Polymer Reaction Engineering
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Lecture – 21
Recycle Reactor and Autocatalytic Reaction

Welcome to the recycle reactor and autocatalytic reaction system under the head of polymer reaction engineering. Now, before we go into detail, let us have a look at what we studied previously. Previously, we discussed about the preference for various kinds of reactor which are being in practice, then we read a discussion about the plug flow reactor in series and a parallel then we discussed about the mixed flow reactor in series. We had a discussion about the different type of reactors in series.

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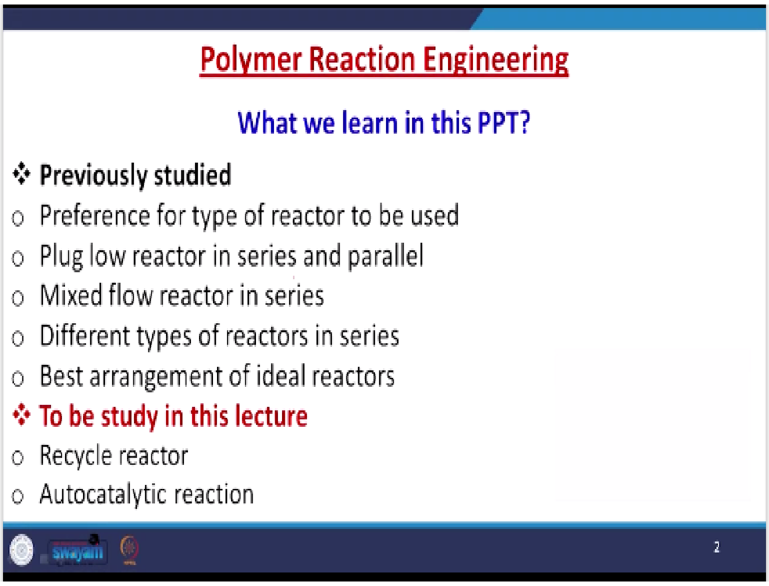

Polymer Reaction Engineering

What we learn in this PPT?

- **Previously studied**
  - Preference for type of reactor to be used
  - Plug low reactor in series and parallel
  - Mixed flow reactor in series
  - Different types of reactors in series
  - Best arrangement of ideal reactors
- **To be study in this lecture**
  - Recycle reactor
  - Autocatalytic reaction

And we had a discussion about the best arrangement to be suited for any kind of ideal reactor system. And in this particular lecture, we are going to discuss about the recycle reactor and autocatalytic reaction system.

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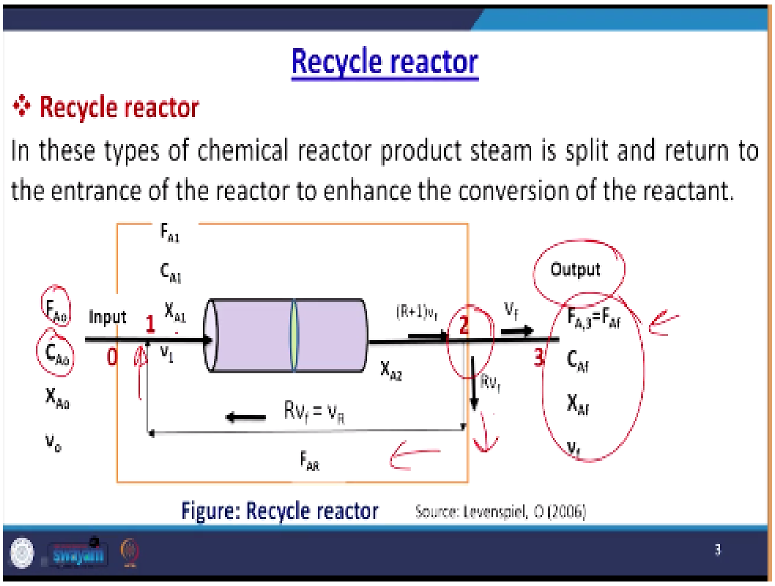

Recycle reactor

- Recycle reactor

In these types of chemical reactor product steam is split and return to the entrance of the reactor to enhance the conversion of the reactant.

