Chemical Reaction Engineering 1
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Lecture 19
Design for Series – Parallel Reactions

Welcome to the 9th lecture of module 4. In this module we are discussing reactor design.

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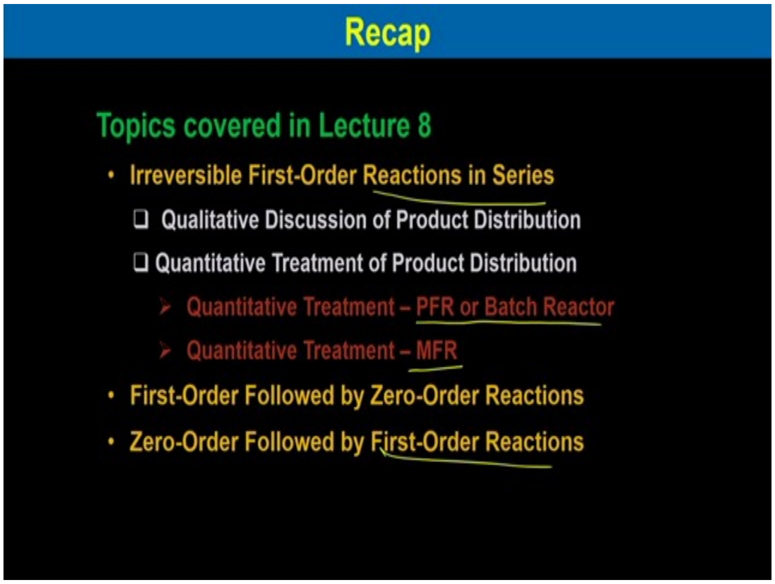

Recap

Topics covered in Lecture 8

- Irreversible First-Order Reactions in Series
  - ❑ Qualitative Discussion of Product Distribution
  - ❑ Quantitative Treatment of Product Distribution
    - ➢ Quantitative Treatment – PFR or Batch Reactor
    - ➢ Quantitative Treatment – MFR
- First-Order Followed by Zero-Order Reactions
- Zero-Order Followed by First-Order Reactions

Before going to this lecture, let us have a brief recap on our previous lecture. In the last lecture we have covered mainly irreversible first order reaction in series. And under which we have quantitatively discussed the product distribution. And then we have quantitatively obtained the productive distribution from the read equations. We have considered two different cases. One is black flow reactor or batch reactor.

And other one is the mixed flow reactor – MFR. Then we have considered different order of the series reaction, like first reaction is first order and the second reaction is zero order, and then we have considered first reaction is zero order and then followed by first order reactions. In these combinations of reactions we have seen how the product distribution changes. In this lecture we will consider design for reversible and series parallel reactions.

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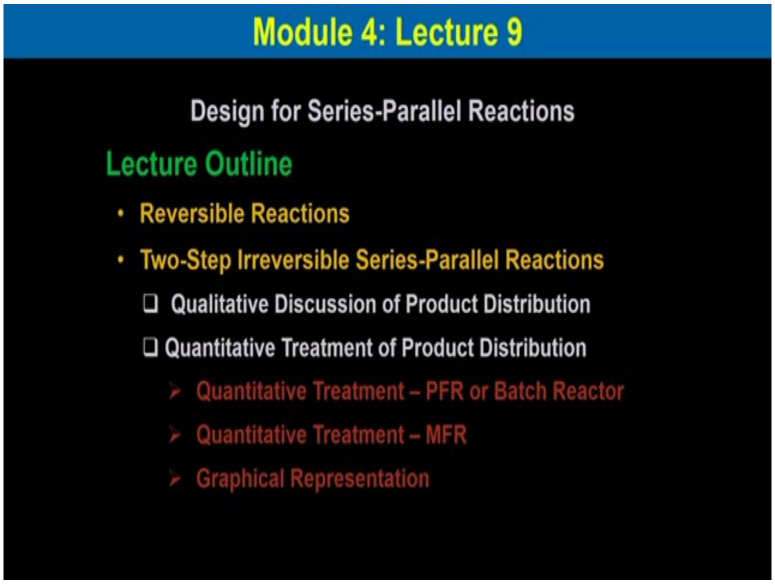

Module 4: Lecture 9

Design for Series-Parallel Reactions

Lecture Outline

- Reversible Reactions
- Two-Step Irreversible Series-Parallel Reactions
  - ☐ Qualitative Discussion of Product Distribution
  - ☐ Quantitative Treatment of Product Distribution
    - ➢ Quantitative Treatment – PFR or Batch Reactor
    - ➢ Quantitative Treatment – MFR
    - ➢ Graphical Representation

So the brief outline of this lecture is reversible reactions, two step irreversible series parallel reactions. Under which we will now discuss the product distribution, qualitative discussion on it, and then we will consider quantitative discussion or quantitative treatment of product distribution for two different cases: one is batch reactor or PFR and the second case is mixed flow reactor. And then we will see that graphical representation of this quantitative treatment.

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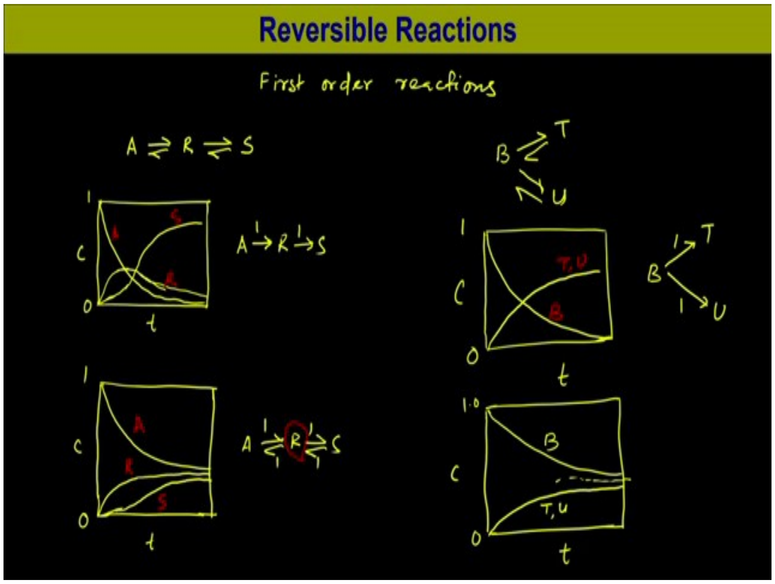

Reversible Reactions

First order reactions

Let us consider reversible reaction the reversible reactions are quite cumbersome to treat them analytically or treat them quantitatively so we will briefly discuss about the product distribution qualitatively. Let us consider first order reversible reactions of two types, one is $A \rightleftharpoons R \rightleftharpoons S$.

