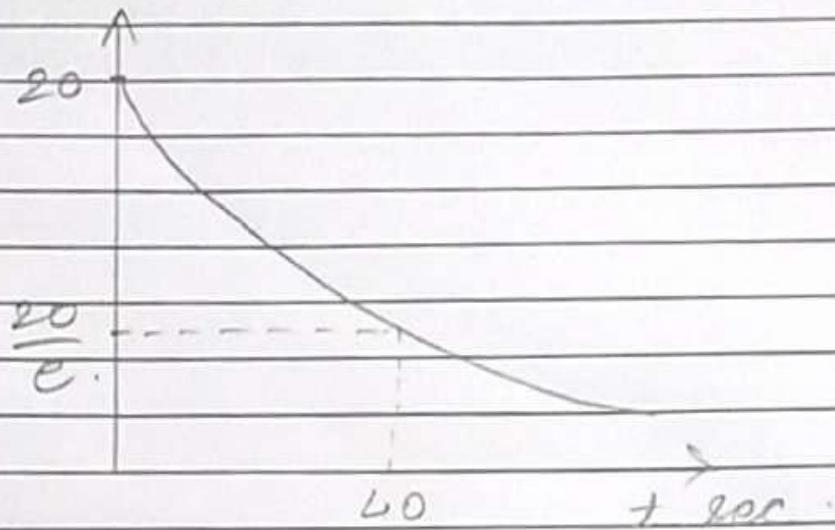
$$V_m = \frac{F_{act}}{F_{tot}} \times V$$

$$= \frac{40}{60} \times 1 = \frac{2}{3} \text{ m}^3$$

$$V_d = \frac{1}{3} \text{ m}^3$$



$$V_d = \frac{1}{3} \text{ m}^3$$



$$V = V_p + V_m + V_d$$

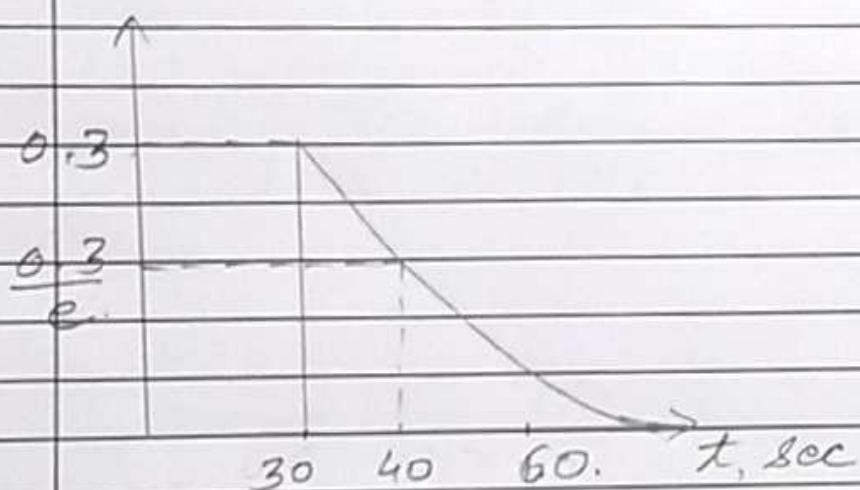
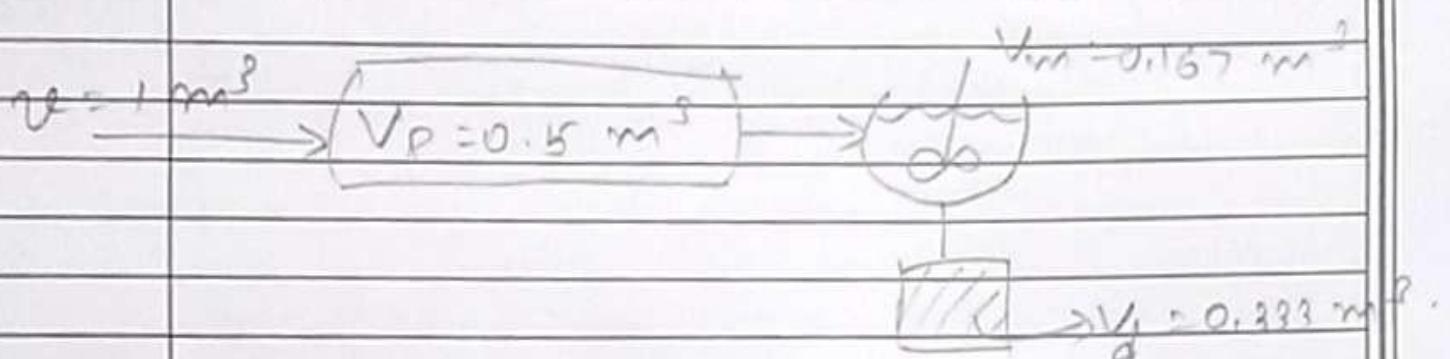
$$V_p = \frac{30}{60} = 0.5 \text{ m}^3$$

$$V_m = \frac{10}{60} = 0.167 \text{ m}^3$$

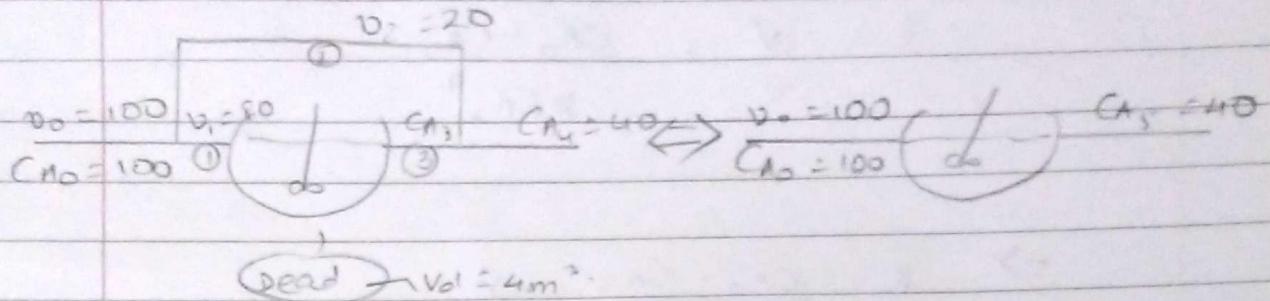
$$V_d = \frac{20}{60} = 0.333 \text{ m}^3$$

$$t_1 = 30 \text{ sec}, \quad t_2 = 10 \text{ sec}.$$

→ Here, All tanks are in series.



12.11



Let,

$$C_{A0} = 100$$

$$\& V_{A0} = 100$$

Taking material balance about the mixing point,

$$V_2 C_{A2} + V_3 C_{A3} = V_4 C_{A4}$$

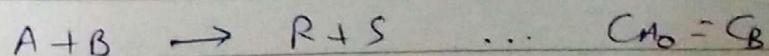
$$\Rightarrow 20(100) + 80C_{A3} = 100(40)$$

$$\Rightarrow C_{A3} = \frac{100(40) + 20(100)}{80} = 75$$

Next evaluate the rate constant

k from the actual 2 m^3 MFR.

For a 2^{nd} order reaction,



We have,

$$t = \frac{V}{v} = \frac{C_{A_0} - C_{A_3}}{k C_{A_3}^2}$$

$$\Rightarrow k = \frac{C_{A_0} - C_{A_3}}{C_{A_3}^2} \cdot \frac{v}{V}$$

$$= \frac{100 - 75}{(75)^2} \cdot \frac{80}{2} = 14.222$$

Finally, for ideal reactor,

$$V_{\text{ideal}} = \frac{C_{A_0} - C_{A_5}}{k C_{A_5}^2} \cdot v$$

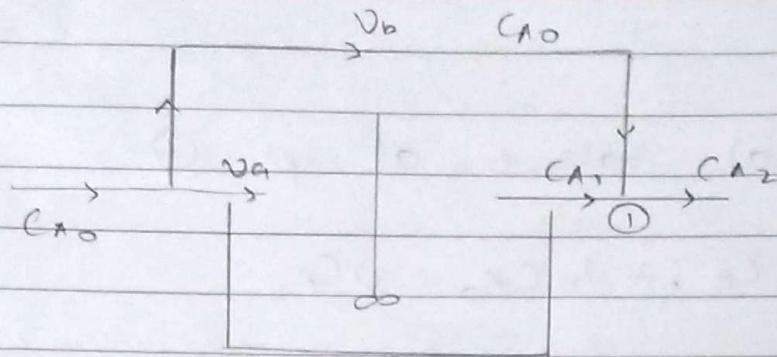
$$\Rightarrow V_{\text{ideal}} = \frac{C_{A_0} - C_{A_5}}{k C_{A_5}^2} \cdot v$$

$$= \frac{100 - 40}{14.22} \cdot \frac{100}{(40)^2}$$

$$= 0.2637 \text{ m}^3$$

which is much smaller than 6 m^3

12.12



Given,

$$\text{Volume, } V = 6 \text{ m}^3$$

Let us assume,

$$V = 90 \text{ m}^3/\text{hr}$$

$$\therefore V_a = 60 \text{ m}^3/\text{hr}$$

$$V_b = 30 \text{ m}^3/\text{hr}$$

$$\& C_A_0 = 100 \text{ kmol/m}^3.$$

Let us assume,

$$V_m = 2 \text{ m}^3. \quad \therefore V_d \text{ (dead vol.)} = 4 \text{ m}^3$$

Now, given $X_A = 75\%$.

$$\therefore C_A_0 = 100$$

$$C_A_1 = ?$$

$$C_A_2 = 25.$$

$$\frac{2}{3}x(C_{A_1}) + \frac{1}{3}(100) = \sqrt{25}$$

$$2C_{A_1} + 100 = 25$$

Now,

Date: 3/1/1
Page No. 3

$$2C_{A_1} = 75 - 100$$

$$C_{A_1} = -\frac{25}{2}$$

material balance at pt. ①

$$V_A C_{A_1} + V_B C_{A_0} = V C_{A_2}$$

$$\Rightarrow 60(C_{A_1}) + 30(100) = 60(25)$$

$$\Rightarrow C_{A_1} = \frac{60 \times 25 - 3000}{60}$$

$$\Rightarrow C_{A_1} = -\frac{750}{60} = -\frac{25}{2} = -12.5$$

But, since C_{A_1} cannot be negative,

∴ We take, $C_{A_1} = 12.5 \text{ kmol/m}^3$.

$$\frac{I}{C_{A_0}} = \frac{X_A}{-r_A}$$

$$\text{Here } I_m = \frac{N_m}{V_A} = \frac{2}{60} = \frac{1}{30}$$

$$\Rightarrow \frac{I}{C_{A_0}} = \frac{X_A}{K C_{A_1}}$$

$$\therefore K = \frac{0.75 \times 100 \times 30}{12.5 \times 1} = 180 \text{ hr}^{-1}$$

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Since this value comes negative,
this question is not possible

CRE-2 Group No-11 Chapter -13
 (13BCH054, 055, 056, 057)

	<p>Ch-13 <u>CRE-2</u> <u>Dispersion Model</u></p>
	<p><u>13.1</u> The flow pattern of gas through blast furnaces was studied by VDEh (Verein Deutscher Eisenhüttenleute Betriebsforschungsinstitut) by injecting Kr-85 into the air streams entering the tuyeres of the 688 m^3 furnace. Assuming that the axial dispersion model applies to flow of gas</p> <p><u>Diagram</u></p> <p><u>Tracer in</u></p> <ul style="list-style-type: none"> - Evaluate the intensity for dispersion of Middle section. Compare D/mid with middle section with expected in an ordinary packed bed.
	<p>Nirma University</p>

$$\bar{E}_2 = 1.665$$

width at 61% maximum height = 0.70

\therefore standard deviation $\sigma_z = 0.35$ (from 13.4)

$$\sigma_z^2 = 0.1225$$

$$\Delta \bar{E} = 1.66 - 0.668 = 0.98$$

$$\Delta(\sigma^2) = 0.1225 - 0.0196 = 0.1029$$

$$\therefore \frac{D}{u_L} = \frac{\Delta(\sigma^2)}{\Delta(\bar{E})^2} = \frac{0.1029}{2(0.98)^2} = 0.0536$$

$$\therefore \frac{D}{u_d p} = \frac{D}{u_L} \left(\frac{L}{dp} \right) = (0.0536) \left(\frac{10.37 - 5.08}{0.028} \right) = 10$$

- From the blast furnace experiment $\frac{D}{u_d p} = 10.5$

- From the fig. 13.17, $\frac{D}{u_d p} = 0.5$

- In practical there are many changes as there is severe channelling of the gas and severe bypassing in the blast furnace.

13.2 Denmark's longest and greatest river, the Gudenaa, certainly deserves study, so pulse tracer tests were run on various stretches of the river using radioactive Ba-82 . Find the annual dispersion coefficient in upper stretch of the river, 8.7 km apart from following data:

t, hr	$C, \text{arbitrary}$	t, hr	$C, \text{arbitrary}$
3.5	0	5.75	440
3.75	3	6	250
4	25	6.25	122
4.25	102	6.5	51
4.5	281	6.75	20
4.75	535	7	9
5	740	7.25	3
5.25	780	7.5	0
5.5	650		

$$\bar{t} = \frac{\sum t_i C_i \Delta t_i}{\sum C_i \Delta t_i}$$

$$= 112.5 + 100 + 433.5 + 1264.5 + 2541.25 + 3700 + \\ 4095 + 3575 + 2530 + 1500 + 762.5 + 331.5 + \\ 135 + 63 + 21.75$$

$$\frac{3 + 25 + 102 + 281 + 535 + 740 + 780 + 650}{+ 440 + 250 + 122 + 51 + 20 + 9 + 3}$$

$$= \frac{21165.5}{4011} = 5.276 \text{ hr.}$$

ans,

$$\sigma^2 = \frac{\sum t_i^2 c_i \Delta t_i}{\sum c_i \Delta t_i} - \bar{t}^2$$

$$= 421.87 + 400 + 1842.37 + 5690.25 + 12070.9 + \\ 18500 + 21498.75 + 19662.5 + 14547.5 \\ + 9000 + 4765.6 + 2154.75 + 911.25 +$$

$$\frac{411 + 157.68}{4011} - (5.276)$$

$$\sigma^2 = 27.93 - 27.83$$

$$\sigma^2 = 0.093$$

Now,

$$\sigma_0^2 = \frac{\sigma^2}{E^2} = \frac{0.093}{5.276} = 0.0176$$

Now,

$$0.0176 = 2 \frac{D}{u_L} + 8 \left(\frac{D}{u_L} \right)^2$$

$$\frac{D}{u_L} = 8.51 \times 10^{-3} \quad \text{or} \quad \frac{D}{u_L} = -0.25$$

So $\frac{D}{u_L} = 0.00851$

Thakkar Parth

13BCH057

Q13.3 RTD Studies were carried out by Jagadish and Satyanarayana in tubular reactor. A squirt of NaCl solution was rapidly injected at reactor entrance, and many cup measurements were taken at exit. From following result calculate dispersion number.

Ans From experiment

t_1 sec	t_2 sec	C
0 - 20	20	0
20 - 25	22.5	60
25 - 30	27.5	210
30 - 35	32.5	170
35 - 40	37.5	75
40 - 45	42.5	35
45 - 50	47.5	10
50 - 55	52.5	5
55 - 70	62.5	0

calculate D/UL :

$$S_C = S_{GJ}$$

$$S_{GJ} = 17687.5$$

$$S_{GJ}^2 = 573781.25$$

$$\bar{t} = 31.31 \text{ sec}$$
$$\sigma^2 = 35.58 \text{ sec}^2$$

$$\frac{D}{n^2} = \frac{\sigma^2}{2(\bar{t})^2} = 0.018$$

Now calculate volume of buffers

$$V = (1.21 \times 10^2) (\pi \times 1.75^2) = 1164 \text{ cm}^3$$

From material balance

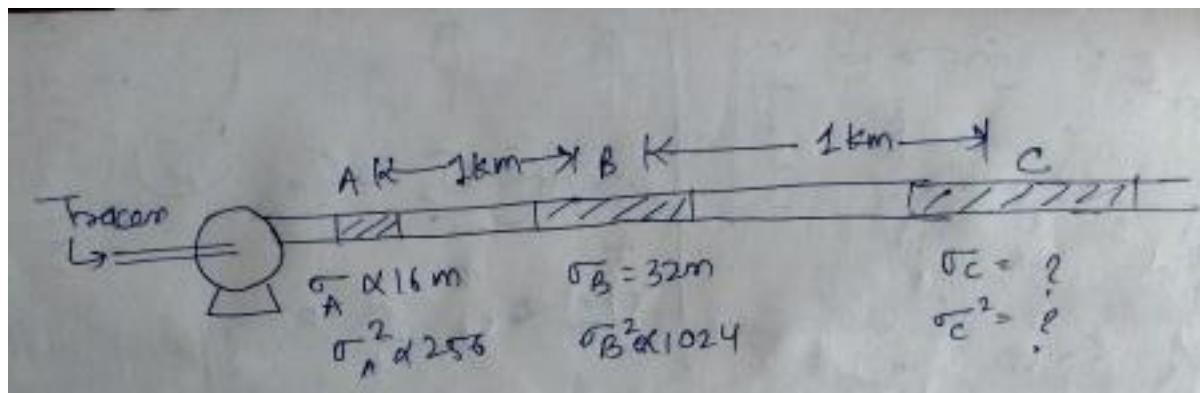
$$u = \frac{1300 \text{ cm}^3}{\text{min}} = 21.67 \frac{\text{cm}^3}{\text{s}}$$

$$\bar{t} = 53.72 \text{ sec}$$

$$\text{Volume of buffers} = \frac{53.72 - 31.31}{53.72} (1164)$$
$$= 986 \text{ cm}^3$$

13.4 is not done as per the talk with you sir

13.5



Solving it with the help of dispersion model –

Using equation 8;

$$\sigma^2 = 2(DL/u^3)$$

Or; σ^2 is proportional to L

Therefore;

$$\sigma_c^2 - \sigma_b^2 = \sigma_b^2 - \sigma_a^2$$

$$\text{Or } \sigma_c^2 - 1024 = 1024 - 256$$

Thus;

$$\sigma_c^2 = 1792$$

Hence Width = $k\sigma_c = 42.3$ meters.

13.6

at refinery pump products A and B successively to receiving stations upto 100 Km away through a 10 cm ID pipeline. The average properties of A and B are

$$\rho = 850 \text{ kg/m}^3$$

$$\mu = 1.7 \times 10^{-3} \text{ kg/ms}$$

$$D = 10^{-4} \text{ m}^2/\text{s}$$

The fluid flows at $u = 20 \text{ cm/s}$, and there are no reservoirs, holding tanks or pipe loops in the line; just a few bends. Estimate the 16% - 84% contaminated width 100 km downstream.

$$\Rightarrow C = \frac{1.7 \times 10^{-3}}{10^{-4}} \frac{\text{kg/m.s}}{\text{m}^2/\text{s}}$$

$$= 1.7 \times 10^6 \frac{\text{kg}}{\text{m}^3}$$

$$= 1.7 \times 10^6 \frac{\text{g}}{\text{L}}$$

$$2\sigma = \sqrt{\frac{8DL}{\mu^3}}$$

$$\sigma = 0.043$$

From graph, taking 16% of contamination

$$16 = \bar{E} - 0.043$$

$$\bar{E} = 16.043$$

$$\sigma_0^2 = \frac{\sigma^2}{t^2} = \frac{2D}{ML} + 8 \left(\frac{D}{ML} \right)^2$$

$$\frac{0.043^2}{16.043^2} = 2 \left(\frac{D}{ML} \right) + 8 \left(\frac{D}{ML} \right)^2$$

$$\therefore \boxed{\frac{D}{ML} = 3.591 \times 10^{-6}}$$

13.7

For finding σ^2 for this flow –

$$Re = (du_p/\mu) = (0.225)(1.1)/(0.9 \times 10^{-6}) = 3.2 \times 10^5$$

$$\text{Now since } (D/ud_t) = 0.22$$

$$\text{From Eqation 8} - (D/uL) = (D/ud_t)(dt/L) = 0.22(0.255/1000000) = 5.61 \times 10^{-8}$$

$$(\sigma^2/t^2) = (\sigma_0)^2 = 2(D/uL) = 2(561 \times 10^{-8}) = 11.22 \times 10^{-8}$$

$$\text{Therefore; } \sigma = (11.22 \times 10^{-8})^{0.5} \times (100000/1.1) = 11022 \times 10^{-8}$$

$$\text{So the width at } 1\sigma = (304.5)(1.1) = 335\text{m}$$

From 5/95 to 95/5 Figure 12 shows that this includes –

(1.65 σ \times 2) of width

Therefore; the 5/95 to 95/5 % width is – (335m)(1.655x2) = 1105m.

13.9

to start assume that a perfect pulse is injected. Then find how far upstream from anammati this pulse was injected.

→ according to any reasonable flow model (dispersion, tank in series, or what have you).

tracer curve \propto (distance from point of injection)

∴ From the anammati reading

$$12 \text{ hrs} = k L^{\frac{1}{2}} \quad \text{(i)}$$

$$\therefore 9 \text{ hrs} = k (L - 119)^{\frac{1}{2}} \quad \text{(ii)}$$

It's From the smooth reading

→ Divide this two eqn:

$$\frac{12}{9}^4 = \frac{L^{\frac{1}{2}}}{(L - 119)^{\frac{1}{2}}}$$

$$\frac{16}{9} = \frac{L}{L - 119}$$

$$\therefore L = 272 \text{ miles}$$

→ Since the dumping may not be instantaneous any location ~~other~~
 $L \leq 278$ miles is suspect.

13.10

$$\left(\frac{\partial}{\partial dp}\right) \frac{dp}{L} = 2$$

$$\therefore \left(\frac{\partial}{\partial dp}\right)_1 = 2 \times \frac{1}{0.002} = 1000$$

$$\left(\frac{\partial}{\partial dp}\right)_2 = \frac{2 \times 9}{0.01} = 1800$$

$$\left(\frac{\partial}{\partial dp}\right)_3 = \frac{2 \times 2}{0.004} = 1000$$

$$E = 2 \text{ min}$$

$$\partial_1 = 0.2 \text{ m/s}$$

$$\partial_2 = 1.8 \text{ m/s}$$

$$\partial_3 = 0.2 \text{ m/s}$$

<u>t</u>	<u>E₁</u>	<u>E₂</u>	<u>E₃</u>
0.5	0.022	0.0291	0.663
1	0.047	0.0473	0.294
2	0.029	0.0224	0.245

$$E = \sqrt{\frac{u^3}{4\pi\partial L}} \exp \left[\frac{(CL - ut)^2}{4\partial L/u} \right]$$

$\Rightarrow t \rightarrow E_2$ give highest area under the curve so it's highest variance

13.11 Length of reactor: 48cm
 $= 0.48\text{ m}$

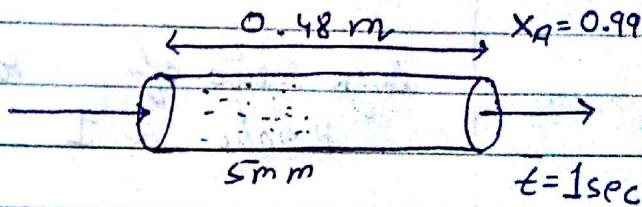
non porous pellets - 5mm

conversion - $X = 99\%$
 $= 0.99$

mean residence time: $\bar{t} = 1\text{ sec.}$

calculate - k .

Assuming plug flow



For 1st order reaction, $E_A = 0$, we have

$$kt = \ln \frac{C_A}{C_A}$$

$$k = \frac{1}{\bar{t}} \ln \frac{C_A}{C_A}$$

$$= \frac{1}{1} \ln \frac{C_A}{C_A}$$

$$= \frac{1}{1\text{ sec}} \times 4.6$$

$$= 4.6\text{ sec}$$

b) Finding K by dispersion model.

From the curve of the figure we find for

$$Re_p = 200 \quad \& \quad \varepsilon = 0.4$$

$$\frac{D\varepsilon}{u_{dp}} = 1$$

$$\text{thus } \frac{D}{u_{dp}} = \frac{1}{\varepsilon} = 2.5$$

size ratio of real to plug flow
 K ratio ≈ 1

$$\frac{K_{true}}{K_{measured}} = \frac{K_{ideal}}{1 + K\varepsilon \left(\frac{D}{u_L} \right)} = 1 + K\varepsilon \left(\frac{D}{u_L} \right) \left(\frac{d_e}{L} \right)$$

$$= 1 + 4.6 \left(2.5 \left(\frac{5}{480} \right) \right)$$

$$= 1.1198$$

$$\therefore K_{true} = (4.6 \text{ sec}^{-1}) \times (1.1198)$$

$$= 5.15 \text{ sec}^{-1}$$

c) Error in assuming plug flow

ideal = 4.6 sec^{-1}

measured = 5.15

$$\text{error} = \left(\frac{5.15 - 4.60}{5.15} \right) \times 100$$

$$= 10.68 \text{ percent.}$$

13.13 For Plug Flow Reactor,

→ 99 % conversion takes place
 $\therefore X_A = 0.99$

→ $C_{A0} = 1000$ is given.