Figure: Recycle reactor

Source: Levenspiel, O (2006)

Now, recycle reactors they are very common in the chemical engineering as well as the polymer engineering aspect and in these types of chemical reactor, product stream is usually split in and returned to the entrance of the reactor to enhance the conversion of the reactor. Now, see sometimes because of the requirement of space because of the requirement of other limitations to cater the need of other limitations, we may have the reactors, which is not as per the required size.

So, in that case there are certain reactant streams those enter into a particular reactor may unreacted. So, at the outlet at this point, you must separate all those things and then you may send back all those things to the inlet of the reactor for the better conversion. And rest remaining thing you can, you may have as an output. So, other things are always same like feed rate, concentration, molar conversion, etcetera.

All these things are remaining same and we have designated all these things in their respective notations over here. Now, if you see that at point 1, we are feeding the fresh feed.

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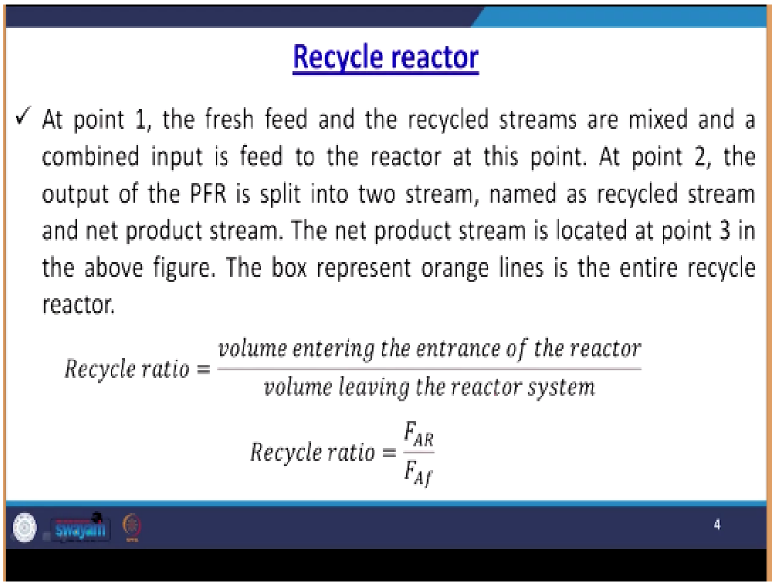

Recycle reactor

- ✓ At point 1, the fresh feed and the recycled streams are mixed and a combined input is feed to the reactor at this point. At point 2, the output of the PFR is split into two stream, named as recycled stream and net product stream. The net product stream is located at point 3 in the above figure. The box represent orange lines is the entire recycle reactor.

$$Recycle\ ratio = \frac{volume\ entering\ the\ entrance\ of\ the\ reactor}{volume\ leaving\ the\ reactor\ system}$$

$$Recycle\ ratio = \frac{F_{AR}}{F_{Af}}$$

And the recycled streams usually they are mixed and a combined input feed is to the reactor at point 1. Now, here you may have to look into a couple of points. One point is that when we talk about the things related to the concentration, when we talk about the things related to the feede,r then we have to look into this aspect that this the return stream or recycling stream is also participating into the input stream.

So, this particular approach we need to be able to address while considering all these things. So, sometimes we need to look into that what should be my recycle ratio and how we can utilise this recycle ratio in respective time. So, recycle ratio is referred as a volume entering the entrance of the reactor divided by the volume leaving the reactor system. So, keeping in view of this particular figure in cognitions, the recycle ratio is referred as F_{AR} upon F_{Af}, F_{Af} is the output feed rate and F_{AR} is the recycle rate.