And in other case, say $\begin{matrix} B \rightleftharpoons T \\ B \rightleftharpoons U \end{matrix}$ So, the concentration profile in a batch or plug flow reactor we can write for this series reversible reaction.

Like we have seen if we consider typical case of $A \xrightarrow{1} R \xrightarrow{1} S$ We can write the product distribution concentration versus time. If we do we have seen that the concentration of A decreases gradually and concentration of R increases and then decreases. And concentration of S initially formation is low and then it is increases. This is the concentration and so this is concentration of A. This is concentration of R. This is concentration of S.

Now, if we consider this reaction, reversible reaction the concentration profile would be, so $A \underset{1}{\overset{1}{\rightleftharpoons}} R \underset{1}{\overset{1}{\rightleftharpoons}} S$. So concentration of A will decrease. Concentration of R will increase and concentration of S initially very low. And then it will increase. And will reach like this. So the concentration profile, this is for A, This is for R, This is for S. So we can see that in this reversible reaction when the rate constraints are of equal in that case the intermediate are it does not reach to the maximum.

So it gradually increased and remains constant after a certain time. So, it very slowly increases but it does not come down so it does not reaches the maximum. Now if we consider this reaction, we know the, for the parallel reaction how the concentration profile look like for A to R to. $B \xrightarrow{1} T \quad B \xrightarrow{1} U$ So the concentration profile would be B will decrease and R and S will be almost similar reaching like this. So, this is for B and this is for T and U.

Now, if we consider the case which is given. So the concentration of B, concentration of B would decrease. And concentration of R and S would increase and it will not cross. So this is the concentration profile for B and this is for T and U. And in both cases we have seen the intermediate does not reach to the maximum.

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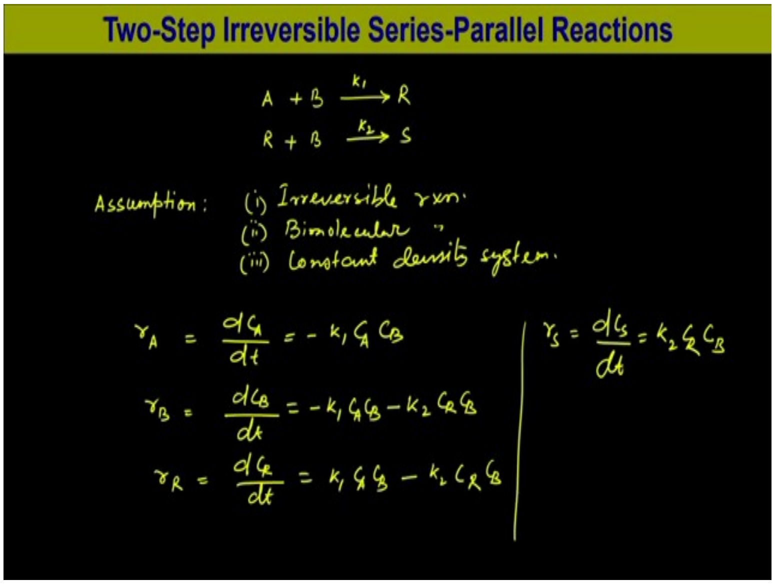

Two-Step Irreversible Series-Parallel Reactions

$A + B \xrightarrow{k_1} R$

$R + B \xrightarrow{k_2} S$

Assumption: (i) Irreversible rxn.
(ii) Bimolecular "
(iii) Constant density system.

$r_A = \frac{dC_A}{dt} = -k_1 C_A C_B$

$r_B = \frac{dC_B}{dt} = -k_1 C_A C_B - k_2 C_R C_B$

$r_R = \frac{dC_R}{dt} = k_1 C_A C_B - k_2 C_R C_B$

$r_S = \frac{dC_S}{dt} = k_2 C_R C_B$

Now, let us consider two step irreversible series parallel reactions. So, in this case if we consider the general case say $A + B \xrightarrow{k_1} R$. Then $R + B \xrightarrow{k_2} S$. So this is a set of reaction and we assume that the reaction, these two reactions are irreversible in nature and this is of biomolecule type and at constant density system. So, our assumption is irreversible reaction.

Second thing is bimolecular and third thing is constant density system. Now, if we based on this, if we write the rate equation, based on this if we write the rate equation, we can write the expression as

$$r_A = \frac{dC_A}{dt} = -k_1 C_A C_B$$

So, $C_A C_B$, for rate of reactions of B we can write

$$r_B = \frac{dC_B}{dt} = -k_1 C_A C_B - k_2 C_R C_B$$

For the rate of reactions of R we can write

$$r_R = \frac{dC_R}{dt} = k_1 C_A C_B - k_2 C_R C_B$$

Now, for S which is forming from the second reaction we can write

$$r_S = \frac{dC_S}{dt} = k_2 C_R C_B$$

So these are the four rate equations we can see from this or we can write from this to two steps irreversible series parallel reaction for constant density system.

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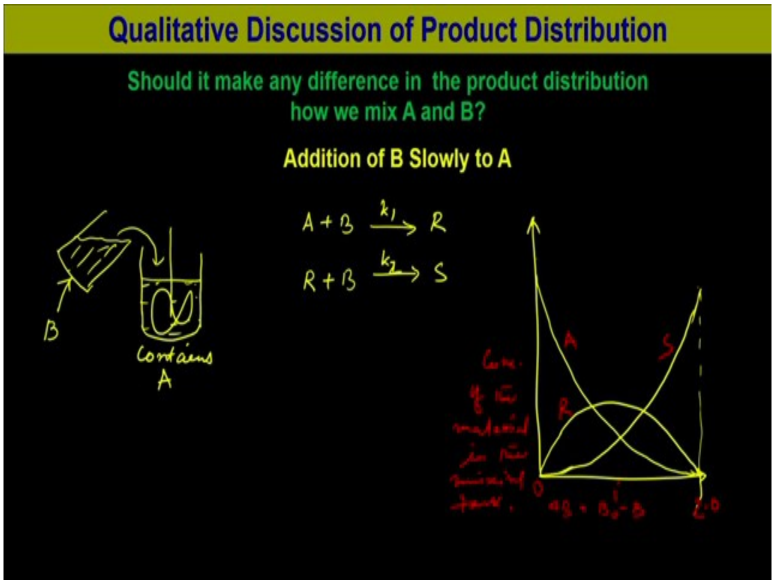

Qualitative Discussion of Product Distribution

Should it make any difference in the product distribution how we mix A and B?

