Chemical Reaction Engineering I
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Lecture 17

Welcome to the seventh lecture of module 4, in this module we are discussing reactor design. Before going to this lecture let us have brief recap on our previous lecture.

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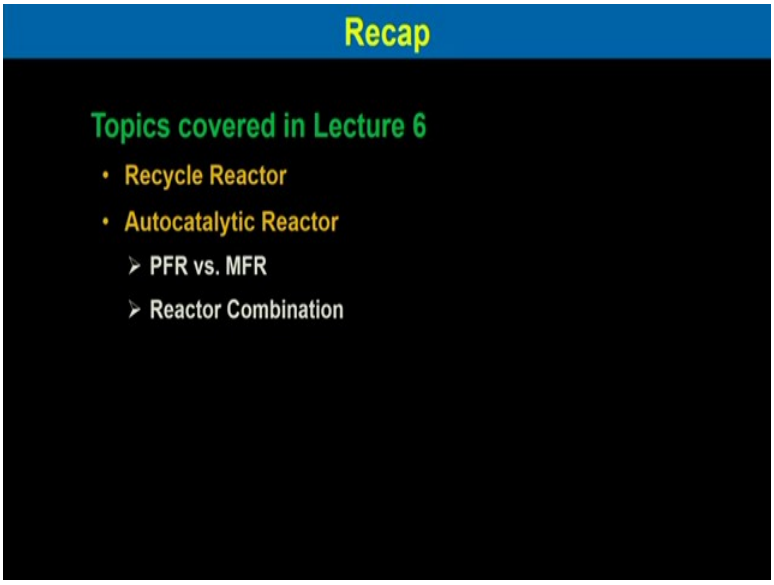

Recap

Topics covered in Lecture 6

- Recycle Reactor
- Autocatalytic Reactor
  - PFR vs. MFR
  - Reactor Combination

In our last lecture we have covered recycle reactor, then we have consider autocatalytic reactor and we have seen, compared between PFR and MFR plug flow reactor and mixed flow reactor and we have seen the reactor combination. And we have noticed that recycle reactor is an good opportunity to change from plug flow reactor to the mixed flow reactor and in case of autocatalytic reactor it gives us impression on the optimization problems, where we have rate concentration curve goes either through maxima or minima.

So, in that case the performance of the plug flow reactor and mixed flow reactor we have compared and if we have reactor combination how to use them.

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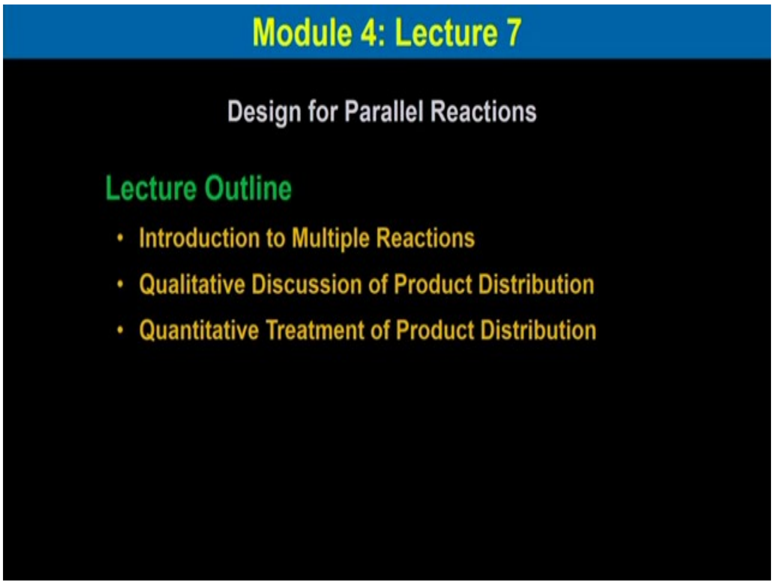

Module 4: Lecture 7

Design for Parallel Reactions

Lecture Outline

- Introduction to Multiple Reactions
- Qualitative Discussion of Product Distribution
- Quantitative Treatment of Product Distribution

Now, we will consider design for parallel reactions, in earlier lectures we have consider single reaction, in that case the product distribution is fixed, so there is no product distribution and we have consider their sizes of the reactor required for a particular job. Now for parallel reactions we will consider the mostly introduction to multiple reaction, qualitative discussing of product distribution, quantitative treatment of the product distribution.

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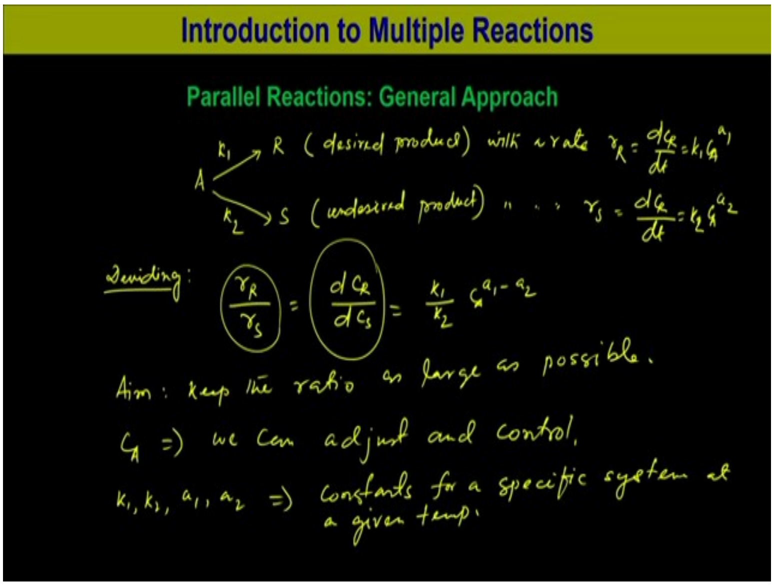

Introduction to Multiple Reactions

Parallel Reactions: General Approach

$$A \xrightarrow{k_1} R \text{ (desired product) with a rate } r_R = \frac{dC_R}{dt} = k_1 C_A^{a_1}$$

$$A \xrightarrow{k_2} S \text{ (undesired product) " " " } r_S = \frac{dC_S}{dt} = k_2 C_A^{a_2}$$

Deviding: $\boxed{\frac{r_R}{r_S}} = \boxed{\frac{dC_R}{dC_S}} = \frac{k_1}{k_2} C_A^{a_1 - a_2}$

Aim: keep the ratio as large as possible.

$C_A \Rightarrow$ we can adjust and control.

$k_1, k_2, a_1, a_2 \Rightarrow$ constants for a specific system at a given temp.

So, let us start with parallel reactions the general approach, say if we consider decomposition of a reactant A it goes either any of the path like

$$A \xrightarrow{k_1} R \text{ (desired product) with } r_R = \frac{dC_R}{dt} = k_1 C_A^{a_1}$$

$$A \xrightarrow{k_2} S \text{ (undesired product) with } r_S = \frac{dC_S}{dt} = k_2 C_A^{a_2}$$

Now if we divide this two relation, so dividing we can obtain

$$\frac{r_R}{r_S} = \frac{dC_R}{dC_S} = \frac{k_1}{k_2} C_A^{a_1 - a_2}$$

Here our aim is to keep this ratio or $\frac{dC_R}{dC_S}$ ratio as large as possible, so as we can see while dividing this two rate equations we have eliminated the time variable and in this to optimize or to increase the ratio we have only one control variables that is C_A.

