Chemical Reaction Engineering-I
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Lecture - 16
Recycle and Autocatalytic Reactors

Welcome to the sixth lecture of module 4. In this module we are discussing reactor design for multiple reactors. Before going to this lecture, let us have brief recap on our previous lecture.

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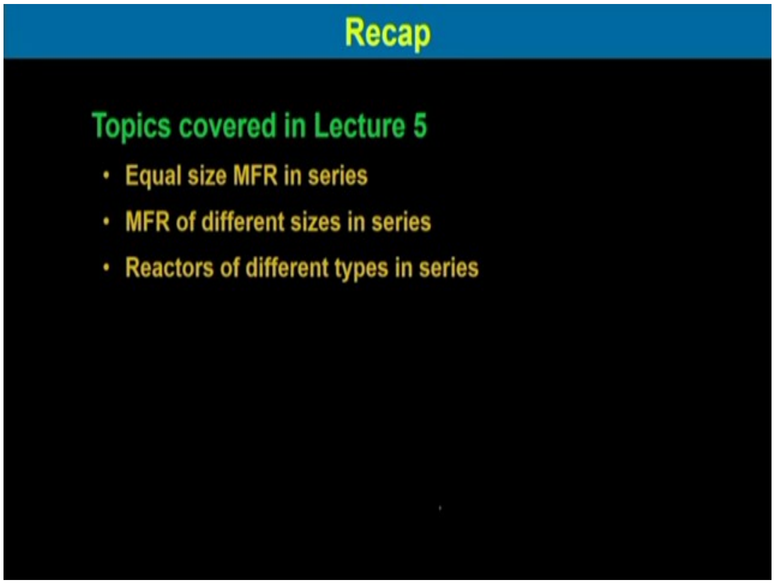

Recap

Topics covered in Lecture 5

- Equal size MFR in series
- MFR of different sizes in series
- Reactors of different types in series

In the previous lecture, we have covered equal size mixed flow reactor connected in series, MFR or mixed flow reactor of different sizes in series, then we have considered reactor of different types connected in series. So, mostly the flow reactors either they are continuous stirred tank reactor or the plug flow reactor. How they are, know how their sizes when they connects in series, how their sizes influence the conversion or for a conversion what are the total volume required that we have covered in our last lecture.

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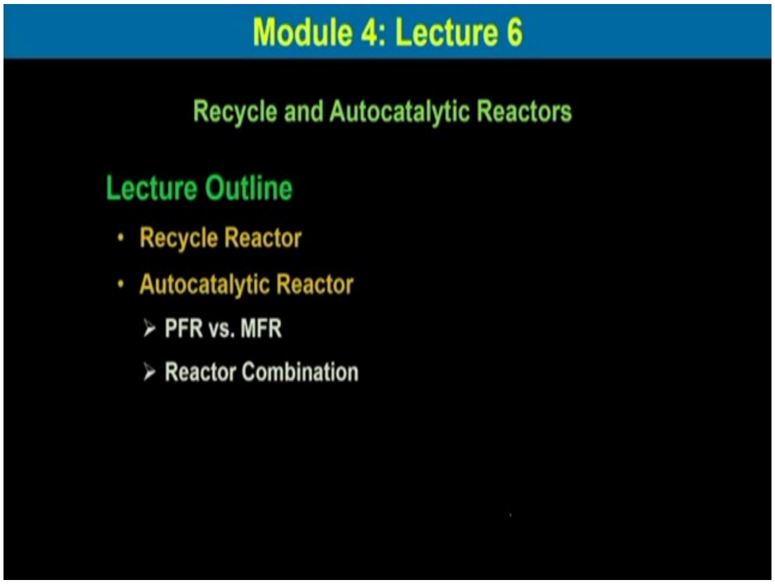

Module 4: Lecture 6

Recycle and Autocatalytic Reactors

Lecture Outline

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

In this lecture, we will consider recycle and autocatalytic reactors. The brief outline of this lecture would be recycle reactor, then autocatalytic reactor and we will compare the sizes for PFR versus MFR, plug flow reactor versus mix flow reactor and different reactor combination.

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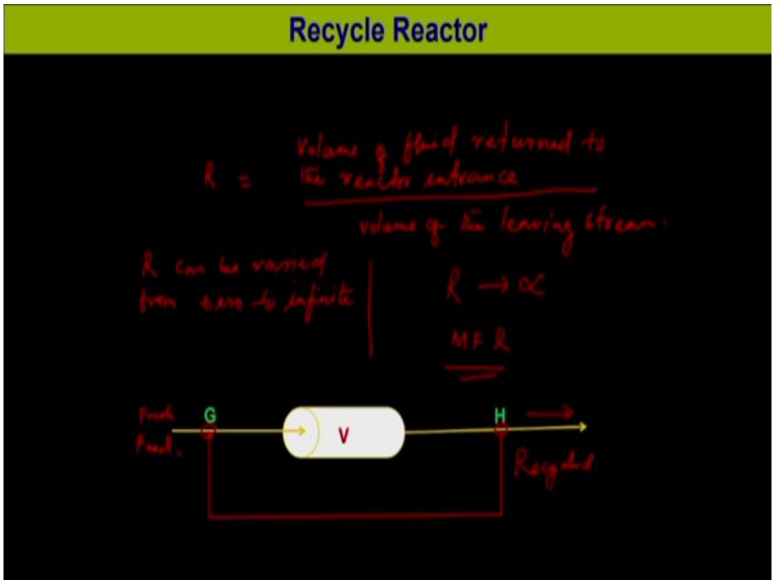

Recycle Reactor

$$R = \frac{\text{Volume of fluid returned to the reactor entrance}}{\text{volume of the leaving stream}}$$

R can be varied from zero to infinite

$R \rightarrow \infty$

MFR

So, let us start with recycle reactor. What is recycled reactor? We can see in certain situations it is advantageous to separate the, or to divide the product stream into two streams and part of the product streams is recycled back to the reactor entrance. So, the part of the liquid which is the recycled can be defined with the recycle ratio. So, let us consider this is the volume of the reactor V and it is recycled part of it to the reactor entrance from point H to point G.

So, the product which is coming out it is divided into two streams, one is the product which is taken and one is recycled which is, and which is comes to point G, which is meeting with the fresh feed. So, the recycled ratio R is defined as volume of feed, returned to the reactor entrance divided by the volume of the, volume of the leaving streams. So, it can be thought of to vary the recycle ratio from 0 to infinity. That means R can be varied from 0 to infinity or infinite.

So this reflection suggests that the plug flow reactor when there is no recycle it behaves a plug flow reactor. When some portion is recycled and fed to the reactor entrance degree of mixing inside the reactor is increased that means as we increase the recycle ratio the behavior of the plug flow reactor approaches to the CSTR. So the degree of mixing increases and at R tends to infinity the behavior of the plug flow reactor will be as MFR mixed flow reactor.