Addition of B Slowly to A

Now, if we qualitatively see how the product distribution changes we could see three different cases. In the product distribution whether should it make any difference in the product distribution how we mix A and B. So, we will see whether additions in different way between A and B change the product distribution. Let us consider addition of A slowly to B and C qualitatively how it happens. Now let us take a beaker where we have B initially in the beaker. So component B is taken in a beaker. Now take another beaker we filled with A. So this contains component A. Now it is added slowly to this beaker.

So, consider the reaction or additional of A into the beaker B in such a way that a small bit of addition of A into the beaker and with continuous studying we should make sure that A, all the A each used up. So as soon as all the A each use stuff in this beaker so product R will form, so as per the reaction, $A + B \xrightarrow{k_1} R$ .So as long as a small bit of A added to this beaker this B reacts with A forms R and the reactions become complete. But as long as R is formed this small bit of R find excess B in the beaker so that $R + B \xrightarrow{k_2} S$

So, finally the product which you will obtain by the addition of A, small bit of A is product S, with no R present in the mixture. So, the concentration profile in this case would be like this. So, concentration of B, moles of A added, so initially at small bit of A is added, B will be used up and finally all the B will be used up, as soon as B will be used up further addition of A would produce would remain only A. So, this is the concentration changes of component B. This is the concentration changes of component A, which will again increase and the product which will form each S, and then since there is no all the B used up so it will remain constant.

So, this is the profile of S. Now, let us look into another way of adding A and B or mixing A and B. If we add B slowly to A, so in a beaker if we take, so this is containing B. This is containing, contains A initially and addition B is slowly done in a beaker contains A with continuous study. Now, let us see how the product distribution changes in this case. Now, as we know the reaction $A + B \xrightarrow{k_1} R$ So, as we add small bit of A or B into A, then A will react with B to go for completion of reaction forming R.

So, we will have R in the reaction, and this R will not find any B initially and hence, it will not produce S. So, as we add on slowly the B, more R will form, and then A and R both will compete to react with B by slowly additions of B into A. So R will find excess of B. And then it will produce the second reaction to produce S $R + B \xrightarrow{k_2} S$. So the product distribution in this case would be A will be used up and R will form and S initially very low. And then S will increase. So this is as we can see the delta B, this is $\Delta B = B_0 - B$.

So, moles of B consumed during the reaction is this side and this is concentration of the material in a mixture. So, this is the concentration of the material in the mixing 4. So, this is say 0 and this is say 1. And this would be 2.0. So, at $2\Delta B$ is to all the A will be used up. And this is the concentration profile for R. R will reach maximum and then it decreased to zero. This is concentration of A and this is concentration profile for S. So, that is how addition of B slowly to A will change the product distribution between, addition of B into A or A into B. So if we add them differently the product distribution changes.

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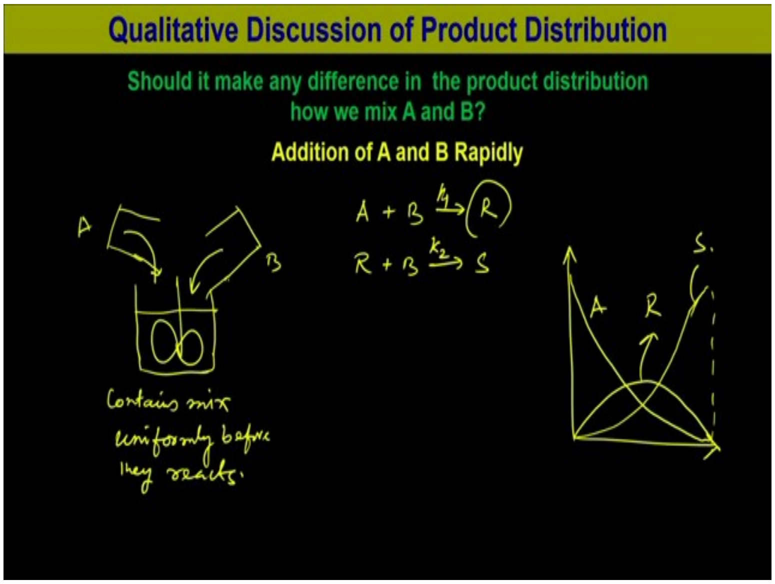

Qualitative Discussion of Product Distribution

Should it make any difference in the product distribution how we mix A and B?

Addition of A and B Rapidly

$A + B \xrightarrow{k_1} R$

$R + B \xrightarrow{k_2} S$

Contains mix uniformly before they reacts.

Now let us consider another case where we can add both A and B simultaneously. If we add both A and B simultaneously and mix them together we obtain say this is our mixing tank and we have, so we can add both A and b component into the beaker so contents mix uniformly before they react. So the reaction is $A + B \xrightarrow{k_1} R$, $R + B \xrightarrow{k_2} S$. Now, if we add A and B together what will happen initially A will react with B and produce R. So this R will initially will find very less.

This R will find B is present. So, A and B both will compete to react with R show both production of R will happen and at the same time S will produce. So it will give the similar concentration profile as we often for the second case the addition of B into A. So if we add an A and B simultaneously the product distribution would be same as that of additional B slowly into container containing A. So the product distribution for this case would be like this. So this is for A, this is for R, and this is for S. So, the product distribution is similar to the earlier case.

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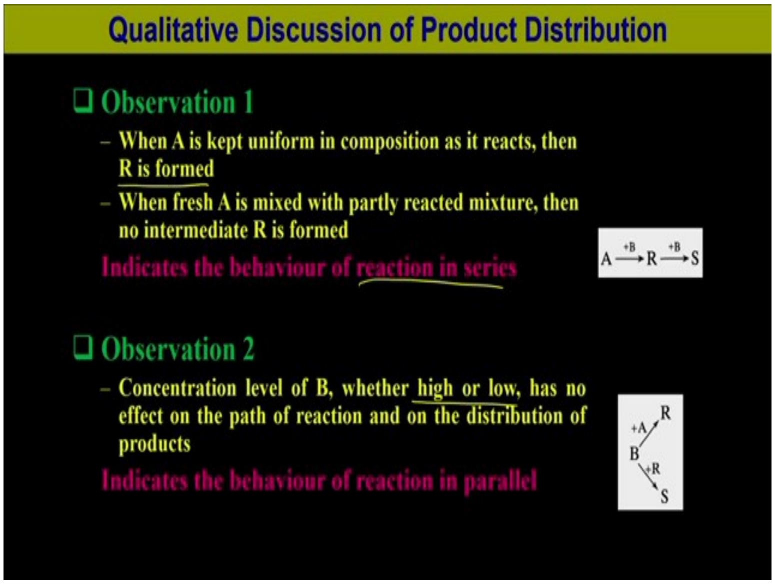