So, C_A which we can adjust and control the other term k_1, k_2, a_1 and a_2 they are constant for a specific system at a given temperature, so k_1, k_2, a_1, a_2 this are constants for a specific system at a given temperature.

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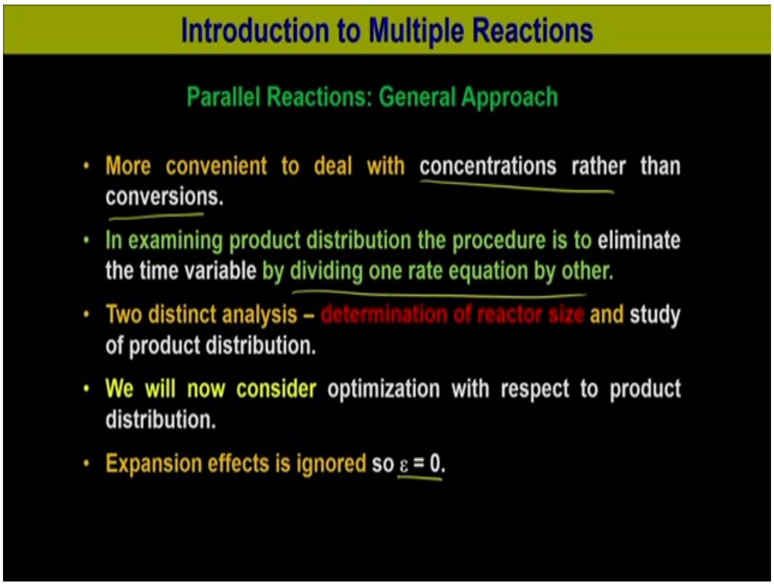

Introduction to Multiple Reactions

Parallel Reactions: General Approach

- More convenient to deal with concentrations rather than conversions.
- In examining product distribution the procedure is to eliminate the time variable by dividing one rate equation by other.
- Two distinct analysis – determination of reactor size and study of product distribution.
- We will now consider optimization with respect to product distribution.
- Expansion effects is ignored so $\varepsilon = 0$.

Now, how we can control this C_A, so for parallel reactions the general approach should be it is more convenient to deal with concentration rather than conversion and secondly in examining the product distribution the procedure is to eliminate the time variables by dividing one of the rate equation by the other, so since this parallel reaction from a particular reactants and forming going through two different path if we divide the rate equation then we can examine the product distribution.

Two distinct analyses can be done determination of the reactors size and study of the product distribution, as we have consider for single reactions the determination of the reactors size here we will consider now the optimization with respect to the product distribution and we will consider expansion effect is ignored so $\varepsilon = 0$.

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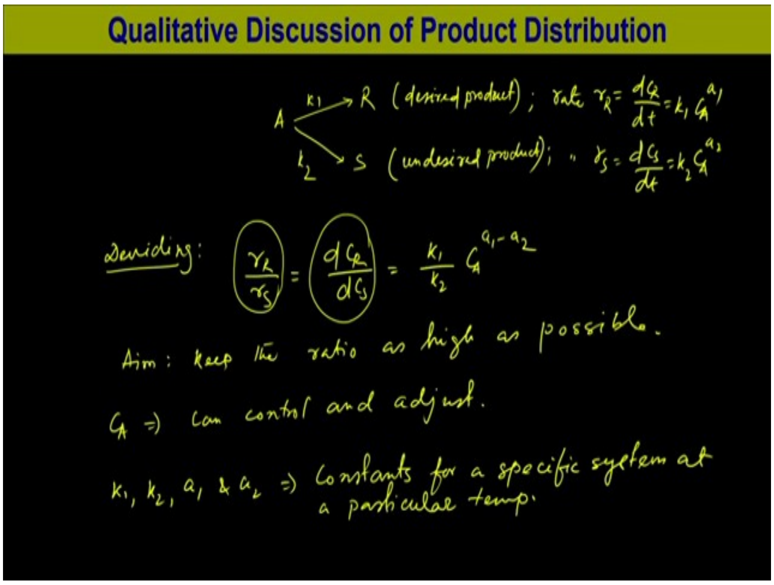

Qualitative Discussion of Product Distribution

$A \xrightarrow{k_1} R$ (desired product); rate $r_R = \frac{dC_R}{dt} = k_1 C_A^{a_1}$

$A \xrightarrow{k_2} S$ (undesired product); " $r_S = \frac{dC_S}{dt} = k_2 C_A^{a_2}$

Dividing: $\boxed{\frac{r_R}{r_S}} = \boxed{\frac{dC_R}{dC_S}} = \frac{k_1}{k_2} C_A^{a_1 - a_2}$

Aim: keep the ratio as high as possible.

$C_A \Rightarrow$ can control and adjust.

k_1, k_2, a_1 & $a_2 \Rightarrow$ Constants for a specific system at a particular temp.

Now, let us qualitative discuss how we can look into the product distribution for a parallel reaction, consider decomposition of component A by either of the two parts that is

$$A \xrightarrow{k_1} R \text{ (desired product) with } r_R = \frac{dC_R}{dt} = k_1 C_A^{a_1}$$

$$A \xrightarrow{k_2} S \text{ (undesired product) with } r_S = \frac{dC_S}{dt} = k_2 C_A^{a_2}$$

Now, if we divide this two rate equation we can obtain

Now our aim is to keep this ratio $\frac{dC_R}{dC_S}$ or their rate ratio of their rate as high as possible.

Now, how we can do that, we have only one control variable that is C_A, C_A we can control and adjust the other parameters here in this relation k_1, k_2, a_1 and a_2 they are constant for a specific system at a particular temperature. So, k_1, k_2, a_1 and a_2 are constants for a specific system at a particular temperature.

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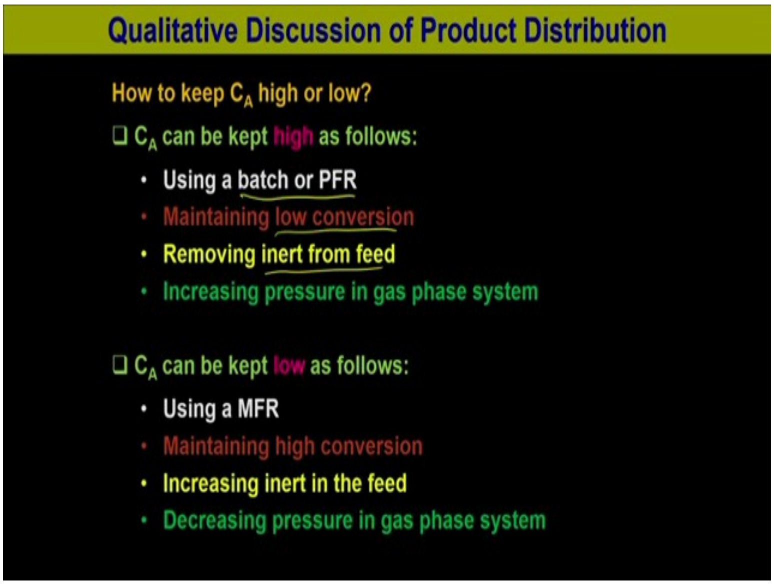

Qualitative Discussion of Product Distribution

How to keep C_A high or low?