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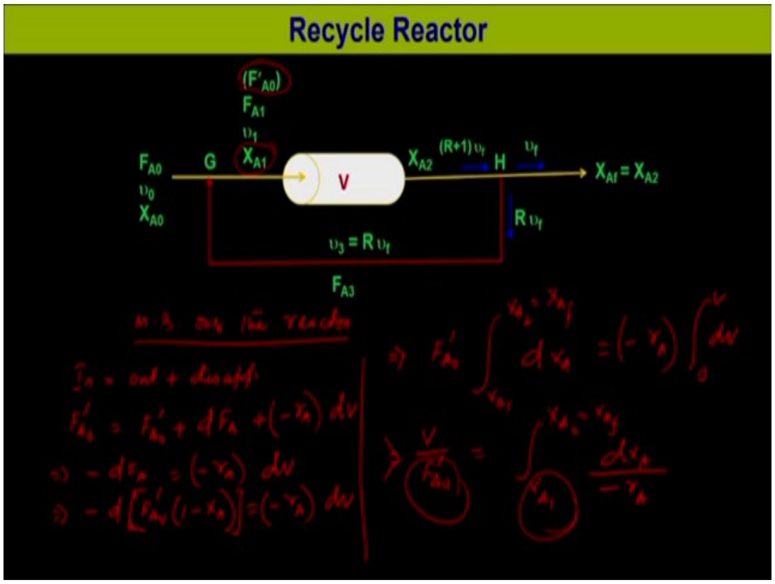

Recycle Reactor

M.B. on the reactor

In = out + disapp.

$F'_{A0} = F'_{A0} + dF_A + (-r_A)\,dV$

$\Rightarrow -dF_A = (-r_A)\,dV$

$\Rightarrow -d[F'_{A0}(1-X_A)] = (-r_A)\,dV$

$\Rightarrow F'_{A0}\int_{X_{A1}}^{X_{A2}=X_{Af}} dX_A = (-r_A)\int_0^V dV$

$\Rightarrow \frac{V}{F'_{A0}} = \int_{X_{A1}}^{X_{A2}=X_{Af}} \frac{dX_A}{-r_A}$

Now, let us quantitatively see how this happens. So, let us take plug flow reactor of volume V and where the inlet to the reactor is F_{A0} is the molar flow rate in, V_0 is the volumetric flow rate of the feed and its conversion is X_{A0}, then the exit to this reactor is X_{A2} and part of the material is recycled here and coming to this point, so from point H and to point G. Now, when part of this material is recycled the volumetric flow rate which is coming out over here is v_f.

So, the material which is recycled back is RV_f part of the total flow which is coming out from this. So V_3 in this A would be equal to RV_f and its molar flow rate is F_{A3}. So due to this addition of the recycle feed this is F_{A1} would be F'_{A0}, which is coming with the fresh feed and with the recycle feed and the volumetric flow rate is V_1 and conversion is X_{A1} because with the fresh feed say with X_{A0} is the conversion, then you have some converted feed which is coming over here.

So, it will change to X_{A1}, the flow which is coming over here is (R plus 1)V_f and the material or the product which is taken out over here is X_{Af} which is equal to X_{A2} which would be equivalent to this over here. Because, same outlet product is recycled back to the reactor entrance. Now, let us do the material balance. So, over the reactor if we do the material balance we can write

in = out + disappearance

So, it would be

$$F'_{A0} = F'_{A0} + dF_A + (-r_A)\,\mathrm{dV}$$

So, we can write from here is

$$-dF_A = (-r_A)\,\mathrm{dV}$$

Now in terms of the conversion this would be

$$-d[F'_{Av}(1 - X_A)] = (-r_A)\,\mathrm{dV}$$

Now, from this we can write, if we integrate this one we can write

$$F'_{A0}\int_{X_{A1}}^{X_{A2}=X_{Af}} dX_A = (-r_A)\int_0^V dV$$

So, from this we can write

$$\frac{V}{F'_{A0}} = \int_{X_{A1}}^{X_{A2}=X_{Af}} \frac{dX_A}{-r_A}$$

Now, here F_{A0} is not known and also the X_{A1} which is over here. So $F_{A0}^{'}$ and X_{A1} is not known. So until these are some relation can be obtained with some known quantities the integration is not possible. So, let us find out how to calculate $F_{A0}^{'}$ and X_{A1}.

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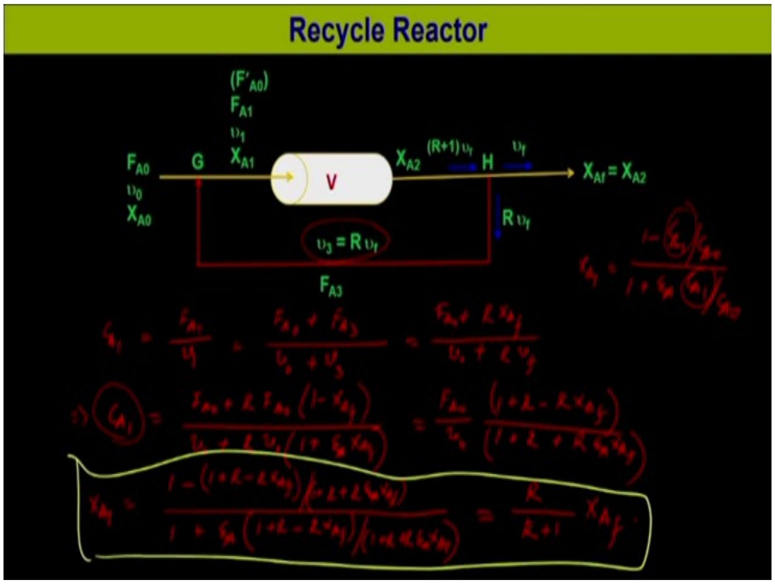
Recycle Reactor

So, $\varepsilon \neq 0$ and there is a split at point H. So we can write

F'_{A0} = (A which would enter in an unconverted recycle stream) + (A entering as fresh feed)

So this is equal to $= RF_{A0} + F_{A0}$

So this would be equal to

$= (R+1)F_{A0}$

And

$$X_{A1} = \frac{1 - C_{A1}/C_{A0}}{1 + \varepsilon_A C_{A1}/C_{A0}}$$

Now,

$$C_{A1} = \frac{F_{A1}}{v_1} = \frac{F_{A0} + F_{A3}}{v_0 + v_3} = \frac{F_{A0} + RX_{Af}}{v_0 + Rv_f}$$

Which is F_{A3} which is v_3.

So, if we write this then

$$C_{A1} = \frac{F_{A0} + RF_{A0}(1 - X_A)}{v_0 + Rv_1(1 + \varepsilon_A X_{Af})} = \frac{F_{A0}(1 + R - RX_{Af})}{v_0(1 + R + R\varepsilon_A X_{Af})}$$

Now, if we substitute this C_{A1} with our earlier relation that is $X_{A1} = \frac{1 - C_{A1}/C_{A0}}{1 + \varepsilon_A C_{A1}/C_{A0}}$.

If we substitute this C_{A1} over here we can get

$$X_{A1} = \frac{1 - \dfrac{(1 + R - RX_{Af})}{(1 + R + R\varepsilon_A X_{Af})}}{1 + \varepsilon_A \dfrac{(1 + R - RX_{Af})}{(1 + R + R\varepsilon_A X_{Af})}} = \frac{R}{R + 1} X_{Af}$$

So, so, we got the relation between X_{A1} which we need and also we got $F_{A0}^{'}$. So both the relations we can put into the integral and then we do the integrations.