∴ For 99 % conversion, $C_A = ?$
 $\therefore C_A = 1$

→ For the 1st order reaction,

$$C_A = C_{A0} \cdot e^{-kt}$$

$$\therefore e^{-kt} = \frac{C_A}{C_{A0}}$$

$$\therefore e^{kt} = \frac{C_{A0}}{C_A} = \frac{1000}{1}$$

$$\therefore kt = \ln 1000$$

$$\therefore kt = 6.907$$

Now $t = 10 \text{ sec.}$

$$\therefore k = 0.6907$$

Now, from the figure,

$$\sigma^2 = \frac{4^2}{24} = \boxed{\frac{2}{3}}$$

∴ Now, $\frac{C_A}{C_{A0}} = \exp \left[(-kt) + \frac{k^2 \sigma^2}{2} \right]$

∴ $\frac{C_A}{C_{A0}} = \exp \left[-6.907 + \frac{0.6907^2 \times \frac{2}{3}}{2} \right]$

∴ $\frac{C_A}{C_{A0}} = 0.001172$

Now $C_{A0} = 1000 \text{ mol/l}$

∴ $C_A = 0.001172 \times 1000$

$$\boxed{C_A = 1.172 \text{ mol/l}}$$

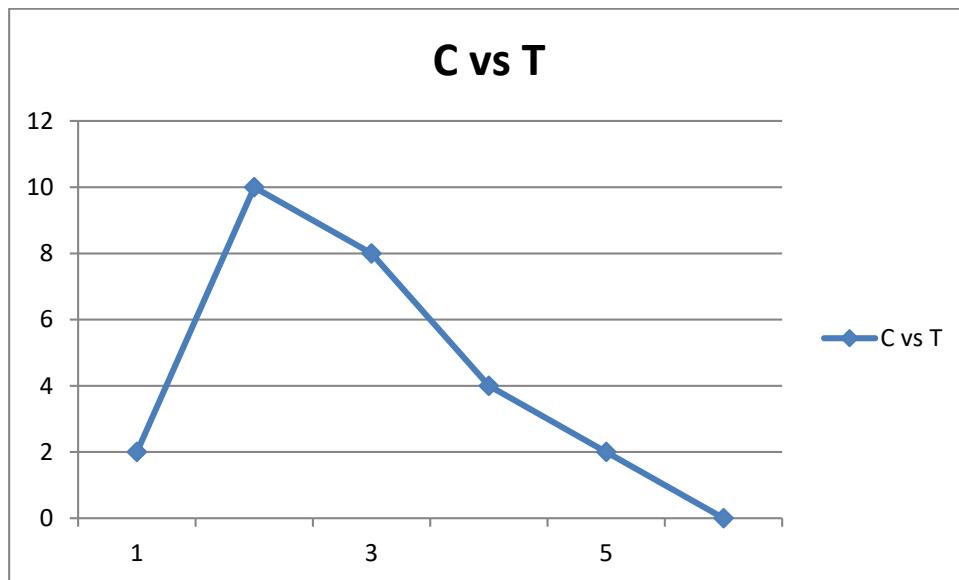
$$\boxed{C_A = 1.172 \text{ mol/l}}$$

Chapter 14: Tanks in Series Model

14.1 From experiment

T	t_{mean}	C
0-2	1	2
2-4	3	10
4-6	5	8
6-8	7	4
8-10	9	2
10-12	11	0

The last observation was interpolated linearly.



$$t_{\text{average}} = \frac{\sum t C}{\sum C} = \frac{1(2) + 3(10) + 5(8) + 7(4) + 9(2) + 11(0)}{2+10+8+4+2} = \frac{118}{26} = 4.538$$

$$\sigma^2 = \frac{\sum t^2 C}{\sum C} - (t_{\text{avg}})^2 = \frac{1^2(2) + 3^2(10) + 5^2(8) + 7^2(4) + 9^2(2) + 11^2(0)}{2+10+8+4+2} - (4.538)^2 = 4.4038$$

$$\frac{1}{N} = \sigma^2_{\theta} = \frac{\sigma^2}{(t_{\text{avg}})^2} = \frac{4.4038}{4.538^2} = 0.2138$$

$$N = 4.68 \text{ tanks}$$

14.2

For N= 10

$$C_{\text{MAX}} = 100 \text{ mmol} ; \sigma^2 = 1 \text{ min.}$$

$$\text{a. } E_{\theta_{\text{MAX}}} \propto C_{\text{MAX}}$$

$$E_{\theta MAX} = \frac{N (N-1)^{(N-1)}}{(N-1)!} e^{-(N-1)}$$

$$E_{\theta MAX} \text{ (for 10 tanks)} = 1.317$$

$$E_{\theta MAX} \text{ (for 20 tanks)} = 1.822$$

$$\frac{E_{\theta MAX} \text{ (for 10 tanks)}}{E_{\theta MAX} \text{ (for 20 tanks)}} = \frac{C_{MAX} \text{ (for 10 tanks)}}{C_{MAX} \text{ (for 20 tanks)}}$$

$$\frac{1.317}{1.822} = \frac{100}{x}$$

$$X = 138.3 \text{ mmol}$$

The maximum concentration of leaving tracer is 138.3 mmol

b. $\sigma^2 \propto N$

$$\frac{\sigma^2 \text{ (for 10 tanks)}}{\sigma^2 \text{ (for 20 tanks)}} = \frac{10}{20}$$

$$\frac{1}{x} = \frac{10}{20}$$

Therefore $x = 2$

The spread is $\sqrt[2]{2} = 1.414 \text{ min.}$

c. The relative spread increases with increase in number of tanks. (ans)

14.3

The above problem is similar to the mixed flow reactor

$V = 1.25 \times 10^9 \text{ bills}$; $v = 10^9 \text{ bills/year}$

$T_{\text{average}} = 1.25 \times 10^9 / 10^9 = 1.25 \text{ years}$

$$E(t) = \frac{\text{Fraction of number of bills}}{\text{Year}} = \frac{b}{b_0}$$

Where b is number of number of bills and b_0 is total number of bills

$$a. F(t) = 1 - e^{t/t(\text{average})} = 1 - e^{t/1.25}$$

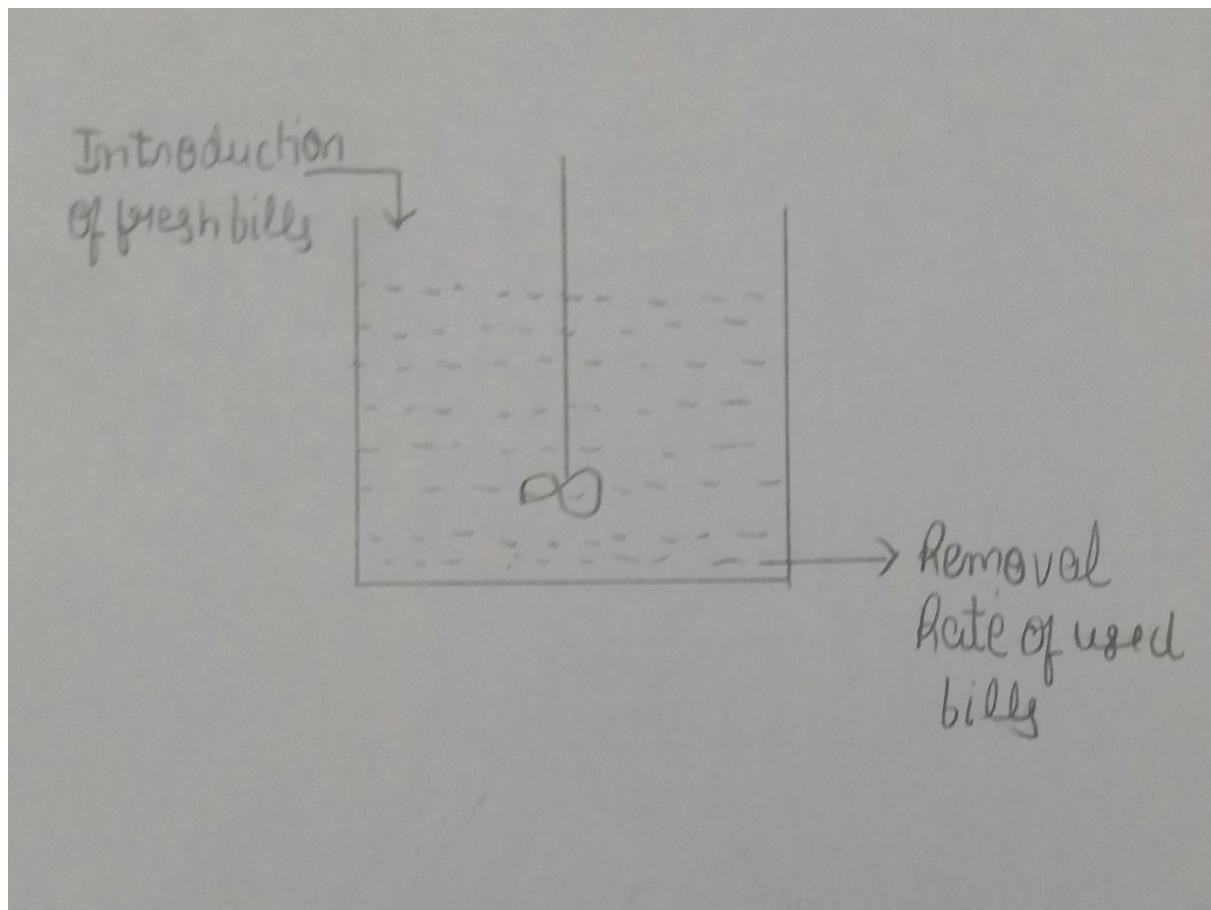
b. The number of bills in circulation which are older than 21 years is by the following formula:

$$b = \int_{21}^{\infty} b_0 E(t) dt \text{ where } b_0 = 1.25 \times 10^9$$

$$E(t) = \int F(t) dt = \int \left(1 - \exp\left(\frac{t}{t(\text{average})}\right)\right) dt$$

$$\text{Therefore } E(t) = \frac{1}{t(\text{average})} e^{t/t(\text{average})} = 0.8 e^{-0.8t}$$

Therefore $b = \int_{21}^{\infty} 0.8 \exp(-0.8t) dt = 63.2$ bills ≈ 63 bills



14.4

$$V = 1.25 \times 10^{15} \text{ bills}$$

$$v = 10^9 \text{ bills}$$

$$T = (V/v) = 1.25 \times 10^6$$

(a)

$$F(t) = e^{-\left(\frac{t}{1.25 \times 10^6}\right)}$$

$$t=0 ; F(t)=0$$

$$t=\infty ; F(t)=1$$

(b)

$$b = \int_{10}^{\infty} b_0 E(t) dt$$

$$\text{Where } b_0 = 1.25 \times 10^{15}$$

$$E(t) = \int F(t) dt = \int 1 - \exp\left(\frac{t}{T}\right) dt$$

$$b = \int_{10}^{\infty} (1.25 * 10^{15}) \left(\frac{1}{1.25*10^6} \exp\left(\frac{-t}{1.25*10^6}\right) \right)$$

$$= 1.009 * 10^9 \text{ bills}$$

$$= 10^9 \text{ bills}$$

14.5

$$kT = \ln \frac{c_{A0}}{c_A} = \ln \frac{1000}{1} = 6.9078$$

For the small deviation from plug flow, by the tanks in series model first calculate σ^2 from the tracer curve.

$$\alpha = 8 - 12 = 4$$

$$\sigma^2 = \frac{\alpha}{24} = \frac{2}{3}$$

$$T = 10$$

$$\frac{1}{N} = \sigma_\phi^2 = \frac{\sigma^2}{T^2} = \frac{\left(\frac{2}{3}\right)}{10^2} = 0.67 * 10^{-2}$$

$$N = 150 \text{ tanks}$$

$$kT = 6.9078 / 150 = 0.0461$$

For tank in series

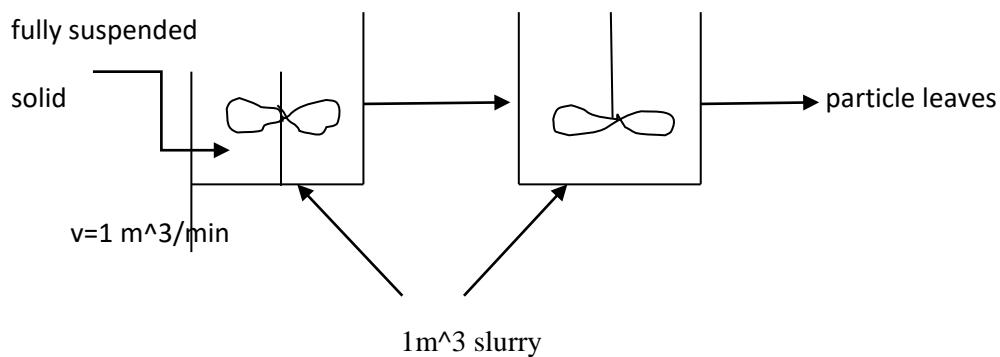
$$\frac{c_{A0}}{c_A} = \frac{1}{(1+kT)^N} = \frac{1}{(1+0.0461)^{150}}$$

$$= 1/863$$

$$\frac{c_{A0}}{c_A} = 0.00116$$

$$c_A = 1.16$$

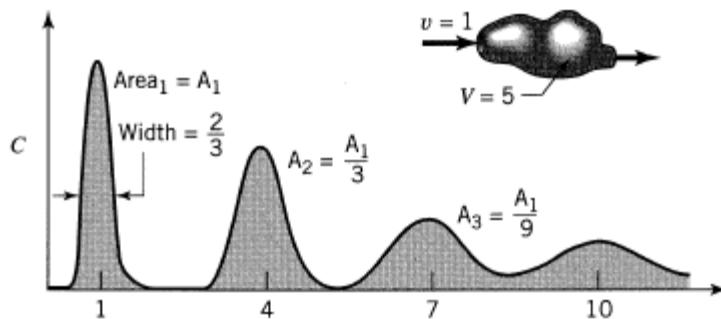
14.6



Conversion complete after 2 minutes in the reactor.

So there is no any dead zone is present because 1 minutes for each reactor.

14.7. Fit the RTD of Fig. P14.7 with the tanks-in-series model.



First approximate each pulse by plug flow pattern.

$$\frac{A_2}{A_1} = \frac{1}{3} = \frac{R}{R+1}$$

$$R=0.5$$

$$\frac{Vp_1}{(R+1)v} = 1;$$

Putting value R;

$$\frac{Vp_1}{(0.5+1)1} = 1;$$

$$Vp_1 = \frac{3}{2};$$

$$\frac{Vp_1}{(R+1)v} + \frac{Vp_2}{Rv} = 3;$$

Putting values and find Vp_2 ;

$$\frac{3/2}{(0.5+1)1} + \frac{Vp2}{(0.5)1} = 3;$$

Vp2=1;

$$V_{actual} = (3/2) + 1 = 2.5;$$

$$V_{dead} = 5 - 2.5 = 2.5;$$

Now considering that the pulse output has width,

$$\frac{\Delta\theta}{\theta_{max}} = \frac{2}{\sqrt{(N1-1)}},$$

$$\frac{2/3}{1} = \frac{2}{\sqrt{(N1-1)}},$$

N1=10 tanks;

$$N2 = (2/3) * N1;$$

N2=6.67 tanks;

$$T_{avg} = \frac{\sum tc}{\sum c};$$

$$T_{avg} = 2.49 = 2.5;$$

$$\frac{V1+V2}{v} = 1.5 + 1.0 = 2.5;$$

14.8

Find out number of tanks.

$$T_{avg} = \frac{\sum tcdt}{\sum cdt};$$

$$= \frac{320}{40};$$

$$= 8 \text{ min}$$

$$\sigma^2 = \frac{\sum tc}{\sum c} - \left[\frac{\sum tcdt}{\sum cdt} \right]^2;$$

$$= \left(\frac{250+490+810+1210}{40} \right) - \left(\frac{320}{40} \right)^2;$$

$$= 5;$$

$$\frac{1}{N} = \frac{\sigma^2}{(tavg)^2};$$

$$N = \frac{64}{5};$$

$$N = 12.8$$

N=13.

14.9 For N tanks in series.

Finding out number of tanks

$$N=1+4\left(\frac{\theta_{max}}{\Delta\theta}\right)^2;$$

N1peak=104 tanks;

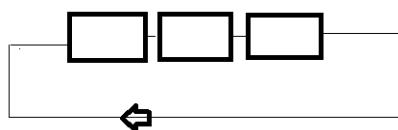
N2peak=101 tanks;

N3peak=101 tanks;

N4peak=97 tanks;

So that average is 100 tanks.

Model



14.10

(a) Area under curve c vs t curve

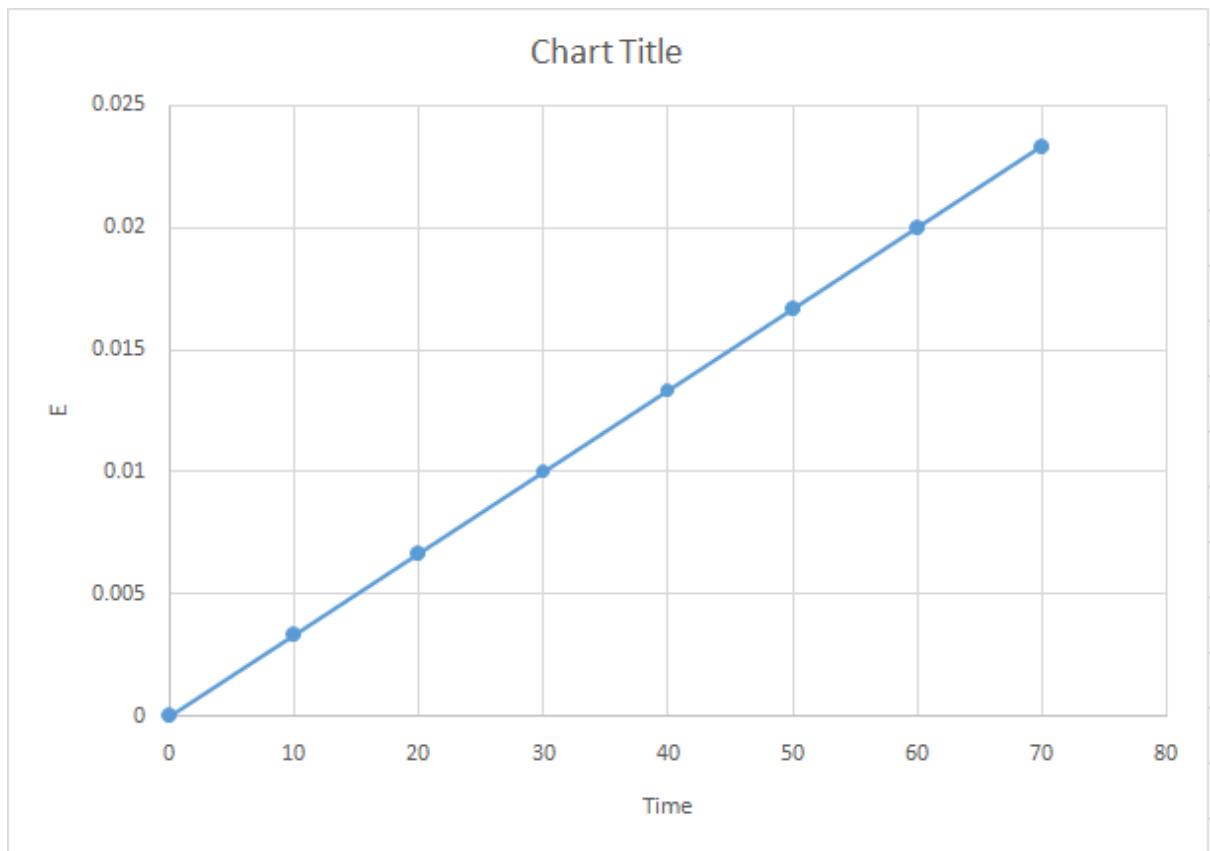
$$\int_0^{\infty} c_i \Delta t_i = \sum c_i \Delta t_i$$

$$=3000$$

$$\text{Mean resident time} = \frac{\sum c_i t_i \Delta t_i}{\sum c_i \Delta t_i} = 34.66$$

(b) E curve

C	Time	E=C/q	CA/CAo
35	0	0	0
38	10	0.00333	0.0202
40	20	0.00666	0.0245
40	30	0.0133	0.0223
39	40	0.0166	0.0183
38	50	0.022	0.0136
35	60	0.0233	0.0099



$$(c) \text{ Variance} = \frac{\sum c_i t_i^2 \Delta t_i}{\sum c_i \Delta t_i} - T_i^2$$

$$= 22.45$$

(d) How many tanks in series in this vessel equipment to?

$$\frac{1}{N} = \sigma_{\emptyset}^2 = \frac{\sigma^2}{T^2} = \frac{(22.45)^2}{34.66^2}$$

$$N = 2.38 \text{ tanks}$$

Example:-14.11

A reactor has flow characteristics given by the nonnormalized C curve in Table P14.11, and by the shape of this curve we feel that the dispersion or tanks-in-series models should satisfactorily represent flow in the reactor.

- (a) Find the conversion expected in this reactor, assuming that the dispersion model holds.
- (b) Find the number of tanks in series which will represent the reactor and the conversion expected, assuming that the tanks-in-series model holds.

Time	Concentration
1	0
2	9
3	57
4	81
5	90
6	90
7	86
8	77
10	67
15	47
20	32
30	15
41	7
52	3
70	0

- (c) Find the conversion by direct use of the tracer curve.
- (d) Comment on the difference in these results, and state which one you think is the most reliable.

Solution:-

To find out non ideal characteristics of reactor determine proper D/uL

To use for dispersion model, or the proper N value to use for tank in series model.

This is done by two way :- matching tracer concentration curve with dispersion model or with tank in series model , or by calculating σ^2 from that D/uL or N .

Lets us use the latter procedure. So first calculate T and σ^2 from the table of data with the help of given equ. $T = \frac{\int_0^\infty tc dt}{\int_0^\infty cd t} = \frac{\sum t_i c_i \Delta t_i}{\sum c_i \Delta t_i}$

$$\sigma^2 = \frac{\int_0^\infty (t - T)^2 cd t}{\int_0^\infty cd t} = \frac{\int_0^\infty t^2 cd t}{\int_0^\infty cd t} - T^2$$

$$\Sigma C = 213$$

$$T = 2149/213 = 10.09 \text{ min}$$

$$\Sigma tc = 2149$$

$$\sigma^2 = \left(\frac{37685}{213} \right) - (10.09)^2 = 75.11$$

$$\Sigma t^2 c = 37685 \quad \sigma_\theta^2 = \frac{\sigma^2}{T^2} = \frac{75.116}{(10.09)^2} = 0.7378$$

Next determine the behavior of ideal PFR

$$k=0.456 \text{ min}^{-1} \quad kT=4.6$$

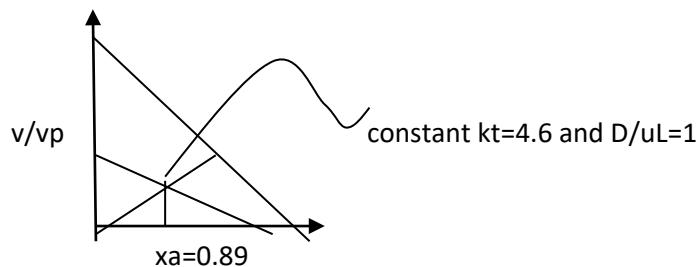
$$\text{so for PFR } x_a = 1 - e^{kT} = 1 - e^{4.6} = 0.99$$

(a) Use the dispersion model

Here related σ_θ^2 with D/uL so,

$$\sigma_\theta^2 = 0.7378 = 2 \left(\frac{D}{uL} \right) - 2 \left(\frac{D}{uL} \right)^2 [1 - e^{-\frac{uL}{D}}]$$

Solve by trial and error. this gives $D/uL=1$



From fig $x(\text{disp})=0.89$

(b) Use tank in series model

$$N = \frac{1}{\sigma_\theta^2} = \frac{1}{0.7385} = 1.35 \text{ Tanks}$$

From fig 6.5 we can find the $X(\text{tank})=83\%$

(c) Use the tracer data directly

$$\text{From } \frac{c}{c_0} = \sum \left(\frac{c}{c_0} \right) E \Delta t$$

To find out E curve make the area under C curve unity,

Time	Concentration	$e^{-0.465(\frac{c_i t_i}{213})}$
1	0	0
2	9	0.0506
3	57	0.0456
4	81	0.0158
5	90	0.0050
6	90	0.0015
7	86	0.0005
8	77	0.0002
10	67	0.0001
15	47	$16*10^{-6}$
20	32	$5*10^{-6}$
30	15	$1*10^{-6}$
41	7	0
52	3	0
70	0	0

$$E = \frac{c}{\text{area}} = \frac{c}{\sum c_i \Delta t}$$

Now we know that

$$\frac{c}{c_0} = \sum \left(\frac{c}{c_0} \right) E \Delta t$$

$$\sum c = 213$$

$$\sum E = 0.1911$$

$$X = 0.88 (\text{from curve})$$

- (d) Which answer is most reliable

Naturally the direct use of tracer gives most reliable answer. In this given model RTD come from dispersion model $D/uL=1$. Thus wind accepted that ans to part (a) and (c) should agree.

Solid Catalysed Reactions

Solution 18.1

We cannot tell just by looking at the reactor and the catalyst bed height whether the reactor is integral or differential. It isn't the depth or the packing or the conversion level that counts but the assumptions used when the data from the reactor are analysed. If we assume it as a constant rate of reaction throughout the reactor, then it is a differential reactor but if we assume a changing rate of reaction with changing position, then it becomes a integral reactor. It is just the matter of how we are looking at the rate.

Solution 18.2

Since the volume is made 3 times the original volume but the temperature, feed flow rate, the amount of the catalyst remains the same, according to the performance equation of the mixed flow reactor,

$$\frac{W}{F_{AO}} = \frac{X_A}{-r_A}$$

Thus there will be no change in the conversion.

Solution 18.3

a) We have been given data for the weight of the catalyst, molar flow rate and the conversion. Since it is a packed bed reactor, the performance equation is as follows.

$$\frac{W}{F_{AO}} = \int_0^{X_A} \frac{dX_A}{-r_A}$$

Writing it in the differential form,

$$\frac{dW}{F_{AO}} = \frac{dX_A}{-r_A}$$

Thus making the subject as $-r_A$,

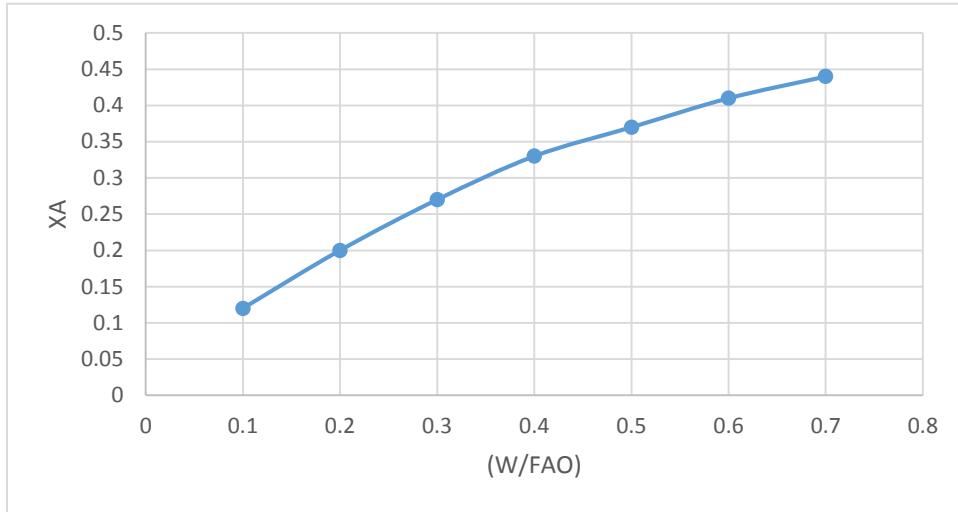
$$-r_A = \frac{dX_A}{d\left(\frac{W}{F_A}\right)}$$

$W, \text{kg cat}$	1	2	3	4	5	6	7
X_A	0.12	0.20	0.27	0.33	0.37	0.41	0.44

Thus we see that the slop of the curve at the $X_A = 0.4$ gives us the rate of the equation.

Thus taking the slope of the curve at the point $X_A = 0.4$

$$-r_A = \frac{0.482 - 0.23}{0.8 - 0.1} = 0.36 \frac{\text{kgmole converted}}{\text{kg cat . hr}}$$



b) For finding the amount of catalyst required if the molar flow is 400 kmol/hr and the conversion required is $X_A=0.4$,

From the curve we can see that for $X_A= 0.4$, the ratio of W/FAO is 0.575.

Therefore, $W= 0.575 \times 400 = 230$ kg Cat.

c) For completely mixed flow reactor,

$$\frac{W}{F_{AO}} = \frac{X_A}{-r_A \text{ at } 0.4}$$

$$\frac{W}{F_{AO}} = \frac{X_A}{-r_A \text{ at } 0.4} = \frac{0.4}{0.36}$$

$$W = 400 \times (0.4/0.36) = 444 \text{ kg catalyst}$$

Solution 18.4

$A \rightarrow R$ n=1/2 th order reaction with infinite (very large) recycle hence $R = \infty$

$W = 3$ kg of catalyst

$C_{A0} = 2 \text{ mol/m}^3$, $C_A = C_{Aout} = 0.5 \text{ mol/m}^3$

$V = 1 \text{ m}^3/\text{hr}$

$\varepsilon_A = 1 - 1/1 = 0$

$$X_A = (C_{A0} - C_A) / (C_{A0} + \varepsilon_A \cdot C_A)$$

$$X_A = \frac{2 - 0.5}{2 + 0 \times 0.5}$$

$$X_A = 0.75$$

F_{A0} = molar flow rate of gas A

$$F_{A0} = 2 \text{ mol/m}^3 \times 1 \text{ m}^3/\text{hr}$$

$$= 2 \text{ mol/hr}$$

$$\therefore \frac{W}{F_{A0}} = \frac{X_{Aout}}{-r_{Aout}} \quad (\text{for MFR}) \quad (1)$$

$$\text{Here, } -r_{Aout} = k' \times C_{Aout}^{1/2} \quad (2)$$

$$\therefore k' = \frac{F_{A0} \times X_{Aout}}{W \times C_{Aout}} \quad (3)$$

$$= \frac{2 \times 0.75}{3 \times 0.5}$$

$$= 1 \text{ m}^3/\text{kg of catalyst} \cdot \text{hr}$$

Put the value of k' in equation (2) to get value of $-r_{Aout}$

$$\therefore -r_{Aout} = 1 \text{ m}^3/\text{kg of catalyst} \cdot \text{hr} \times 0.5^{1/2} \text{ mol/m}^3$$

$$\therefore -r_{Aout} = 0.707 \text{ mol / kg of catalyst} \cdot \text{hr}$$

$$\text{Hence, } -r_A \text{ (mol / kg of catalyst} \cdot \text{hr}) = (1 \text{ m}^3/\text{kg of catalyst} \cdot \text{hr}) (C_A \text{ mol / m}^3)^{1/2}$$

SOLUTION 18.5

Very large recycle, $A \rightarrow 3R$, $n=1$ and feed contains 50% A and 50% inert.