❑ C_A can be kept high as follows:

- Using a batch or PFR
- Maintaining low conversion
- Removing inert from feed
- Increasing pressure in gas phase system

❑ C_A can be kept low as follows:

- Using a MFR
- Maintaining high conversion
- Increasing inert in the feed
- Decreasing pressure in gas phase system

Now, how we can control this concentration C_A, C_A can be kept high by the following ways if we use a batch reactors or PFR where we can keep C_A as high as possible, we can also do maintaining low conversion or we can remove the inert from the feed or we can also increase the pressure in a gas phase reaction, so if we have this are the four means by which we can keep our know concentration high one is by batch or plug flow reactor or we can go up to a low concentration know conversion.

Then we can remove the inert if present in the feed that we will also keep the concentration high or if it is gas phase reactions we can pressurize to high pressure so that the concentration becomes higher. We can keep concentration low by either of the following ways one is instead of batch and PFR we can use mixed flow reactor then we can maintain high conversion we can increase the inert in the feed or we can decrease the pressure in the gas phase systems, so this way we can control the concentration C_A of a particular system.

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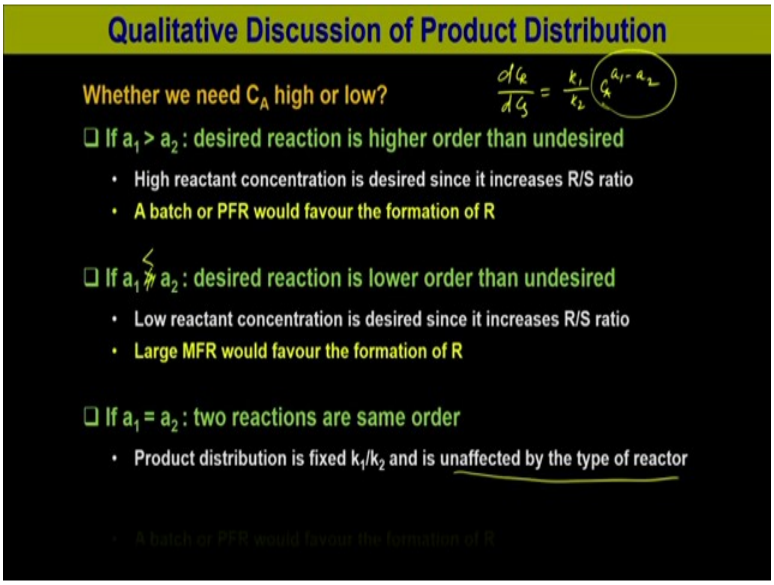

Qualitative Discussion of Product Distribution

Whether we need C_A high or low? $\frac{dC_R}{dC_S} = \frac{k_1}{k_2} C_A^{a_1 - a_2}$

❑ If $a_1 > a_2$: desired reaction is higher order than undesired

- High reactant concentration is desired since it increases R/S ratio
- A batch or PFR would favour the formation of R

❑ If $a_1 \overset{<}{\cancel{>}} a_2$: desired reaction is lower order than undesired

- Low reactant concentration is desired since it increases R/S ratio
- Large MFR would favour the formation of R

❑ If $a_1 = a_2$: two reactions are same order

- Product distribution is fixed k_1/k_2 and is unaffected by the type of reactor
- A batch or PFR would favour the formation of R

Now, whether we need C_A high or low for a particular reactions how we will judge,

If a_1 is greater than a_2, So basically if we consider our relation say

$$\frac{dC_R}{dC_S} = \frac{k_1}{k_2} C_A^{a_1 - a_2}$$

Now if a_1 is greater than a_2 the desired reaction is of higher order than the undesired one, so high reactants concentration is desired since it increases R by S ratio, so if we wanted to increase the ratio high reactant concentration from this relation we can see would help to keep the ratio higher, a batch or PFR would favor the formation of R.

Now, if a_1 is less than a_2 the desired reaction is of lower order than the undesired one so in that case low reactants concentration is desired since it increases the R by S ratio, so depending on the order of the reaction we can decide whether we need high or low concentration.

So, in that case we can use know if a_1 is less than a_2 large mixed flow reactor would favor the formation of R, now if a_1 and a_2 both are same if we look into this relation a_1 and a_2 same so dCR by dCS will be the ratio of $\frac{k_1}{k_2}$, so two reactions are of the same order and product distribution is fixed with $\frac{k_1}{k_2}$ and is unaffected by the type of the reactor because both the reaction of the parallel reactions are of the same order.

So a batch or PFR would favor the formation of R, so if it is same order although the reactor type are unaffected for this we should use the so if product distribution is fixed k_1 no, if a_1 and a_2 the order of the reactions are of the same order then we can see from here the ratio between the product CR and CS the desired product with respect to the undesired product is fixed by the term $\frac{k_1}{k_2}$ and is unaffected by the type of reactor, since the reactor type is by is unaffected we can use any type of reactor.

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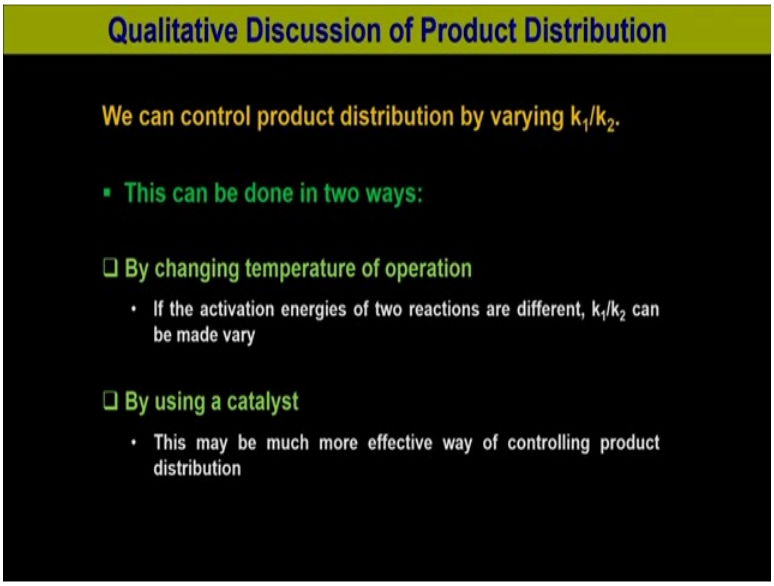

Qualitative Discussion of Product Distribution

We can control product distribution by varying k_1/k_2.

- This can be done in two ways:

☐ By changing temperature of operation

- If the activation energies of two reactions are different, k_1/k_2 can be made vary

☐ By using a catalyst

- This may be much more effective way of controlling product distribution

Now, how we can control the product distribution by varying $\frac{k_1}{k_2}$, so for equal order of the reaction the product distribution is fixed by $\frac{k_1}{k_2}$ so how can we control k_1 and k_2 this can be done in two ways one is by changing the temperature of operation so if temperature is fixed we can change the temperature of operation and if the activation energies of the two reactions are different k_1 and k_2 can be made vary but if the activation energy for both the reaction are same we cannot change $\frac{k_1}{k_2}$ by varying the temperature.

Now, another way is to change $\frac{k_1}{k_2}$ by using a catalyst, this may be much more effective way of controlling product distribution, so if we use the catalyst the rate constant values will know change significantly, so by this way we can know control the product distribution by varying k_1 and k_2.