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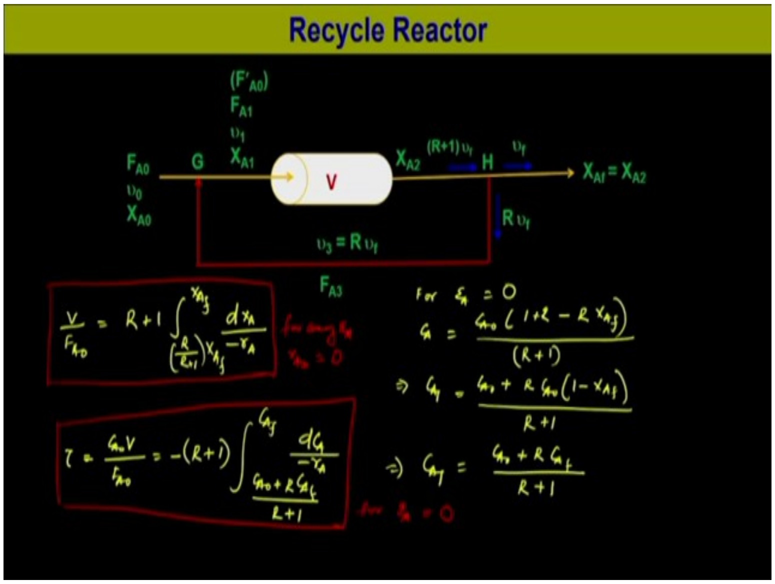

Recycle Reactor

$$\frac{V}{F_{A0}} = R+1 \int_{\left(\frac{R}{R+1}\right)X_{Af}}^{X_{Af}} \frac{dX_A}{-r_A}$$

for any ε_A
$X_{A0} = 0$

For $\varepsilon_A = 0$

$$C_{A1} = \frac{C_{A0}(1+R-RX_{Af})}{(R+1)}$$

$$\Rightarrow C_{A1} = \frac{C_{A0} + R C_{A0}(1-X_{Af})}{R+1}$$

$$\Rightarrow C_{A1} = \frac{C_{A0} + R C_{Af}}{R+1}$$

$$\tau = \frac{C_{A0}V}{F_{A0}} = -(R+1)\int_{\frac{C_{A0}+RC_{Af}}{R+1}}^{C_{Af}} \frac{dC_A}{-r_A}$$

for $\varepsilon_A = 0$

So finally, with this X_{A1} values if we consider for any ε_A and the conversion initial conversion is 0, we can write the performance equation for CSTR as $\frac{V}{F_{A0}} = (\mathrm{R}+1)\int_{\frac{R}{R+1}X_{Af}}^{X_{Af}} \frac{dX_A}{-r_A}$ and this relation is valid for any ε_A and $X_{A0} = 0$. Now, if we consider C_{A1} for $\varepsilon_A = 0$, we can write, so for $\varepsilon_A = 0$.

Then this C_{A1} we can write

$$C_{A1} = \frac{C_{A0}(1+R-RX_{Af})}{R+1}$$

$$C_{A1} = \frac{C_{A0} + RC_{A0}(1-X_{Af})}{R+1}$$

$$C_{A1} = \frac{C_{A0} + RC_{Af}}{R+1}$$

So, with this limit if we write for any ε_A the Performance Equation for the recycle reactor we can write as

$$\tau = \frac{C_{A0}V}{F_{A0}} = -(\mathrm{R}+1)\int_{\frac{C_{A0}+RC_{Af}}{R+1}}^{C_{Af}} \frac{dC_A}{-r_A}$$

This relation as we said is valid for $\varepsilon_A = 0$. Now, this two expression, this in terms of the conversion and in terms of the concentration we can show graphically.

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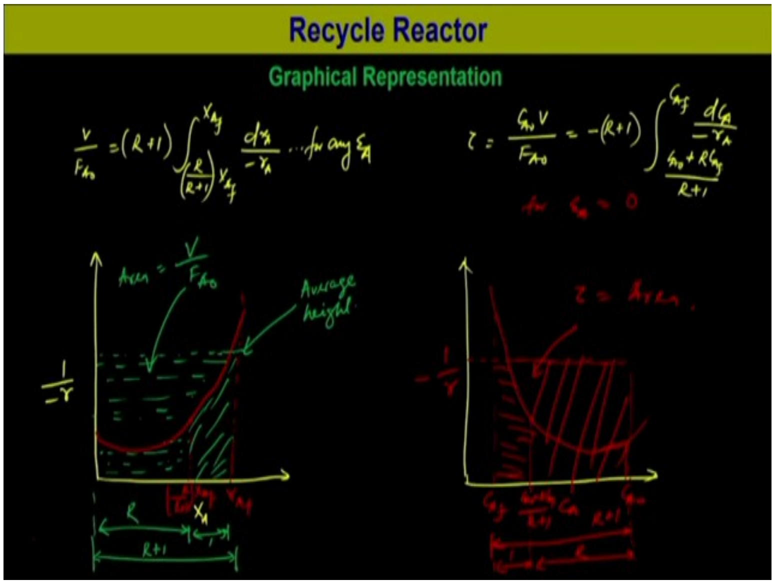

Recycle Reactor

Graphical Representation

So, for V, $\frac{V}{F_{A0}} = (\mathrm{R}+1)\int_{\frac{R}{R+1}X_{Af}}^{X_{Af}} \frac{dX_A}{-r_A}$ and this is for any ε_A. So, if we do the general representation graphically and if we plot $\frac{1}{-r}$ versus X_A. So this would be initially the conversion is because it is recycle reactor there is some conversion and conversion will. So initially because of recycled reactor there would be some conversion at the beginning and conversion will little bit drop and then it will increase.

So the values of this would be X_{Af}. Now, if it is plug flow reactor, the integral term, this is the integral term of the Performance Equation of the recycle reactor, so in that case from it is limit from $\frac{R}{R+1}X_{Af}$ to X_{Af}. So, if we consider this is $\frac{R}{R+1}X_{Af}$. So this gives the volume, the area under this curve is represents the conversion under this area under this integral and if recycle is increased. So at the, if we consider the overall $\frac{V}{F_{A0}}$ it will take the volume which closely resembles to the CSTR the other part.

So this would be probably the average height and the total volume requirement for this recycle reactor and this part from here to this is $R+1$ and this part is 1 and this part is R. Now, if we plot for the specific case when $\varepsilon_A = 0$. So we can see this is for the special case and the Performance Equation is $\tau = \frac{C_{A0}V}{F_{A0}} = -(\mathrm{R}+1)\int_{\frac{C_{A0}+RC_{Af}}{R+1}}^{C_{Af}} \frac{dC_A}{-r_A}$ and this is for $\varepsilon_A = 0$.

Now, if we plot this $-r_A$, $-\frac{1}{r}$ versus C_{A1}. So the plot could be like this. So means you start with certain concentration that is C_{A0} and the final conversion is at say C_{Af}. So the integral term is from $\frac{C_{A0}+RC_{Af}}{R+1}$. So this is the integral part area under this curve. So this would be C_{Af}, $\frac{C_{A0}+RC_{Af}}{R+1}$. So the average area requirement for this is about this. So this is the τ which is the area and recycle ratio.

So from here from this point to this point is $R+1$ and this part is R, this part is 1 and these part is R. So, this is for the special case when $\varepsilon_A = 0$ and this is the general representation of the recycle reactor Performance Equation graphically.