Here $\xi=1$, $F_{A0}=2 \text{ mol/hr}$, $W=3 \text{ kg}$, $C_{Aout}=0.5 \text{ mol/m}^3$, $C_{Ao}=2 \text{ mol/m}^3$

With large recycle, use the performance equation of a mixed flow reactor,

$$\frac{W}{F_{A0}} = \frac{X_{Aout}}{-r_{Aout}}, \quad -r_{Aout} = k' C_{Aout} \dots \text{first order decomposition of A}$$

$$\therefore \frac{W}{F_{A0}} = \left(\frac{1 - \frac{C_{Aout}}{C_{Ao}}}{1 + \frac{C_{Aout}}{C_{Ao}}} \right) \times \frac{1}{k' C_{Aout}}$$

$$\therefore k' = 0.8 \text{ m}^3/(\text{h} \cdot \text{kg} \cdot \text{cat})$$

$$\text{Therefore, } -r_A = -\frac{1}{W} \frac{dN_A}{dt} = 0.8 \text{ m}^3/(\text{h} \cdot \text{kg} \cdot \text{cat}) \cdot C_A \text{ mol/m}^3$$

SOLUTION 18.6

No recycle, $A \rightarrow 3R$, $n=2$ and feed contains 25% A and 75% inert, 4 volumes

$$\xi_A = (6-4)/4 = 0.5$$

$$C_A = C_{Ao} \left(\frac{1-X_A}{1+0.5X_A} \right)$$

With No recycle, it becomes a plug flow reactor.

$$\text{So, } \frac{W}{FA_0} = \int_0^{XA} \frac{dXA}{-r_A}$$

$$-r_A = k' C_A^2$$

$$\frac{W}{FA_0} = \int_0^{XA} \frac{dXA}{\left(\frac{1-XA}{1+0.5XA}\right)^2}$$

$$= \int_0^{XA} \frac{(1+0.5XA)^2 dXA}{(1-XA)^2}$$

$$= \int_0^{XA} \frac{(1+XA+0.25XA^2) dXA}{(1-XA)^2}$$

$$= \int_0^{XA} \frac{dXA}{(1-XA)^2} + \int_0^{XA} \frac{(XA) dXA}{(1-XA)^2} + 0.25 \int_0^{XA} \frac{XA^2 dXA}{(1-XA)^2}$$

$$I = \int_0^{XA} \frac{dXA}{(1-XA)^2} = \frac{XA}{(1-XA)}$$

$$II = \int_0^{XA} \frac{(XA) dXA}{(1-XA)^2} = \frac{XA}{(1-XA)} + \ln(1-XA)$$

$$III = 0.25 \int_0^{XA} \frac{XA^2 dXA}{(1-XA)^2} = 0.25 \frac{XA}{(1-XA)} + 0.50 \ln(1-XA) + 0.25XA$$

$$I+II+III = 2.25 \frac{XA}{(1-XA)} + 1.50 \ln(1-XA) + 0.25XA$$

$$\frac{W}{FA_0} = \frac{1}{k' C_{AO}} \left[2.25 \frac{XA}{(1-XA)} + 1.50 \ln(1-XA) + 0.25XA \right]$$

$$X_A = 0.67$$

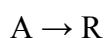
$$k' = \left[2.25 \frac{XA}{(1-XA)} + 1.50 \ln(1-XA) + 0.25XA \right] \times \frac{FA_0}{C_{AO}^2 \times W}$$

$$k' = 0.512 \text{ m}^6 / (\text{mol} \cdot \text{h} \cdot \text{kg} \cdot \text{cat})$$

$$-r_A = -\frac{1}{W} \frac{dNA}{dt} = 0.512 \text{ m}^6 / (\text{mol} \cdot \text{h} \cdot \text{kg} \cdot \text{cat}) \cdot (C_A \text{ mol/m}^3)^2$$

Solution 18.7

Mixed Flow Behaviour



$$\epsilon_a = \frac{1-1}{1} = 0$$

$$C_{AO} = 10 \frac{\text{mol}}{\text{m}^3}; W = 4 \text{ gm}$$

Performance Equation

$$\frac{W}{F_{AO}} = \frac{X_A}{-r_A}$$

For No. 1:

$$V_o = 3 \frac{m^3}{h}, X_A = 0.2$$

$$F_{AO} = V_o * C_{AO}$$

$$= 3 * 10$$

$$= 30 \frac{mol}{h}$$

$$-r_A = X_A * \frac{F_{AO}}{W}$$

$$= 0.2 * 30/4$$

$$= 1.5 \frac{mol}{h g cat}$$

$$C_A = C_{AO} * (1-X_A) \text{ since } \epsilon a = 0$$

$$= 10 (0.8)$$

$$C_A = 8 \frac{mol}{m^3}$$

For No. 2:

$$V_o = 2 \frac{m^3}{h} \quad X_A = 0.3$$

$$F_{AO} = V_o * C_{AO}$$

$$= 2 * 10$$

$$= 20 \frac{mol}{h}$$

$$-r_A = X_A * \frac{F_{AO}}{W}$$

$$= 0.3 * 20/4$$

$$= 1.5 \frac{mol}{h g cat}$$

$$C_A = C_{AO} * (1-X_A) \text{ since } \epsilon a = 0$$

$$= 10 (0.7)$$

$$C_A = 7 \frac{mol}{m^3}$$

V_o	3	2	1.2
F_{AO}	30	20	12
X_A	0.2	0.3	0.5
C_A	8	7	5
$-r_A$	1.5	1.5	1.5

So the reaction is independent of C_A (0th Order)

$$-r_A = K C_A^n$$

$$-r_A = 1.5 \frac{\text{mol}}{\text{h g cat}}$$

Solution 18.8

Plug Flow

$$C_{AO} = 60 \frac{\text{mol}}{\text{m}^3} \quad v_O = 3 \frac{\text{lt}}{\text{min}} = 3 * 10^{-3} \frac{\text{m}^3}{\text{min}}$$

$$F_{AO} = v_O * C_{AO}$$

$$= 60 * 3 * 10^{-3}$$

$$= 0.18 \frac{\text{mol}}{\text{min}}$$

$$\frac{W}{F_{AO}} = \int_0^{X_A} \frac{dX_A}{-r_A}$$

$$A \rightarrow R \quad , \quad \epsilon_a = \frac{1-1}{1} = 0$$

$$C_A = C_{AO} * (1-X_A)$$

$$X_A = 1 - \frac{C_A}{C_{AO}}$$

$$X_{A1} = 1 - \frac{30}{60} = 0.5$$

$$\frac{W_1}{F_{AO}} = \frac{0.5}{0.18} = 2.78$$

$$X_{A2} = 1 - \frac{20}{60} = 0.67$$

$$\frac{W_2}{F_{AO}} = \frac{1}{0.18} = 5.56$$

$$X_{A3} = 1 - \frac{10}{60} = 0.833$$

$$\frac{W_3}{F_{AO}} = \frac{2.5}{0.18} = 13.89$$

Guessing the rate as

First order

$$-r_A = k * C_A$$

$$= k * C_{AO} * (1-X_A)$$

$$\frac{W}{F_{AO}} = \int_0^{X_A} \frac{dX_A}{-r_A}$$

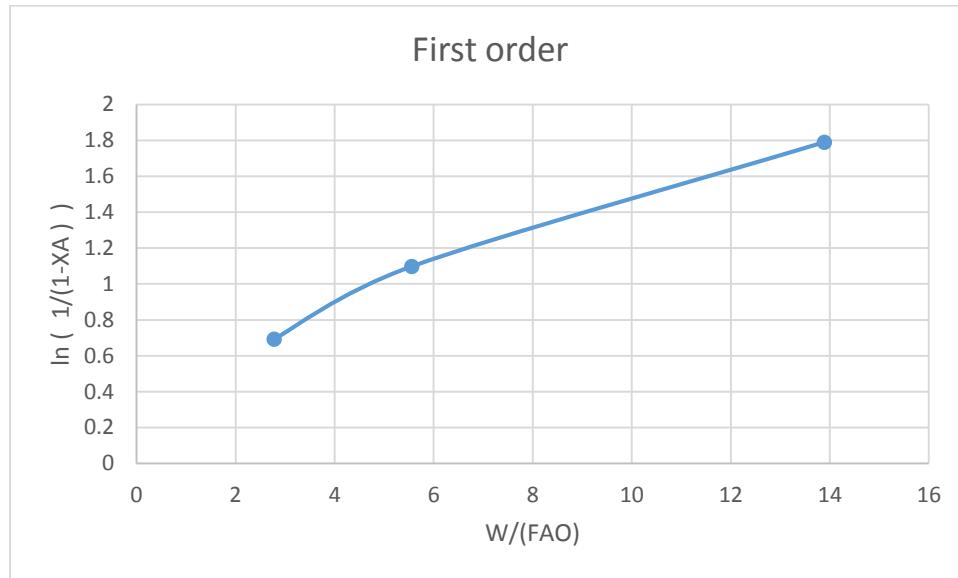
$$= \int_0^{X_A} \frac{dX_A}{k * C_{AO} * (1 - X_A)}$$

$$= \frac{-\ln(1 - X_A)}{k * C_{AO}}$$

$$\frac{W}{F_{AO}} = \frac{1}{k * C_{AO}} * \ln \left(\frac{1}{1-X_A} \right)$$

$y = mx$

	1	2	3
$\frac{W}{F_{AO}}$	2.78	5.56	13.89
$\ln \left(\frac{1}{1-X_A} \right)$	0.693	1.098	1.79



$\frac{W}{F_{AO}}$ vs $\ln \left(\frac{1}{1-X_A} \right)$ is not coming straight line. So our assumption of First order is wrong.

Guessing Second order:

$$-r_A = k * C_A^2$$

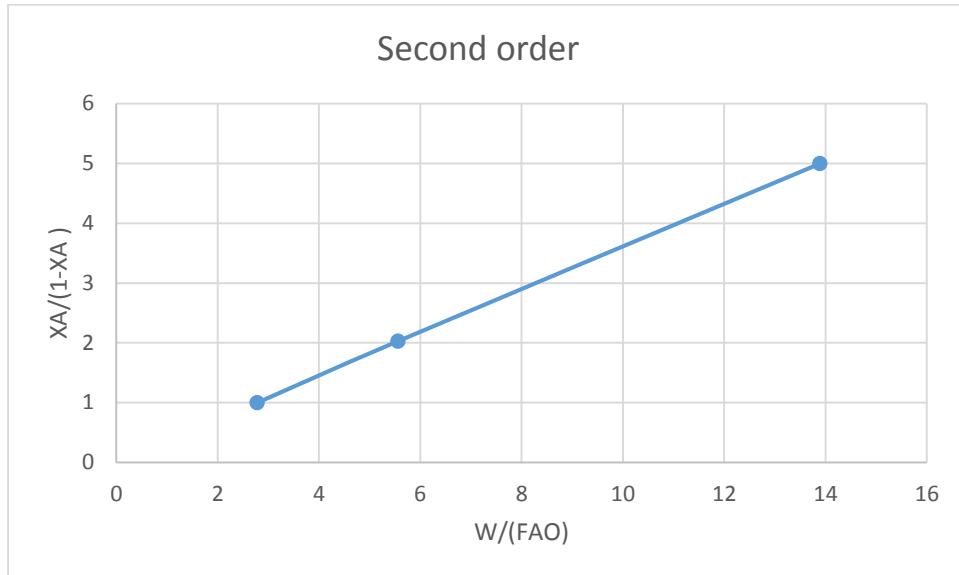
$$= k * C_{AO}^2 * (1-X_A)^2$$

$$\frac{W}{F_{AO}} = \int_0^{X_A} \frac{dX_A}{-r_A}$$

$$= \int_0^{X_A} \frac{dX_A}{k * C_{AO}^2 * (1-X_A)^2}$$

$$\frac{W}{F_{AO}} = \frac{1}{k * C_{AO}^2} * \frac{X_A}{1-X_A}$$

	1	2	3
$\frac{W}{F_{AO}}$	2.78	5.56	13.89
$\frac{X_A}{1-X_A}$	1	2.03	4.998



$\frac{W}{F_{AO}}$ vs $\frac{X_A}{1-X_A}$ is coming straight line. So our assumption of Second order is correct.

$$\text{Slope} = \frac{1}{k * C_{AO}^2} = 2.773$$

$$\frac{1}{k * 60^2} = 2.773$$

$$k = 10^{-4} \frac{m^6}{\text{mol min g cat}}$$

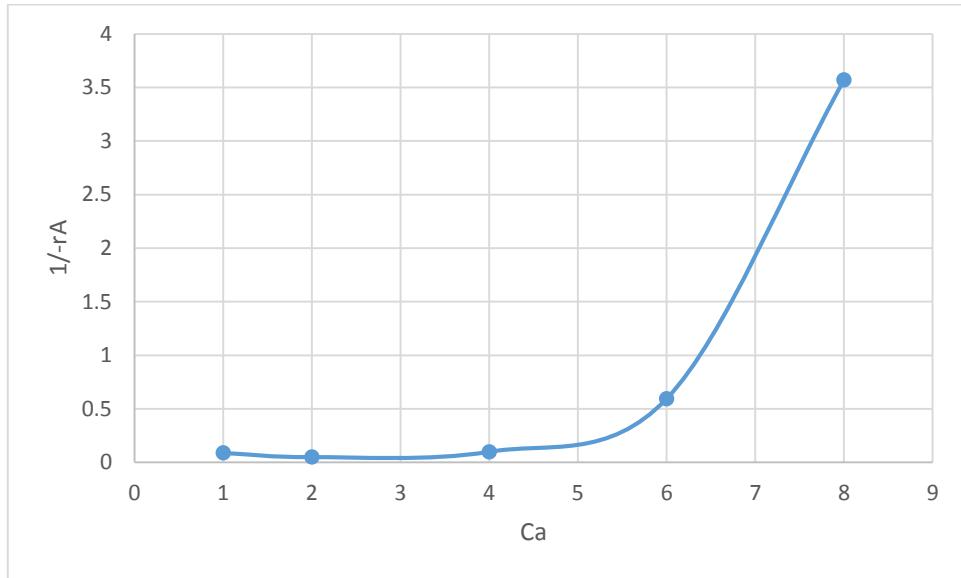
$$-r_A = 10^{-4} * C_A^2$$

Solution 18.9

We have reaction A \rightarrow R, $C_{AO} = 10 \text{ mol/m}^3$

F_{AO} , mol/min	0.14	0.42	1.67	2.5	1.25
C_A , mol/m ³	8	6	4	2	1

C_A	X_A	F_{AO}	$1/-r_A$
8	0.2	0.14	3.571429
6	0.4	0.42	0.595238
4	0.6	1.67	0.0998
2	0.8	2.5	0.05
1	0.9	1.25	0.088889



For packed bed reactor with $C_{AO} = 8 \text{ mol/m}^3$ and $X_A = 0.75$, $C_A = 2 \text{ mol/m}^3$.

Also the area under the curve for $1/-r_A$ vs C_A from $C_{AO} = 8 \text{ mol/m}^3$ to $C_A = 2 \text{ mol/m}^3$ is 5.08.

According to the performance equation of the Packed bed reactor,

$$\frac{W}{F_{AO}} = \int \frac{dX_A}{-r_A}$$

We get, $W = 1000 \times 5.08/8 = 615 \text{ kg}$ of catalyst is required.

Solution 18.10

For Mixed Flow reactor, the concentration inside the reactor will be same as that of the leaving stream. Given that the initial reactant concentration is 10 mol/m^3 and the conversion is 90 %, the outlet concentration of the stream will be 1 mol/m^3 . Thus from the above tabulated data, the rate constant can be found out.

$$k = \frac{-r_A}{C_A}$$

$$\text{Thus } k = \frac{11.25}{1} = 11.25 \text{ m}^3/\text{mol. Min}$$

Thus the amount of the catalyst required is given by

$$W = \frac{F_{AO}}{k} X \frac{X_A}{C_A}$$

$$W = 1000 \times 0.9 / (11.25 \times 1)$$

$$W = 80 \text{ kg}$$

Term Paper
Of Cre-II,
Chapter No:18
Solid Catalysed Reactions
Sum No: 18.11-18.20

Submitted By:

Samarpita Chakraborty
(13BCH013)

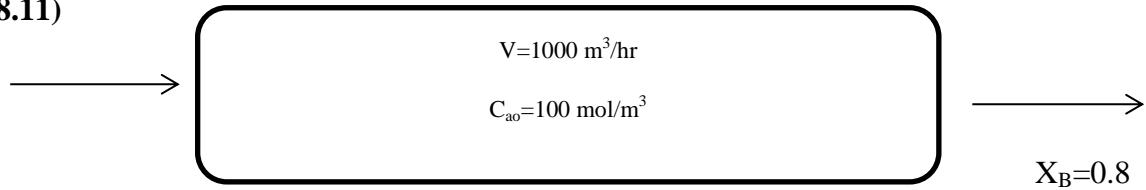
Harsh Dodia
(13BCH014)

Nirav Donga
(13BCH015)

Harshit Goyal
(13BCH018)



18.11)



$$-r_A = \frac{50CA}{1+0.02CA} \text{ Mol/kg.hr}$$

For Plug Flow

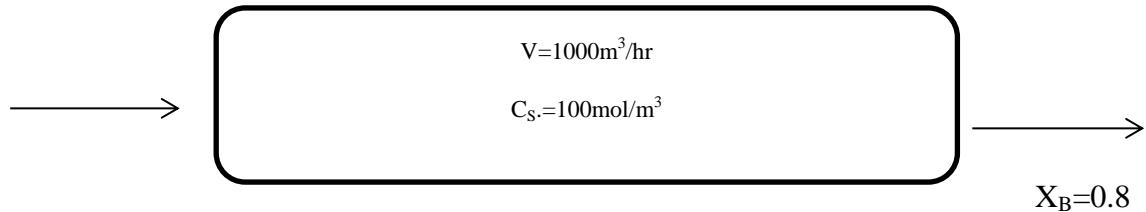
$$T' = \frac{W}{v} = \int_0^{X_A f} dX_A / -r' A = 1/k' \int_{20}^{100} \frac{1+0.02Ca}{50Ca} dCa$$

$$K'T' = [\ln(C_{ao}/Ca) + k(C_{ao}-Ca)]$$

$$\Rightarrow \frac{1000}{50} [\ln \frac{100}{20} + .02 (100-20)]$$

$$\Rightarrow W = 64.19 \text{ Kcal}$$

18.12)



$$-r_A = 8 C_A^2 \text{ Mol/kg.hr}$$

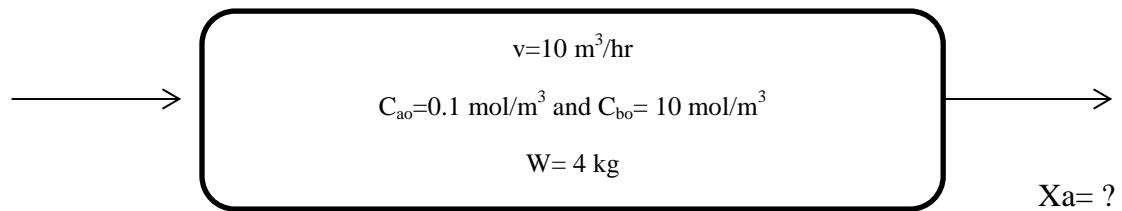
For Plug Flow

$$T' = \frac{W}{v} = \int_0^{X_A f} dX_A / -r' a = 1/k' \int_{20}^{100} dCa / -r' a$$

$$T' = 1/8 \frac{\int_{20}^{100} dCa}{8Ca^2}$$

- $\Rightarrow -1/8 [1/C_{a0} - 1/C_a]$
- $\Rightarrow -1/8 [1/100 - 1/20]$
- $\Rightarrow T' = W/V = 0.005$
- $\Rightarrow W = 0.005 \times 1000 = 5 \text{ kg catalyst}$

18.13)



$$-r_a' = .6 C_A C_B$$

$$\text{For } C_{Ao}=0.01 C_{Bo}$$

We can assume that $C_B = \text{Constant}$

$$\Rightarrow -r_A' = C_A C_B = .6 C_A \cdot 10 = 6 C_A$$

$$\Rightarrow T' = \frac{W}{v} = \frac{4}{10} = .4 \text{ kg.hr/m}^3$$

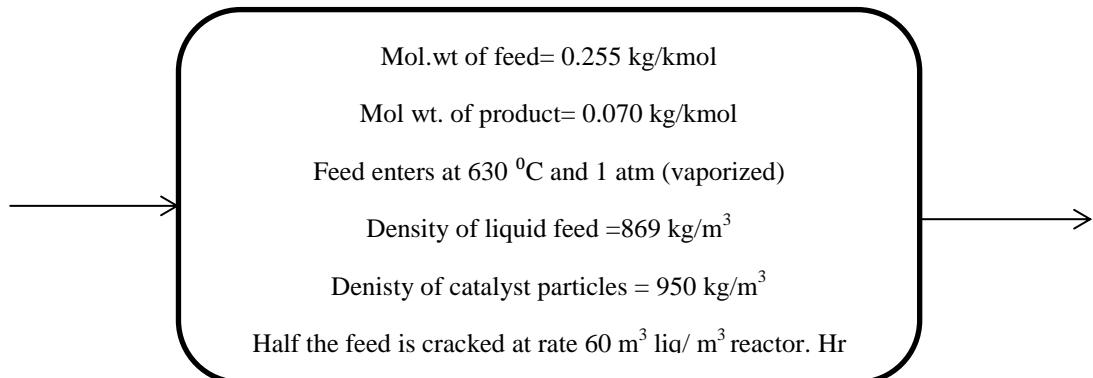
\Rightarrow For First order

$$\Rightarrow \frac{C_A}{C_{Ao}} = e^{-k' T'} = e^{-6 \cdot .4} = .0907$$

$$\Rightarrow X_A = 90.9\%$$

$$\Rightarrow X_B = .909\%$$

18.14)



For Plug flow

$$\tau/C_{ao} = V/W \int \frac{dx}{-ra'}$$

Where V = volume of catalyst and W = weight of catalyst

We know, $C_{ao} = P_{ao}/RT$

$$= 1 \text{ atm}/0.082 \times (630 + 273)$$

$$= 0.01350 \text{ mol/litre}$$

$$= 13.50 \text{ mol / m}^3$$

For Plug flow and 1st order kinetics,

$$k''' \tau''' = \ln[C_{ao}/C_a]$$

$$k''' (1/60) = \ln (13.5/7.75)$$

$$k''' = 41.5888 \text{ hr}^{-1}$$

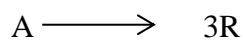
We know,

$k''' \tau''' = k' \tau'$ [τ' is $\tau'''x$ (Density of the catalyst particles-bulk Density of packed bed) - as in solid catalyzed reactions volume of catalysts can be taken as the void volume of reactor.]