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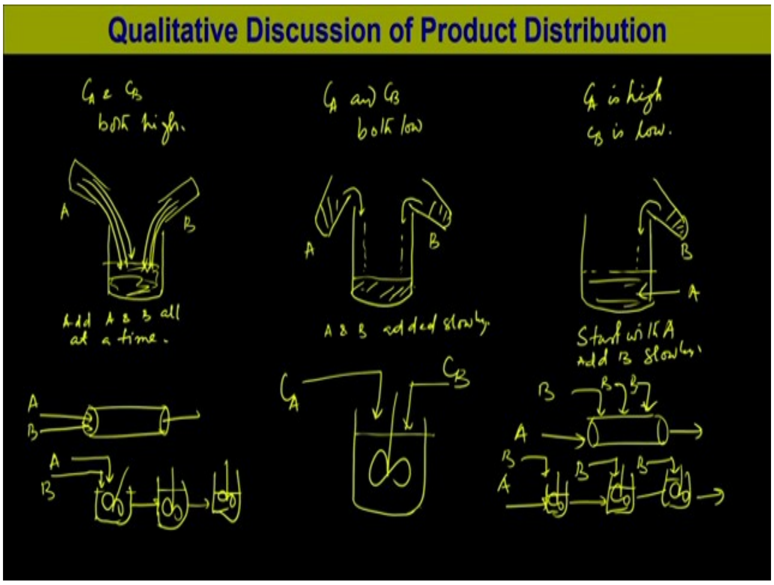

Qualitative Discussion of Product Distribution

Now, let us see if we consider two different type of reactors one is batch reactor another is flow reactor how we can keep the concentration in the reactor system at a different, say If we take a beaker or the batch reactor and we add A and B two reactant together, so if we add A and B all at a time so this C_A and C_B both high, the second case we can consider and we add slowly with in the in the batch reactor, so A and B added slowly, now in the third case start with A and add B slowly so this is A and add B slowly.

So, in this case since A and B both are added slowly the concentration of C_A and C_B both low, C_A and C_B both low and in this case C_A is high and C_B is low, so this way we can control the concentration of the reactant at different levels. Now, if we consider flow reactor say if we take CSTR or plug flow reactor we can take PFR and both A and B flows together, so at A and B now if we take CSTR here also we can add A and B and they need flows through the second reactor and third reactor and so on, but if we wanted to keep the concentration low both A and B we can take know bigger size CSTR and add C_A and C_B together.

Now if we want to keep C_A high and C_B low in that case we can take plug flow reactor and we can start with A and we can add at different location B so B we can add at different location or we can use CSTR in series and we start with A flow and we add slowly B to ease of that of the CSTR, so this way we can keep concentration of A at different level using the know batch and continuous reactor.

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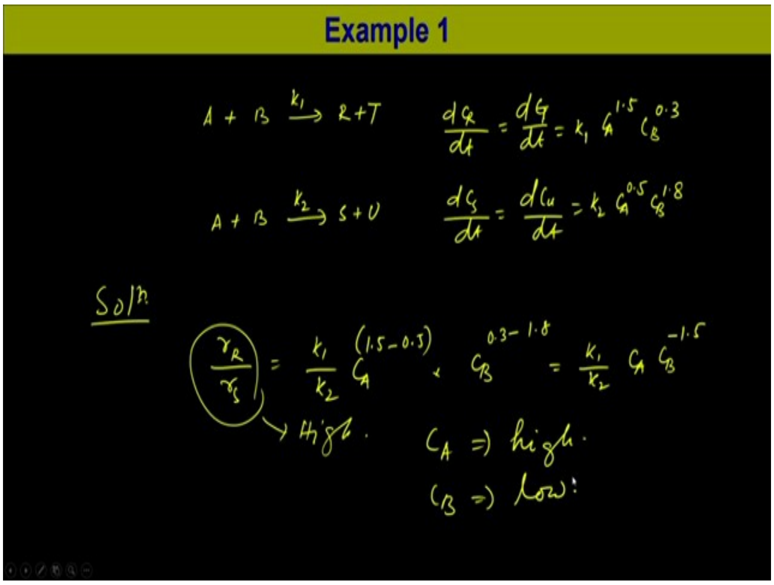

Example 1

$A + B \xrightarrow{k_1} R+T \qquad \frac{dC_R}{dt} = \frac{dC_T}{dt} = k_1 C_A^{1.5} C_B^{0.3}$

$A + B \xrightarrow{k_2} S+U \qquad \frac{dC_S}{dt} = \frac{dC_U}{dt} = k_2 C_A^{0.5} C_B^{1.8}$

Soln.

$\boxed{\frac{r_R}{r_S}} = \frac{k_1}{k_2} C_A^{(1.5-0.3)} \times C_B^{0.3-1.8} = \frac{k_1}{k_2} C_A C_B^{-1.5}$

→ High.

$C_A \Rightarrow$ high.

$C_B \Rightarrow$ low.

Now, let us look into a simple example, suppose if a liquid phase reactions is occurring where

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

And the rate

$$\frac{dC_R}{dt} = \frac{dC_T}{dt} = k_1 C_A^{1.5} C_B^{0.3}$$

Now if this reaction is accomplished when it by another side reaction which is unwanted reaction that is

$$A + B \xrightarrow{k_2} S + U$$

And the rate is

$$\frac{dC_S}{dt} = \frac{dC_U}{dt} = k_1 C_A^{0.5} C_B^{1.8}$$

Now, we have to find out the favorable product distribution condition and look into the probable contacting scheme in the flow reactor say now if we divide this to rate equations we will obtain

$$\frac{r_R}{r_S} = \frac{k_1}{k_2} C_A^{1.5-0.5} C_B^{0.3-1.8}$$

So this is equal to

$$\frac{r_R}{r_S} = \frac{k_1}{k_2} C_A C_B^{-1.5}$$

So, as we can see that to keep this ratio high we need to keep C_A as high as possible, C_A should be high and C_B should be low now let us see how to keep CA and C_B low.

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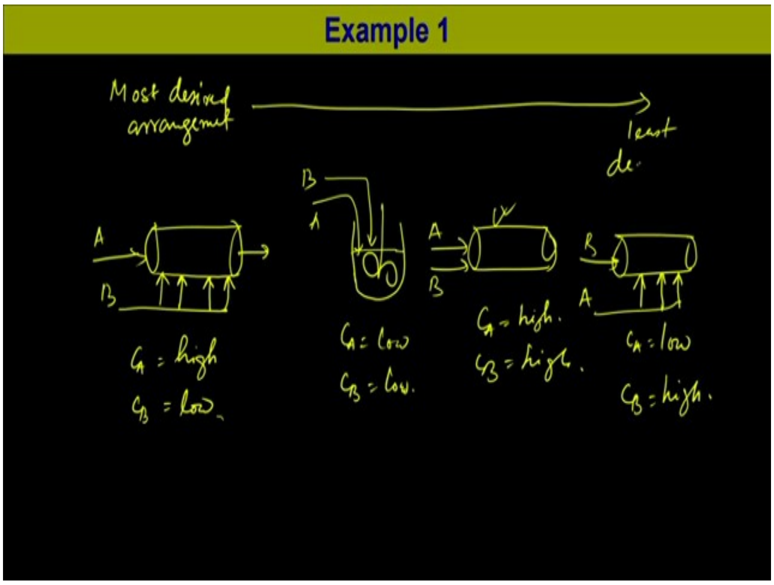

Example 1

So, if have say plug flow reactor and if we pass A and with prime with no different location if we fit B then we can keep the concentration of C_A high at most of the times C_B low, if we only use CSTR what will happen we add both A and B together, so in this case C_A would be low and C_B would be low if we take PFR and flow both A and B so C_A high C_B also high, now if we take PFR flow B at A at different location so here C_A low and C_B high as we need C_A high and C_B low so this is the most desired arrangement and then C_B is low in this case and C_A becomes low.