Qualitative Discussion of Product Distribution

❑ Observation 1

- When A is kept uniform in composition as it reacts, then R is formed
- When fresh A is mixed with partly reacted mixture, then no intermediate R is formed

Indicates the behaviour of reaction in series

$A\xrightarrow{+B}R\xrightarrow{+B}S$

❑ Observation 2

- Concentration level of B, whether high or low, has no effect on the path of reaction and on the distribution of products

Indicates the behaviour of reaction in parallel

$B\xrightarrow{+A}R$, $B\xrightarrow{+R}S$

Now from this qualitative discussion we have two major observations. Observation 1 – when A is kept uniform in composition as it reacts, then R is formed. So we can see R intermediate each formed. And fresh A is mixed with partly reacting mixture then no intermediate are each formed. The first case which we each which we have discussed we have taken. Fresh A is mixed partly reacted mixture then intermediate R is not formed. So this is the typical trend of B no reaction in theory. So this is the A to R to S with addition of B in each of the reaction $A\xrightarrow{+B}R\xrightarrow{+B}S$.

So that is called behavior typical behavior of the series reaction. In the second observation we can see; if we keep the concentration level of B. Whether it is high or low whatever concentration we can keep, there is no effect on the path of the reactions and on the product distribution as we have seen if we add B slowly with A and both a and b together ten the product distribution does not change. So this is the, this indicates the behavior of reaction in parallel. So it indicates $\begin{matrix}B\xrightarrow{+A}R\\ B\xrightarrow{+R}S\end{matrix}$ with the addition of A and R to different reactions path it follows and so it considered as Parallel reaction.

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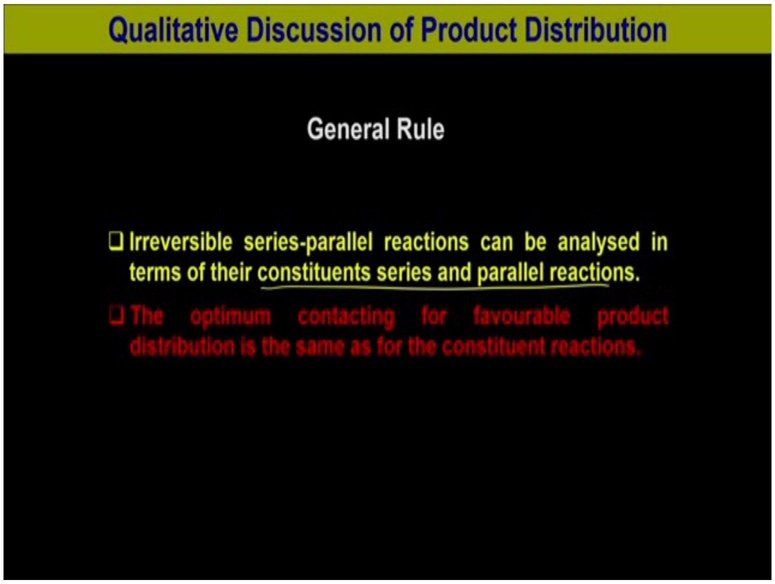

Qualitative Discussion of Product Distribution

General Rule

- ☐ Irreversible series-parallel reactions can be analysed in terms of their constituents series and parallel reactions.
- ☐ The optimum contacting for favourable product distribution is the same as for the constituent reactions.

So the general rule we can write irreversible series parallel reactions can be analyzed in terms of their constituency series parallel reaction. And the optimum contacting for favorable product distribution is the same for the constituent reactions. So, we can treat the series parallel reactions which can be analyzed in terms of their series reactions as well as parallel reactions and that our optimum contacting pattern would be similar to their individual constituent reactions.

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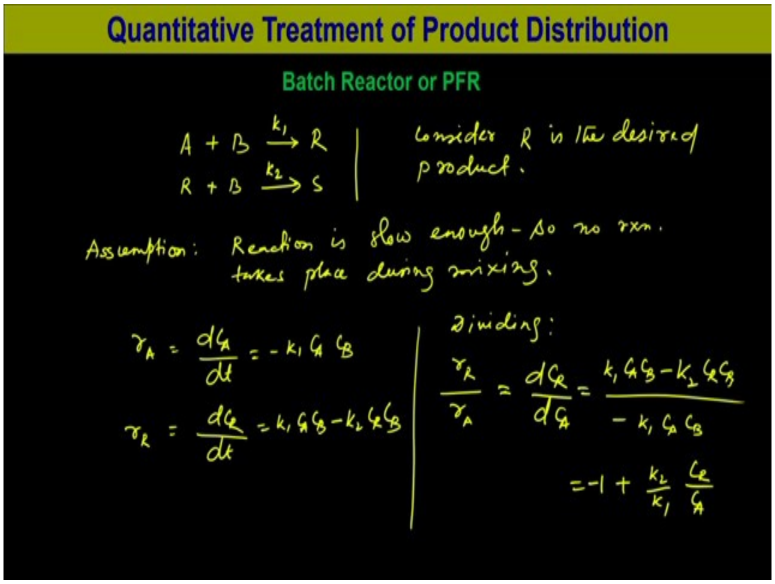

Quantitative Treatment of Product Distribution

Batch Reactor or PFR

$$A + B \xrightarrow{k_1} R$$
$$R + B \xrightarrow{k_2} S$$

Consider R is the desired product.

Assumption: Reaction is slow enough - so no rxn. takes place during mixing.

$$r_A = \frac{dC_A}{dt} = -k_1 C_A C_B$$

$$r_R = \frac{dC_R}{dt} = k_1 C_A C_B - k_2 C_R C_B$$

Dividing:

$$\frac{r_R}{r_A} = \frac{dC_R}{dC_A} = \frac{k_1 C_A C_B - k_2 C_R C_B}{-k_1 C_A C_B}$$

$$= -1 + \frac{k_2}{k_1}\frac{C_R}{C_A}$$

Now, let us quantitatively discuss the product distribution for two different cases, one is Batch reactor or PFR and second case is the mixed flow reactor. Now, let us consider the earlier reactions that is $A + B \xrightarrow{k_1} R$, $R + B \xrightarrow{k_2} S$. So, here we consider R is the desired product and assumption is that the reaction is slow enough, so no reaction takes place during mixing. Now, for this case, let us write

$r_A = \frac{dC_A}{dt} = -k_1 C_A C_B$ and $r_R = \frac{dC_R}{dt} = k_1 C_A C_B - k_2 C_R C_B$ Now, if we divide these two rates expression we obtain, $\frac{r_R}{r_A} = \frac{dC_R}{dC_A} = \frac{k_1 C_A C_B - k_2 C_R C_B}{-k_1 C_A C_B}$. So, this we can simplify would be equal to $\frac{r_R}{r_A} = \frac{dC_R}{dC_A} = -1 + \frac{k_2}{k_1}\frac{C_R}{C_A}$. So, the solution method of these is already discussed earlier.