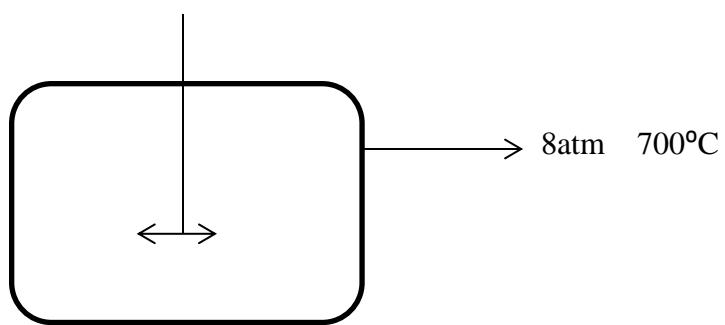
$$(41.588)(1/60) = k' ((950-700)/60)$$

$$k' = 0.166 \text{ m}^3 \text{ liquid/kg catalyst. Hr}$$

18.15)



$$\varepsilon = 2$$



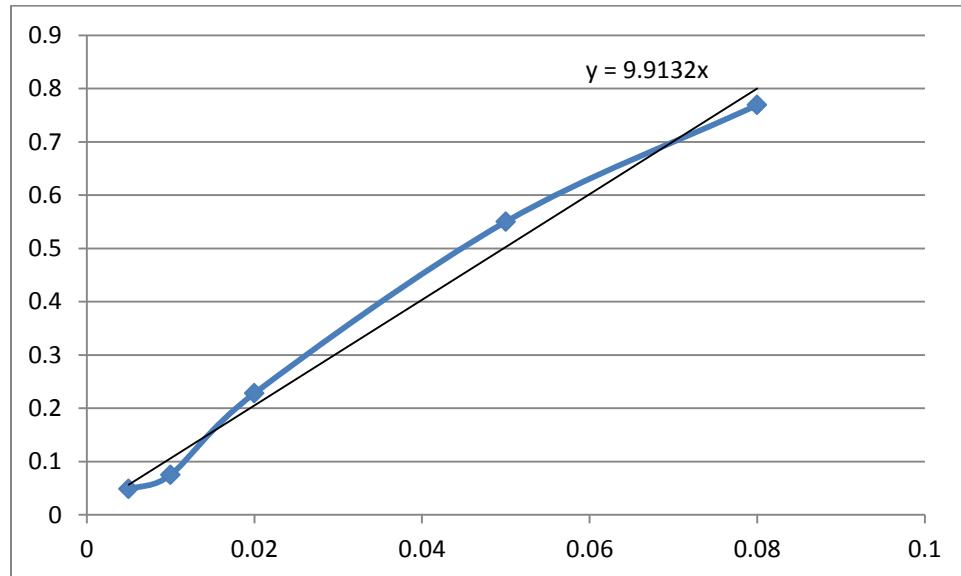
$$\frac{W}{Fao} = \frac{Xa}{-ra'}$$

$$\frac{Ca}{Cao} = \frac{1-Xa}{1+2Xa}$$

$$Ca = P_A/RT = \frac{8}{.08206*973} = 0.1 \text{ mol/lit}$$

Ca	Ca/Cao	Xa = (1 - Ca/Cao) / (1 + 2Ca/Cao)	Fao = vCao	-ra = Xa / Fao / W
0.08	0.8	0.076923077	10	0.769
0.05	0.5	0.25	2.2	0.55
0.02	0.2	0.571428571	0.4	0.228
0.01	0.1	0.75	0.1	0.075
0.005	0.005	0.863636364	0.05	0.0482

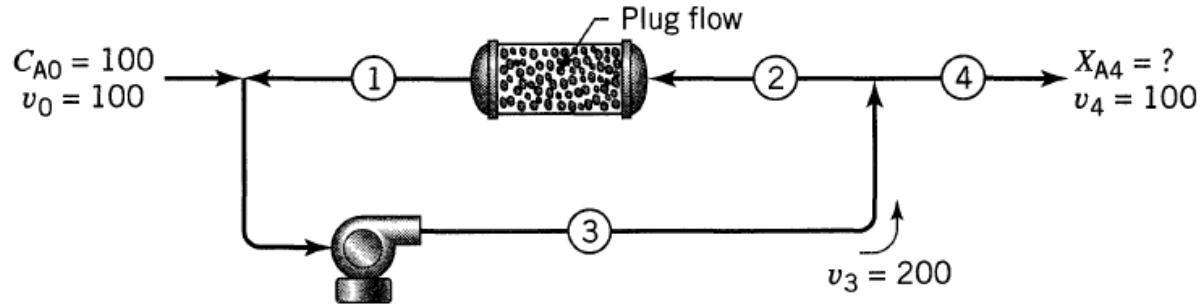
-r_a vs C_a



The Trendline of the curve gives us the relation:

$$-r_A' = 9.9132 C_A$$

18.16)



For 1st order solid catalyzed reaction, without any complex piping conversion is $X_A = 0.8$ and thus

$$\Rightarrow k' \tau' = \ln [C_{AO}/C_A]$$

$$\Rightarrow k' \tau' = -\ln [1-X_a]$$

$$\Rightarrow k' \tau' = -\ln[1-0.8]$$

⇒ $k' \tau' = 1.6094$ (Damkohler number for 1st order reactions)

at points 2, 3, 4 the conversion is same at steady state.

$$\tau'/C_{A0} = \int \frac{dXa}{-ra} = \int \frac{dXa}{k' Ca}$$

$$\Rightarrow k' \tau' / C_{A0} = \int_{Xa2}^{Xa1} \frac{dXa}{C_{ao}(1-Xa)}$$

$$\Rightarrow k' \tau' = -\ln [(1-X_{a1})/(1-X_{a2})]$$

Taking mole balance,

$$C_{A0}v_0 + C_{A1}v_1 = C_{A3}v_3$$

And $C_{A2} = C_{A3} = C_{A4}$

$$\Rightarrow C_{A0}v_0 + C_{A1}v_1 = C_{A3}v_3$$

Solving equation 1 and 2,

$$1.6094 = -\ln \left[\frac{(1-X_{a1})}{(1-X_{a2})} \right]$$

$$\Rightarrow e^{1.6094} = [(1-X_{a2})/(1-X_{a1})]$$

$$\Rightarrow 5(1 - XA1) = 1 - XA2$$

$$\Rightarrow 5C_{A1}/C_{A0} \equiv C_{A2}/C_{A0}$$

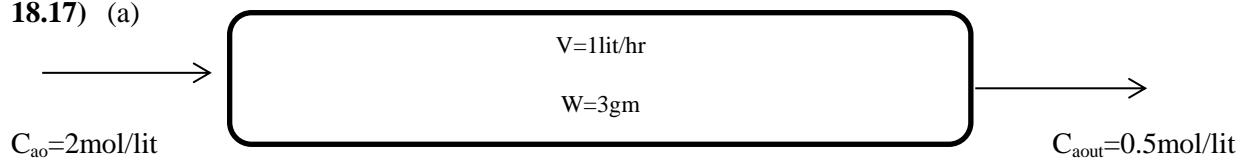
$$\Rightarrow C_{A2}/C_{A1} \equiv C_{A3}/C_{A1} \equiv C_{A4}/C_{A1} \equiv 5$$

Therefore solving equation 2 we get,

$$C_{A4} \equiv 11.11 \times 5 \equiv 55.55$$

Thus, $X_{A1} = 1 - (55.55/100) = 0.444$

18.17) (a)



1000.111

$$\nabla \equiv \text{Im} / \text{Re}$$

$$W=3gm$$

$$C_{aout}=0.5\text{mol/lit}$$

Second order

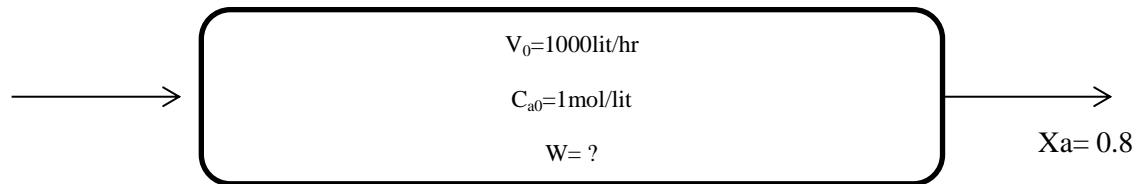
$$- r_a' = k' C_a^2$$

$$T' = \frac{W_{Cao}}{Fao} = \frac{W}{v_0} = \frac{C_{ao} - C_a}{-ra'}$$

$$k' = \frac{V_0}{W} \cdot \frac{Ca_0 - Ca}{Ca * Ca}$$

$$= \frac{1}{3} \cdot \frac{2-0.5}{0.5*0.5} = 2 \text{lit}^2/\text{mol.gm.hr}$$

(b) For packed bed (assume plug flow)



For plug flow

$$T' = \frac{W}{V_0} = \int_{C_a}^{C_{ao}} \frac{dC_a}{kC_a \cdot C_a} = \frac{1}{k} \left[\frac{1}{C_a} - \frac{1}{C_{ao}} \right]$$

$$W = \frac{1000}{2} \cdot \left[\frac{1}{0.2} - \frac{1}{1} \right] = 2000 \text{ gm} = 2 \text{ kg}$$

(c) Add inert solid

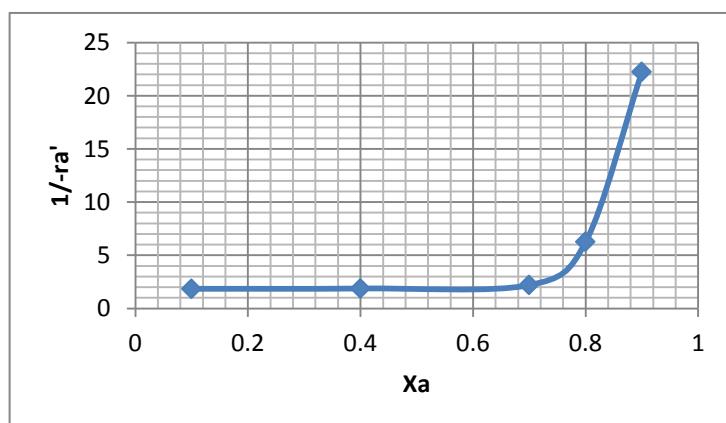
This does not change the rate equation or performance equation

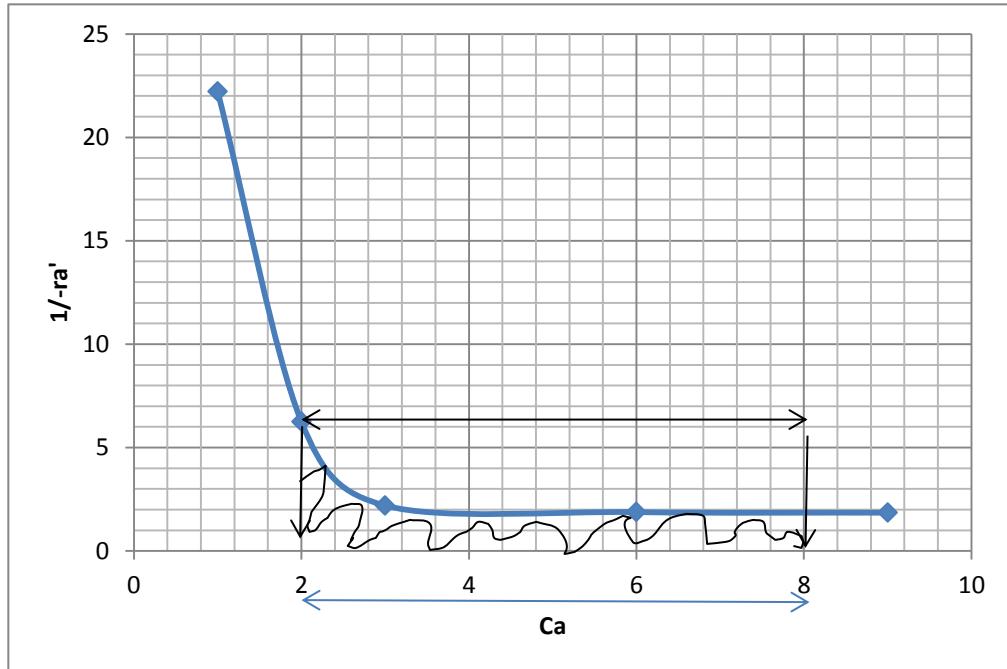
Therefore, adding inert make the reactor bigger but does not change the weight of the catalyst needed for the process

18.18)

$A \rightarrow R$ in a packed bed reactor.

C_{ao} mol/m ³	C_a mol/m ³	V_0 (lit/hr)	F_{ao}	X_a	$(-r_a')$	$1/(-r_a')$
10	1	5	0.05	0.9	0.045	22.22222
W kg cat	2	20	0.2	0.8	0.16	6.25
1	3	65	0.65	0.7	0.455	2.197802
	6	133	1.33	0.4	0.532	1.879699
	9	540	5.4	0.1	0.54	1.851852





$$\int \frac{dCa}{-ra} = 14$$

(Area under the curve for PFR i.e with no recycle of exit fluid for $X_a = 0.75$)

$$(C_{a0} - C_a) / -ra = 36$$

(Area under the curve for CSTR i.e with very high recycle and for $X_a = 0.75$)

Hence,

Part 1: For PFR,

$$W = F_{AO}/C_{AO} \int \frac{dCa}{-ra} = (1000 \times 14)/8 = 1750 \text{ kg catalyst}$$

Part 2 : For CSTR,

$$W = F_{AO}/C_{AO} \times (C_{a0} - C_a) / -ra$$

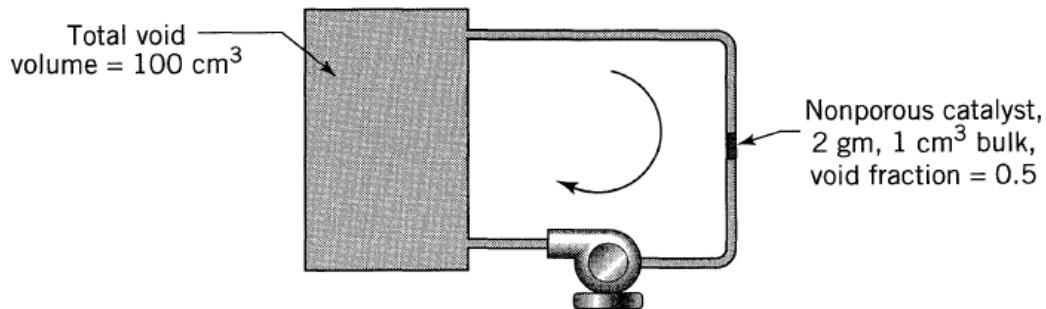
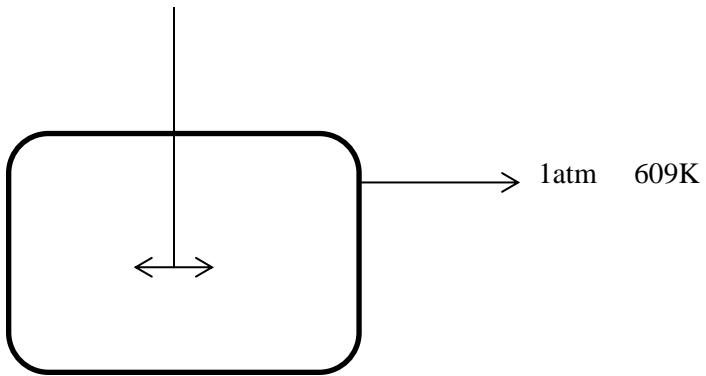
$$= (1000/8) \times 36$$

$$= 4500 \text{ kg catalyst}$$

18.19)



$$V=100 \text{ cm}^3$$



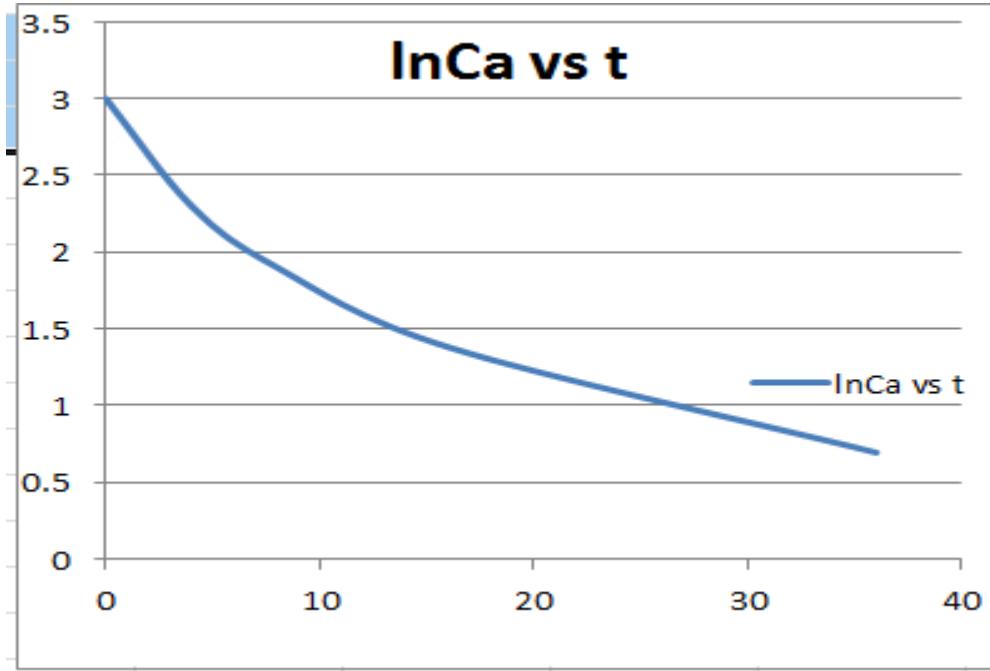
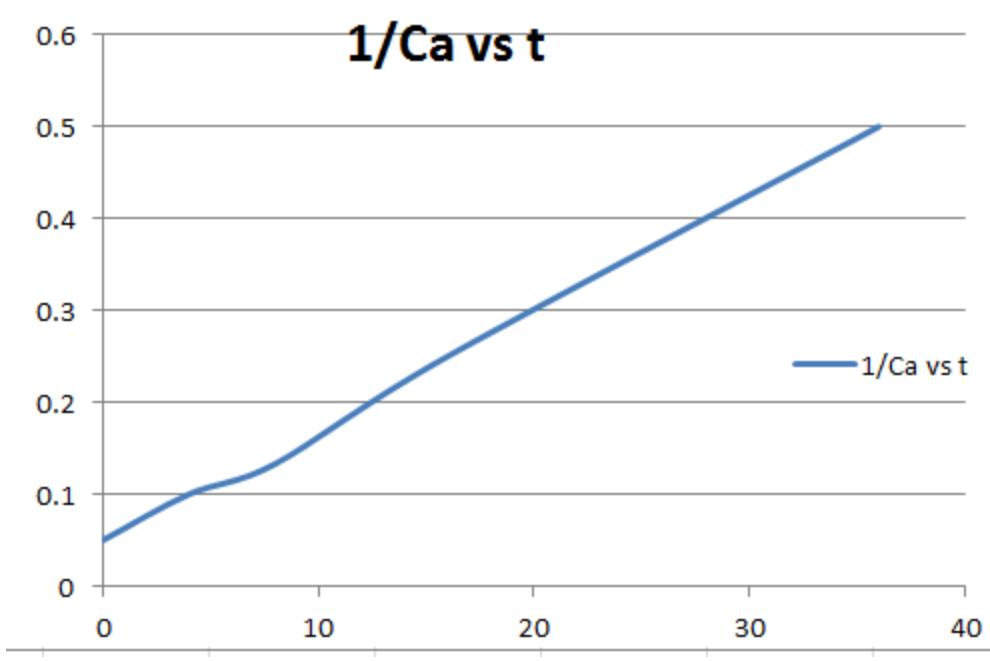
This batch circulation system is a constant volume system, so $\dot{\epsilon}_a=0$

$$C_A = P_{A0}/RT = \frac{101325}{8.314 \times 609} = 20 \text{ mol/m}^3$$

$$P_A = P_{A0} + \frac{a}{\lambda n} (\pi o - \pi)$$

$$= 1 + \frac{2}{-1} (1 - \pi)$$

t	π	P _A	C _a	lnC _a	1/C _a	
0	1	1	20	3	0.05	
4	0.75	0.5	10	2.3	0.1	
8	0.67	0.33	6.67	1.9	0.135	
6	0.60	0.2	4	1.38	0.25	
36	0.55	0.1	2	0.693	0.5	



Slope of 1/Ca vs t is 0.0125.

Therefore rate equation is $r_a = 0.0125 Ca^2$

18.20)

$$M_w = \mu_T^2 \epsilon = L^2 (-r_A''' / C_A)_{obs} / D_e$$

$$M_w = .15$$

$$-r_A''' / C_A = .88$$

$$D_e = 2 \times 10^{-6}$$

$$.15 = L^2 \times .88 / 2 \times 10^{-6}$$

$$L = 5.83 \times 10^{-4} \text{ m}$$

$$= 58.3 \text{ mm}$$

$$L = R/3 \quad (\text{Sphere})$$

$$L = D/6$$

$$D = \mathbf{350 \text{ mm}}$$

18.21. A reaction $A \rightarrow R$ is to take place on a porous catalyst pellet ($d = 6\text{mm}$, $d_e = 10\text{m}^3/\text{m cat. s}$). How much is the rate slowed by pore diffusional resistance if the concentration of reactant bathing the particle is 100 mol/m^3 and the diffusion-free kinetics are given by

$$-r_a = 0.1 c_a^2 \frac{\text{mol}}{\text{m}^3 \cdot \text{cal} \cdot \text{s}}$$

ans.

$$\text{For } n^{\text{th}} \text{ order reaction } M_T = \frac{d_p}{6} \sqrt{\frac{(n+1)*K'' C_a^{n-1}}{2*D_e}}$$

$$= \frac{6*10^{-3}}{6} \sqrt{\frac{(2+1)*0.1*100^{2-1}}{2*10^{-6}}} \\ = 3.873$$

From the Graph value of $E = 0.23$

18.22 In the absence of pore diffusion resistance a particular first-order gas- phase reaction proceeds as reported below.

$$-r_A''' = 10^{-6} \text{ mol/cm}^3 \text{ cat} \cdot \text{s}$$

$$C_A = 10^{-5} \text{ mol/cm}^3, \quad \text{at 1 atm and } 400^\circ\text{C}$$

What size of spherical catalyst pellets ($g e 10^{-3} = \text{cm}^3/\text{cm cat as}$) would ensure that pore resistance effects do not intrude to slow the rate of re- action?

Given $P = 1\text{ atm}$

$$C_{Ao} = P/RT$$

$$C_{Ao} = 1/(0.08206*673)$$

$$C_{Ao} = 1.8*10^{-5} \text{ mol/cm}^3$$

$$X_{Ae} = C_{Ao} - C_A / C_{Ao}$$

$$X_{Ae} = (1.8-1)10^{-5} / 1.8 \cdot 10^{-5}$$

$$X_{Ae} = 0.444$$

$$M_t = L(K''/D_e * X_{Ae})^{(1/2)}$$

$$M_T = 0.4$$

By Solving above equation

We get

$$L = 0.4 \text{ cm}$$

For Spherical particle

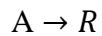
$$R = 3L$$

$$R = 0.0795 \text{ cm}$$

$$R = 0.8 \text{ mm}$$

18.23. The first-order decomposition of A is run in an experimental mixed flow reactor. Find the role played by pore diffusion in these runs in effect determine whether the runs were made under diffusion-free, strong resistance or intermediate conditions.

d_p	w	C_{ao}	v	x_a
3	1	100	9	0.4
12	4	300	8	0.6



ans.

No	d_p	w	C_{AO}	v	x_a	C_A	K'
1	3	1	100	9	0.4	60	6
2	12	4	300	8	0.6	120	3

For Mixed Flow

(1)

$$\begin{aligned} C_A &= C_{A0}(1 - X_A) \\ &= 100(1 - 0.4) \\ &= 60 \end{aligned}$$

(2)

$$\begin{aligned} C_A &= C_{A0}(1 - X_A) \\ &= 300(1 - 0.6) \\ &= 120 \end{aligned}$$

For No diffusion

$$\frac{K_2}{K_1} = 1$$

For Strong resistance

$$\frac{K_2}{K_1} = \frac{d_{p2}}{d_{p1}} = \frac{1}{4}$$

From the given data :

$$\tau' = \frac{w}{v} = \frac{C_{A0} - C_A}{W' C_A}$$

$$\begin{aligned} K_1' &= \frac{V * (C_{A0} - C_A)}{W' * C_A} \\ &= \frac{(100 - 60) * 9}{1 * 60} \\ &= 6 \end{aligned}$$

$$\begin{aligned} K_2' &= \frac{V * (C_{A0} - C_A)}{W' * C_A} \\ &= \frac{(300 - 120) * 8}{4 * 120} \\ &= 3 \end{aligned}$$

$$\frac{K_2}{K_1} = \frac{3}{6} = \frac{1}{2}$$

So that, diffusion take place at intermediate condition

18.24 The first-order decomposition of A is run in an experimental mixed flow reactor. Find the role played by pore diffusion in these runs in effect determine whether the runs were made under diffusion-free, strong resistance or intermediate conditions.

d_p	w	C_{ao}	v	x_a
4	1	300	60	0.8
8	3	100	160	0.6

$A \rightarrow R$

ans

No	d_p	w	C_{A0}	V	x_a	C_A	K'
1	4	1	300	60	0.8	60	240
2	8	3	100	160	0.6	40	80

For Mixed Flow

(1)

$$\begin{aligned} C_A &= C_{A0}(1 - X_A) \\ &= 300(1 - 0.8) \\ &= 60 \end{aligned}$$

(2)

$$\begin{aligned} C_A &= C_{A0}(1 - X_A) \\ &= 100(1 - 0.6) \\ &= 40 \end{aligned}$$

For No diffusion

$$\frac{K_2}{K_1} = 1$$

For Strong diffusion

$$\frac{K_2}{K_1} = \frac{d_{p2}}{d_{p1}} = \frac{1}{2}$$

From the given data :

$$\tau' = \frac{w}{v} = \frac{C_{A0} - C_A}{W' C_A}$$

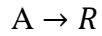
$$\begin{aligned} K_1' &= \frac{V * (C_{A0} - C_A)}{W' * C_A} \\ &= \frac{(300 - 60) * 60}{1 * 60} \\ &= 240 \end{aligned} \quad \begin{aligned} K_2' &= \frac{V * (C_{A0} - C_A)}{W' * C_A} \\ &= \frac{(100 - 40) * 160}{3 * 40} \\ &= 80 \end{aligned}$$

$$\frac{K_2}{K_1} = \frac{80}{240} = \frac{1}{3}$$

So that, diffusion take place at strong resistance condition

18.25 The first-order decomposition of A is run in an experimental mixed flow reactor. Find the role played by pore diffusion in these runs in effect determine whether the runs were made under diffusion-free, strong resistance or intermediate conditions.

d _p	w	C _{ao}	v	x _a
2	4	75	10	0.2
1	6	100	5	0.6



ans

No	d _p	w	C _{A0}	V	x _a	C _A	K'
1	2	4	75	10	0.2	60	
2	1	6	100	5	0.6	40	

For Mixed Flow

(1)

$$\begin{aligned} C_A &= C_{A0}(1 - X_A) \\ &= 75(1 - 0.2) \\ &= 60 \end{aligned}$$

(2)

$$\begin{aligned} C_A &= C_{A0}(1 - X_A) \\ &= 100(1 - 0.6) \\ &= 40 \end{aligned}$$

For No diffusion

$$\frac{K_2}{K_1} = 1$$

For Strong diffusion

$$\frac{K_2}{K_1} = \frac{d_{p2}}{d_{p1}} = \frac{1}{2}$$

From the given data :

$$\tau' = \frac{w}{v} = \frac{C_{A0} - C_A}{W' C_A}$$

$$\begin{aligned}
 K_1' &= \frac{V*(C_{A0} - C_A)}{W'*C_A} & K_2' &= \frac{V*(C_{A0} - C_A)}{W'*C_A} \\
 &= \frac{(75-60)*10}{4*60} & &= \frac{(100-40)*5}{6*40} \\
 &= 0.625 & &= 1.25
 \end{aligned}$$

$$\frac{K_2}{K_1} = \frac{1.25}{0.625} = 2$$

So that, diffusion take place at strong pore diffusion

18.26. Find the activation energy of the first-order reaction from the following data:

d_p	C_A	$-r'_A$	T, K	
1	20	1	480	$A \rightarrow R$
2	40	1	480	$C_{A0} = 50$
2	40	3	500	

Solution 18.26

d_p	C_A	$-r'_A$	T, K
1	20	1	480
2	40	1	480
2	40	3	500



$$\text{Now, } d_{p2} / d_{p1} = k_1 / k_2 = k_0 e^{-E/RT_1} / k_0 e^{-E/RT_2} = 2$$

Similarly,

$$d_{p3} / d_{p2} = k_2 / k_3 = k_0 e^{-E/RT_2} / k_0 e^{-E/RT_3} = 1$$

$$d_{p3} / d_{p1} = k_1 / k_3 = e^{-E/RT_1} / e^{-E/RT_3} = 2$$

On solving we get,

$$E = -69139.224 \text{ J} = -69.13 \text{ kJ}$$

- 18.27.** What can you tell about the influencing resistances for the porous catalyst from the data of Table P18.27 obtained in a recycle type mixed flow reactor. In all runs the leaving stream has the same composition, and conditions are isothermal throughout.

Table P18.27

Quantity of Catalyst	Pellet Diameter	Flow Rate of Given Feed	Recycle Rate	Measured Reaction Rate, $-r'_A$
1	1	1	High	4
4	1	4	Higher still	4
1	2	1	Higher still	3
4	2	4	High	3

Solution 18.27

Quantity of Catalyst	Pellet Diameter	Flow rate of given feed	Recycle Rate	Measured reaction rate
1	1	1	High	4
4	1	4	Higher still	4
1	1	1	Higher still	3
4	2	4	High	3

All these runs were made at the same W/F_{AO} . We are also told that the recycle rate is high enough to have mixed flow throughout. Thus changing the recycle rate from run 1 to run 2, or from run 3 to run 4 with no change in rate shows that film resistance doesn't influence the rate.

Next, if particles were non-porous then the smaller size (runs 1 & 2) should have double the rate of the larger size (runs 3 & 4). This is not what is measured hence the results are not consistent with the guess of non-porous particles. (1) If in the regime of no pore diffusion resistance the rates should be same for large and small pellets. (2) If in the regime of strong pore diffusion the rate should halve from going 4 to 2 in going to the larger particle.

Our results are half-way between these two extremes, hence we must be operating under conditions where pore diffusion is just beginning to influence the rate. Hence we can conclude that, porous particles, no film resistance, pore resistance just beginning to intrude and effect the rate.

- 18.28.** Experiments at 300°C in a packed bed reactor with very large recycle stream give the results shown below for the first order catalytic decomposition $A \rightarrow R \rightarrow S$. Under the best possible conditions (always at 300°C) what $C_{R,\text{max}}/C_{A0}$ may we expect, and how do you suggest we get this (what flow pattern and particle size, large or small)?

d_p	W/F_{A0}	$C_{R,\text{max}}/C_{A0}$	
4	1	0.5	No recycle
8	2	0.5	

Solution 18.28

d_p	W/F_{A0}	$C_{R,\text{max}}/C_{A0}$
4	1	0.5
8	2	0.5



Under the best possible condition we may accept $C_{R,\text{max}}/C_{A0}$ to be 0.5 and to obtain that we may use the plug flow pattern and catalyst size to be small.