So, this is less preferred compared to this and then C_A is high and C_B is high as the power of C_B is 1.5 this is the third case is less desired this is less desired over the CSTR with simultaneous addition of A and B, and similarly the fourth case where C_B is very high and C_A is low which is also the least preferred one, so the preference is goes in this order and his would be the least desired.

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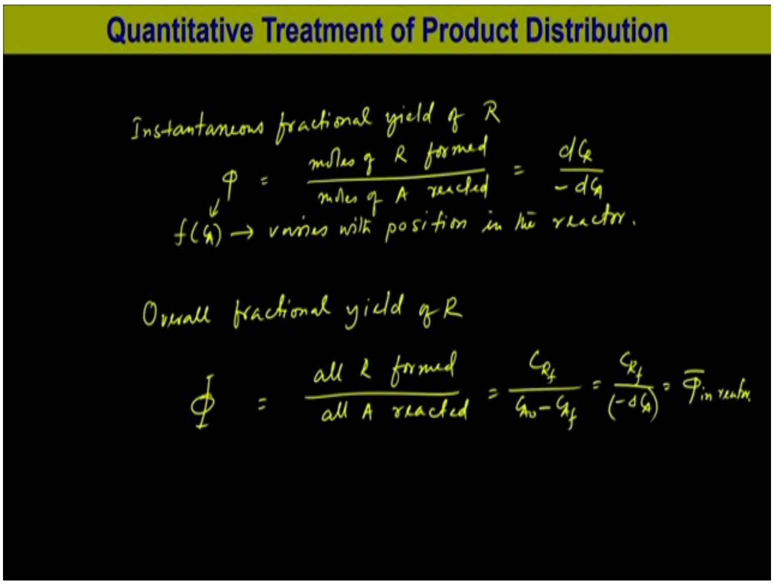

Quantitative Treatment of Product Distribution

Instantaneous fractional yield of R

$$\varphi = \frac{\text{moles of R formed}}{\text{moles of A reacted}} = \frac{dC_R}{-dC_A}$$

$f(C_A) \rightarrow$ varies with position in the reactor.

Overall fractional yield of R

$$\Phi = \frac{\text{all R formed}}{\text{all A reacted}} = \frac{C_{Rf}}{C_{A0}-C_{Af}} = \frac{C_{Rf}}{(-\Delta C_A)} = \bar{\varphi}_{\text{in reactor}}$$

So, now we will look into the quantitative treatment of the product distribution, if the rates of the individual reactions are known we can quantitatively determine the product distribution so in this respect we will define two terms one is instantaneous fraction yield that is represented by, instantaneous fractional yield of R which is defined by

$$\phi = \frac{\text{moles of } R \text{ formed}}{\text{moles of } A \text{ reacted}}$$

And then we can write this is

$$\phi = \frac{dC_R}{-dC_A}$$

So, this is function of concentration so it varies with position in the reactor, so another term is used is the overall fractional yield and this is defined with

$$\Phi = \frac{\text{all } R \text{ formed}}{\text{all } A \text{ reacted}}$$

This we can write

$$\Phi = \frac{C_{Rf}}{C_{A0} - C_{Af}} = \frac{C_{Rf}}{\left(-\Delta C_A\right)} = \bar{\phi}_{\text{in reactor}}$$

So, the overall fractional yield is the average or mean of all the instantaneous react know fractional yield because small phi is the know the fractional yield at a particular location and which will vary inside the reactor, so the overall fractional yield can be calculated with the mean values of the instantaneous fractional yield in the reactor.

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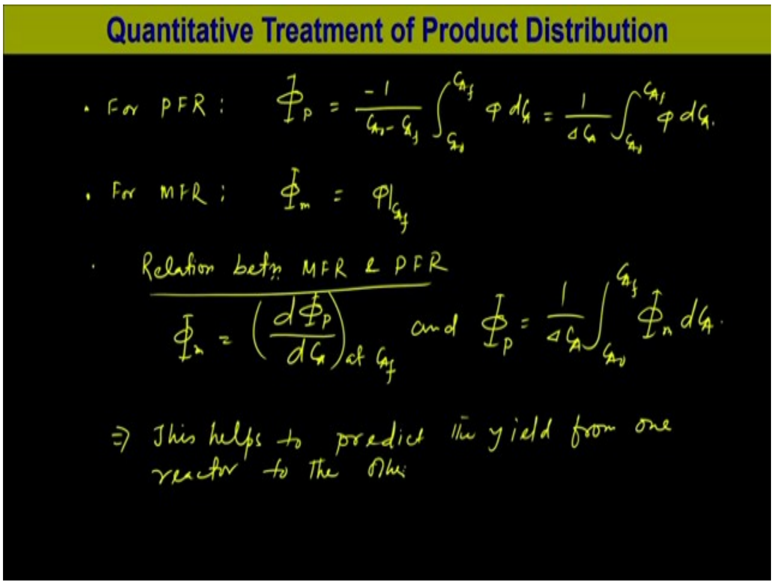

Quantitative Treatment of Product Distribution

- For PFR : $\Phi_p = \frac{-1}{C_{A0}-C_{Af}}\int_{C_{A0}}^{C_{Af}} \varphi \, dC_A = \frac{1}{\Delta C_A}\int_{C_{A0}}^{C_{Af}} \varphi \, dC_A.$
- For MFR : $\Phi_m = \varphi\big|_{C_{Af}}$
- Relation betn MFR & PFR

$\Phi_m = \left(\frac{d\Phi_p}{dC_A}\right)_{at\ C_{Af}}$ and $\Phi_p = \frac{1}{\Delta C_A}\int_{C_{A0}}^{C_{Af}} \Phi_m \, dC_A.$

⇒ This helps to predict the yield from one reactor to the other

Now, if you consider PFR we can write

$$\Phi_P = \frac{-1}{C_{A0} - C_{Af}} \int_{C_{A0}}^{C_{Af}} \phi dC_A = \frac{1}{\Delta C_A} \int_{C_{A0}}^{C_{Af}} \phi dC_A$$

And same for MFR mixed flow reactor we can write

$$\Phi_M = \phi\big|_{C_{Af}}$$

The relation between MFR and PFR we can write in terms of the overall fractional yield we can write

$$\Phi_M = \left(\frac{d\Phi_P}{C_A}\right)_{at\ C_{Af}} \text{ and } \Phi_P = \frac{1}{\Delta C_A} \int_{C_{A0}}^{C_{Af}} \Phi_M dC_A$$

So this type of relations allowed us to predict the yield from one reactor to the other, so this helps to predict the yield from one reactor to the other.