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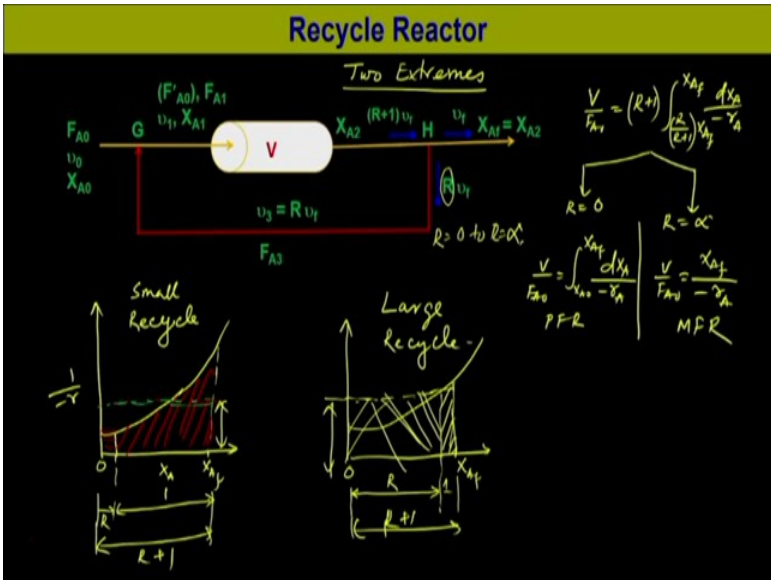

Recycle Reactor

Now, if we consider recycle reactors, there are two extremes we can consider, two extremes. What are those 2 extremes? One is this recycle ratio we can vary R equal to 0 to R is equal to infinity. So for this special case, if we ride this Performance Equation $\frac{V}{F_{A0}} = (\mathrm{R}+1)\int_{\frac{R}{R+1}X_{Af}}^{X_{Af}} \frac{dX_A}{-r_A}$ the two special case we can write R is equal to 0 and R equal to infinite; two extremes.

So, if R is equal to 0 it will behave completely plug flow reactor. So we will get the Performance Equation $\frac{V}{F_{A0}} = \int_{X_{A0}}^{X_{Af}} \frac{dX_A}{-r_A}$. So this is PFR and this equation would be $\frac{V}{F_{A0}} = \frac{dX_A}{-r_A}$ So this is mixed flow reactor. Now, this can be seen graphically, we can see the overall volume requirement as we have done before, if we have very small recycle, it will behave like a plug flow reactor and we can plot say $\frac{1}{-r}$ versus X_A.

So, which will vary from 0 to X_{Af} and the conversion will change like this and this is X_{Af}. And so, if our recycle is very small, so we can consider this is our recycle up to this. So this is R and this is there is no recycle this is 1. So this is behave like a plug flow reactor and the total is $R+1$. So the area under this curve is the plug flow reactor area volume requirement and this area would be the CSTR area. So the average area requirement would be something about this, this is the average area requirement.

But in this case, if we consider large recycle. So this is for small recycle, for large recycle it would be 0 to X_{Af} say over here and our recycle is very large. So we will keep up to this say. So this is recycle and this part is 1 not recycle. So total is $R+1$. So the rate versus conversion curve under this, this would be the PFR volume requirement and the rest of the part because of large recycle it would be the area requirement would be high. So because it will be like a CSTR, so the average area requirement would be high compared to small recycle. So this is for large recycle.

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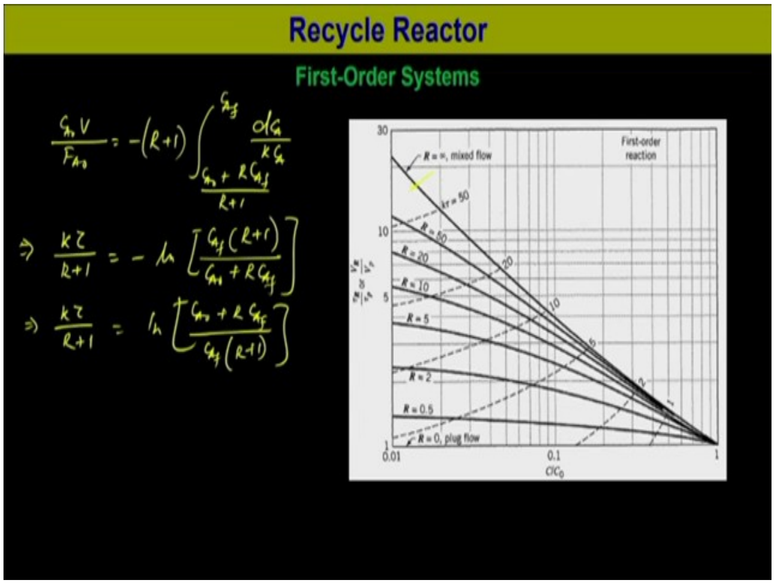

Recycle Reactor

First-Order Systems

$$\frac{C_{A0}V}{F_{A0}} = -(R+1)\int_{\frac{C_{A0}+RC_{Af}}{R+1}}^{C_{Af}} \frac{dC_A}{kC_A}$$

$$\Rightarrow \frac{k\tau}{R+1} = -\ln\left[\frac{C_{Af}(R+1)}{C_{A0}+RC_{Af}}\right]$$

$$\Rightarrow \frac{k\tau}{R+1} = \ln\left[\frac{C_{A0}+RC_{Af}}{C_{Af}(R+1)}\right]$$

Now, if we consider first order reaction, for first order reaction, we can write the Performance Equation

$$\frac{C_{A0}V}{F_{A0}} = -(\mathrm{R}+1)\int_{\frac{C_{A0}+RC_{Af}}{R+1}}^{C_{Af}} \frac{dC_A}{kC_A}$$

This is for first order. So if we integrate we will get

$$\frac{k\tau}{R+1} = -\ln[\frac{C_{Af}(\mathrm{R}+1)}{C_{Af}+RC_{Af}}]$$

So this is nothing but

$$\frac{k\tau}{R+1} = -\ln[\frac{C_{Af}(\mathrm{R}+1)}{C_{Af}(R+1)}]$$

So now, if we take the ratio between the phase time or residence time or their volume ratio of recycle reactor and the plug flow reactor we could see for the first order reaction from here this is Levenspiel plot and we can see that when there is recycle is large it behave like a mixed flow reactor MFR when R tends to infinite. So over here the volume requirement becomes large, when recycle ratio is reduced it goes to close to plug reactor, when R tends to 0 it behaves like a plug flow reactor. So this is Levenspiel plot.

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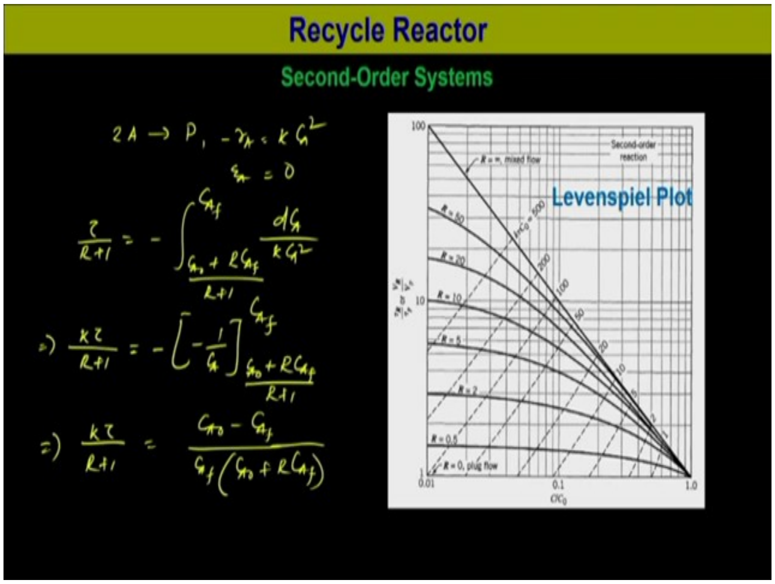

Recycle Reactor

Second-Order Systems

$2A \rightarrow P, \; -r_A = kC_A^2$

$\varepsilon_A = 0$

$\frac{\tau}{R+1} = -\int_{\frac{C_{A0}+RC_{Af}}{R+1}}^{C_{Af}} \frac{dC_A}{kC_A^2}$

$\Rightarrow \frac{k\tau}{R+1} = -\left[-\frac{1}{C_A}\right]_{\frac{C_{A0}+RC_{Af}}{R+1}}^{C_{Af}}$

$\Rightarrow \frac{k\tau}{R+1} = \frac{C_{A0}-C_{Af}}{C_{Af}(C_{A0}+RC_{Af})}$

Now, for the second order system also we can get similar information for the Levenspiel plot. So for second order system if we consider say $2A \rightarrow P$. So with $-r_A = kC_A^2$ and $\varepsilon_A = 0$.