- 18.29.** Experiments with a basket type mixed flow reactor on the solid catalyzed decomposition $A \rightarrow R \rightarrow S$ give the results of Table P18.29. Under the best possible reaction conditions (always at 300°C) what is the maximum concentration of R we may expect? How do you suggest that this be obtained?

Table P18.29

Size of Porous Pellets	Temperature	W/F_{A0}	$C_{R\text{max}}/C_{A0}$
6 mm	300°C	25	23%
12 mm	300°C	50	23%

Solution 18.29

For mixed flow the reactor performance equation is: $W/F_{A0} = X_A/-r_A$ and since the data show that the rate is inversely proportional to pellet size shows that pore diffusion controls in both runs shows:

$k_2/k_1 = 0.5$ and by eliminating pore diffusion in backmix flow we can get $-C_R/C_{A0} = 0.44$

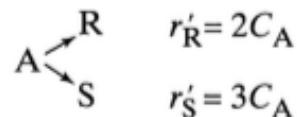
and by eliminating pore diffusion and using plug flow we can get $-C_R/C_{A0} = 0.63$

So, use smaller pellets in a packed and we should be able to achieve as high as $C_R/C_{A0} = 0.63$

18.30. Reactant A at $C_{A0} = 10 \text{ mol/m}^3$ is to be passed through a packed bed catalytic reactor where it will decompose into either R or S. To maximize the formation of R and for 90% decomposition of A determine

- whether to operate in the strong pore diffusion regime or in the diffusion-free regime
- whether to use plug flow or mixed flow (high recycle)
- C_R expected in the exit stream.

The kinetics of the decomposition, when free of pore diffusion resistance, is given by



Solution 18.30

$$C_{A0} = 10 \text{ mol/m}^3$$

A packed bed catalytic reactor is used.

- It should be operated in the strong diffusion regime.
- We should use a plug flow.

- 18.31.** A packed bed reactor converts A to R by a first-order catalytic reaction, $A \rightarrow R$. With 9-mm pellets the reactor operates in the strong pore diffusion resistance regime and gives 63.2% conversion. If these pellets were replaced by 18-mm pellets (to reduce pressure drop) how would this affect the conversion?

Solution: First order catalytic reaction, $A \rightarrow R$ (Strong pore diffusion resistance)

$$-\ln \frac{C_A}{C_{A0}} = kt$$

$$-\ln(1-X_a) = kt$$

$$1 - X_a = e^{-kt}$$

In the strong pore diffusion resistance, Double the pellet size rate constant is same

$$K_1 = K_2 = K$$

$$X_{a1} = 0.632, k_1 = ?$$

$$1 - X_{a1} = e^{-k_1 t_1}$$

$$1 - 0.632 = e^{-k t_1}$$

$$Kt_1 = 1$$

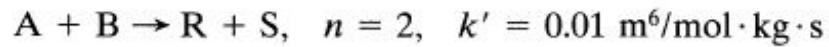
For 18 mm pellets, $t_2 = 0.5t_1$ so $Kt_2 = 0.5$.

$$1 - X_{a2} = e^{-k_2 t_2}$$

$$1 - X_{a2} = e^{-0.5}$$

$$X_{a2} = 0.393$$

- 18.32.** We want to build a packed bed reactor filled with 1.2-cm porous catalyst particles ($\rho_s = 2000 \text{ kg/m}^3$, $D_e = 2 \times 10^{-6} \text{ m}^3/\text{m cat}\cdot\text{s}$) to treat 1 m^3/s of feed gas (1/3 A, 1/3 B, 1/3 inert) at 336°C and 1 atm to 80% conversion of A. Experiments with fine catalyst particles which are free from diffusional resistance show that



How much catalyst must we use?

Solution:

$$P = 1 \text{ atm}, \quad T = 336 \text{ }^\circ\text{C}, \quad X_a = 0.8, \quad D_e = 2 \times 10^{-6} \frac{\text{m}^3}{\text{m cat.s}}$$

$$L = \frac{1.2 \times 10^{-2}}{2 \times 3} = 0.002 \text{ m}$$

$$C_{ao} = \frac{P_{ao}}{RT} = \frac{101325}{8.314 \times (336 + 273)} = 20 \frac{\text{mol}}{\text{m}^3}$$

$$\frac{\tau}{C_{ao}} = \int \frac{dX_a}{-r_a}$$

$$\frac{\tau}{C_{ao}} = \frac{2000}{0.01} \int \frac{X_a * (1 + \epsilon_a X_a)^2}{C_{ao}^2 * (1 - X_a)^2}$$

$$\tau = \frac{1}{20 * C_{ao}} \int \frac{dX_a}{(1 - X_a)^2} = \frac{1}{40} \left[\frac{1}{1 - X_a} - 1 \right] = \frac{1}{40} \left[\frac{1}{1 - 0.8} - 1 \right] = 0.1$$

$$\tau = \frac{W}{F_{Ao}} \rightarrow W = 0.1 * 1 = 0.1 \text{ m}^3 = 200 \text{ kg}$$

- 18.33.** In an experimental mixed flow reactor with 10 gm of 1.2-mm catalyst particles and a feed of 4 cm³/s of pure A at 1 atm and 336°C we get 80% conversion for the first-order reaction



We want to design a commercial-sized reactor to treat large amounts of feed to 80% conversion at the above temperature and pressure. Our choice is between a fluidized bed of 1-mm particles (assume mixed flow of gas) and a packed bed of 1.5-cm particles. Which should we choose so as to minimize the amount of catalyst needed? How much advantage is there in this choice?

Additional Data: For the catalyst particles:

$$\rho_s = 2000 \text{ kg/m}^3 \quad D_e = 10^{-6} \text{ m}^3/\text{m cat} \cdot \text{s}$$

Solution:

P= 1 atm, T= 336 °C, v= 4 cm³/s, X_a= 0.8 when 10 gm of 1.2 mm catalyst

Design a fluidized bed of 1-mm particles (assume mixed flow of gas) and packed bed of 1.5 cm particles which need minimum catalyst?

$$C_{ao} = \frac{P_{ao}}{RT} = \frac{101325}{8.314 * (336 + 273)} = 20 \frac{\text{mol}}{\text{m}^3} \quad k = \frac{-r_a}{C_a} = \frac{12.8}{20 * (1 - 0.8)} = 3.2 \text{ sec}^{-1}$$

$$\frac{\tau}{C_{ao}} = \frac{X_a}{-r_a}$$

$$\tau = \frac{W}{F_{Ao}} = \frac{0.01}{4 * 10^{-6}} = 2500 \text{ sec}$$

$$-r_a = \frac{20 * 0.8}{2500} = 6.4 * 10^{-3} \frac{\text{mol}}{\text{kg} \cdot \text{s}} = 12.8 \frac{\text{mol}}{\text{m}^3 \cdot \text{s}}$$

$$M_w = \frac{L^2 * (-r_a)}{C_a * D_e} = \frac{12.8 * (0.0002)^2}{20 * 0.2 * 10^{-6}} = 0.128$$

For Packed bed:

$$L = 2.5 * 10^{-3} \text{ m}$$

$$M_T = L \sqrt{\frac{K}{D}} = 2.5 * 10^{-3} \sqrt{\frac{3.2}{10^{-6}}} = 4.472 \rightarrow \xi = \frac{\tanh M_T}{M_T} = \frac{\tanh(4.472)}{4.472} = 0.2236$$

$$\frac{W}{V} = \frac{1}{k * \epsilon} \ln \frac{C_{ao}}{C_a} = 4500 \frac{kg}{m^3 \cdot s}$$

For Fluidized Bed:

$$L = 1.67 \times 10^{-4} \text{ m}$$

$$M_T = L \sqrt{\frac{K}{D}} = 1.67 \times 10^{-4} \sqrt{\frac{3.2}{10^{-6}}} = 0.2987 \rightarrow \xi = \frac{\tanh M_T}{M_T} = \frac{\tanh(0.298)}{0.298} = 0.98$$

$$\frac{W}{V} = \frac{1}{k * \epsilon} \frac{C_{ao} X_a}{C_a (1 - X_a)} = 2500 \frac{kg}{m^3 \cdot s}$$

Fluidized bed is better because it's required less amount of catalyst. It needs only 55.55% of the packed bed catalyst.

Problem 18.34 & 18.35

In aqueous solution, and in contact with the right catalyst, reactant A is converted to product R by the elementary reaction $A \rightarrow R$. Find the mass of catalyst needed in a packed bed reactor for 90% conversion of 10^4 mol A/hr of feed having $C_{A0} = 10^3$ mol/m³. For this reaction

34. $k''' = 8 \times 10^{-4} \text{ m}^3/\text{m}^3 \text{ bed. s}$

35. $k''' = 2 \text{ m}^3/\text{m}^3 \text{ bed. s}$

Additional data:

Diameter of porous catalyst pellets = 6 mm

Effective diffusion coefficient of A in the pellet = $4 \times 10^4 \text{ m}^3/\text{m cat. s}$

Void age of packed bed = 0.5

Bulk density of packed bed = 2000 kg/m³ of bed

Solution 35:

$$k''' = 2 \left(\frac{\text{m}^3}{\text{m}^3 \text{ bed sec}} \right) * 2 \left(\frac{\text{m}^3 \text{ bed}}{1 \text{ m}^3 \text{ catalyst}} \right)$$

$$= 4 \left(\frac{\text{m}^3}{\text{m}^3 \text{ cat sec}} \right)$$

$$MT = L \sqrt{\frac{k'''}{D}}$$

$$= \frac{6 * 10^{-3}}{6} \sqrt{\frac{4}{4 * 10^{-8}}}$$

$$= 10$$

$$\varepsilon = \frac{1}{MT}$$

$$= .1$$

$$\tau''' = \frac{CA_0 * V_{cat}}{FA_0}$$

$$= \int \frac{dCA}{k''' * CA * \varepsilon}$$

$$\begin{aligned}
&= \frac{1}{k'''' * \varepsilon} \ln \frac{CA_0}{CA} \\
v_{\text{cat}} &= \frac{FA_0}{CA_0 * k'''' * \varepsilon} \ln \frac{CA_0}{CA} \\
&= \frac{10^{4}}{3600*1000*4*1} \ln \frac{10}{1} \\
&= 0.016
\end{aligned}$$

$$W = V_{\text{cat}} * P_{\text{cat}}$$

$$\begin{aligned}
&= V_{\text{cat}} * \left(\frac{P_{\text{bulk}}}{\text{voidage}} \right) \\
&= 0.016 * \frac{2000}{0.5} \\
&= 64 \text{ kg}
\end{aligned}$$

Solution 34:

$$\begin{aligned}
k''' &= 8 * 10^{-4} \left(\frac{\text{m}^3}{\text{m}^3 \text{ bed sec}} \right) * 2 \left(\frac{\text{m}^3 \text{ bed}}{1 \text{ m}^3 \text{ catalyst}} \right) \\
&= 16 * 10^{-4} \left(\frac{\text{m}^3}{\text{m}^3 \text{ cat sec}} \right)
\end{aligned}$$

$$\begin{aligned}
MT &= L \sqrt{\frac{k''''}{D}} \\
&= \frac{6 * 10^{-3}}{6} \sqrt{\frac{16 * 10^{-4}}{4 * 10^{-8}}} \\
&= 0.2
\end{aligned}$$

$$\varepsilon = 1$$

$$\begin{aligned}
\tau''' &= \frac{CA_0 * V_{\text{cat}}}{FA_0} \\
&= \int \frac{dCA}{k'''' * CA * \varepsilon} \\
&= \frac{1}{k'''' * \varepsilon} \ln \frac{CA_0}{CA}
\end{aligned}$$

$$V_{\text{cat}} = \frac{FA_0}{CA_0 * k'''' * \varepsilon} \ln \frac{CA_0}{CA}$$

$$= \frac{10^4}{3600*1000 * 16*10^{-4}*1} \ln \frac{10}{1}$$

$$= 4$$

$$W = V_{\text{cat}} * P_{\text{cat}}$$

$$= V_{\text{cat}} * \left(\frac{P_{\text{bulk}}}{\text{voidage}} \right)$$

$$= 4 * \frac{2000}{0.5}$$

$$= 16000 \text{ kg}$$

Problem 18.36

A first-order catalytic reaction $A(l) \rightarrow R(l)$ is run in a long, narrow vertical reactor with up flow of liquid through a fluidized bed of catalyst particles. Conversion is 95% at the start of operations when the catalyst particles are 5 mm in diameter. The catalyst is friable and slowly wears away, particles shrink and the fine powder produced washes out of the reactor. After a few months each of the 5-mm spheres has shrunk to 3-mm spheres. What should be the conversion at this time? Assume plug flow of liquid.

- (a) Particles are porous and allow easy access for reactants (no resistance to pore diffusion).
- (b) Particles are porous and at all sizes provide a strong resistance to pore diffusion.

Solution 18.36:

$$a) \frac{-r_{A0}}{r_{A'}} = \frac{kCA}{kCA'} = 1 = \frac{CA_0(1-X_A)}{CA_0(1-X_{A'})}$$

$$1 - X_A = 1 - X_{A'}$$

$$1 - X_{A'} = 1 - 0.05$$

$$X_{A'} = 0.95$$

$$b) r_A = k C_A$$

$$\frac{rA1}{rA2} = \frac{k CA1}{kCA2} = \frac{R2}{R1}$$

$$\frac{CA0(1-XA)}{CA0(1-XA')} = \frac{3}{5}$$

$$\frac{1-95}{1-XA'} = 0.6$$

$$1 - X_A' = 0.0833$$

$$X_A' = \mathbf{0.916}$$

18.37. At present we are running our catalytic first-order reaction in the strong pore diffusion regime in a packed bed reactor filled with platinum impregnated 6-mm particles of uniform size. A catalyst manufacturer suggests that we replace our catalyst with 6-mm pellets consisting of fused 0.06-mm grains. The voidage between grains in the pellet would be about 25%. If these new pellets were free of pore diffusion resistance in their large voids (between grains), but if the grains were still in the strong diffusional resistance regime, how would this change affect the weight of catalyst needed and the reactor volume?

Solⁿ: Denoting catalyst palate without grains as 1 and with grains as 2. Therefore, in strong pore diffusion regime (as grains are having strong pore diffusion);

$$\frac{M_{T_2}}{M_{T_1}} = \frac{\varepsilon_1}{\varepsilon_2} = \frac{R_2}{R_1} = 0.01 = \frac{r'_{A_1}}{r'_{A_2}} = \frac{W_2}{W_1} = \frac{V_2 * .75}{V_1}$$

- Reason for last 3 terms;

$$r'_{A_2} = \frac{X_A * F_A}{W}$$

But,

$$F_A = C_A * v_A = \frac{N_A * v_A}{V}$$

- As between grains there is 25% of void age and there exist free pore diffusion hence in only 75% of total volume there will be strong pore resistance.

$$\frac{W_2}{W_1} = 0.01$$

- Hence **1% of earlier catalyst weight is required to obtain same results.**

$$\frac{V_2 * .75}{V_1} = 0.01$$

$$\frac{V_2}{V_1} = 0.0133$$

- Therefore **1.33% of earlier volume is required.**

18.38. Instead of impregnating the whole porous particle uniformly with platinum (see Problem 18.37), suppose we only impregnate the outer layer of the spherical particle to a thickness of 0.3 mm. How much platinum do we save by this change? Assume that we are in the strong pore diffusion regime throughout.

Solⁿ: As catalyst is still in strong pore diffusion regime even after impregnating only outer surface hence formulas used in previous numerical are applicable. Denoting throughout impregnated catalyst as 1 and catalyst impregnated only at outer surface as 2.

$$\frac{M_{T_2}}{M_{T_1}} = \frac{6.3}{6} = 1.05$$

$$\frac{\varepsilon_2}{\varepsilon_1} = \frac{1}{1.05} = 0.9524 = \frac{W_2}{W_1}$$

$$W_2 = 0.9524 * W_1$$

- Assuming W kg of Pt was used earlier then amount of Pt saved by impregnating only outer surface will be;

$$= W_1 - W_2 = 0.0476 * W$$

- Means **4.76% kg of earlier amount of Pt used can be saved.**

18.39. Because the catalytic reaction $A \rightarrow R$ is highly exothermic with rate highly temperature-dependent, a long tubular flow reactor immersed in a trough of water, as shown in Fig. P18.39, is used to obtain essentially isothermal kinetic data. Pure A at 0°C and 1 atm flows through this tube at 10 cm³/sec, and the stream composition is analyzed at various locations.

Distance from feed input, meters	0	12	24	36	48	60	72	84	(∞)
Partial pressure of A, mm Hg	760	600	475	390	320	275	240	215	150

Determine what size of plug flow reactor operating at 0°C and 1 atm would give 50% conversion of A to R for a feed rate of 100 kmol/hr of pure A.

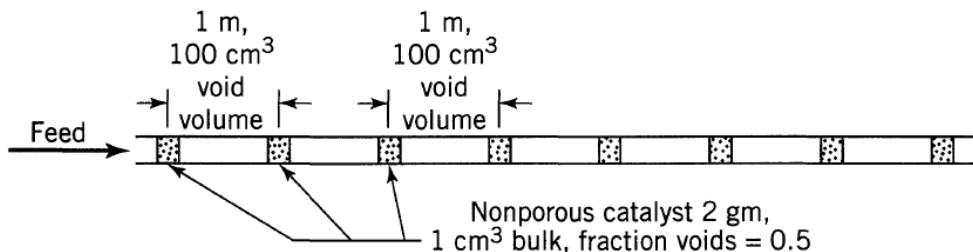


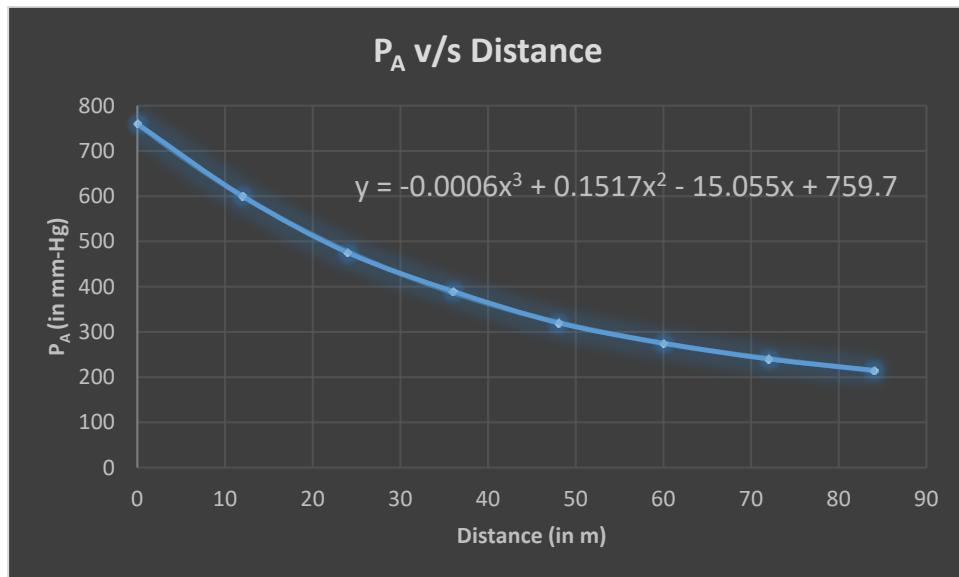
Figure P18.39

Solⁿ:

$$C_A = \frac{p_A}{R * T}$$

$$X_A = 0.5 = 1 - \frac{p_{A_0}}{p_A}$$

- Therefore, p_A at 50% conversion is $361.9 \cong 362$ mm-Hg.



- From given data we can obtain above curve and 50% conversion (362 mm-Hg) is achieved at distance 39.97 m.
- Now each 1m length of tube consists 1cm^3 of bulk catalyst. Hence till distance 39.97 cm^3 of bulk catalyst will be there.

Now,

$$\frac{V_r}{F_{A_0}} = \frac{V_{catalyst}}{C_{A_0} * v_0}$$

- From ideal gas law,

$$PV=nRT$$

$$C_{A_0} = \frac{n}{V} = \frac{P_{A_0}}{R * T} = \frac{1}{22400} \frac{mol}{cm^3}$$

Therefore,

$$\frac{V_r}{\frac{100 * 10^3}{3600} \frac{mol}{s}} = \frac{39.97 \text{ cm}^3}{\frac{1}{22400} \frac{mol}{cm^3} * 10 \frac{cm^3}{s}}$$

$$V_r = 2.48 * 10^6 \text{ cm}^3$$

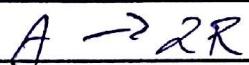
$$V_r = 2.48 \text{ m}^3$$

Solution 18.40 :

$\rightarrow A \rightarrow 2R, X_A = 0.50 \text{ & } F_{A0} = 100 \text{ kmol/h}$

$$\frac{t}{C_{A0}} = \int_0^{X_A} \frac{dx_A}{-r_A} = \frac{V}{W} \int_0^{X_A} \frac{dx_A}{-r_A'}$$

$$\frac{t}{C_{A0}} = \frac{V}{W} \int_0^{X_A} \frac{dx_A}{-r_A'}$$



$$| \quad \epsilon_A = \frac{2-1}{1} = 1 |$$

$$C_A = \frac{C_{A0}(1-X_A)}{(1+\epsilon_A X_A)}$$

or

$$X_A = \frac{1 - \frac{C_A}{C_{A0}}}{1 + \frac{\epsilon_A C_A}{C_{A0}}}$$

$$\therefore \epsilon_A = 1$$

$$\Rightarrow X_A = \frac{1 - \frac{C_A}{C_{A0}}}{1 + \frac{C_A}{C_{A0}}}$$

$$C_A = \frac{P_A}{RT} ; \quad C_{A0} = \frac{P_{A0}}{RT}$$

$$\therefore \frac{C_A}{C_{A_0}} = \frac{P_A}{P_{A_0}}$$

P_A is partial pressure of A at any time t
 P_{A_0} is initial partial pressure of A()

$P_{A_0} = 760 \text{ mm Hg}$ as pure A feed

$$X_A = \frac{1 - \frac{P_A}{760}}{1 + \frac{P_A}{760}}$$

t	0	2	4	6	8	10	12	14
P_A	760	600	475	390	320	275	240	215
X_A	0	0.12	0.23	0.32	0.41	0.47	0.47	0.56

$$P_A = 600 \text{ mm Hg}$$

$$X_A = \frac{1 - \left(\frac{600}{760}\right)}{1 + \left(\frac{600}{760}\right)} = 0.1176 = 0.12$$

Try for 1st order rate equation

$$-r_A' = k' C_A = k' C_{A_0} (1 - X_A), \quad \epsilon_A = 1$$

$$(1 + X_A)$$

$$\therefore \frac{t}{C_{A_0}} = \frac{V}{W} \quad \left. \begin{array}{l} X_A \\ \frac{dX_A}{k' C_{A_0} (1 - X_A)} \\ (1 + X_A) \end{array} \right\}$$

$$\Rightarrow t = \frac{V}{Wk'} [-2 \ln(1-x_A) - x_A]$$

$$y = mx$$

$$\therefore y = t ; x = [-2 \ln(1-x_A) - x_A] ; m = \frac{V}{Wk'}$$

t	0	2	4	6	8	10	12	14
x_A	0	0.12	0.23	0.32	0.41	0.47	0.52	0.56
x	0	0.136	0.293	0.45	0.645	0.80	0.95	1.082

$$\text{Slope} = \frac{V}{Wk'} = 12.31 \text{ min}$$

$$k' = \frac{V}{12.31 W}$$

$$W = \rho g, V = 100 \text{ cm}^3$$

$$k' = \frac{100}{12.31 \times 2} = 4.06 \text{ l} \\ (\text{kgcat.min})$$

$$[-2x_A'] = (4.06) (A)$$

Determining size of PFR

$$W = \int \frac{dx_A}{-2x_A'} ; -2x_A' = k' C_{A0} \frac{(1-x_A)}{(1+x_A)}$$

$$\frac{W}{F_{A0}} = \int_0^{X_A} \frac{(1+X_A) dX_A}{k' C_{A0} (1-X_A)}$$

$$\frac{W}{F_{A0}} = \frac{1}{k' C_{A0}} [-R \ln(1-X_A) - X_A]$$

$$C_{A0} = \frac{P_{A0}}{RT}$$

$$P_{A0} = 760 \text{ mm Hg}$$

$$T = 0 + 273 = 273 \text{ K}$$

$$\Rightarrow C_{A0} = \frac{1}{0.08206 \times 273} = 0.0446 \text{ mol/l}$$

$$\text{Now, } F_{A0} = 10^5 \text{ mol/h} = 1666.67 \text{ mol/min}$$

$$X_A = \frac{50}{100} = 0.5$$

$$W = \frac{1666.67}{4.06 \times 0.0446} [-R \ln(1-0.5) - 0.5]$$

$$W = 8157 \text{ Kg}$$

(ii) Size of PFR when:

Partial pressure of inert = 1 atm

Total pressure at start = 2 atm

partial pressure of A at start = $2 - 1 = 1 \text{ atm}$

$$\therefore \frac{F_A}{F_{A0}} = \frac{3-2}{2} = 0.50$$

$$F_A = 4.06$$

$$W = \frac{F A_0}{k' C_{A_0}} [- (1 + \Sigma A) \ln(1 - X_A) - \Sigma A X_A]$$

$$\bar{F} A_0 = 1666.67 \text{ mol/min}$$

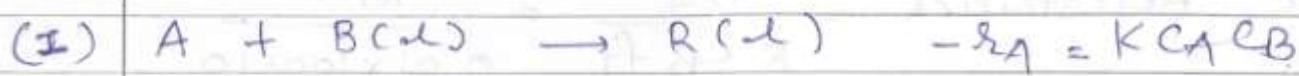
$$C_{A_0} = \frac{1}{0.08206 \times 273} = 0.0446 \text{ mol/l}$$

$$P_{A_0} = 1 \text{ atm} ; X_A = 0.50 ; \Sigma A = 0.50$$

$$W = \frac{1666.67}{4.06 \times 0.0446} [- (1 + 0.5) \ln(1 - 0.5) - 0.5 \times 0.5]$$

$$\Rightarrow W = 7269 \text{ kg}$$

Amount of Catalyst needed = 7269 kg



$$K_A g^a = 0.1$$

$$P_A = 100 \text{ Pa}$$

$$K_A l^a = 100$$

$$C_B = 100 \text{ mol}$$

$$f_L = 0.01 \text{ m}^3$$

$$K = 10$$

$$a = 100$$

$$H_A = 10^5$$

$$D_{A1} = D_{B1} = 10^{-6} \text{ m}^2/\text{hr}$$

$$\text{gas film Resistance} = \frac{1}{K_A g^a} = \frac{1}{0.1} = 10$$

$$\text{liquid film Resistance} = \frac{H_A}{K_A l^a E} = \frac{10^5}{100 \times 1} = 10^3$$

$$MH = \frac{\sqrt{D_A K C_B}}{K_A l^a} = \sqrt{\frac{10^{-6} \times 10 \times 100}{1}} = 0.0316$$

$$E_F = 1 + \frac{D_B C_B H_A}{b D_A P_A} \quad \text{Here } P_A = P_A^* = 100$$

$$= 1 + \frac{10^{-6} \times 100 \times 10^5}{1 \times 100 \times 100}$$

$$= 1.001$$

$$E_F > 5 MH$$

$$\therefore E = MH$$

But E cannot be < 1

$$\therefore E = 1$$

$$\text{If } PA_f = 0 \quad E_i = 0 \\ E = mH \quad \text{so } \underline{E = 1}$$

$$\text{Kinetic Resistance} = \frac{HA}{K_{CB} f_l} = \frac{10^5}{0.01 \times 100 \times 10} \\ = 10,000$$

$$-r_A = \frac{10^5}{0.01 \times 100 \times 10000} = \frac{P_A}{K_{Ag}^d + K_{Al}^{cl} E + \frac{HA}{K_{CB} f_l}} \\ = 0.00908$$

(a) Resistance $r_A = 0.00908 \frac{\text{mol}}{\text{hr. m}^2 \text{ reactor}}$

(b) Resistance :- Kinetic & Liquid film
 Location :- Main body of liquid film
 Behaviour in liquid film :- Physical transport.