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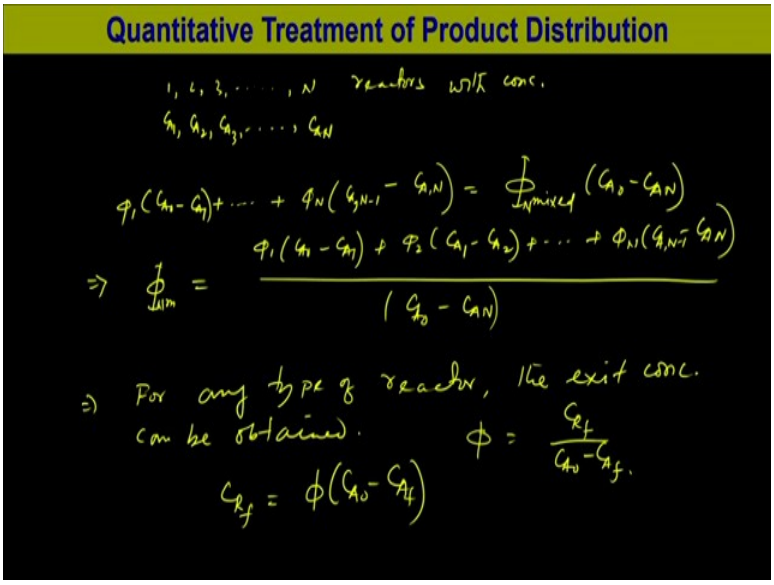

Quantitative Treatment of Product Distribution

1, 2, 3, ..., N reactors with conc.

$C_{A1}, C_{A2}, C_{A3}, \ldots, C_{AN}$

$$\phi_1(C_{A0}-C_{A1}) + \cdots + \phi_N(C_{AN-1}-C_{AN}) = \Phi_{N\,mixed}(C_{A0}-C_{AN})$$

$$\Rightarrow \Phi_{Nm} = \frac{\phi_1(C_{A0}-C_{A1}) + \phi_2(C_{A1}-C_{A2}) + \cdots + \phi_N(C_{AN-1}-C_{AN})}{(C_{A0}-C_{AN})}$$

⇒ For any type of reactor, the exit conc. can be obtained. $\Phi = \frac{C_{Rf}}{C_{A0}-C_{Af}}$.

$$C_{Rf} = \phi(C_{A0}-C_{Af})$$

Now for a series of MFR reactor which is connected in series say N numbers of reactors connected in series we can write say we have

$$1,2,3.........N \text{ reactors}$$

With concentrations

$$C_{A1}, C_{A2}, C_{A3} ....C_{AN}$$

we can write

$$\phi_1(C_{A1} - C_{Af}) + ...\phi_N(C_{AN-1} - C_{AN}) = \Phi_{Mixed}(C_{A0} - C_{AN})$$

So, from here we can write

$$\Phi_{Mixed} = \frac{\phi_1(C_{A0} - C_{A1}) + \phi_2(C_{A1} - C_{A2}) + ...\phi +_N (C_{AN-1} - C_{AN})}{(C_{A0} - C_{AN})}$$

So for any type of reactor the exit concentration can be obtained from the relation that is

$$\Phi = \frac{C_{Rf}}{C_{A0} - C_{Af}}$$

So we can write

$$C_{Rf} = \Phi(C_{A0} - C_{Af})$$

So that is from the definition of the overall fractional yield, so we can calculate the exit concentration C_{Rf} for any kind of reactor.

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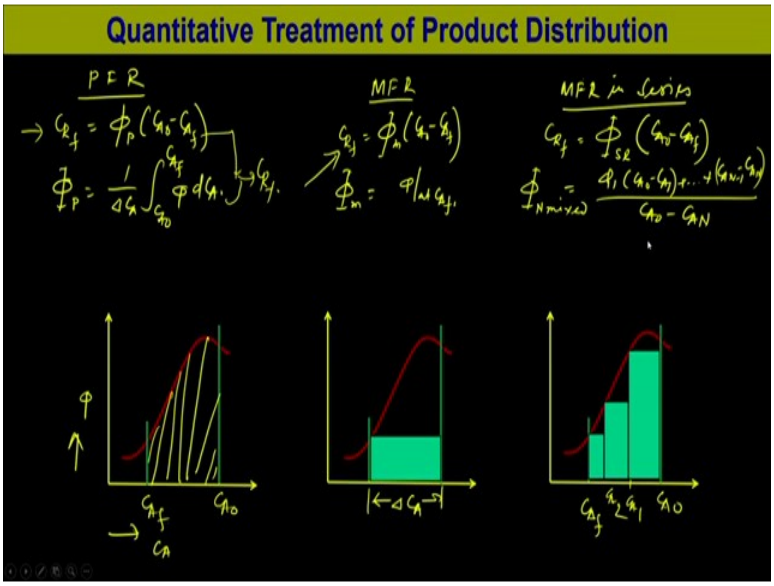

Quantitative Treatment of Product Distribution

PFR

$\rightarrow C_{Rf} = \Phi_p (C_{A0} - C_{Af})$

$\Phi_p = \frac{1}{\Delta C_A} \int_{C_{A0}}^{C_{Af}} \varphi \, dC_A \rightarrow C_{Rf}$

MFR

$C_{Rf} = \Phi_m (C_{A0} - C_{Af})$

$\Phi_m = \varphi |_{at\ C_{Af}}$

MFR in series

$C_{Rf} = \Phi_{SR} (C_{A0} - C_{Af})$

$\Phi_{N\,mixed} = \frac{\varphi_1 (C_{A0} - C_{A1}) + \dots + (C_{AN-1} - C_{AN})}{C_{A0} - C_{AN}}$

Now, if we consider PFR we can write

$$C_{Rf} = \Phi(C_{A0} - C_{Af})$$

And so from here

$$\Phi_P = \frac{1}{\Delta C_A} \int_{C_{A0}}^{C_{Af}} \Phi dC_A$$

So for this case we can know take a contradiction C_{A0} and then to C_{Af} and this would give the area under this curve would give know C_{Rf} , so this is Φ and this is concentration this are plotted for PFR and then the area under this curve we can calculate here and we can calculate Φ_p and if we substitute Φ_p over here in the C_{Rf} equation we can calculate know C_{Rf} from here so using this two relation we can calculate C_{Rf} relation.

Now, if we consider mixed flow reactor that is MFR, this is

$$C_{Rf} = \Phi_m (C_{A0} - C_{Af})$$

$$\Phi_m = \Phi|_{C_{Af}}$$

Now if we consider the similar arrangement so the area under this that is ΔC_A this is from here to this it is ΔC_A, so we can calculate Φ_m over here from this area and then finally we can calculate C_{Rf} .

Now if we consider staged reactors not only CSTR one CSTR but N numbers of CSTR connected in series in that case we can write C_{Rf} MFR in series,

$$C_{Rf} = \Phi_{SR}(C_{A0} - C_{Af})$$

$$\text{and } \Phi_{N\,mixed} = \frac{\phi_1(C_{A0} - C_{A1}) + ...\phi +_N (C_{AN-1} - C_{AN})}{(C_{A0} - C_{AN})}$$

So if we plot from the concentration between C_{A0} to C_{Af} s this is C_{A0} this is C_{Af}.

So, first it will go to C_{A1} up to this and then this is the volume required this is the second reactor and this is the third reactor, so this is and so on so this way it will continue say if we have three reactor connected in series, so C_{A2} would be this and so on. So from here this way we can calculate the C_{Rf} that is the products desired product distribution C_{Rf} we can calculate from this.