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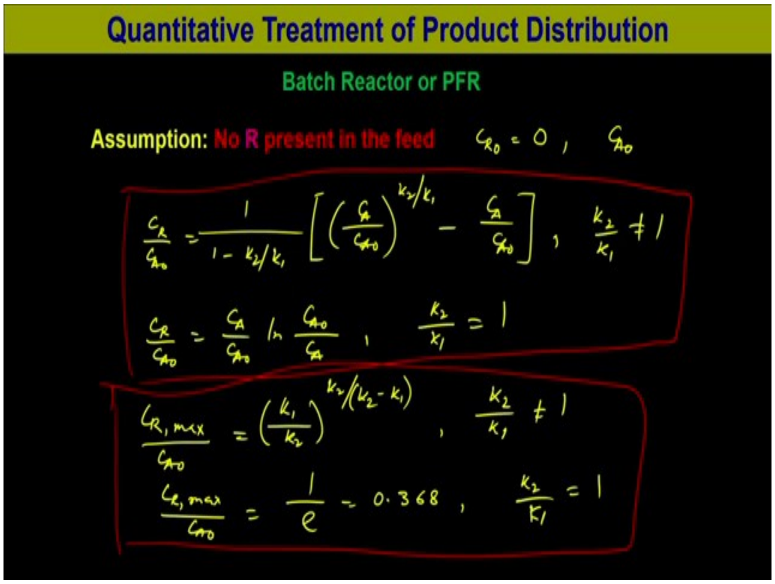

Quantitative Treatment of Product Distribution

Batch Reactor or PFR

Assumption: No R present in the feed $C_{R0} = 0$, C_{A0}

$$\frac{C_R}{C_{A0}} = \frac{1}{1 - k_2/k_1}\left[\left(\frac{C_A}{C_{A0}}\right)^{k_2/k_1} - \frac{C_A}{C_{A0}}\right], \quad \frac{k_2}{k_1} \neq 1$$

$$\frac{C_R}{C_{A0}} = \frac{C_A}{C_{A0}} \ln \frac{C_{A0}}{C_A}, \quad \frac{k_2}{k_1} = 1$$

$$\frac{C_{R,max}}{C_{A0}} = \left(\frac{k_1}{k_2}\right)^{k_2/(k_2-k_1)}, \quad \frac{k_2}{k_1} \neq 1$$

$$\frac{C_{R,max}}{C_{A0}} = \frac{1}{e} \approx 0.368, \quad \frac{k_2}{k_1} = 1$$

Now, if we assume no R present in the feed, that means $C_{R0} = 0$ initially. And CA initially present is C_{A0}, so we can integrate and get the solutions of the differential equations, which is

$\frac{C_R}{C_{A0}} = \frac{1}{1 - \frac{k_2}{k_1}}\left[\left(\frac{C_A}{C_{A0}}\right)^{\frac{k_2}{k_1}} - \frac{C_A}{C_{A0}}\right]$. This is valid for $\frac{k_2}{k_1} \neq 1$.

So, for $\frac{k_2}{k_1} = 1$, we can write $\frac{C_R}{C_{A0}} = \frac{C_A}{C_{A0}} \ln \frac{C_{A0}}{C_A}$ and this is for $\frac{k_2}{k_1} = 1$. So these are the operation profile of R our relations between C_R and C_A. Now the maximum concentrations we know how to obtain which we have discussed earlier just differentiate and set it to zero.

So, you will obtain, $\frac{C_{R\max}}{C_{A0}} = \left(\frac{k_1}{k_2}\right)^{\left(\frac{k_2}{k_2 - k_1}\right)}$ this is for $\frac{k_2}{k_1} \neq 1$, and $\frac{C_{R\max}}{C_{A0}} = \frac{1}{e} = 0.368$ that is for $\frac{k_2}{k_1} = 1$. So, this is how we can obtain the relation between C_R and C_A. At the same time we can calculate the maximum concentration of intermediate which is obtained. So from this we can calculate the optimum concentration or maximum concentration of C_R can be often at different ratio of $\frac{k_2}{k_1}$.

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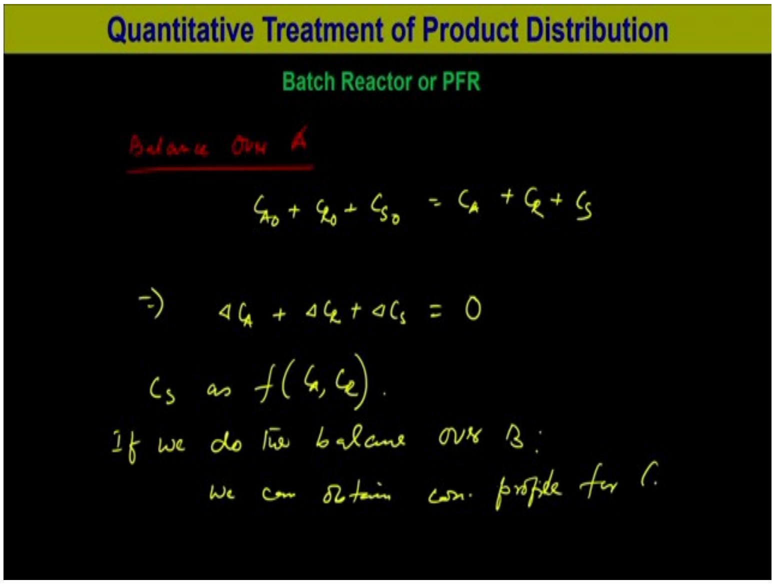

Quantitative Treatment of Product Distribution

Batch Reactor or PFR

Balance over A

$$C_{A0} + C_{R0} + C_{S0} = C_A + C_R + C_S$$

$$\Rightarrow \quad \Delta C_A + \Delta C_R + \Delta C_S = 0$$

C_S as $f(C_A, C_R)$.

If we do the balance over B:
we can obtain con. profile for C.

The concentration for other species for plug or batch reactor we can obtain form the component balance, so if we do the component balance over A, we can get $C_{A0} + C_{R0} + C_{S0} = C_A + C_R + C_S$. From here we can write $\Delta C_A + \Delta C_R + \Delta C_S = 0$. So, from here we can put the relations between R and A, C_A, C_R and C_A, and we can obtain the C_S as $f(C_{A,} C_R)$. Now, if we do the balance over B, we can obtain concentration profile for C.