So we can write

$$\frac{\tau}{R+1} = -\int_{\frac{C_{A0}+RC_{Af}}{R+1}}^{C_{Af}} \frac{dC_A}{kC_A^2}$$

Now, if we integrate it would be

$$\frac{k\tau}{R+1} = -\left[-\frac{1}{C_A}\right]_{\frac{C_{A0}+RC_{Af}}{R+1}}^{C_{Af}}$$

$$\frac{k\tau}{R+1} = \frac{C_{A0}-C_{Af}}{C_{Af}(C_A + RC_{Af})}$$

similar to the first order reaction we can also take the ratio of the volume required between the recycled reactor and plug flow reactor.

And if we can see that if we change the recycle ratio then it will goes from when recycled ratio is like it is behave like a plug flow, when it is high it will behave like a mixed flow reactor.

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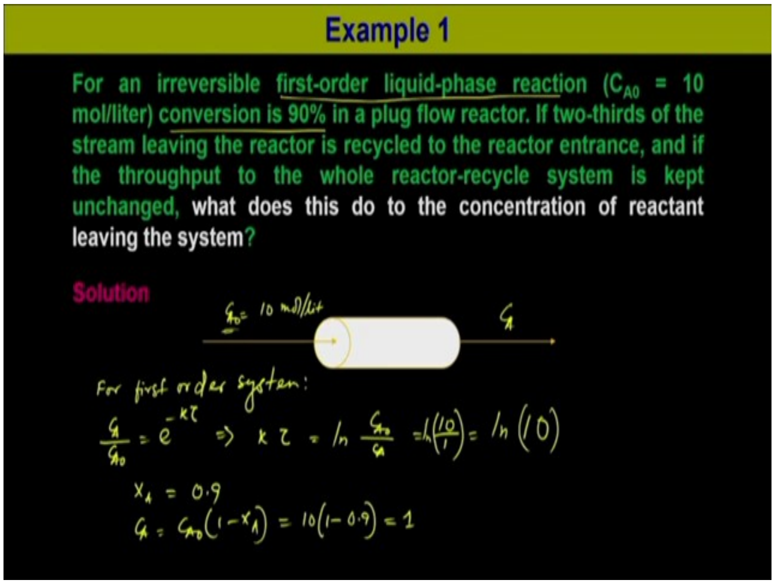

Example 1

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

Solution

For first order system:

$$\frac{C_A}{C_{A0}} = e^{-k\tau} \Rightarrow k\tau = \ln\frac{C_{A0}}{C_A} = \ln\left(\frac{10}{1}\right) = \ln(10)$$

$$X_A = 0.9$$

$$C_A = C_{A0}(1-X_A) = 10(1-0.9) = 1$$

Now, let us take an example. For an irreversible first order liquid phase reaction, where $C_{A0} = 10\ \frac{mol}{L}$, conversion is 90% in a plug flow reactor, if two third of the stream leaving the reactor is recycled to the reactor entrance, and if the throughput to the whole recycle reactor system is kept unchanged, what does this do to the concentration of the reactant leaving the systems?

Now, let us solve it. Say initially we had $C_{A0} = 10\frac{mol}{L}$ and this is exit is say C_A. Now, as it said this is for first order irreversible liquid phase reaction, so for first order system we know that,

$$\frac{C_A}{C_{A0}} = e^{-k\tau}$$

From here we can write

$$k\tau = \ln\frac{C_{A0}}{C_A} = \ln\frac{10}{1} = \ln(10)$$

$$X_A = 0.9$$

So conversion is 90%. So, $X_A = 0.9$.

So, this is equal to, C_A would be equal to for 90 percent conversion, C_A would be C

$$C_A = C_{A0}(1 - X_A) = 10(1 - 0.9) = 1$$

So $k\tau = \ln\frac{10}{1} = \ln(10)$

Now, as it is said two third of the stream leaving the reactor is recycled to the reactor entrance.

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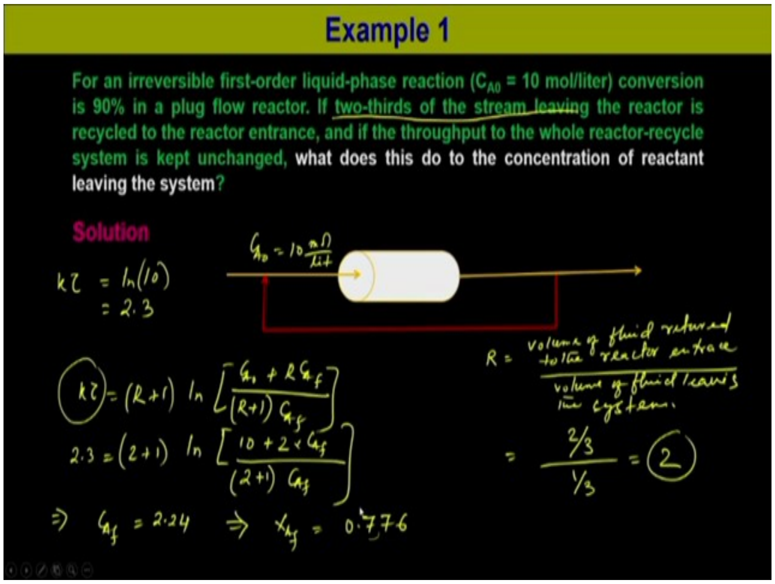

Example 1

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

Solution

$k\tau = \ln(10)$
$= 2.3$

$C_{A0} = 10 \frac{mol}{lit}$

$R = \frac{\text{volume of fluid returned to the reactor entrance}}{\text{volume of fluid leaving the system.}}$

$= \frac{2/3}{1/3} = \boxed{2}$

$\boxed{k\tau} = (R+1) \ln\left[\frac{C_{A0} + RC_{Af}}{(R+1)C_{Af}}\right]$

$2.3 = (2+1) \ln\left[\frac{10 + 2 \times C_{Af}}{(2+1)C_{Af}}\right]$

$\Rightarrow C_{Af} = 2.24 \Rightarrow X_{Af} = 0.776$

So, from the definition we can write R is equal to volume of fluid returned to the reactor entrance divided by volume of fluid leaving the system. So now, as it is said two third of the stream leaving the reactor that means is recycled. So two third is recycled and so the volume of fluid which is leaving the system is one third.

$$R = \frac{2/3}{1/3} = 2$$

So recycle ratio we can get over here is 2.