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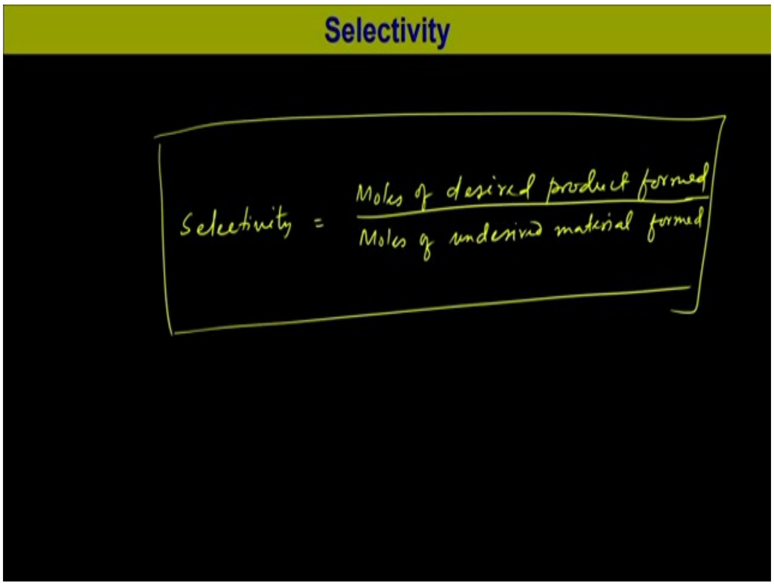

Selectivity

$$\text{Selectivity} = \frac{\text{Moles of desired product formed}}{\text{Moles of undesired material formed}}$$

Now, another important term is the selectivity which we use generally in place of the fractional yield, so it is defined

$$selectivity = \frac{moles\ of\ desired\ product\ formed}{moles\ of\ undesired\ material\ formed}$$

So this is sometimes helpful to use in place of the fractional yield the selectivity, so if the selectivity is higher so as high as possible is the selectivity our desired product would be much more compared to the undesired product, so this will give us how much our maximum quantity of the desired product we are producing for a parallel reaction.

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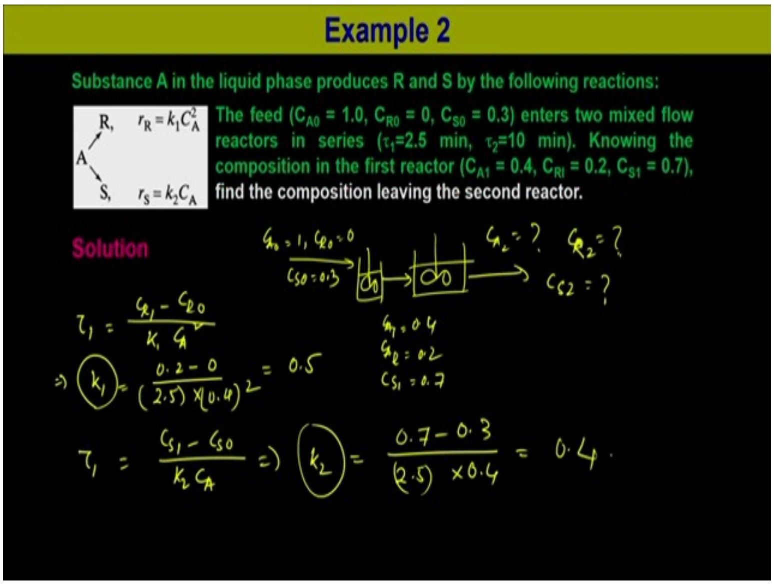

Example 2

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

$A \nearrow R,\ r_R = k_1 C_A^2$

$A \searrow S,\ r_S = k_2 C_A$

The feed (C_{A0} = 1.0, C_{R0} = 0, C_{S0} = 0.3) enters two mixed flow reactors in series (τ_1=2.5 min, τ_2=10 min). Knowing the composition in the first reactor (C_{A1} = 0.4, C_{RI} = 0.2, C_{S1} = 0.7), find the composition leaving the second reactor.

Solution

$C_{A0} = 1,\ C_{R0} = 0$

$C_{S0} = 0.3$

$C_{A2} = ?\ C_{R2} = ?$

$C_{S2} = ?$

$C_{A1} = 0.4$

$C_{R1} = 0.2$

$C_{S1} = 0.7$

$$\tau_1 = \frac{C_{R1} - C_{R0}}{k_1 C_A^2}$$

$$\Rightarrow k_1 = \frac{0.2 - 0}{(2.5) \times (0.4)^2} = 0.5$$

$$\tau_1 = \frac{C_{S1} - C_{S0}}{k_2 C_A} \Rightarrow k_2 = \frac{0.7 - 0.3}{(2.5) \times 0.4} = 0.4.$$

Now, let us take an example say substance A in the liquid phase produces R and S by the following reaction $\begin{array}{c} A \to R \\ A \to S \end{array}$ and the rate of reactions is given $r_R = k_1 C_A^2$ and $r_S = k_2 C_A$, now the feed conditions is given C_R is 0 and C_S is 0.3 and C_{A0} is 1, enters to mixed flow reactor in series knowing the composition in the first reactor find the composition leaving the second reactor.

So, let us solve it so we have two reactors as their τ is different so the volume is different so the inlet to this is

$$C_{A1} C_{A0} = 1,\ C_{RS} C_{R0} = 0 \text{ and } C_{S0} = 0.3$$

now C_{A1} from here which is going to this

$$C_{A1} = 0.4$$
$$C_{R1} = 0.2$$
$$C_{S1} = 0.7$$

Now we have to find out the exit concentration C_{A2}, C_{R2} and C_{S2}.

Now for the first mixed flow reactor here if we write

$$\tau_1 = \frac{C_{R1} - C_{R0}}{k_1 C_A^2}$$

So second order reaction, so from here we can write

$$k_1 = \frac{0.2 - 0}{2.5 \times 0.4^2} = 0.5$$

And same for the undesired product is, so we can write

$$\tau_1 = \frac{C_{S1} - C_{S0}}{k_2 C_A}$$

So from here

$$k_1 = \frac{0.7 - 0.3}{2.5 \times 0.4} = 0.4$$

So k_1 and k_2 we have obtained for the first reactor.

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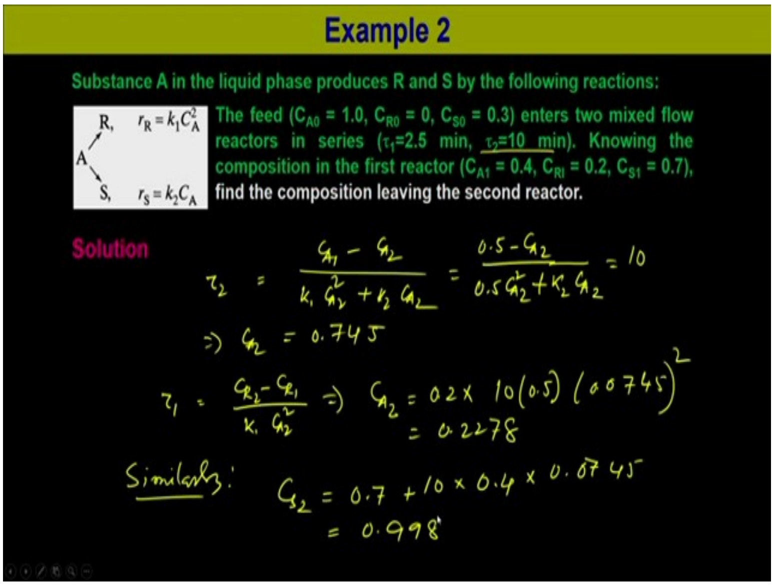