2) $K = 10^6 \quad H_A = 10^4$

gas film resistance :- $\frac{I}{K_{Ag}^d} = \frac{1}{0.1} = 10$

Liquid film resistance :- $\frac{HA}{K_{Al}^{cl} E} = \frac{10^4}{100 \times 1} = 100$

$$MH = \sqrt{\frac{10^6 \times 10^4 \times 100}{1}} = 10$$

$$E_f = 1 + \frac{100 \times 10^6 \times 10^4}{1 \times 100 \times 100} \quad P_A = P_A^0 = 100 \text{ Pa}$$

$$E_f^0 = I \times 10^{-2} \quad \text{Here } MH > 5 E_f^0$$

$$E_i = 1.01 \quad \therefore E_f^0 = E = I$$

IF $PAi^{\circ} = 0$

$$Ei^{\circ} = \infty$$

$$Ei^{\circ} > 5 \text{ MH}$$

$$\therefore E = \text{MH} = 10$$

∴ our Assumption Ps

wrong Here.

$$\text{Kinetic resistance} = \frac{10^4}{10^6 \times 100 \times 0.01} = 0.01$$

$$-r_A^{\text{lim}} = \frac{10^2}{0.01 + 10 + 100} = 0.909$$

(a) Resistance Rate = $0.909 \frac{\text{mol}}{\text{hr m}^2 \text{ reactor}}$

(b) Resistance :- $\frac{2}{3}$ liquid film, $\frac{1}{3}$ gas film

(c) Location :- liquid film

(d) Behaviour in liquid film :- Fast reaction.

$$(3) K = 10 \quad H_A = 10^3$$

$$\text{gas film Resistance} = \frac{1}{K_A g^{\alpha}} = \frac{1}{10} = 0.1$$

$$\text{liquid film Resistance} = \frac{H_A}{K_A g^{\alpha} \cdot E} = \frac{10^3}{10^2 \times 1} = 10$$

$$\text{Here } \text{MH} = \frac{10^6 \times 10 \times 10^2}{1} = 3.16 \times 10^2$$

$$Ei^{\circ} = 1 + \frac{DB CB H_A}{b D_A PAi^{\circ}} \quad PA = PAi^{\circ}$$

$$Ei^{\circ} = 1 + \frac{10^6 \times 100 \times 10^3}{1 \times 100 \times 100} = 1.00001$$

$E_f > 5 \text{ MH}$

$E = \text{MH}$ But E can not be ≤ 1

$$\therefore \underline{E_f = 1}$$

And $P_f \cdot R_f = P A f = 0$

$$\therefore E_f = \infty$$

$$\therefore E = \text{MH} \quad \underline{\text{so } E = 1}$$

$$\text{Kinetic Resistance} = \frac{HA}{K_{CB} f_l} = \frac{10^3}{10(0.8)(0.01)} = 10$$

$$\text{Rate} = -\frac{dN}{dt} = \frac{PA}{\frac{1}{K_A g^a} + \frac{HA}{K_A l^a E} + \frac{HA}{K_{CB} f_l}} = \frac{10^2}{\frac{1}{0.1} + \frac{10^3}{10^2} + \frac{10^3}{10(0.8)(0.01)}} = 3.33$$

(a) Reaction Rate = $3.33 \frac{\text{mol}}{\text{hr m}^3 \text{ reactor}}$

(b) Resistance = $1/3$ in gas, $1/3$ in liquid film
 $1/3$ in kinetic

(c) location = main body liquid

(d) behaviour = physical transport

CRE-2

4.
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Given

$$K_{M_A} a = 0.1 \text{ mol/hr m}^2 \text{ of reactor pa}$$

$$K_{M_B} a = 100 \text{ m}^2 \text{ lig/m}^3 \text{ reactor hr}$$

$$f_t = 0.01 \text{ m}^3 \text{ lig/m}^3 \text{ reactor}$$

$$D_{AE} = D_{B1} = 10^{-6} \text{ m}^2/\text{hr}$$

$$a = 100 \text{ m}^2/\text{m}^3$$

$$P_A = 100 \text{ Pa}$$

$$C_B = 100 \text{ mol (m}^3 \text{ lig)}$$

$$\text{Req } K = 10^{-4} \text{ m}^2 \text{ lig/mol hr} \quad H_A = 1 \text{ Pa m}^3 \text{ lig/mol}$$

$$M_H = \sqrt{\frac{D_A K C_B}{K_{M_A}}} = \sqrt{\frac{(10^{-6})(10^{-4})(100)}{1}} = 10^{-4}$$

$$E_i = 1 + \frac{D_B C_B H_A}{b D_A P_A} = 1 + 1 = 2$$

$$E_i > 5M_H$$

$$\therefore E = M_H$$

$$\begin{aligned}
 -r_{A'''} &= \frac{P_A}{\frac{1}{K_{M_A} a} + \frac{H_A}{K_{M_B} a E} + \frac{H_A}{K C_B f_t}} \\
 &= \frac{100}{\frac{1}{0.1} + \frac{1}{100(10^{-4})} + \frac{1}{(10^{-4})(10^2)(10^{-2})}} \\
 &= \frac{100}{10 + 100 + 10000} \\
 &= 9.8911 \times 10^{-3} \text{ mol/hr m}^3 \text{ reactor}
 \end{aligned}$$

(a) Reaction Rate = 9.81×10^{-3} mol/m² m³ reactor

(b) Resistance: In main body - 99%.
Reaction zone - main body of liquid

Behaviour of liquid film = physical transport

5.
→

$$K = 10^{-2} \text{ m}^3 \text{ liquid/mol hr} \quad H_A = 1 \text{ Pa} \cdot \text{m}^3 \text{ liquid/mol}$$

$$M_H = \sqrt{\frac{DKC_B}{k_{Ae}}} = \sqrt{\frac{(10^{-6})(10^2)(10^2)}{1}} = 10^3$$

$$\Sigma = 1$$

$$\therefore -r_A''' = \frac{P_A}{K_{Ae}^a} + \frac{H_A}{K_{Ae}^a F} + \frac{H_A}{k_{Bf}^a} = \frac{10^2}{\frac{1}{0.1} + \frac{1}{10^2(0.1)} + \frac{1}{(10^{-2})(0)^2(0.1)}} = 50\%$$

$$-r_A''' = 5 \text{ mol/m}^2 \text{ m}^3 \text{ reactor}$$

(a) Reaction rate = 5 mol/m² m³ reactor

(b) Resistance: 50% in film
50% in main body of liquid

Reaction zone - main body of liquid

Behaviour of liquid film - physical transport

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$$k_{AL} a = 0.1 \text{ mol/m}^3 \text{ hr of reactor } P_A$$

$$k_{AL} a = 100 \text{ m}^3/\text{leg/m}^3 \text{ reactor } P_A$$

$$a = 100 \text{ m}^2/\text{m}^3 \text{ reactor}$$

$$D_{AL} = \frac{k_{AL} a}{P_{BL}} = 0.01 \text{ m}^3 \text{ leg/m}^3 \text{ reactor}$$

$$a = 100 \text{ m}^2/\text{m}^3 \text{ reactor}$$

$$\text{where } P_A = 100 \text{ Pa} \quad C_B = \frac{100 \text{ mol}}{\text{m}^3}$$

$$k = 10^8 \text{ m}^3 \text{ leg/mol} \cdot \text{hr} \quad H_A = 1 \frac{\text{Pa}}{\text{m}^3 \text{ leg/mol}}$$

$$-r_A = k C_A C_B$$

First find

$$M_H = \sqrt{\frac{D_A k C_B^2}{K_{AL}}}$$

$$= \sqrt{\frac{10^{-6} \times 10^8 \times 100}{1}} = 100$$

Assuming

$$R_i = 1 + \frac{D_B C_B H_A}{b D_A P_A}$$

$$= 1 + \frac{100 \times 1}{100 \times 1} = 2$$

$$\text{thus } E_i \leq \frac{M_H}{5}$$

So this is an instantaneous reaction at a plane on the leg film in which case $E \leq E_i$

25. 7

$$C_B = 1 \text{ mol/m}^3$$

$$M_H = \sqrt{\frac{2kC_B}{K_{dL}}} = \sqrt{\frac{10^{-6} \times 10^6 \times 1}{1}} = 1$$

$$E_i = 1 + \frac{1(1)10^5}{2 \times 5 \times 10^3} = 51$$

Since $E_i > 5M_H$, we have pseudo 1st order reaction in film

$$E = M_H = 1$$

Now rate expression

$$\begin{aligned} -r_A''' &= \frac{P_A}{\frac{1}{k_{dL}^A} + \frac{H_A}{k_{dL}^A E} + \frac{H_m}{K C_B^2 F_L}} \\ &= \frac{3 \times 10^5}{\frac{1}{0.01} + \frac{10^5}{20(1)} + \frac{10^5}{10^6(1)(0.98)}} \end{aligned}$$

$$= \frac{5000}{5001} \approx 1 \frac{\text{mol}}{\text{m}^3 \text{hr}}$$

Main reaction resistance is in lig film
Reaction zone is in lig film as well
and the rate is $1 \frac{\text{mol}}{\text{hr} \cdot \text{m}^3}$

$$08. \quad P_A = 1.8 \times 10^{-9} \quad K = 10 \quad C_B = 500$$

$$M_H = \sqrt{\frac{D K C_B}{K_{AL}^2}} = \sqrt{\frac{1.8 \times 10^{-9} \times 10 \times 500}{(10^{-4})^2}}$$

$$= \frac{3 \times 10^{-3}}{10^{-4}} = 30$$

$$\therefore M_H = 30$$

$$F_i = 1 + \frac{D_B C_B \cdot H_A}{b \cdot D_A P_{Ai}}$$

$$= 1 + \frac{3.06 \times 10^{-9} \times 500 \times 25000}{2 \times 1.8 \times 10^{-9} \times 10^5} \quad (\text{For } P_{Ai} = P_A)$$

$$= 107.25$$

$$\text{For } P_{Ai} = 0$$

$$F_i = \infty$$

from graph $F = M_H = 83$ so taking $M_H = 30$

$$- \gamma_A''' = \frac{P_A}{\frac{1}{KgA} + \frac{H_A}{K_{AL} \cdot a \cdot F} + \frac{H_A}{K \cdot C_B \cdot f}}$$

$$= \frac{10^5}{\frac{1}{10^{-4}} + \frac{25000}{10^4 \times 30} + \frac{25000}{10 \times 500 \times 0.1}}$$

$$= \frac{10^5}{10000 + 833333.3 + 50}$$

$$= 0.1198$$

Q9. Since it's a instantaneous reaction $K = \infty$.

$$\begin{aligned} F_i &= 1 + \frac{D_B C_B H_A}{D_A P_A} \\ &= 1 + \frac{0.64 \times 250 \times 10^{-4}}{0.02 \times 10^{-3}} \\ &= 1 + 800 = 801 \end{aligned}$$

$$\text{gas phase resistance } \frac{1}{K_{g,a}} = \frac{1}{60} = 0.0166$$

$$\text{liq. film resistance } = H_A = \frac{10^{-4}}{K_{L,A} \cdot e} = \frac{10^{-4}}{0.03 \times 801} = 4.16 \times 10^{-6}$$

$$\text{kinetic} = \infty$$

\therefore gas film controls

$$-r_A''' = \frac{K_{g,a} \cdot P_A}{60 \times 0.02} = 1.2 \text{ mol/m}^3 \text{s}$$

b) straight Axis

$$\begin{aligned} -r_A''' &= \frac{P_A}{\frac{1}{K_{g,a}} + \frac{H_A}{K_{L,A}}} \\ &= \frac{0.02}{0.0166 + 3.3 \times 10^{-3}} = 1.005 \text{ mol/m}^3 \text{s} \end{aligned}$$

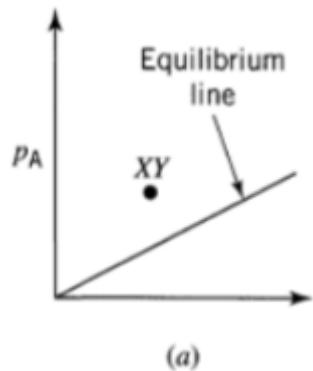
$$\text{so rate} = \frac{1.2 - 1.005}{1.005} = 19.4\% \text{ by adding MEA}$$

Group no: 7: 13bch036, 13bch037, 13bch038, 13bch040

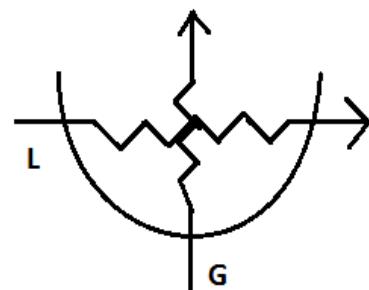
Cre II- term paper II

Chapter 24: Fluid-Fluid reactors design

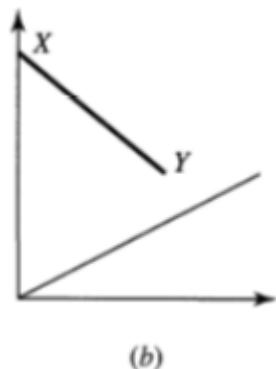
24.1



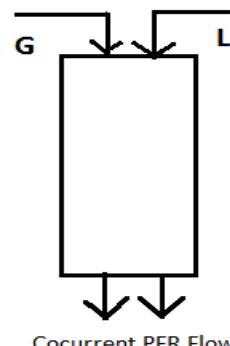
(a)



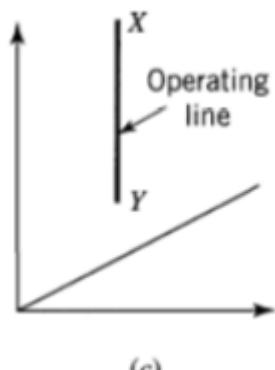
Gas bubbled in well stirred liquid
---Mixed-Mixed pattern



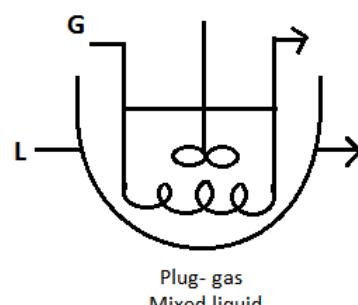
(b)

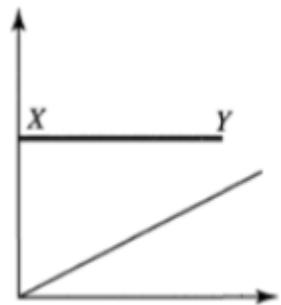


Cocurrent PFR Flow

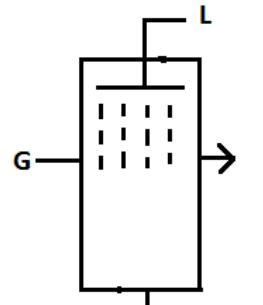


(c)

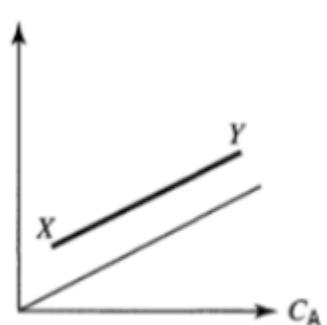




(d)



Mixed gas- PLug liquid



(e)



Counter current PRF

24.2

$A = \text{agitated tank}$ $H_A=0, K=0$

$$M_H = \frac{\sqrt{D_{ab} * k * C_b}}{K_{al}} = \frac{\sqrt{3.6 * 10^{-6} * 0 * C_b}}{0.114} = 0$$

$$Ei = 1 + \frac{C_b * Ha}{PA_1} = 1$$

$Ei \geq 1$, therefore $Ei = E = 1$

$$\text{Gas film resistance} = \frac{1}{K_{ag} * a} = \frac{1}{0.36} = 2.778$$

$$\text{kinetic resistance} = \frac{Ha}{k * C_b * f_l} = 0$$

$$\text{Liquid film resistance} = \frac{Ha}{k_{al} * a * E} = 0$$

$$-r_A = \frac{PA}{\frac{1}{K_{ag} * a}} = \frac{1000}{2.778} = 360$$

$$F_g (Y_{in} - Y_{out}) = -r_a * V_r = F_g * (P_{Ain} - P_{Aout})/\Pi$$

(i) Volume:

$$V_r = \frac{90000}{360} \frac{(1000 - 100)}{10^5} = 22.5 \text{ m}^3$$

(ii) 100% gas film resistance

24.3

Straight mass transfer, counter current, $H_A = 18$, $P_{A2} = 100$

By material balance between points 1 & 2, we can find C_{A1}

$$\frac{90000}{10^5} (1000 - 100) = \frac{900000}{55556} (C_{A1} - 0)$$

Or $C_{A1} = 50 \text{ mol/m}^3$

At equilibrium, $P_A^* = H_A * C_A$ or $P_{A1}^* = 18 * 50 = 900 \text{ Pa}$

Now from the P_A vs C_A diagram we can see that the operating and equilibrium lines are parallel. Thus the rate of transfer is the same everywhere. Hence,

$$-rA''' = \frac{1}{\frac{1}{kag * a} + \frac{HA}{kal * a}} (PA - PA^*) = \frac{1}{\frac{1}{0.36} + \frac{18}{72}} (1000 - 900)$$

$$-rA''' = 33 \text{ mol/(m}^3 * \text{hr)}$$

(i) Volume

$$V_r = \frac{Fg}{\Pi} \int \frac{dpa}{-ra'''} = \frac{90000}{10^5} \frac{(1000 - 100)}{33} = 24.5 \text{ m}^3$$

(ii) 100% gas film resistance

24.4

Tower

$$(K_{Ag} * a * P_A)_{top} = 0.36 * 100 = 36$$

$$(K_{Ag} * a * P_A)_{bottom} = 0.36 * 1000 = 360$$

$$(K_{Al} * a * C_B)_{top} = 5.556 * 72 = 400$$

$$(K_{Al} * a * C_B)_{bottom} = 72 * 555556 = 4000$$

$$C_{Bin} = 55.55 \text{ mol/m}^3$$

$$C_{Bout} = 10\% \text{ of } C_{bin} = 5.55 \text{ mol/m}^3$$

$$(K_{Al} * a * C_B)_{bottom} > (K_{Ag} * a * P_A)_{bottom}$$

$$(K_{Al} * a * C_B)_{top} > (K_{Ag} * a * P_A)_{top}$$

Therefore gas film resistance is controlling one.

$$-rA'''' = \frac{1}{\frac{1}{kag * a}} PA$$

(i) Volume

$$Vr = \frac{Fg}{\Pi} \int \frac{dXa}{-ra} = \frac{Fg}{kag * a * \Pi} \int_{10^2}^{10^3} \frac{dpa}{pa} = \frac{90000}{0.36} \ln \frac{10}{1} = 5.75 \text{ m}^3$$

(ii) 100% gas film resistance

24.5

By doing material balance,

$$Fg (Y_{A1} - Y_{A2}) = F_l (X_{A1} - X_{A2})$$

$$90000 \left(\frac{0.01}{0.99} - \frac{0.001}{0.999} \right) = 900000 (0.001 - X_{B1})$$

$$C_{B1} = 5 \text{ mol/m}^3$$

We need to calculate Ei and M_H to find out the rate

$$Ei = 1 + \frac{Db * Cb}{b * Da * Ca} = 1 + \frac{Cb}{Ca} = 1 + \frac{Cb * Ha}{Pai} = 1 + \frac{10^5 * Cb}{Pai}$$

$$M_H = \frac{\sqrt{Dab*k*Cb}}{Kal^2} = \infty$$

Since $Ei \ll M_H$, we have $E=Ei$

At top point 2,

Assuming that all the resistance lies in the gas film and liquid film resistance is negligible so taking $P_{A2}^* = P_{A2}$

$$Ei = 1 + \frac{55.56 * 10^5}{100} = 5.556 * 10^4$$

Hence $E = 5.556 * 10^4$. Now rate equation,

$$\begin{aligned} -rA'''' &= \frac{1}{\frac{1}{kag*a} + \frac{HA}{kal*a*e} + \frac{HA}{k*Cb*fl}} PA \\ &= \frac{1}{\frac{1}{0.36} + \frac{10^5}{72(5.556 * 10^4)} + \frac{10^5}{\infty}} PA = 0.36 * PA \end{aligned}$$

We can see that gas film resistance is not negligible.

At bottom (point 1),

$$Ei = 1 + \frac{5 * 10^5}{1000} = 501$$

$$M_H = \frac{\sqrt{Dab*k*Cb}}{Kal^2} = \infty$$

Since $Ei \ll M_H$, we have $E=Ei$ so rate equation is,

$$-rA'''' = \frac{1}{\frac{1}{0.36} + \frac{10^5}{72(501)} + \frac{10^5}{\infty}} PA = 0.18 * PA = \frac{1}{\frac{1}{0.36} + \frac{1}{0.36} + 0} PA = 0.18 * PA$$

This shows that gas and liquid film resistance is 50-50%

Trying 2nd time,

Guessing $P_{Ai} = 500$, and repeating the procedure, we get $E_i = 1001$ and from the rate expression 1/3rd of the resistance is in the gas film. Thus our guess was wrong.

Trying 3rd time, guessing $P_{Ai} = 500$ or 10% resistance in the gas film. Then $E_i = 5001$

$$-rA'''' = \frac{1}{\frac{1}{0.36} + \frac{1}{3.6} + 0} PA = 0.32 * PA$$

So $-rA''''$ mean = $(0.36+0.33)/2 = 0.345 \text{ PA}$

Hence,

(i) Volume

$$Vr = \frac{Fg}{\pi} \int \frac{dpa}{-ra''''} = \frac{90000}{10^5} \int_{10^2}^{10^3} \frac{dpa}{0.345 * pa} = \frac{90000}{34500} \ln \frac{10}{1} = 6 \text{ m}^3$$

(ii) Gas film resistance is 91% of total, and 9% is from liquid film.

24.6

Agitated Tank, $H_A = 10^5$, $k = 2.6 * 10^7$

$$F_g (Y_{\text{OUT}} - Y_{\text{IN}}) = F_l (X_{\text{IN}} - X_{\text{OUT}})$$

$$90000 \left(\frac{1000}{10^5} - \frac{100}{10^5} \right) = 900 \left(\frac{5556}{55556} - \frac{C_{\text{Bout}}}{55556} \right)$$

$$C_{\text{Bout}} = 555.96 \text{ mol/m}^3$$

$$M_H = \frac{\sqrt{D_{ab} * k * C_b}}{k a l^2} = \frac{\sqrt{3.68 * 10^{-6} * 2.6 * 10^7 * 555.96}}{0.72^2} = 300.46$$

$$P_{\text{Ai}} = 100 \text{ KPa}$$

$$Ei = 1 + \frac{C_b * H_a}{P_{\text{Ai}}} Ei = 1 + \frac{500 * 10^5}{100} = 5 * 10^5$$

$$Ei \geq M_H, M_H = E = 300.46$$

$$-rA'''' = \frac{1}{\frac{1}{kag * a} + \frac{HA}{kal * a} + \frac{HA}{k * Cb * fl}} PA$$

$$-rA'''' = \frac{1}{\frac{1}{0.72} + \frac{10^5}{144 * 300} + \frac{10^5}{2.6 * 10^5 * 555.56 * 0.9}} PA = 0.710 * PA$$

(i) Volume

$$Vr = \frac{Fg}{\pi} \int \frac{dpa}{-ra''''} = \frac{90000}{10^5} \left(\frac{1000 - 100}{100 * 0.719} \right) = 11.26 \text{ m}^3$$

$$(ii) \text{Thus gas film resistance} = \frac{\frac{1}{0.72}}{\left(\frac{1}{0.719}\right)} = 99\%$$

24.7

$$F_g (Y_{\text{OUT}} - Y_{\text{IN}}) = F_l (X_{\text{IN}} - X_{\text{OUT}})$$

$$90000 \left(\frac{0.01}{0.99} - \frac{0.001}{0.999} \right) = \frac{900000}{55556} (55.56 - C_{b\text{out}})$$

$$C_B = 5 \text{ mol/m}^3$$

$$\text{At exit conditions, } M_H = \frac{\sqrt{3.68*10^{-6}*2.6*10^5*500}}{0.72^2} = 30$$

$$Ei = 1 + \frac{10^5 * 500}{1000} > MH$$

Therefore, Ei = M_H = 30

$$-rA'''' = \frac{PA}{\frac{1}{0.72} + \frac{10^5}{144 * 40} + \frac{10^5}{2.6 * 10^5 * 500 * 0.9}}$$

$$-rA'''' = 0.041 * P_A$$

Therefore,

$$Vr = \frac{Fg}{\Pi} * \frac{\Delta P}{-rA''''} = \frac{90000(1000 - 100)}{10^5(0.041) * 100} = 197.6 \text{ m}^3$$

(i) Volume = 197.6 m³

(ii) Liquid film dominates (94.3%)

24.8

H_A = 1000, k = 2.6 * 10³, Tower

$$\frac{Fg}{\Pi} (PA_1 - PA_2) = \frac{Fl}{b * Ct} (Cb_2 - Cb_1)$$

$$\frac{90000}{10^5} (1000 - 900) = \frac{900000}{55556} (Cb_2 - Cb_1)$$

$$C_{b\text{out}} = 5.556 \text{ mol/m}^3$$

$$\text{At top, } M_H = \frac{\sqrt{3.68 \times 10^{-6} \times 2.6 \times 10^3 \times 55.56}}{0.72} = 1$$

$$Ei = 1 + \frac{55.56 \times 10^5}{100} = 55561 > MH$$

$$-rA'''' = \frac{1}{\frac{1}{kag * a} + \frac{HA}{kal * a} + \frac{HA}{k * Cb * fl}} PA$$

$$-rA'''' = \frac{100}{\frac{1}{0.36} + \frac{10^5}{0.72 * 100} + \frac{10^5}{2.6 * 1000 * 55.56 * 0.9}}$$

$$-rA'''' = 0.0718$$

$$1/-rA'''' = 13.92$$

$$\text{At bottom, } M_H = \frac{\sqrt{3.68 \times 10^{-6} \times 2.6 \times 10^3 \times 55.56}}{0.72^2} = 0.3167$$

But M_H can't be less than 1. Therefore it is equal to 1.