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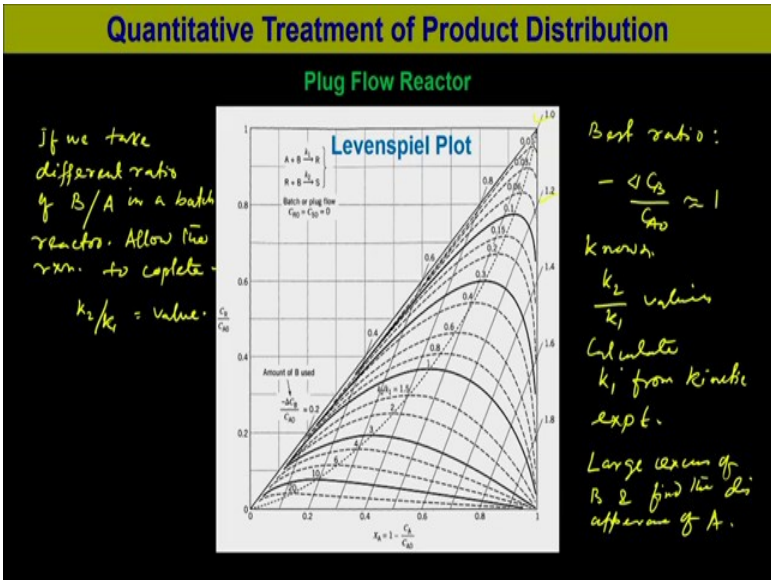

Quantitative Treatment of Product Distribution

Plug Flow Reactor

If we take different ratio of B/A in a batch reactor. Allow the rxn. to complete.

k_2/k_1 = value.

Best ratio:

$-\frac{\Delta C_B}{C_{A0}} \approx 1$

known.

$\frac{k_2}{k_1}$ values

Calculate k_1 from kinetic expt.

Large excess of B & find the disappearance of A.

Now, let us see the Levenspiel plot for different $\frac{k_2}{k_1}$ values and different $\frac{C_B}{C_A}$ ratio, how the product distribution changes or how the product distribution can be calculated from the Levenspiel plot for series parallel reaction in a batch or plug flow reactor. So, in this case you can see this plot source at different $\frac{k_2}{k_1}$ values, how the changing with the concentrate, no mole fraction or conversion of A changes the product distribution.

So the y axis is $\frac{C_R}{C_{A0}}$ which is shown over here. And these lines, these at source the $\frac{\Delta C_B}{C_{A0}}$. So at $\frac{\Delta C_B}{C_{A0}}$ values these are plotted. So, to obtain this plot this is plotted based on the equations we have derived, so kinetically we can calculate for a particular reaction $\frac{k_2}{k_1}$ values we can calculate.

So this is can be done from the experiments. So, if we take different ratio of $\frac{B}{A}$ in a batch reactor, and allow the reaction to complete, so then we can obtain for each run (44:09) we can obtain $\frac{k_2}{k_1}$ values.

The best ratio delta $\frac{\Delta C_B}{C_{A0}}$ would be when it is 1. So you can see, that means $-\frac{\Delta C_B}{C_{A0}} \approx 1$ If we look into this curve over here, you can see that $\frac{k_2}{k_1}$ values they are far apart from each other. So this would be the best ratio to be considered for the reaction.

So, with a known $\frac{k_2}{k_1}$ values what we need to calculate k_1 from kinetic experiments. How, we can do from the kinetic experiments k_1, how we can obtain? If we take large excess of B and then follow the disappearance of A. Take large access of B and find the disappearance of A. So, this will behave like a first order reaction, so we can obtain k_1 values. So, that means it is pseudo fast order reaction, so we can calculate k_1 and with that we can calculate k_2 as well.

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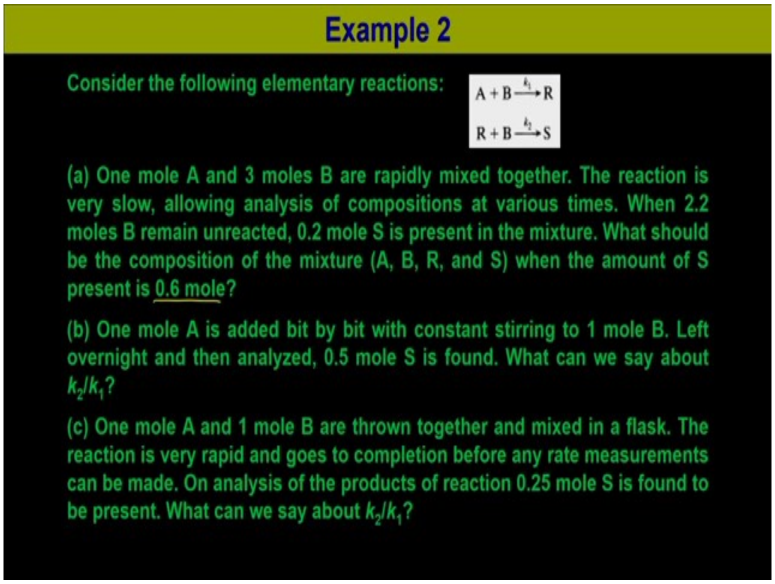

Example 2

Consider the following elementary reactions: $A + B \xrightarrow{k_1} R$, $R + B \xrightarrow{k_2} S$

(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?

Let us take an example consider the following elementary reactions. That is $A + B \xrightarrow{k_1} R$ and $R + B \xrightarrow{k_2} S$ with the example which we have consider. 1 mole of A and 3 moles of B are rapidly mixed together the reaction is very slow allowing analysis of the composition at various times. When 2.2 moles of B remain unreacted 0.2 moles of S is present in the mixture. What should be the composition of the mixture at A, B, R and S when the amount of S present is 0.6 moles.

The second problem is that one mole of A is added bit by bit with constant stirring to one mole of B. Left over night and then analyzed 0.5 moles of S is found, what we can see about the $\frac{k_2}{k_1}$ values. And the third problem is that one mole of A, and one mole of B are thrown together and mixed in a flux, 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 of S is found to be present. What can we say about $\frac{k_2}{k_1}$?