Example 2

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

$$A \nearrow R, \quad r_R = k_1 C_A^2$$
$$A \searrow S, \quad r_S = k_2 C_A$$

The feed (C_{A0} = 1.0, C_{R0} = 0, C_{S0} = 0.3) enters two mixed flow reactors in series (τ_1=2.5 min, τ_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

$$\tau_2 = \frac{C_{A1} - C_{A2}}{k_1 C_{A2}^2 + k_2 C_{A2}} = \frac{0.5 - C_{A2}}{0.5 C_{A2}^2 + k_2 C_{A2}} = 10$$

$$\Rightarrow C_{A2} = 0.745$$

$$\tau_1 = \frac{C_{R2} - C_{R1}}{k_1 C_{A2}^2} \Rightarrow C_{A2} = 0.2 \times 10(0.5)(0.0745)^2 = 0.2278$$

Similarly:

$$C_{S2} = 0.7 + 10 \times 0.4 \times 0.0745 = 0.998$$

Now if we go to the second reactor we can write

$$\tau_2 = \frac{C_{A1} - C_{A2}}{k_1 C_{A2}^2 + k_2 C_{A2}}$$

So if we substitute this is

$$\tau_2 = \frac{0.5 - C_{A2}}{0.5 C_{A2}^2 + k_2 C_{A2}} = 10$$

So from here we can calculate

$$C_{A2} = 0.745.$$

Now

$$\tau_1 = \frac{C_{R2} - C_{R1}}{k_1 C_{A2}^2}$$

So from here we can write

$$C_{A2} = 0.2 \times 10(0.5)(0.745)^2 = 0.2278$$

Similar way we can calculate

$$C_{S2} = 0.7 + 10 \times 0.4 \times 0.0745 = 0.98$$

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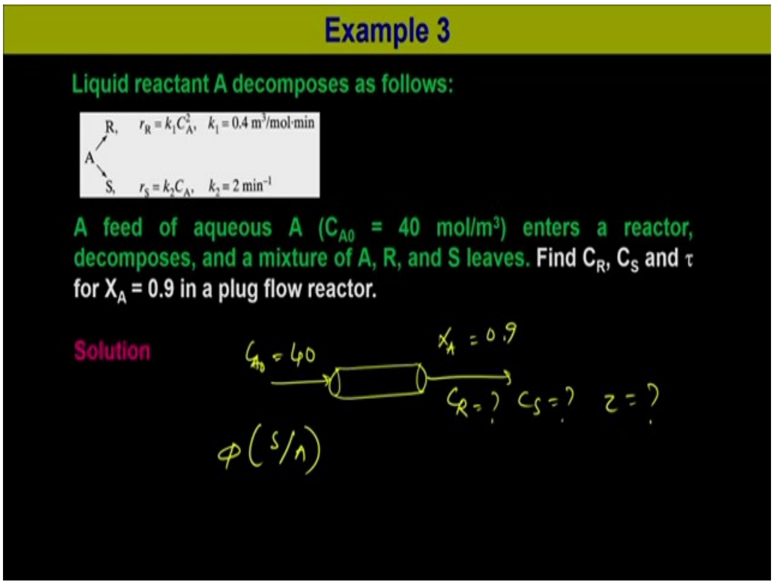

Example 3

Liquid reactant A decomposes as follows:

$$A \rightarrow R, \quad r_R = k_1 C_A^2, \quad k_1 = 0.4\ \text{m}^3/\text{mol}\cdot\text{min}$$
$$A \rightarrow S, \quad r_S = k_2 C_A, \quad k_2 = 2\ \text{min}^{-1}$$

A feed of aqueous A (C_{A0} = 40 mol/m^3) enters a reactor, decomposes, and a mixture of A, R, and S leaves. Find C_R, C_S and τ for X_A = 0.9 in a plug flow reactor.

Solution

$C_{A0} = 40$

$X_A = 0.9$

$C_R = ?$ $C_S = ?$ $\tau = ?$

$\phi(S/A)$

Now, let us take another small example liquid reactant A decomposes as follows, so this path and a feed of aqueous A which is 40 mol/m^3 enters a reactor decomposes and a mixture of A, R and S leaves find C_R , C_S and τ for $X_A = 0.9$ in a plug flow reactor. So, reactor is given which is plug flow, so it is $C_{A0} = 40$ and $X_A = 0.9$ we have to find out C_R is equal to how much, C_S is equal to how much, and τ is equal to what. So, from this what we can see we have to determine $\Phi\left(\frac{S}{A}\right)$.

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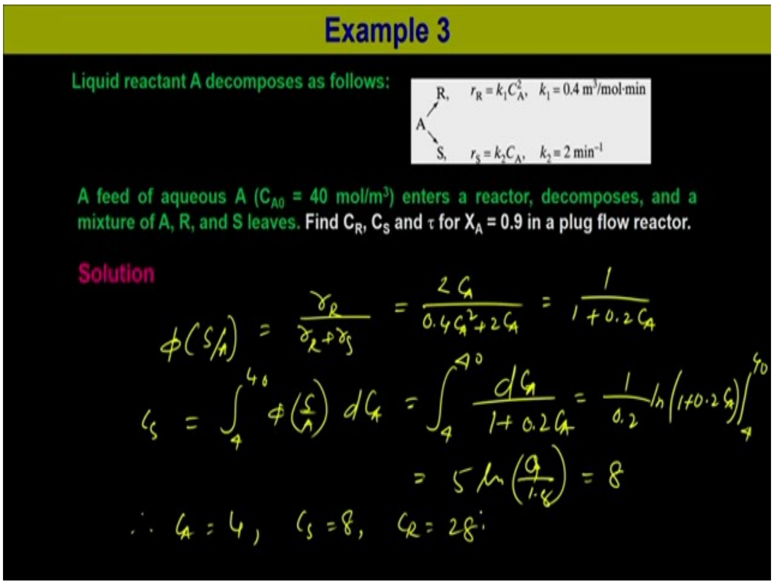

Example 3

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A feed of aqueous A (C_{A0} = 40 mol/m^3) enters a reactor, decomposes, and a mixture of A, R, and S leaves. Find C_R, C_S and τ for X_A = 0.9 in a plug flow reactor.

Solution

$$\phi(S/A) = \frac{r_R}{r_R + r_S} = \frac{2C_A}{0.4C_A^2 + 2C_A} = \frac{1}{1+0.2C_A}$$

$$C_S = \int_4^{40} \phi\left(\frac{S}{A}\right) dC_A = \int_4^{40} \frac{dC_A}{1+0.2C_A} = \frac{1}{0.2}\ln(1+0.2C_A)\Big|_4^{40}$$

$$= 5\ln\left(\frac{9}{1.8}\right) = 8$$

$$\therefore C_A = 4, \quad C_S = 8, \quad C_R = 28.$$

So, we can write

$$\Phi\left(\frac{S}{A}\right)=\frac{r_R}{r_R+r_S}$$

$$\Phi\left(\frac{S}{A}\right)=\frac{2C_A}{0.4C_A^2+2C_A}$$

$$\Phi\left(\frac{S}{A}\right)=\frac{1}{1+0.2C_A}$$

So now if we substitute the values it would be

$$C_S=\int_4^{40}\Phi\left(\frac{S}{A}\right)dC_A$$

$$C_S=\int_4^{40}\frac{1}{1+0.2C_A}dC_A$$

$$C_S=\frac{1}{0.2}\ln\left(1+0.2C_A\right)\Big|_4^{40}$$

So this would be equal to

$$C_S=5\ln\left(\frac{9}{1.8}\right)=8$$

So therefore $C_A=4$, $C_S=8$ and $C_R=28$

So this way we can calculate the products distribution. So thank you very much for attending this lecture and we will continue our discussion on the reactant design for multiple reactions in the next lecture.