$$Ei = 1 + \frac{10^5 * 5.556}{1000} = 55561 > MH$$

$$-rA'''' = \frac{100}{\frac{1}{0.36} + \frac{10^5}{0.72} + \frac{10^5}{2.6 * 1000 * 5.556 * 0.9}}$$

$$-rA'''' = 0.714$$

$$1/-rA'''' = 1.4$$

At the middle, at $P_A = 3000 \text{ Pa}$, $C_A = 44.44 \text{ mol/m}^3$

$$M_H = \frac{\sqrt{3.68 \times 10^{-6} \times 2.6 \times 10^3 \times 44.44}}{0.72^2} = 0.895$$

$$Ei = 1 + \frac{10^5 * 44.44}{1000} > MH$$

So $E = M_H = 1$

$$-rA'''' = \frac{100}{\frac{1}{0.36} + \frac{10^5}{0.72} + \frac{10^5}{2.6 * 1000 * 44.44 * 0.9}}$$

$$-rA'''' = 0.359$$

$$1/-rA'''' = 2.58$$

$$Vr = \frac{Fg}{\Pi} \int_{10^2}^{10^3} \frac{dpa}{-rA''}$$

$$Vr = 2685.6 \text{ m}^3$$

$$24.9$$

$$F_g (Y_{in} - Y_{out}) = F_I (X_{BOUT} - X_{BIN})$$

$$90000 \left(\frac{0.01}{0.99} - \frac{0.001}{0.999} \right) = \frac{900000}{55556} (55.56 - C_{b,out})$$

$$C_B = 5 \text{ mol/m}^3$$

$$\text{At top, } M_H = \frac{\sqrt{3.68 \times 10^{-6} \times 2.6 \times 10^7 \times 55.56}}{0.72^2} = 100$$

$$Ei = 1 + \frac{10^5 * 55.56}{1000} > MH$$

Therefore, Ei = M_H = 100

$$-rA'''' = \frac{100}{\frac{1}{0.36} + \frac{10^5}{0.72 * 100} + \frac{10^5}{2.6 * 10^7 * 55.56 * 0.9}}$$

$$-rA'''' = 6$$

$$\text{At bottom, } M_H = \frac{\sqrt{3.68 \times 10^{-6} \times 2.6 \times 10^7 \times 5}}{0.72^2} = 30$$

$$Ei = 1 + \frac{10^5 * 5}{1000} > MH$$

Therefore, Ei = M_H = 30

$$-rA'''' = \frac{100}{\frac{1}{0.36} + \frac{10^5}{0.72 * 30} + \frac{10^5}{2.6 * 1000 * 5 * 0.9}}$$

$$-rA'''' = 20.4$$

In the middle, at P_A = 547 Pa, C_A = 30.56 mol/m^3

$$M_H = \frac{\sqrt{3.68 \times 10^{-6} \times 2.6 \times 10^7 \times 30.56}}{0.72^2} = 74$$

$$Ei = 1 + \frac{10^5 \times 30.56}{1000} > MH$$

So E = M_H = 74

$$-rA'''' = \frac{100}{\frac{1}{0.36} + \frac{10^5}{0.72 \times 74} + \frac{10^5}{2.6 \times 10^7 \times 30.56 \times 0.9}}$$

$$-rA'''' = 25.4$$

$$1/-rA'''' = 0.0393$$

$$Vr = \frac{Fg}{\Pi} \int_{10^2}^{10^3} \frac{dpa}{-rA''}$$

(i) Volume

$$Vr = (9000/10^5) \times 66 = 59.4 \text{ m}^3$$

(ii) liquid film dominates (84%)

24.10

H_A = 1000, k = 2.6 × 10⁵, Tower

$$\frac{Fg}{\Pi} (PA1 - PA2) = \frac{Fl}{b * Ct} (Cb2 - Cb1)$$

$$\frac{90000}{10^5} (1000 - 900) = \frac{900000}{55556} (Cb2 - Cb1)$$

$$C_{Bout} = 5.556 \text{ mol/m}^3$$

$$\text{At top, } M_H = \frac{\sqrt{3.63 \times 10^{-6} \times 2.6 \times 10^5 \times 55.56}}{0.72} = 10$$

$$Ei = 1 + \frac{55.56 \times 10^3}{100} = 556.6 > MH$$

Therefore, Ei = M_H = 10

$$-rA'''' = \frac{100}{\frac{1}{0.36} + \frac{10^3}{0.72 \times 10} + \frac{10^3}{2.6 \times 10^5 \times 55.56 \times 0.9}}$$

$$-rA'''' = 23.95 \text{ mol/m}^3\text{hr}$$

$$1/-rA'''' = 0.0417$$

$$\text{At bottom, } M_H = \frac{\sqrt{3.68 \times 10^{-6} \times 2.6 \times 10^5 \times 5.56}}{0.72^2} = 3.16$$

But M_H can't be less than 1. Therefore it is equal to 1.

$$Ei = 1 + \frac{10^3 * 5.556}{1000} = 6.55 > MH$$

Therefore, $Ei = M_H = 3.16$

$$-rA'''' = \frac{100}{\frac{1}{0.36} + \frac{10^3}{0.72 * 3.16} + \frac{10^5}{2.6 * 10^5 * 5.556 * 0.9}}$$

$$-rA'''' = 137.93$$

$$1/-rA'''' = 0.0073$$

At the middle, at $P_A = 300 \text{ Pa}$, $C_A = 44.44 \text{ mol/m}^3$

$$M_H = \frac{\sqrt{3.68 \times 10^{-6} \times 2.6 \times 10^7 \times 44.44}}{0.72^2} = 8.95$$

$$Ei = 1 + \frac{10^5 * 44.44}{1000} > MH$$

So $E = M_H = 8.95$

$$-rA'''' = \frac{300}{\frac{1}{0.36} + \frac{10^5}{0.72 * 8.95} + \frac{10^5}{2.6 * 10^5 * 44.44 * 0.9}}$$

$$-rA'''' = 69.136$$

$$1/-rA'''' = 0.0144$$

$$Vr = \frac{Fg}{\Pi} \int_{10^2}^{10^3} \frac{dpa}{-rA''}$$

$$Vr = 0.9 * 10.8 = 9.72 \text{ m}^3$$

24.11

$$CA = \frac{PAin}{HA} = \frac{101325}{3500} = 28.95 \text{ mol/m}^3$$

$C_{B_{in}} = 300 \text{ mol/m}^3$, since C_B is greater than C_A we have excess of B, so C_B can be taken as 300 mol/m³

$$M_H = \frac{\sqrt{1.4 \cdot 10^{-9} \cdot 0.433 \cdot 300 \cdot 120}}{0.25} = 2.05$$

$$Ei = 1 + \frac{300 \cdot 3500}{101325} = 11.36 > MH$$

So $E = M_H = 2.05$

$$-rA'''' = \frac{101325}{0 + \frac{3500}{0.025 \cdot 2.05} + \frac{3500}{0.433 \cdot 300 \cdot 0.08}}$$

$$-rA'''' = 1.476$$

$$1/-rA'''' = 0.677$$

$$Vr = FA0 \int_0^{XA} \frac{dXA}{-rA''''}$$

$$F_{A0} = V_0 \cdot C_{A0} = 0.0363 \cdot 18.95 = 1.05 \text{ m}^3/\text{hr}$$

$$XA = \frac{Vr}{FA0} (-rA''') = \frac{0.6042}{1.05} * 1.48 = 85\% \text{ conversion}$$

24.12



$$K = 2.6 \cdot 10^9 \text{ km}^3/\text{mol.hr}, H_A = 10^5 \text{ Pa m}^3/\text{mol.hr}$$

$$A_{cs} = 55 \text{ m}^3$$

$$F_g = 100, F_l = 250 \text{ mol/s} \cdot \text{m}^2$$

$$D = 1.5 \cdot 10^9 \text{ m}^2/\text{s}$$

$$C_B (\text{IN}) = 10\% * 250 = 25 \text{ mol/m}^3$$

$$\frac{Fg}{\Pi} (PA1 - PA2) = \frac{Fl}{b * Ct} (Cb2 - Cb1)$$

$$\frac{100}{10^5} (2.36 * 0.99) = \frac{250}{2 * 2736} (25 - CB2)$$

$$C_{B2} = 24.9 \text{ m}^3 / \text{mol}$$

$$M_H = \frac{\sqrt{1.5 \cdot 10^{-9} \cdot 2.6 \cdot 10^9 \cdot 24.9}}{0.45} = 0.218$$

$$Ei = 1 + \frac{24.5 \cdot 10^5}{0} = \infty > MH$$

But M_H can't be less than 1. Therefore E is equal to 1.

When $P_A = 1000$,

$$-rA'''' = \frac{PA}{\frac{1}{133} + \frac{10^5}{133 \cdot 1} + \frac{10^5}{2.6 \cdot 10^9 \cdot 24.9 \cdot 0.9}} = 1.329 \cdot 10^{-3} PA$$

$$H = \frac{Fg}{Acs \cdot \pi} \int_{10^2}^{10^3} \frac{dPa}{0.1329 \cdot Pa} = \frac{100}{55 \cdot 1} \cdot \frac{\ln 10}{0.1329} = 3.14 \text{ m}$$

24.13

For agitated tank,

$$K = 2.6 \cdot 10^5, H_A = 10^5$$

At the beginning, $C_B = 555.6 \text{ mol/m}^3$

$$M_H = \frac{\sqrt{3.6 \cdot 10^{-6} \cdot 2.6 \cdot 10^5 \cdot 555.6}}{1.44} = 15.84$$

$$Ei = 1 + \frac{555.6 \cdot 10^5}{1000} = 55561 > MH$$

So $E = M_H = 15.84$

$$-rA'''' = \frac{PAin}{\frac{\pi \cdot Vr}{Fg} + \frac{1}{Kag \cdot a} + \frac{Ha}{Kal \cdot a \cdot E} + \frac{Ha}{K \cdot Cb \cdot fl}}$$

$$-rA'''' = \frac{1000}{\frac{10^5 \cdot 1.62}{9000 \cdot 0.9} + \frac{1}{0.72} + \frac{10^5}{144 \cdot 15.84} + \frac{10^5}{2.6 \cdot 10^5 \cdot 555.6 \cdot 0.9}}$$

$$-rA'''' = 15.33 \text{ mol/m}^3 \cdot \text{hr}$$

$$1/-rA'''' = 0.0652$$

$$\text{At the end of the run, } M_H = \frac{\sqrt{3.68 \times 10^{-6} \times 2.6 \times 10^5 \times 55.6}}{1.44} = 5.01$$

$$Ei = 1 + \frac{10^5 * 55.56}{1000} = 5561 > MH$$

Therefore, $Ei = M_H = 5.01$

$$-rA'''' = \frac{1000}{20 + 1.3889 + \frac{10^5}{10^5 * 144 * 5.01} + 0}$$

$$-rA'''' = 6.25 \text{ mol/m}^3 \cdot \text{hr}$$

$$1/-rA'''' = 0.16$$

At some intermediate run, $C_A = 138.9 \text{ mol/m}^3$

$$M_H = 15.84/2 = 7.92$$

$$Ei = 1 + \frac{10^5 * 138.9}{1000} = 13890 > MH$$

So $E = M_H = 7.92$

$$-rA'''' = \frac{1000}{20 + 1.3889 + \frac{10^5}{144 * 7.92} + 0}$$

$$-rA'''' = 9.168 \text{ mol/m}^3 \cdot \text{hr}$$

$$1/-rA'''' = 0.109$$

The length of the time that we have to bubble gas through the liquid is

$$t = \frac{Fl}{b} \int_{10^2}^{10^3} \frac{dCb}{-rA''} = Fl * \text{area} = 0.9 * 51.38 = 46.2 \text{ hr}$$

The minimum time needed if all the A reacts with B,

$$t \text{ min} = \frac{Vl(Cb0 - Cbf)}{Fg(PA/(\Pi - Pa))} = \frac{1.62(555.6 - 55.56)}{9000(1000/99000)} = 8.91 \text{ hr}$$

Therefore, the efficiency of the use of A = $8.91/46.24 = 19.26\%$

24.14

For agitated tank,

$$K = 2.6 \times 10^9, H_A = 10^5$$

At the beginning, $C_B = 555.6 \text{ mol/m}^3$

$$M_H = \frac{\sqrt{3.6 \times 10^{-6} \times 2.6 \times 10^9 \times 555.6}}{1.44} = 1583.6$$

$$Ei = 1 + \frac{555.6 \times 10^5}{1000} = 55561 > MH$$

So $E = M_H = 1583.6$

$$-rA'''' = \frac{PAin}{\frac{\pi \times Vr}{Fg} + \frac{1}{Kag \times a} + \frac{Ha}{Kal \times a \times E} + \frac{Ha}{K \times Cb \times fl}}$$

$$-rA'''' = \frac{1000}{\frac{10^5 \times 1.62}{9000 \times 0.9} + \frac{1}{0.72} + \frac{10^5}{144 \times 1583.6} + \frac{10^5}{2.6 \times 10^9 \times 555.6 \times 0.9}}$$

$$-rA'''' = 45.81 \text{ mol/m}^3 \cdot \text{hr}$$

$$1/-rA'''' = 0.0218$$

$$\text{At the end of the run, } M_H = \frac{\sqrt{3.68 \times 10^{-6} \times 2.6 \times 10^9 \times 55.6}}{1.44} = 506.5$$

$$Ei = 1 + \frac{10^5 \times 55.56}{1000} = 5561 > MH$$

Therefore, $Ei = M_H = 506.5$

$$-rA'''' = \frac{1000}{20 + 1.3889 + \frac{10^5}{144 \times 506.5} + 0}$$

$$-rA'''' = 43.93 \text{ mol/m}^3 \cdot \text{hr}$$

$$1/-rA'''' = 0.0227$$

At some intermediate run, $C_A = 138.9 \text{ mol/m}^3$

$$M_H = 1583.6/2 = 791.8$$

$$Ei = 1 + \frac{10^5 * 138.9}{1000} = 13890 > MH$$

So $E = M_H = 395.9$

$$-rA'''' = \frac{1000}{20 + \frac{10^5}{144 * 791.8} + 0}$$

$$-rA'''' = 44.9 \text{ mol/m}^3 \cdot \text{hr}$$

$$1/-rA'''' = 0.022$$

The length of the time that we have to bubble gas through the liquid is

$$t = \frac{Fl}{b} \int \frac{dCb}{-rA''} = Fl * area = 0.9 * 10.987 = 9.88 \text{ hr}$$

The minimum time needed if all the A reacts with B,

$$t_{\min} = \frac{Vl(Cb_0 - Cbf)}{Fg(PA/(\Pi - Pa))} = \frac{1.62(555.6 - 55.56)}{9000(1000/99000)} = 8.91 \text{ hr}$$

Therefore, the efficiency of the use of A = $8.91/9.88 = 90.1\%$

24.15

For agitated tank,

$$K = 2.6 * 10^3, H_A = 10^5$$

At the beginning, $C_B = 555.6 \text{ mol/m}^3$

$$M_H = \frac{\sqrt{3.6 * 10^{-6} * 2.6 * 10^3 * 555.6}}{1.44} = 1.584$$

$$Ei = 1 + \frac{555.6 * 10^5}{1000} = 55561 > MH$$

So $E = M_H = 1.58$

$$-rA'''' = \frac{PAin}{\frac{\Pi * Vr}{Fg} + \frac{1}{Kag * a} + \frac{Ha}{Kal * a * E} + \frac{Ha}{K * Cb * fl}}$$

$$-rA'''' = \frac{1000}{\frac{10^5 * 1.62}{9000 * 0.9} + \frac{1}{0.72} + \frac{10^5}{144 * 1.584} + \frac{10^5}{2.6 * 10^5 * 555.6 * 0.9}}$$

$$-rA'''' = 2.175 \text{ mol/m}^3\text{hr}$$

$$1/-rA'''' = 0.459$$

$$\text{At the end of the run, } M_H = \frac{\sqrt{3.68 \times 10^{-6} \times 2.6 \times 10^3 \times 55.6}}{1.44} = 0.5$$

$$Ei = 1 + \frac{10^5 * 55.56}{1000} = 5561 > MH$$

$$\text{Therefore, } Ei = M_H = 0.5$$

$$-rA'''' = \frac{1000}{20 + 1.3889 + \frac{10^5}{10^5 * 144 * 0.5} + 0}$$

$$-rA'''' = 0.7096 \text{ mol/m}^3\text{hr}$$

$$1/-rA'''' = 1.41$$

$$\text{At some intermediate run, } C_A = 555.6/4 = 138.9 \text{ mol/m}^3$$

$$M_H = 15.84/4 = 0.792$$

$$Ei = 1 + \frac{10^5 * 138.9}{1000} = 13890 > MH$$

$$\text{So } E = M_H = 1$$

$$-rA'''' = \frac{1000}{20 + 1.3889 + \frac{10^5}{144 * 1} + 0}$$

$$-rA'''' = 1.66 \text{ mol/m}^3\text{hr}$$

$$1/-rA'''' = 0.6$$

The length of the time that we have to bubble gas through the liquid is

$$t = \frac{Fl}{b} \int_{10^2}^{10^3} \frac{dCb}{-rA''} = Fl * \text{area} = 0.9 * 350 = 315 \text{ hr}$$

The minimum time needed if all the A reacts with B,

$$t \text{ min} = \frac{Vl(Cb0 - Cbf)}{Fg(PA/(\Pi - Pa))} = \frac{1.62(555.6 - 55.56)}{9000(1000/99000)} = 8.91 \text{ hr}$$

Therefore, the efficiency of the use of A = 8.91/315 = 2.82%

24.16

$$K = 2.6 \times 10^{11} \text{ m}^3/\text{mol} \cdot \text{hr}, H_A = 10^3 \text{ Pa/m}^3 \cdot \text{mol}$$

$$M_H = \frac{\sqrt{1.5 \times 10^{-9} \times 2.6 \times 10^{11} \times 24.9}}{45} = 2.18$$

$E_i = \infty$, therefore, $E_i = M_H = 2.18$

$$\begin{aligned} -rA'''' &= \frac{1}{\frac{1}{kag * a} + \frac{HA}{kal * a * E} + \frac{HA}{k * Cb * fl}} PA \\ &= \frac{1}{\frac{1}{133} + \frac{10^3}{133} + \frac{10^3}{2.6 \times 10^{11} \times 24.09 \times 0.9}} PA = 0.1328 * PA \end{aligned}$$

$$H = \frac{Fg}{Acs * \pi} \int_{10^2}^{10^3} \frac{dPa}{0.1328 * Pa} = \frac{100}{55 * 1} * \frac{\ln 10}{0.1328} = 31.524 \text{ m}$$

Chapter 25 : Fluid-Particle Reactions:Kinetics

Roll Number : Rohan Patel (13BCH041)
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Q 25.1 A batch of solids of uniform size is treated by gas in a uniform environment. Solid is converted to give a nonflaking product according to the shrinking-core model. Conversion is about 7/8 for a reaction time of 1 h, conversion is complete in two hours. What mechanism is rate controlling?

A 25.1

Assume spherical particles
 $\tau=2$ hr $t=1$ hr, $X_b=0.875$

Film Diffusion

$$\frac{t}{\tau} = \frac{1}{2} = 0.5 \neq 0.875 = X_b$$

Film Diffusion not dominating.

Ash Diffusion

$$1 - 3(1 - X_b)^{\frac{2}{3}} + 2(1 - X_b) = 0.5 = \frac{t}{\tau}$$

Ash Diffusion is dominating.

Reaction

$$1 - (1 - X_b)^{\frac{1}{3}} = 0.5 = \frac{t}{\tau}$$

Reaction control is also dominating

Hence, Ash Diffusion and Reaction controls are dominating.

Q 25.2 In a shady spot at the end of Brown Street in Lewisburg, Pennsylvania, stands a Civil War memorial-a brass general, a brass cannon which persistent undergraduate legend insists may still fire some day, and a stack of iron cannonballs. At the time this memorial was set up, 1868, the cannonballs were 30 inches in circumference. Today due to weathering, rusting, and the once-a-decade steel wire scrubbing by the DCW, the cannonballs are only 29.75 in. in circumference. Approximately, when will they disappear completely?

A 25.2

R=4.78 inch

r_c=4.74 inch t=148 years

As it is a reaction controlling mechanism.

$$X_b = 1 - \left(\frac{r_c}{R}\right)^3 = 0.025$$

$$\text{Now, } \frac{t}{\tau} = 1 - (1 - X_b)^{\frac{1}{3}} = 8.4 \times 10^3$$

$$\tau = 17,686 \text{ years}$$

Hence the time in another 17,538 years.

Q 25.3 Calculate the time needed to burn to completion particles of graphite (R, = 5 mm, p, = 2.2 gm/cm³, k" = 20 cm/sec) in an 8% oxygen stream. For the high gas velocity used assume that film diffusion does not offer any resistance to transfer and reaction. Reaction temperature = 900°C.

A 25.3

As it is a shrinking core particle ash film diffusion will not participate in the reaction. Also it is given that film diffusion is negligible. Hence only reaction control is applicable.

R=5 mm

$$\rho_b = 2.2 \text{ gm/cm}^3 = 0.1833 \text{ mol/cm}^3$$

$$k'' = 20 \text{ cm/sec}$$

$$C_{ag} = \frac{1}{22400} \times \frac{273}{273 + 900} \times 0.08 = 8.3 \times 10^{-7}$$

$$b=1$$

$$\tau = \rho_b \times \frac{R}{b k'' C_{ag}} = 5512 \text{ sec} = 1.53 \text{ hr}$$

Hence 1.53 hours are needed for complete combustion of graphite particles.

Q 25.4 Spherical particles of zinc blende of size $R = 1$ mm are roasted in an 8% oxygen stream at 900°C and 1 atm. The stoichiometry of the reaction is Assuming that reaction proceeds by the shrinking-core model calculate the time needed for complete conversion of a particle and the relative resistance of ash layer diffusion during this operation.

Data

Density of solid, $p_s = 4.13 \text{ gm/cm}^3 = 0.0425 \text{ mol/cm}^3$

Reaction rate constant, $k'' = 2 \text{ cm/sec}$

For gases in the ZnO layer, $D_e = 0.08 \text{ cm}^2/\text{sec}$

Note that film resistance can safely be neglected as long as a growing ash layer is present.

A 25.4

For the reaction, $b = 2/3$

$$\tau_{\text{total}} = \tau_{\text{ash}} + \tau_{\text{reaction}}$$

For ash layer control,

$$C_{\text{AG}} = P_a / RT = 0.08 * 101325 / (8.314 * 1173) = 0.83118 * 10^{-2} \text{ mol/L}$$

$$\tau_{\text{ash}} = \frac{0.0425 * 1 * 10^{-2}}{6 * 2 / 3 * 0.08 * 0.83118 * 10^{-6}} = 1598.02 \text{ sec}$$

For Reaction control,

$$\tau_{\text{reaction}} = \frac{0.0425 * 1 * 10^{-1}}{2/3 * 2 * 0.83118 * 10^{-6}} = 3834.90 \text{ sec}$$

$$\tau_{\text{total}} = 1598.02 + 3834.90 = 5432.94 \text{ sec}$$

$$= 90.54 \text{ min}$$

$$\begin{aligned} \text{Relative Resistance of ash layer} &= \frac{1598.02}{5432.94} * 100 \\ &= 29.41 \% \end{aligned}$$

Q On doubling the particle size from R to $2R$ the time for complete conversion triples. What is the contribution of ash diffusion to the overall resistance for particles of size,

Q 25.5 R?

A 25.5

Let 1 refer to particle size of R

2 refer to particle size of $2R$

Then, $\tau_2 = 3\tau_1 \dots \dots \dots (1)$

$$\tau_1 = \tau_{1\text{ash}} + \tau_{1\text{reaction}} \dots \dots \dots (2)$$

$$\tau_2 = \tau_{2\text{ash}} + \tau_{2\text{reaction}} \dots \dots \dots (3)$$

Put $\tau_{2\text{ash}} = 4\tau_{1\text{ash}}$(4)

$$\tau_{2\text{reaction}} = 2\tau_{1\text{reaction}}$$
.....(5)

So, from equation (1),(2),(3),(4) and (5),

$$3\tau_1 = 4\tau_{1\text{ash}} + 2\tau_{1\text{reaction}}$$
.....(6)

So from equation (2) and (6),

$$\tau_{1\text{ash}} = \tau_{1\text{reaction}}$$

therefore % contribution of ash diffusion for $R = 50\%$

Q 25.6 R?

A 25.6

Let 1 refer to particle size of R

2 refer to particle size of $2R$

Then, $\tau_2 = 3\tau_1$(1)

$$\tau_1 = \tau_{1\text{ash}} + \tau_{1\text{reaction}}$$
.....(2)

$$\tau_2 = \tau_{2\text{ash}} + \tau_{2\text{reaction}}$$
.....(3)

Put $\tau_{2\text{ash}} = 4\tau_{1\text{ash}}$(4)

$$\tau_{2\text{reaction}} = 2\tau_{1\text{reaction}}$$
.....(5)

So, from equation (1),(2),(3),(4) and (5),

$$3\tau_1 = 4\tau_{1\text{ash}} + 2\tau_{1\text{reaction}}$$
.....(6)

So from equation (2) and (6),

$$\tau_{1\text{ash}} = \tau_{1\text{reaction}}$$

put values from equation (4) and (5),

$$\tau_{2\text{ash}}/4 = \tau_{2\text{reaction}}/2$$

$$\text{so, } \tau_{2\text{reaction}} = \tau_{2\text{ash}}/2$$

therefore % contribution of ash diffusion for $R = 66.66\%$

Q Spherical solid particles containing B are roasted isothermally in an oven with gas of constant composition. Solids are converted to a firm nonflaking product according to the SCM as follows:



From the following conversion data (by chemical analysis) or core size data (by slicing and measuring) determine the rate controlling mechanism for the transformation of solid.

Q 25.7

D_p (mm)	X_b	t (min)
1	1	4
1.5	1	6

A 25.7

For finding out the corresponding rate control mechanism, considering the constant size spherical particles if it is:

Film diffusion controlling : The value of R/τ will remain constant for both cases.

Reaction controlling: The value of R/τ will remain constant for both cases.

Ash diffusion control : The value of R^2/τ will remain constant for both cases.

Substituting the value of τ from both cases:

D_p (mm)	X_b	t (min)	Film Diffusion control	Ash film diffusion control	Reaction Control
			$\frac{R}{t} X_b$	$\frac{R^2}{t} [1 - 3(1 - X_b)^{\frac{2}{3}} + 2(1 - X_b)]$	$\frac{R}{t} [1 - (1 - X_b)^{1/3}]$
1	1	4	0.25	0.0625	0.125
1.5	1	6	0.1667	0.0938	0.125

From the above table it implies that the rate controlling mechanism for the transformation of solid is **Reaction Control**.

Q 25.8

D_p (mm)	X_b	t (sec)
1	0.3	2
1	0.75	5

A 25.8

For finding out the corresponding rate control mechanism, considering the constant size spherical particles if it is:

Film diffusion controlling : The value of R/τ will remain constant for both cases.

Reaction controlling: The value of R/τ will remain constant for both cases.

Ash diffusion control : The value of R^2/τ will remain constant for both cases.

Substituting the value of τ from both cases:

D_p (mm)	X_b	t (sec)	Film Diffusion control	Ash film diffusion control	Reaction Control
			$\frac{R}{t} X_b$	$\frac{R^2}{t} [1 - 3(1 - X_b)^{\frac{2}{3}} + 2(1 - X_b)]$	$\frac{R}{t} [1 - (1 - X_b)^{1/3}]$
1	0.3	2	0.15	0.00436	0.0280
1	0.75	5	.015	0.01547	0.037

From the above table it implies that the rate controlling mechanism for the transformation of solid is **Film diffusion control**.

Q 25.9

D_p (mm)	X_b	t (sec)
1	1	200
1.5	1	450

A 25.9

For finding out the corresponding rate control mechanism, considering the constant size spherical particles if it is:

Film diffusion controlling : The value of R/τ will remain constant for both cases.

Reaction controlling: The value of R/τ will remain constant for both cases.

Ash diffusion control : The value of R^2/τ will remain constant for both cases.

Substituting the value of τ from both cases:

D_p (mm)	X_b	t (sec)	Film Diffusion control	Ash film diffusion control	Reaction Control
			$\frac{R}{t} X_b$	$\frac{R^2}{t} [1 - 3(1 - X_b)^{\frac{2}{3}} + 2(1 - X_b)]$	$\frac{R}{t} [1 - (1 - X_b)^{1/3}]$
1	1	200	0.005	0.00125	0.0025
1	1	450	0.0022	0.00125	0.00167

From the above table it implies that the rate controlling mechanism for the transformation of solid is **Ash film diffusion control**.

Q 25.10

D_p (mm)	X_b	t (sec)
2	0.875	1
1	1	1

A 25.10

For finding out the corresponding rate control mechanism, considering the constant size spherical particles if it is:

Film diffusion controlling : The value of R/τ will remain constant for both cases.