Now with recycle, for the cycle reactor we know

$$\frac{k\tau}{R+1} = (R+1)\ln\left[\frac{C_{A0} + RC_{Af}}{(R+1)C_{Af}}\right]$$

this is for first order reaction, we have derived this relation. So if we substitute the values say C_{Af} we have to calculate. So, $k\tau$ we have calculated earlier,

$$k\tau = \ln\frac{10}{1} = \ln(10) = 2.3$$

So if we substitute

$$2.3 = (2+1)\ln\left[\frac{10+2C_{Af}}{(2+1)\mathrm{C}_{Af}}\right]$$

So if we simplify this would give

$$C_{Af} = 2.24$$

Or we can write from here

$$X_{Af} = 0.776$$

So if we keep the throughput through the whole recycle reactor unchanged it will change the exit conversion to 0.776. So, the final conversion will be reduced.

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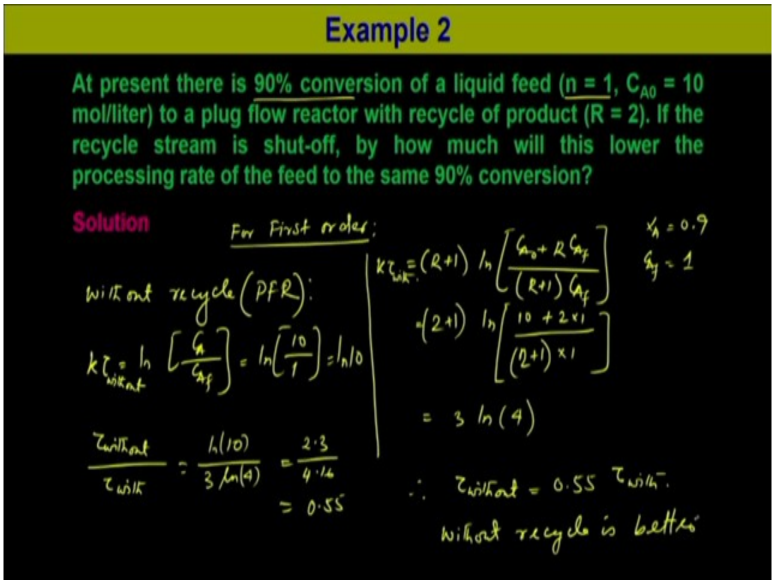

Example 2

At present there is 90% conversion of a liquid feed (n = 1, C_{A0} = 10 mol/liter) to a plug flow reactor with recycle of product (R = 2). If the recycle stream is shut-off, by how much will this lower the processing rate of the feed to the same 90% conversion?

Solution

For First order:

$X_A = 0.9$

$C_{Af} = 1$

without recycle (PFR):

$k\tau_{without} = \ln\left[\frac{C_{A0}}{C_{Af}}\right] = \ln\left(\frac{10}{1}\right) = \ln 10$

$k\tau_{with} = (R+1)\ln\left[\frac{C_{A0}+RC_{Af}}{(R+1)C_{Af}}\right]$

$= (2+1)\ln\left[\frac{10+2\times1}{(2+1)\times1}\right]$

$= 3\ln(4)$

$\frac{\tau_{without}}{\tau_{with}} = \frac{\ln(10)}{3\ln(4)} = \frac{2.3}{4.16} = 0.55$

$\therefore \tau_{without} = 0.55\,\tau_{with}$.

without recycle is better

Now take another example. At present there is 90% conversion of a liquid feed (n=1, C_{A0} = 10 $\frac{mol}{L}$) to a plug flow reactor with recycle of product and recycle ratio is given R=2, if the recycle stream is shut off, by how much will this lower the processing rate of the feed to the same 90% conversion? So, basically recycled reactor later converted to the plug flow reactor.

So, let us solve this. So this since n = 1. So this is first order reaction. So for first order reaction, we know that

$$k\tau = (R+1)\ln\left[\frac{C_{A0}+RC_{Af}}{(\mathrm{R}+1)\mathrm{C}_{Af}}\right]$$

Now, if we substitute the values

$$k\tau = (2+1)\ln\left[\frac{10+2\times1}{(2+1)\times1}\right]$$

Now with recycle this is with the recycle. Now, without recycle. That means it is PFR, we can write

$k\tau = 3\ln(4)$

$$k\tau = \ln\left(\frac{C_A}{C_{Af}}\right)\ln\frac{10}{1} = \ln(10)$$

So, if we take the ratio their $k\tau$. So this is without and this is with recycled. So, if we take

$$\frac{\tau_{without}}{\tau_{with}} = \frac{\ln(10)}{3\ln(4)} = \frac{3.4}{4.16} = 0.55$$

So hence, we can write

$\tau_{without} = 0.55\tau_{with}$

So that means, we can see that without recycle is better. So without recycle is better.

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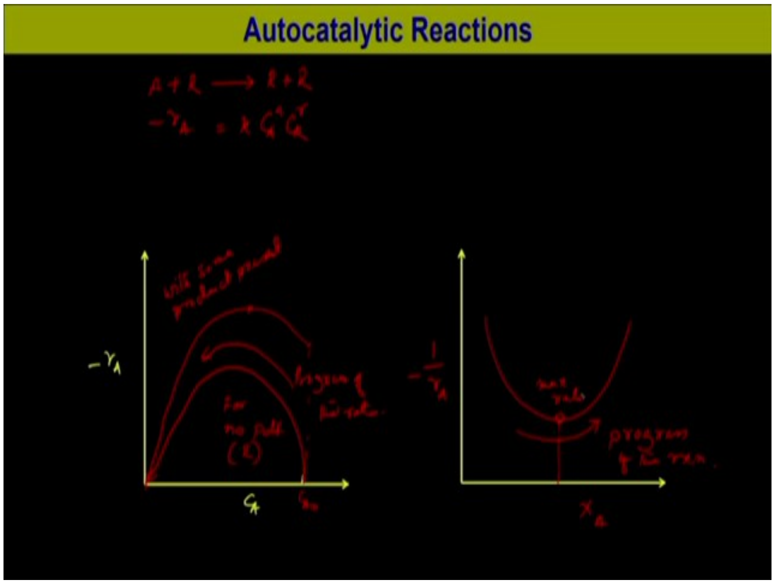

Autocatalytic Reactions

$A + R \longrightarrow R + R$

$-r_A = k C_A^a C_R^r$

So now, we will discuss autocatalytic reaction. As we have seen for any positive order reaction for batch reactor we have seen that as the reaction proceeds, the concentration drops and the reaction rate decreases. So the rate changes progressively, as the rate decreases progressively as the reactant concentration is decreased.

But, in case of autocatalytic reaction, the reactants reacts with the product which is formed and then the reaction proceeds. So reactions become faster. So in this case what happens at the beginning we need to have certain products, so that which can react reactant and form the product again.

So, autocatalytic reactions if we consider the rate versus concentration change, say this is minus $-r_A$ versus C_A initially when the reaction starts at a high concentration, starts with C_{A0} and the reaction rate increases progressively and then it decreases. So basically it starts with C_{A0}, initially there are very small quantities of the product is present, then the reaction starts, the rate increases progressively and then it reaches maximum.

So this is basically if reaction can start without any product, say if we consider with the rate $-r_A = kC_A^a C_R^r$, and if the reactions can start without the product, it will be very low rate initially and as soon as the product will form then they will react and the rate will be faster. So this is for no product R, if we have some product present at the start of the reaction, so this rate could have been started at higher and then the rate could have been like this.