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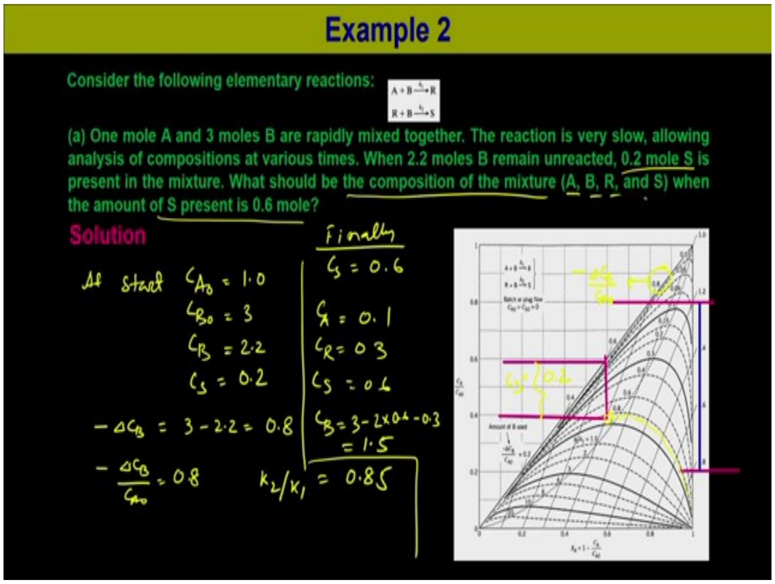

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Solution

At start $C_{A0} = 1.0$

$C_{B0} = 3$

$C_B = 2.2$

$C_S = 0.2$

$-\Delta C_B = 3 - 2.2 = 0.8$

$-\frac{\Delta C_B}{C_{A0}} = 0.8$

Finally

$C_S = 0.6$

$C_A = 0.1$

$C_R = 0.3$

$C_S = 0.6$

$C_B = 3 - 2\times0.6 - 0.3$
$= 1.5$

$k_2/k_1 = 0.85$

So, in this case, at the start of the reaction for the first case, so at start $C_{A0} = 1.0$ $C_{B0} = 3$ and B you can write C_{A0}, C_{B0} and C_B is 2.2 and C_S is 0.2. Now, we can do from the material balance, we can calculate $-\Delta C_B = 3 - 2.2$ which is 0.8. Now, if we consider this figure we have to find out this point.

So, this is the line for 0.8 ΔC_B by, so here we can write $-\frac{\Delta C_B}{C_{A0}} = 0.8$ so we can locate this. This is the curve. So, this is for $-\frac{\Delta C_B}{C_{A0}} = 0.8$. Now, we have to C_S is given 0.2. So, following this line we can locate 0.2 which is this one. This is the distance of delta S. This is C_S which is equal to 0.2.

So with this we can obtain this point which is no $\frac{k_2}{k_1}$ which is equal to 0.85.

So once we obtain $\frac{k_2}{k_1}$, 0.85 over here, now we can follow this curve. This will be over here. So, then we can take this is 0.6, $S = 0.6$ at this value. So, since finally C_S is, $C_S = 0.6$ finally. So, with this 0.6 we can locate at this point. We can calculate A. C_A Would be 0.1, C_R would be 0.3 and C_S

is given 0.6 and B, $C_B = 3 - 2 \times 0.6 - 0.3 = 1.5$. So, we can obtain the No composition of the mixture that is A, B, R and S.

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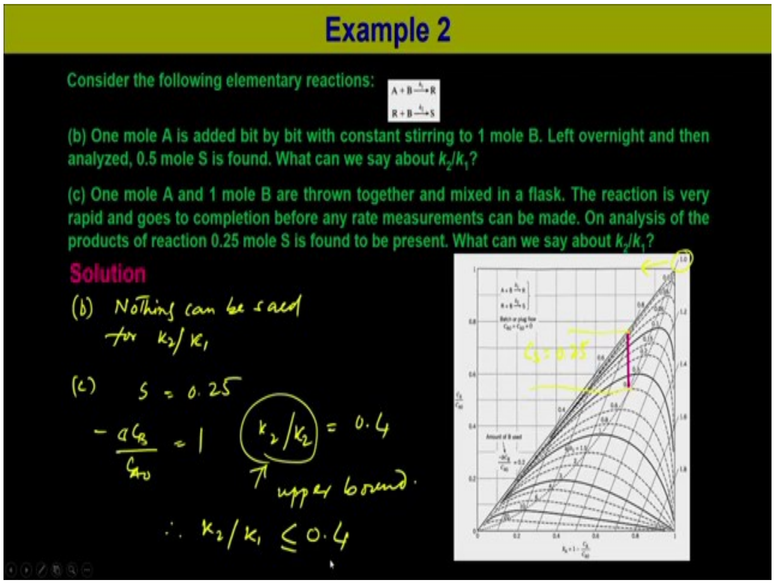

Example 2

Consider the following elementary reactions: $A + B \xrightarrow{k_1} R$, $R + B \xrightarrow{k_2} S$

(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

(b) Nothing can be said for k_2/k_1

(c) $S = 0.25$

$-\frac{\Delta C_B}{C_{A0}} = 1$ $\boxed{k_2/k_2} = 0.4$ ↑ upper bound.

$\therefore k_2/k_1 \leq 0.4$

Now for the second case one mole of A is added bit by bit with constant stirring to one mole of B left overnight and then analyzed and obtained 0.5 mole of S is found. And what can we say about $\frac{k_2}{k_1}$. From this we cannot say. So solution of B we cannot obtain any values of or we cannot say anything. Nothing can be said for $\frac{k_2}{k_1}$. Now if you consider C which is one mole of A. And one mole B are thrown together and mix in a flask, the reaction is very rapid and goes to completion before any rate measurements meet.

So we have, it is given so 0.25 of S. So, this is 0.25 which is over here, we can calculate. So, this is $S = 0.25$ and with $-\frac{\Delta C_B}{C_{A0}} = 1$ because one mole is added to one mole of B. So, since, this is 1 we will follow this line. This is value of $C_S = 0.6$ And we can obtain $\frac{k_2}{k_1} = 0.4$. Since, the reaction is very rapid and R actually formed place, then what could be formed. So, this $\frac{k_2}{k_1}$ is the upper bound. So, we can say, therefore, $\frac{k_2}{k_1} \leq 0.4$.