Reaction controlling: The value of R/τ will remain constant for both cases.

Ash diffusion control : The value of R^2/τ will remain constant for both cases.

Substituting the value of τ from both cases:

D_p (mm)	X_b	t (sec)	Film Diffusion control	Ash film diffusion control	Reaction Control
			$\frac{R}{t} X_b$	$\frac{R^2}{t} [1 - 3(1 - X_b)^{\frac{2}{3}} + 2(1 - X_b)]$	$\frac{R}{t} [1 - (1 - X_b)^{1/3}]$
2	0.875	1	0.875	0.5	0.5
1	1	1	0.5	0.25	0.5

From the above table it implies that the rate controlling mechanism for the transformation of solid is **Reaction control**.

Q 25.11 Uniform-sized spherical particles UO₂ are reduced to UO, in a uniform environment with the following results:

t , hr	0.180	0.347	0.453	0.567	0.733
X_B	0.45	0.68	0.80	0.95	0.98

If reaction follows the SCM, find the controlling mechanism and a rate equation to represent this reduction.

A 25.11

Method : 1

For

Gas Film Controlling : $\frac{t}{\tau} = X_b$

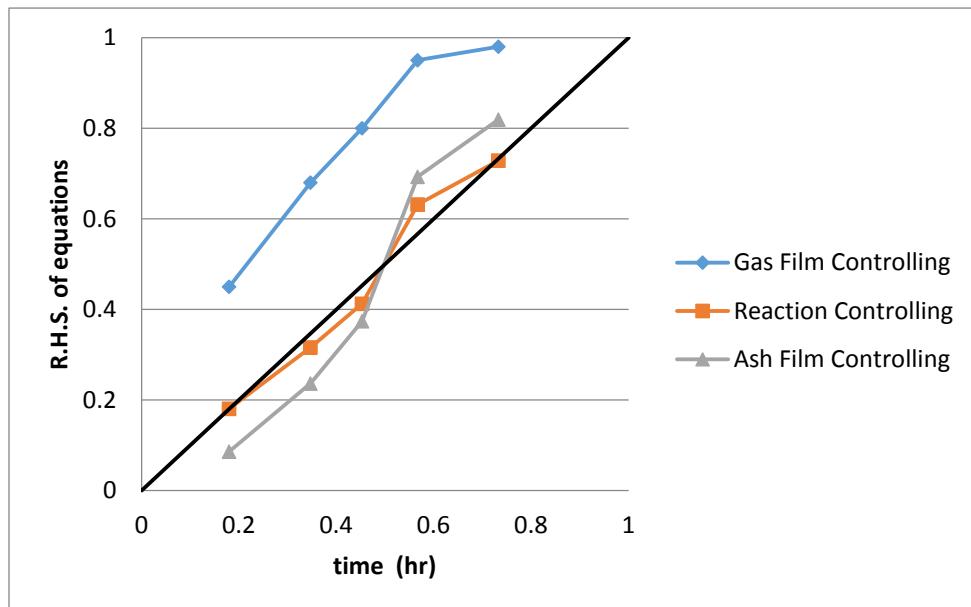
Reaction Controlling : $\frac{t}{\tau} = 1 - (1 - X_b)^{1/3}$

Ash Film Controlling : $\frac{t}{\tau} = 1 - 3(1 - X_b)^{\frac{2}{3}} + 2(1 - X_b)$

Now, Find the value of R.H.S of all equation...

t , hr	X_b	$1 - (1 - X_b)^{1/3}$	$1 - 3(1 - X_b)^{\frac{2}{3}} + 2(1 - X_b)$
0.18	0.45	0.1807	0.0861
0.347	0.68	0.316	0.2365
0.453	0.8	0.4125	0.374
0.567	0.95	0.6316	0.6928
0.733	0.98	0.7286	0.819

Then, Plot R.H.S. vs time(hr) and whichever is nearer to diagonal line it will be controlling mechanism.



The assumption of reaction control gives a better straight line fit than does the assumption for gas film and ash film.

Method 2 :

Find the value of τ for any 2 or 3 time for all three mechanism and in whichever mechanism all τ are same then it will be controlling mechanism.

Time,hr	0.18	0.453	0.733
Xb	0.45	0.8	0.98
Gas Film Controlling	0.4	0.56625	0.7479
Reaction Controlling	0.996	1.09	1.004
Ash Film Controlling	2.09	1.211	0.894

From the above table it implies that the rate controlling mechanism for the transformation of solid is **Reaction control**.

Q 25.12 A large stockpile of coal is burning. Every part of its surface is in flames. In a 24-hr period the linear size of the pile, as measured by its silhouette against the horizon, seems to decrease by about 5%.

- (a) How should the burning mass decrease in size?
- (b) When should the fire burn itself out?
- (c) State the assumptions on which your estimation is based.

A 25.12

- (a). As it is written that surface is in flames, the burning mass should decrease in size by Shrinking Core Model (SCM)

(b). The coal fire will burn out when entire coal will be covered by the ash layer and it will no longer be able to diffuse oxygen through the ash layer and the fire should burn itself out.

(c). The outer surface of the solid particle and the deeper layers do not take part in the reaction until all the outer layer has transformed into solid or gaseous product. The reaction zone then moves inward(into solid), constantly reducing the size of core of unreacted solid and leaving behind completely converted solid(solid product) and inert material (inert constituent of the solid reactant). And we refer to converted solid and inert material as ash. At any time the solid comprises of a core surrounded by a envelope. The envelope consist of a solid product and inert material. Ash layer may contribute to resistance.

CHAPTER 26

FLUID-PARTICLE REACTORS: DESIGN

SOLUTION OF UNSOLVED EXAMPLES

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A stream of particles of one size are 80% converted (SCM/ash diffusion control, uniform gas environment) on passing through a reactor. If the reactor is made twice the size but with the same gas environment, same feed rate, and same flow pattern of solids, what would be the conversion of solids? The solids are in

26.1. plug flow.

26.2. mixed flow.

26.1

Solution

Given: Shrinking core model with ash diffusion as controlling mechanism

Conversion = 80%

To find conversion when the size of reactor is doubled

Feed rate, flow pattern, gas environment are considered constant

For plug flow, SCM, Ash diffusion

$$\begin{aligned}\frac{t_p}{\tau} &= 1 - 3(1 - X_B)^{2/3} + 2(1 - X_B) \\ &= 1 - 3(1 - 0.8)^{2/3} + 2(1 - 0.8) \\ &= 0.374\end{aligned}$$

On doubling the size of reactor $t_p' = 2t_p$

$$\frac{2t_p}{\tau} = 1 - 3(1 - X_B')^{2/3} + 2(1 - X_B')$$

$$\text{So, } X_B' = 96.5\%$$

26.2

Solution

For MFR same gas environment and same feed rate so no change in conversion.

A solid feed consisting of
20 wt% of 1-mm particles and smaller
30 wt% of 2-mm particles
50 wt% of 4-mm particles
passes through a rotating tubular reactor somewhat like a cement kiln where it reacts with gas to give a hard nonfriable solid product (SCM/reaction control, $\tau = 4$ h for 4-mm particles).

26.3. Find the residence time needed for 100% conversion of solids.

26.4. Find the mean conversion of the solids for a residence time of 15 min.

26.3

Solution

Reactor type: tubular

Hard solid product (SCM/Reaction control)

$\tau = 4$ hr for 4mm particles

To find: residence time for 100% conversion of solids

For plug flow SCM/reaction control

$$\tau = \frac{\rho_B R}{k'' b C_{Ag}}$$

This shows that $\tau \propto R$

$$\tau_{2mm} = 2 \text{ hours}$$

$$\tau_{1mm} = 2 \text{ hours}$$

For 100% conversion residence time should be more than 4hours.

26.4

Solution

We need to find conversion of 1 mm, 2mm & 4mm particle sizes in 15 min of time.

- For 4mm particle

$$\frac{15}{4 * 60} = 1 - (1 - x_b)^{\frac{1}{3}}$$

$$(1 - x_b) = 0.824$$
$$x_b = 0.176$$

- For 2 mm particle

$$\frac{15}{2 * 60} = 1 - (1 - x_b)^{\frac{1}{3}}$$

$$(1 - x_b) = 0.669$$
$$x_b = 0.331$$

- For 1mm particle

$$\frac{15}{1 * 60} = 1 - (1 - x_b)^{\frac{1}{3}}$$

$$(1 - x_b) = 0.423$$

$$x_b = 0.577$$

- Over all conversion

$$(1 - x_b) = 0.5 * 0.176 + 0.3 * 0.331 + 0.2 * 0.577$$
$$x_b = 0.6973$$

26.5. Particles of uniform size are 60% converted on the average (shrinking core model with reaction controlling) when flowing through a single fluidized bed. If the reactor is made twice as large but contains the same amount of solids and with the same gas environment what would be the conversion of solids?

Solution

Given: SCM with reaction control

Conversion 60%

To find: conversion when reactor is made twice as large keeping amount of solids and gas environment constant

$W_1=W_2$ (Amount of solids)

Concentration $C_{A01}=C_{A02}$

$$\frac{W}{F_{A0}} = \frac{\bar{t}}{C_{A0}}$$

Here same gas environment so $F_{A01}=F_{A02}$

Therefore, $\bar{t}_1 = \bar{t}_2$

Conversion is same

Size of reactor does not play role but the weight of solids passed play a role in changing conversion in this case.

26.6. Solids of unchanging size, $R = 0.3$ mm, are reacted with gas in a steady flow bench scale fluidized reactor with the following result.

$$\bar{t} = \frac{w}{F_0} = 100 \text{ sec}$$

$$1 - x_b = \frac{1}{4} * \frac{\tau}{\bar{t}} - \frac{1}{20} \left(\frac{\tau}{\bar{t}} \right)^2 + \frac{1}{120} * \left(\frac{\tau}{\bar{t}} \right)^3$$

$$\frac{\tau}{\bar{t}} = 1.246$$

$$\tau = 124.65$$

$$1 - x_b = 0.02$$

$$0.02 = \frac{1}{4} * \frac{\tau}{\bar{t}} - \frac{1}{20} \left(\frac{\tau}{\bar{t}} \right)^2 + \frac{1}{120} * \left(\frac{\tau}{\bar{t}} \right)^3$$

$$\bar{t} = \frac{124.6}{0.081} = 1538.27$$

$\bar{t} > \tau$ because of presence of non idealities.

$$w = \bar{t} * F_0$$

$$\underline{w = 15382.7 \text{ g}}$$

26.7. Solve Example 26.3 with the following modification: the kinetics of the reaction is ash diffusion controlled with $\tau(R = 100 \mu\text{m}) = 10 \text{ min}$.

Information from Example 26.3	Modification
<ul style="list-style-type: none"> ➤ 30% of 50μm radius particles ($\tau=5\text{min}$) ➤ 40% of 100μm radius particles ($\tau=10\text{min}$) ➤ 30% of 200μm radius particles ($\tau=20\text{min}$) ➤ Reactor type: Fluidized bed reactor (MFR) ➤ Unchanging particle (SCM) with reaction control ➤ Feed rate = 1kg solids/min ➤ Solids in bed = 10kg ➤ Mean residence time = 10min 	<ul style="list-style-type: none"> ➤ Ash film control ➤ $\tau(R=100\mu\text{m}) = 10\text{min}$

Solution

For ash controlling mechanism $\tau \propto R^2$

$$\text{So, } \tau(R=50\mu\text{m}) = \frac{\tau(R=100\mu\text{m})*(50^2)}{100^2} = \frac{10*(50^2)}{100^2} = 2.5\text{min}$$

$$\text{And, } \tau(R=200\mu\text{m}) = \frac{\tau(R=100\mu\text{m})*(200^2)}{100^2} = \frac{10*(200^2)}{100^2} = 40\text{min}$$

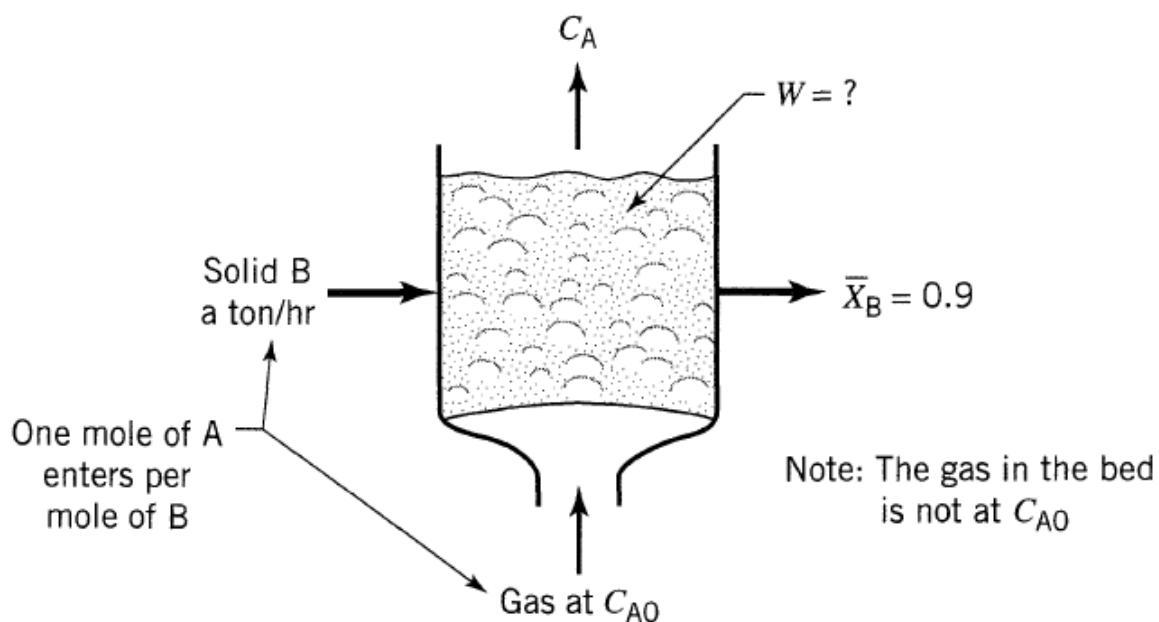
For ash diffusion

$$\begin{aligned}
 1 - \bar{\bar{X}}_B &= \sum \left\{ \frac{1}{5} \frac{\tau(R_i)}{\bar{t}} - \frac{19}{420} \left(\frac{\tau(R_i)}{\bar{t}} \right)^2 \right\} \frac{F(R_i)}{F} \\
 &= 0.3 \left\{ \left[\frac{1}{5} * \frac{2.5}{10} \right] - \left[\frac{19}{420} * \left(\frac{2.5}{10} \right)^2 \right] \right\} + 0.4 \left\{ \left[\frac{1}{5} * \frac{10}{10} \right] - \left[\frac{19}{420} * \left(\frac{10}{10} \right)^2 \right] \right\} + \\
 &\quad 0.3 \left\{ \left[\frac{1}{5} * \frac{40}{10} \right] - \left[\frac{19}{420} * \left(\frac{40}{10} \right)^2 \right] \right\} \\
 &= 0.0989
 \end{aligned}$$

Conversion = 0.901 = 90.1%

26.8. Repeat Example 26.4 if twice the stoichiometric ratio of gas to solid, still at C_{A0} , is fed to the reactor.

Information from Example 26.4	Modification
<ul style="list-style-type: none"> ➤ $A(\text{gas}) + B(\text{solid}) \rightarrow R(\text{gas}) + S(\text{solid})$ ➤ $\tau = 1\text{hr}$ (with environment of C_{A0} gas concentration) ➤ Gas and solid both in mixed flow ➤ $C_{A0} = C_{B0}$ ➤ $\bar{X}_B = 0.9$ ➤ $F_{B0} = 1\text{ ton/hr}$ ➤ Stoichiometric feed rate of A and B 	<ul style="list-style-type: none"> ➤ Twice gas to solid ➤ Stoichiometric ratio



Solution

Material balance

$$2(C_{A0} - C_A) F_{A0} = (C_{B0} - C_B) F_{B0}$$

$$2(C_{A0} - C_A) = 0.9 C_{A0}$$

$$\text{Therefore, } C_A = 0.55 C_{A0}$$

The solid will be in the environment of the gas of concentration $0.55C_{A0}$

$$\tau \propto \frac{1}{C_{A0}} \text{ from equation } \tau = \frac{\rho_B R}{b k C_{A0}}$$

$$\text{So } \tau = \frac{1}{0.55} = 1.818 \text{ h}$$

For reaction control;

$$1 - \bar{X}_B = \frac{1}{4} \frac{\tau}{\bar{t}} - \frac{1}{20} \left(\frac{\tau}{\bar{t}} \right)^2 = 0.1$$

$$\text{On solving this equation } \frac{\tau}{\bar{t}} = 0.435$$

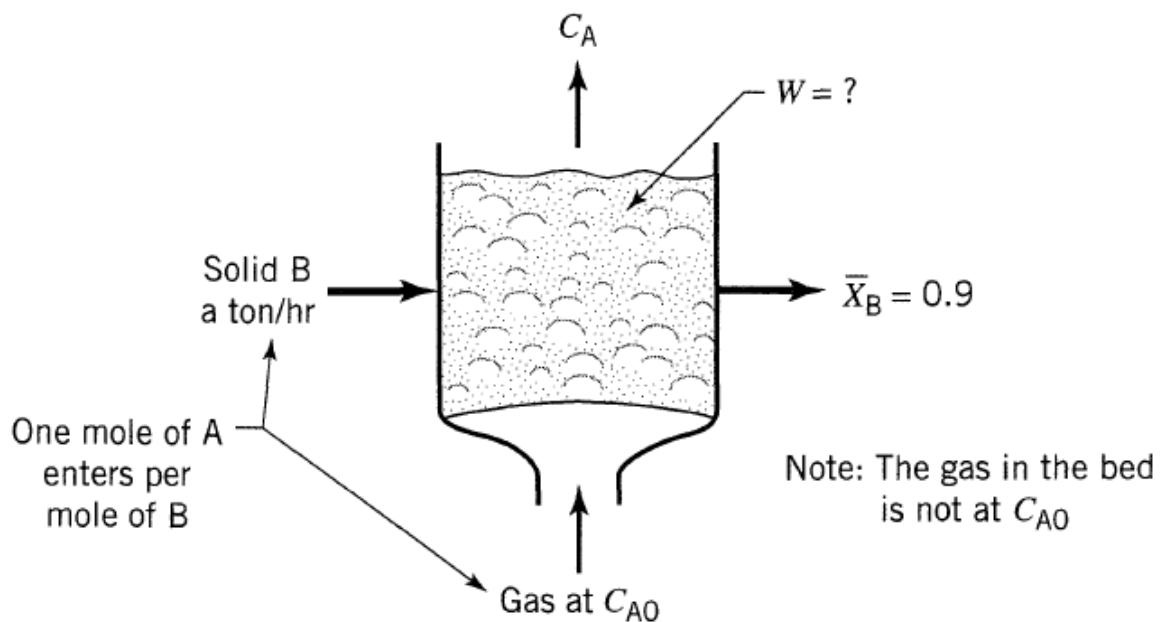
$$\bar{t} = \frac{\tau}{0.435} = \frac{1.818}{0.435} = 4.18 \text{ hr}$$

$$W = \bar{t} F_{B0} = 4.18 \text{ tons}$$

Weight of bed required is 4.18tons.

26.9. Repeat Example 26.4 if the gas is assumed to pass in plug flow through the reactor.

Information from Example 26.4	Modification
<ul style="list-style-type: none"> ➤ $A(\text{gas}) + B(\text{solid}) \rightarrow R(\text{gas}) + S(\text{solid})$ ➤ $\tau = 1\text{hr}$ (with environment of C_{A0} gas concentration) ➤ Gas and solid both in mixed flow ➤ $C_{A0} = C_{B0}$ ➤ $\bar{X}_B = 0.9$ ➤ $F_{B0} = 1 \text{ ton/hr}$ ➤ Stoichiometric feed rate of A and B 	<ul style="list-style-type: none"> ➤ Gas is in plug flow



Solution

$$C_{Af} = 0.1C_{A0}$$

Taking logarithmic mean for the gas

$$C_A = \frac{C_{A0} - C_{Af}}{\ln \frac{C_{A0}}{C_{Af}}} = \frac{C_{A0} - 0.1C_{A0}}{\ln \frac{C_{A0}}{0.1C_{A0}}} = 0.39C_{A0}$$

The solid will be in the environment of the gas of concentration $0.55C_{A0}$

$$\tau \propto \frac{1}{C_{A0}} \text{ from equation } \tau = \frac{\rho_B R}{b k} \frac{1}{C_{A0}}$$

$$\text{So } \tau = \frac{1}{0.39} = 2.564 \text{ h}$$

For reaction control;

$$1 - \bar{X}_B = \frac{1}{4} \frac{\tau}{\bar{t}} - \frac{1}{20} \left(\frac{\tau}{\bar{t}} \right)^2 = 0.1$$

$$\text{On solving this equation } \frac{\tau}{\bar{t}} = 0.435$$

$$\bar{t} = \frac{\tau}{0.435} = \frac{2.564}{0.435} = 5.89 \text{ hr}$$

$$W = \bar{t} F_{B0} = 5.89 \text{ tons}$$

Weight of bed required is 5.89 tons.

- 26.10.** Consider the following process for converting waste shredded fibers into a useful product. Fibers and fluid are fed continuously into a mixed flow reactor where they react according to the shrinking core model with the reaction step as rate controlling. Develop the performance expression for this operation as a function of the pertinent parameters and ignore elutriation.

Reaction step is rate controlling (SCM)

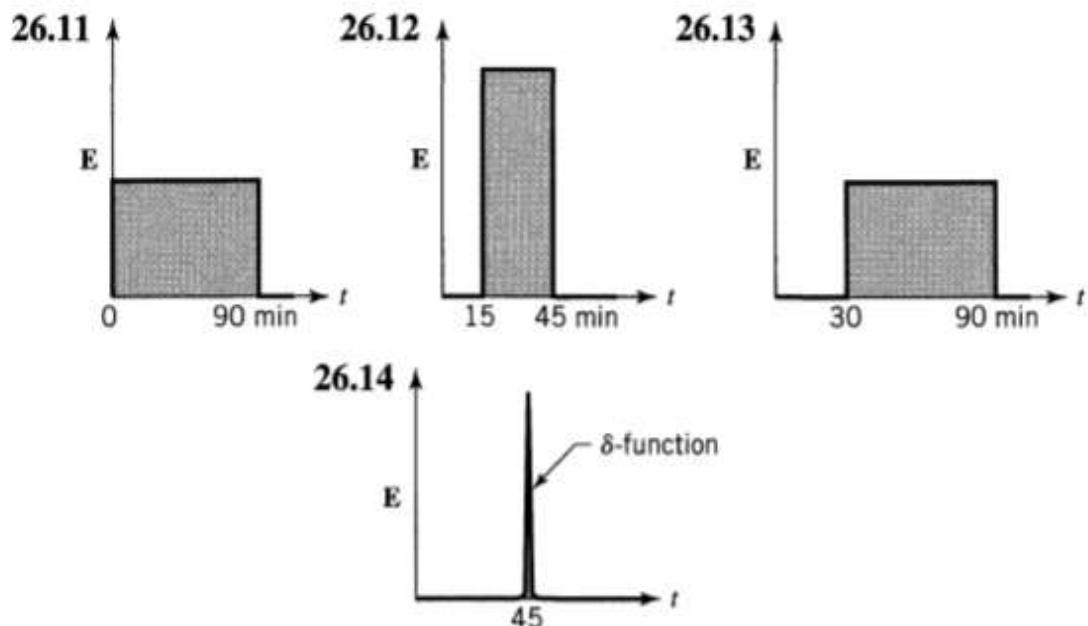
Assuming that Fibers are cylinder in shape with same particle size and the useful product is solid (unchanging particle size)

Solution

$$1-X_B = \left[1 - \frac{t}{\tau}\right]^2$$

$$\begin{aligned}
 1-\bar{X}_B &= \int_0^\tau (1-X_B) E \, dt \\
 &= \int_0^\tau \left[1 - \frac{t}{\tau}\right]^2 e^{-t/\bar{t}} \, dt \\
 &= \int_0^\tau \left[1 - \frac{2t}{\tau} + \left(\frac{t}{\tau}\right)^2\right] e^{-t/\bar{t}} \, dt \\
 &= \left[\left[1 + \left(\frac{t}{\tau}\right)^2 - \frac{2t\bar{t}}{\tau^2} - \frac{2\bar{t}^2}{\tau^2} + \frac{2t}{\tau} + \frac{\bar{t}}{\tau}\right] e^{-t/\bar{t}} \right]_0^\tau \\
 &= -e^{-T} + e^{-T} - \frac{2e^{-T}}{T} - \frac{2e^{-T}}{T^2} + 2e^{-T} + \frac{e^{-T}}{T} + 1 - \frac{1}{T} - \frac{2}{T^2} \quad [\text{where } T = \frac{\tau}{\bar{t}}] \\
 1-\bar{X}_B &= -\frac{e^{-T}}{T} + \frac{2(1-e^{-T})}{T^2} + 2e^{-T} + 1 - \frac{1}{T}
 \end{aligned}$$

Hydrogen sulfide is removed from coal gas by passing the gas through a moving bed or iron oxide particles. In the coal gas environment (consider uniform) the solids are converted from Fe_2O_3 to FeS by the SCM/reaction control, $\tau = 1 \text{ hr}$. Find the fractional conversion of oxide to iron sulfide if the RTD of solids in the reactor is approximated by the E curves of Figs. P26.11–P26.14.



Figures P26.11–P26.14

Solution

26.11	23.12
<p>For SCM/Reaction Control, $t/\tau = 1 - (1 - X_B)^{1/3}$</p> <p>so from above equation $\tau = 1 \text{ hr} (60 \text{ min})$</p> $1 - \bar{X}_B = \int_0^\tau (1 - X_B) E dt$ $1 - \bar{X}_B = \int_0^\tau (1 - t/\tau)^3 * (60/90) dt$ $= (2/3) * \int_0^1 (1 - t)^3 * dt$ $= (2/3) * (1/4)$ $= 0.167$ $\bar{X}_B = 83.3\%$	<p>For SCM/Reaction Control, $t/\tau = 1 - (1 - X_B)^{1/3}$</p> <p>so from above equation $\tau = 1 \text{ hr} (60 \text{ min})$</p> $1 - \bar{X}_B = \int_0^\tau (1 - X_B) E dt$ $1 - \bar{X}_B = \int_{0.25}^{0.75} (1 - t/\tau)^3 * (60/30) dt$ $= 2 * \int_{0.25}^{0.75} (1 - t)^3 * dt$ $= 2 * 0.078$ $= 0.156$ $\bar{X}_B = 0.8437$

26.13	26.14
<p>For SCM/Reaction Control, $t/\tau = 1 - (1 - X_B)^{1/3}$ so from above equation $\tau = 1 \text{ hr}(60\text{min})$</p> $1 - \bar{X}_B = \int_0^{\tau} (1 - X_B) E dt$ $1 - \bar{X}_B = \int_{0.5}^1 (1 - t/\tau)^3 * (60/60) * dt$ $= \int_{0.5}^1 (1 - t)^3 * dt$ $= 0.0156$ $\bar{X}_B = 0.9843$	<p>For SCM/Reaction Control, $t/\tau = 1 - (1 - X_B)^{1/3}$ so from above equation $\tau = 1 \text{ hr}(60\text{min})$</p> $1 - \bar{X}_B = \int_0^{\tau} (1 - X_B) E dt$ $1 - \bar{X}_B = \int_0^{\tau} (1 - t/\tau)^3 * 1 * dt$ $= 1 * \int_0^{0.75} (1 - t)^3 * dt$ $= 1 * 0.4687$ $= 0.4687$ $\bar{X}_B = 0.5313$

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