So this is with some product present and the progress of the rate is like this. Now this autocatalytic reactions leads to a very interesting optimization problem as we can see because it gives maxima or minima once it reacts and starts, it reaches to a maxima or minima and then goes to completion. So if we plot minor $-\frac{1}{r_A}$ versus X_A conversion, the plot would be like this. So this would be the maximum point of rate. So this is the progress of the reaction and this point is the maximum rate.

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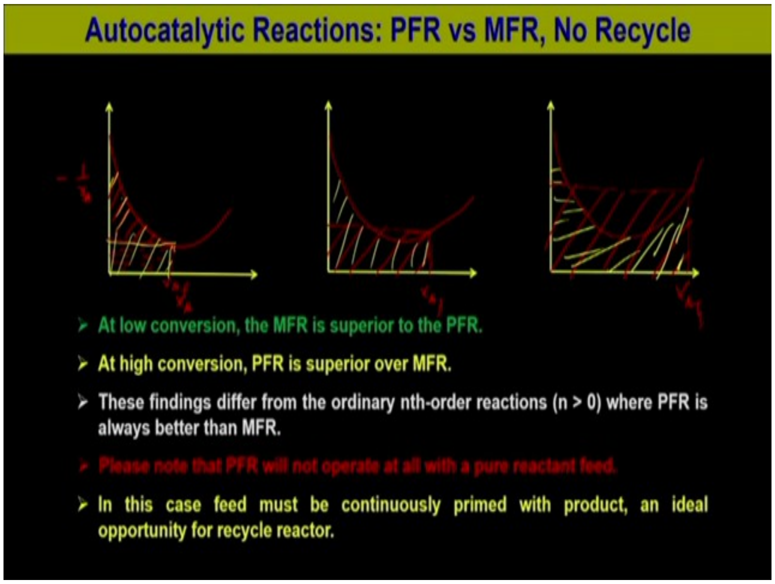

Autocatalytic Reactions: PFR vs MFR, No Recycle

- At low conversion, the MFR is superior to the PFR.
- At high conversion, PFR is superior over MFR.
- These findings differ from the ordinary nth-order reactions (n > 0) where PFR is always better than MFR.
- Please note that PFR will not operate at all with a pure reactant feed.
- In this case feed must be continuously primed with product, an ideal opportunity for recycle reactor.

If we consider plug flow versus mixed flow and no recycle. In this case, we can see that if we plot $-\frac{1}{r_A}$ versus X_A. So the plot would be like this and the conversion if we take this is X_{Af}. So this is MFR and this is PFR. Now 3 cases we will see. In another case, so if we take the conversion initial conversion is high say X_{Af}. So the CSTR would take the volume this much, whereas PFR will take the volume this 1.

Now, if we take very high conversion say so this is the volume required for CSTR and the PFR, PFR volume would be this much. So we can see that at low conversion the MFR would be superior as we can see that the volume requirement for CSTR would be small compared to the plug flow reactor volume. So, if we go to moderate conversion say X_{Af}, at high conversion here we can see PFR is superior compared to the CSTR because the volume requirement for PFR is small compared to the CSTR.

And this finding differ for ordinary nth order reaction that is n greater than 0, where PFR is always greater than MFR. So it may be noted that PFR will not operate at all with pure reactant feed. As we can see for autocatalytic reaction, the reaction should start with certain percentage or certain concentration, minimum concentration of the product because which will initiate the autocatalytic reaction. So this is ideal for the recycle reactor. So in this case feed must be continuously primed with product an ideal opportunity for the recycle reactor.

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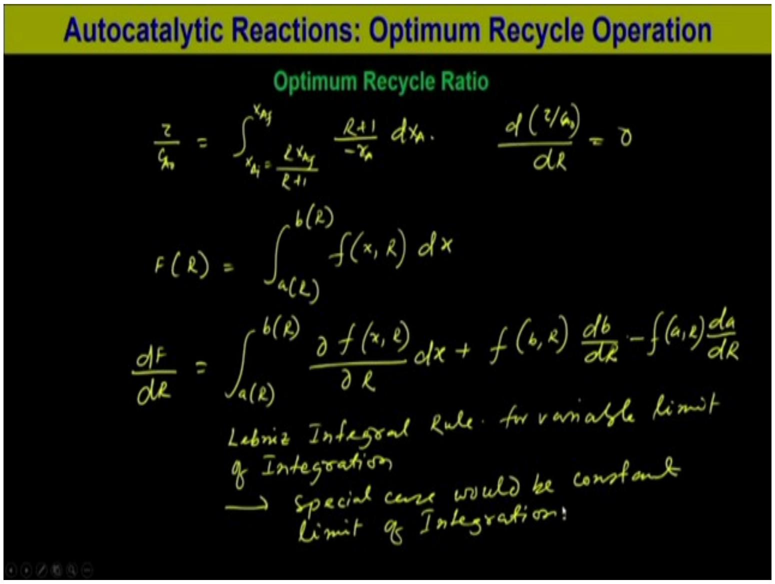

Autocatalytic Reactions: Optimum Recycle Operation

Optimum Recycle Ratio

$$\frac{\tau}{C_{A0}} = \int_{X_{Ai}=\frac{RX_{Af}}{R+1}}^{X_{Af}} \frac{R+1}{-r_A}\, dX_A . \qquad \frac{d(\tau/C_{A0})}{dR} = 0$$

$$F(R) = \int_{a(R)}^{b(R)} f(x,R)\, dx$$

$$\frac{dF}{dR} = \int_{a(R)}^{b(R)} \frac{\partial f(x,R)}{\partial R} dx + f(b,R)\frac{db}{dR} - f(a,R)\frac{da}{dR}$$

Lebniz Integral Rule. for variable limit of Integration

→ special case would be constant limit of Integration!

Now, we can calculate the optimum recycle ratio, the optimum recycle ratio we can calculate from the earlier equation that we have derived $\frac{\tau}{C_{A0}}$ for recycled reactor would be equal to $\frac{\tau}{C_{A0}} = \int_{X_{Ai}=\frac{RX_{Af}}{R+1}}^{X_{Af}} \frac{R+1}{-r_A} dX_A$ and if we differentiate this equation that means $\frac{d(\tau / C_{A0})}{dR} = 0$ we can obtain the optimum recycle ratio. And this can be done using the differentiation under the integral which can be done from theorem of calculus.

As we know

$$\frac{dF}{dR} = \int_{a(R)}^{b(\mathrm{R})} \frac{\partial f(\mathrm{x,R})}{\partial R} dx + f(\mathrm{b,R})\frac{db}{dR} - f(\mathrm{a,R})\frac{da}{dR}$$

So, this is Leibniz integral rule for variable limit of integration and special case would be constantly limit of integration.