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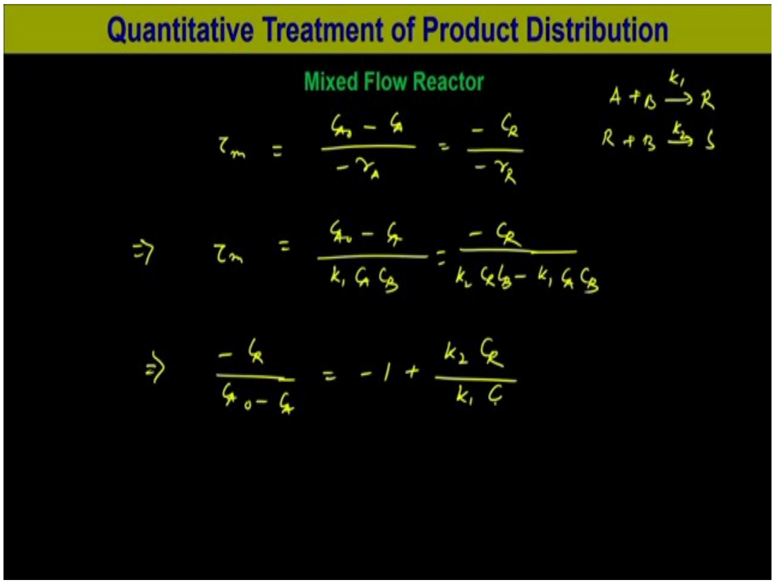

Quantitative Treatment of Product Distribution

Mixed Flow Reactor

$$A + B \xrightarrow{k_1} R$$

$$R + B \xrightarrow{k_2} S$$

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

$$\Rightarrow \tau_m = \frac{C_{A0} - C_A}{k_1 C_A C_B} = \frac{-C_R}{k_2 C_R C_B - k_1 C_A C_B}$$

$$\Rightarrow \frac{-C_R}{C_{A0} - C_A} = -1 + \frac{k_2 C_R}{k_1 C_A}$$

Now, if we consider mixed flow reactor we can write the design equation as we have done before,

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

From here we can write

$$\tau_m = \frac{C_{A0} - C_A}{k_1 C_A C_B} = \frac{-C_R}{k_2 C_R C_B - k_1 C_A C_B}$$

Now, if we rearrange, from here we can write from this, we can write

$$\frac{-C_R}{C_{A0} - C_A} = -1 + \frac{k_2}{k_1}\frac{C_R}{C_A}$$

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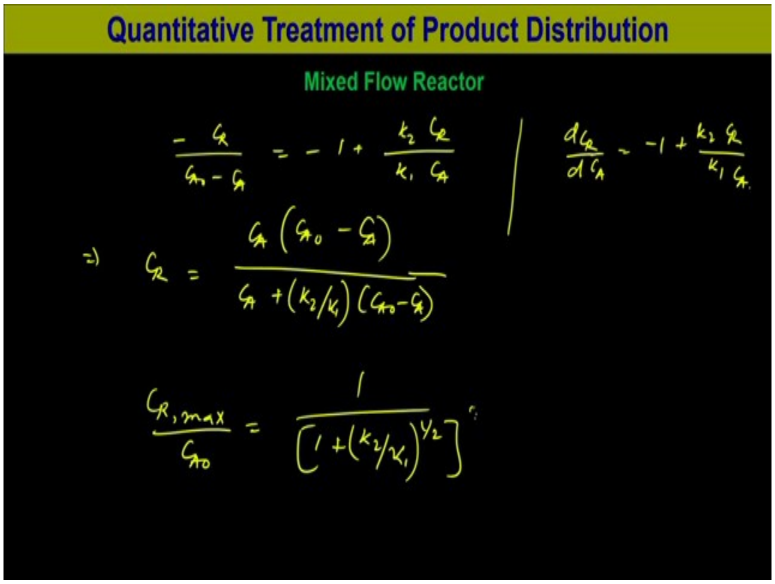

Quantitative Treatment of Product Distribution

Mixed Flow Reactor

$$\frac{-C_R}{C_{A0}-C_A} = -1 + \frac{k_2 C_R}{k_1 C_A} \qquad \frac{dC_R}{dC_A} = -1 + \frac{k_2 C_R}{k_1 C_A}$$

$$\Rightarrow C_R = \frac{C_A(C_{A0}-C_A)}{C_A + (k_2/k_1)(C_{A0}-C_A)}$$

$$\frac{C_{R,max}}{C_{A0}} = \frac{1}{\left[1+(k_2/k_1)^{1/2}\right]}$$

So $\frac{-C_R}{C_{A0}-C_A} = -1 + \frac{k_2}{k_1}\frac{C_R}{C_A}$

So this is nothing but the difference forms of the differential equation which we have obtained earlier that is

$$\frac{dC_R}{dC_A} = -1 + \frac{k_2}{k_1}\frac{C_R}{C_A}$$

we can write

$$C_R = \frac{C_A(C_{A0}-C_A)}{C_A + \left(\frac{k_2}{k_1}\right)(C_{A0}-C_A)}$$

And we can find out maximum by the earlier procedure, so we can write

$$\frac{C_{R\max}}{C_{A0}} = \frac{1}{\left[1+\left(\frac{k_2}{k_1}\right)^{1/2}\right]}$$

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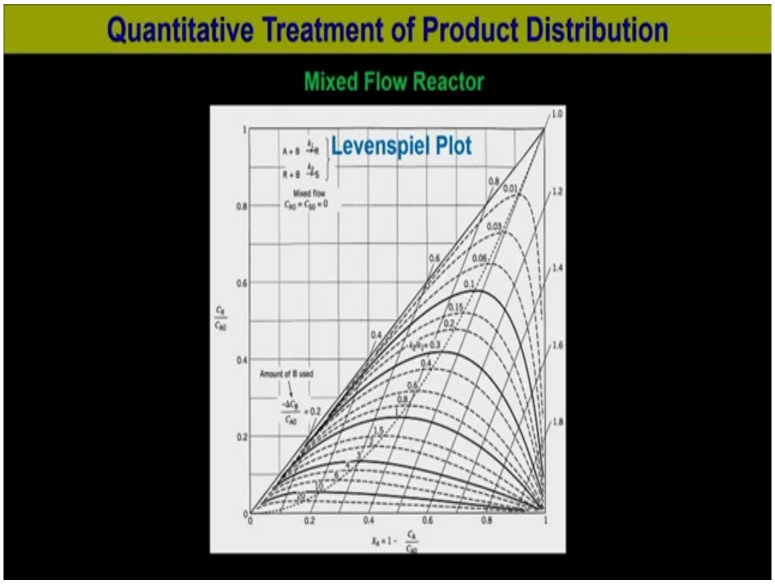

Quantitative Treatment of Product Distribution

Mixed Flow Reactor

So, graphically we can see the Levenspeil plot for the mixed flow reactor. So, it is similar to the earlier plot as we have done for the plug flow reactor, the Levenspeil plot of our various $\frac{k_2}{k_1}$ values and $\frac{\Delta C_B}{C_{A0}}$. We can see the Levenspeil plot for the distribution of the products. So, thank you very much for attending this lecture and we will continue our discussion in the next lecture.