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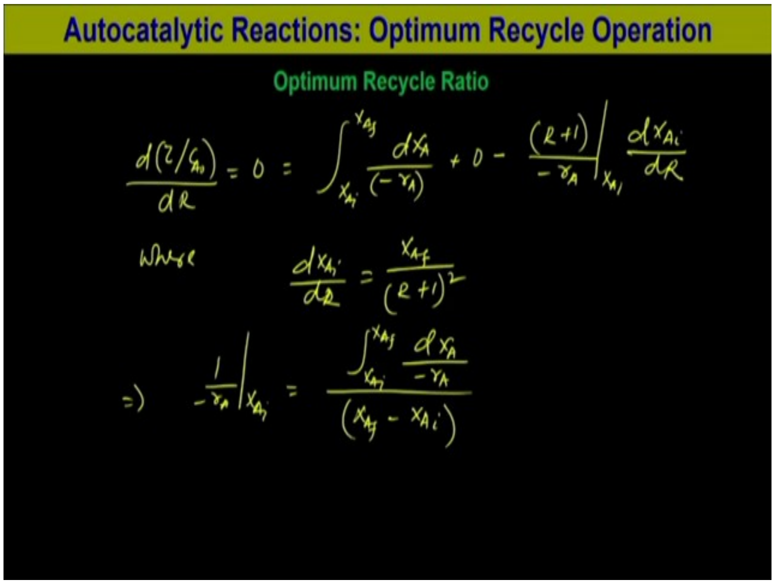

Autocatalytic Reactions: Optimum Recycle Operation

Optimum Recycle Ratio

$$\frac{d(\tau/C_{A0})}{dR} = 0 = \int_{X_{Ai}}^{X_{Af}} \frac{dX_A}{(-r_A)} + 0 - \left.\frac{(R+1)}{-r_A}\right|_{X_{Ai}} \frac{dX_{Ai}}{dR}$$

Where $\frac{dX_{Ai}}{dR} = \frac{X_{Af}}{(R+1)^2}$

$$\Rightarrow \left.\frac{1}{-r_A}\right|_{X_{Ai}} = \frac{\int_{X_{Ai}}^{X_{Af}} \frac{dX_A}{-r_A}}{(X_{Af} - X_{Ai})}$$

Now, if we apply this same thing in this case, this would be

$$\frac{d\left(\tau/C_{A0}\right)}{dR} = 0 = \int_{X_{Ai}}^{X_{Af}} \frac{dX_A}{-r_A} + 0 - \left.\frac{(R+1)}{-r_A}\right|_{X_{Ai}} \frac{dX_{Ai}}{dR}$$

$$\text{Where } \frac{dX_{Ai}}{dR} = \frac{X_{Af}}{(R+1)^2}$$

So, if we combine this and rearrange this relation we will obtain

$$\left.\frac{1}{-r_A}\right|_{X_{Ai}} = \frac{\int_{X_{Ai}}^{X_{Af}} \frac{dX_{Ai}}{-r_A}}{(X_{Af} - X_{Ai})}$$

So in other words, we can see that the optimum recycle ratio introduces to the reactor if it whose

$-\frac{1}{r_A}$ value equals to the average value.

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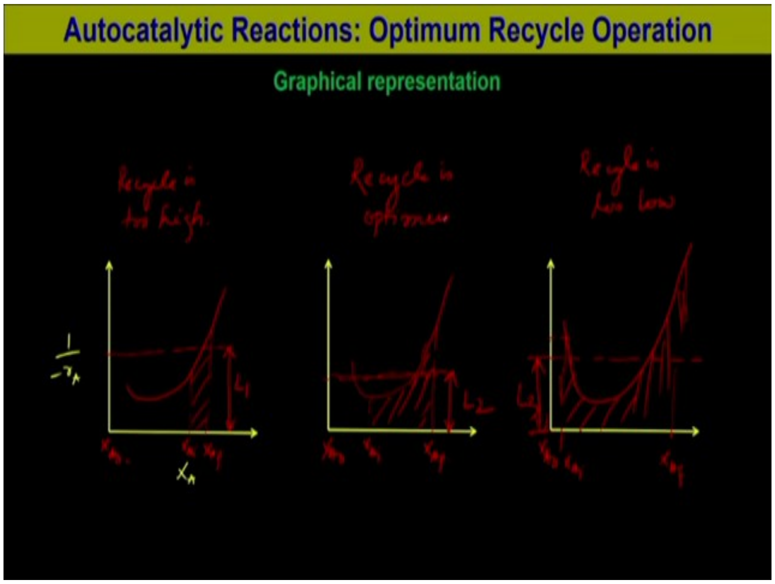

Autocatalytic Reactions: Optimum Recycle Operation

Graphical representation

This can be seen graphically. So, if we plot $-\frac{1}{r_A}$ versus $-\frac{1}{r_A}$ we could see that if recycle is very high, then for this particular type of rate concentration curve, this is say X_{Ai} to X_{Af} and this is X_{A0}, this is area under the integral. So the average height would be say this much say L1 and if we take, see high X_{Ai} values to X_{Af} and this is X_{A0} this is the area under the curve and this is the average height say L2 and recycle is very low. So that means say X_{Ai} to X_{Af}.

So the area requirement which is X_{A0}, so this is PFR and the average height is say somewhere here say L3. The first case is recycle is too high, this is recycle is too low and this is recycle is optimum.

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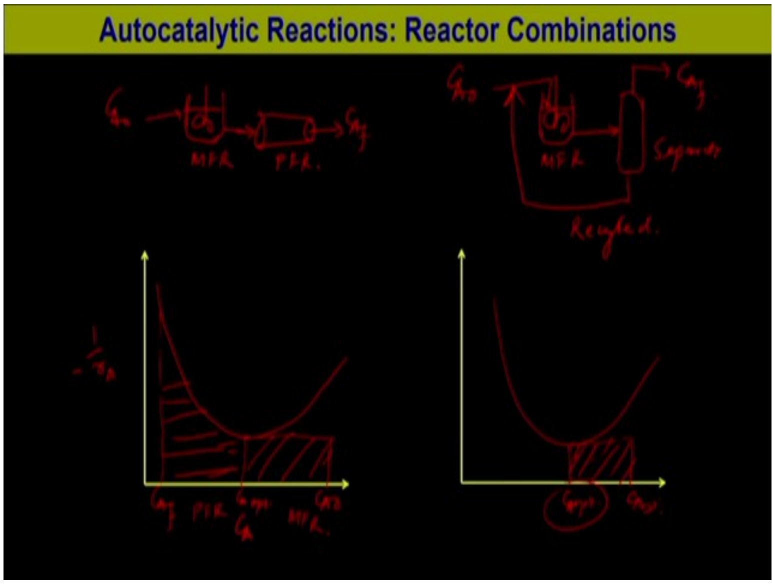

Autocatalytic Reactions: Reactor Combinations

Now, if we consider combination of the reactors say if we have plug flow and CSTR, we can always look into the arrangement of the PFR and CSTR arrangement in such a way that the total volume requirement for autocatalytic reaction is minimum. Say, if we consider these 2 cases, say we have mixed flow reactor, where we have C_{A0} this is MFR, then outlet from here is going to PFR. And finally, we are getting C_{Af}, this is PFR. In this case the product which is, we are getting is not separated and is fed to the PFR. So the overall volume requirement in this case is $-\frac{1}{r_A}$ versus concentration if we plot and the nature of the curve is like this autocatalytic reaction.

So we can, say this is optimum. So this and our initial start of the concentrations is C_{A0}. So we will look for CSTR this 1, and rest to C_{Af}. So this is PFR. Now, if we have option to separate the product and recycle back, in this case we can see that say if we have CSTR and the product which is coming out is separated here and recycled back to the reactor entrance. So this is recycled reactor MFR and this is separator.

So you can separate the product C_{Af}, so in this case, we can see that the volume requirement would be; so this is optimum and this is the C_{A0}. So we can see that only MFR volume upto optimum concentration we can run with the CSTR with recycle. So looking into the rate concentration curve and the options available in hand, whether we can separate the product and then recycle back or without recycle whether we can process it depending on that we can decide which option to choose or which would be more desired design or optimum design.

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THANK YOU

So, thank you very much for attending this lecture and we will continue our discussion on the reactor design part in the next lecture.