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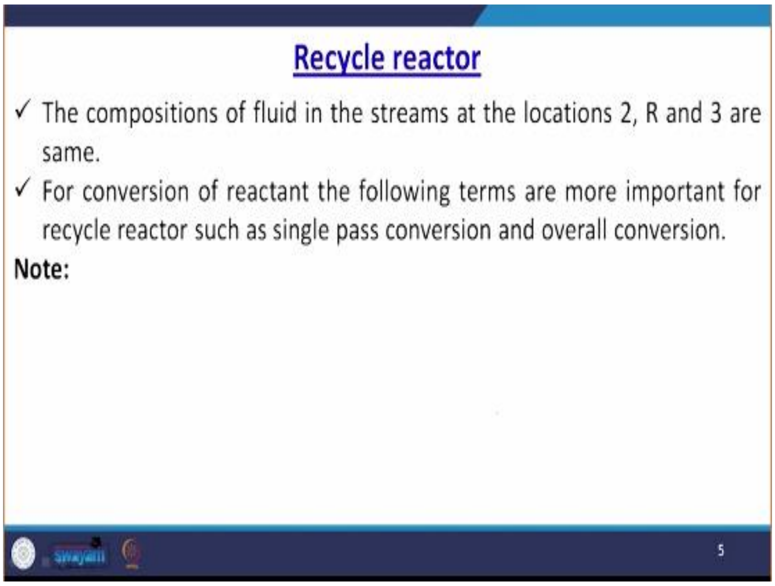

Recycle reactor

- ✓ The compositions of fluid in the streams at the locations 2, R and 3 are same.
- ✓ For conversion of reactant the following terms are more important for recycle reactor such as single pass conversion and overall conversion.

Note:

Now, when we talk about the composition of the fluid in the stream usually which is situated at this location number 2, then R and 3 are the same, then for the conversion of the reactant in the various terms can be given and they attract more important aspects comparatively, there is a recycle reactor system. And sometimes you may need to address the things related to the single pass conversion and overall conversion system.

Now, let us have a look about this particular thing that when we talk about the single pass conversion.

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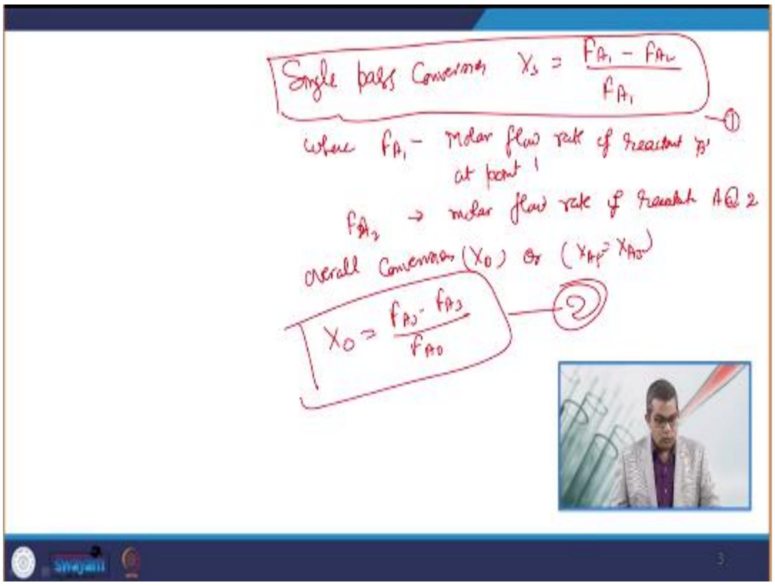

$$\boxed{\text{Single pass Conversion } X_s = \frac{F_{A_1} - F_{A_2}}{F_{A_1}}} \quad \text{—①}$$

where F_{A_1} – molar flow rate of reactant 'A' at point 1

F_{A_2} → molar flow rate of reactant A @ 2

overall Conversion (X_0) or $(X_{Af} = X_{A0})$

$$\boxed{X_0 = \frac{F_{A0} - F_{A3}}{F_{A0}}} \quad \text{—②}$$

Now, single pass conversion F_{A1}. This is my equation number 1. Now, where we can say that F_{A1} that is equal to the molar flow rate of reactant A at point 1 and F_{A2} is the molar flow rate of reactant A at point 2. So, we can write the overall conversion X_o or we can say X_{Af} is equal to X_{A3}. So, we can write more general equation that X_0 is equal to $F_{A0} - F_{A3}$ upon F_{A0}, this can be represented as equation number 2.

$$\text{Single pass conversion } (X_S) = \frac{F_{A_1} - F_{A_2}}{F_{A_1}}$$

$$\text{Overall conversion } (X_O) = \frac{F_{A_o} - F_{A_3}}{F_{A_o}}$$

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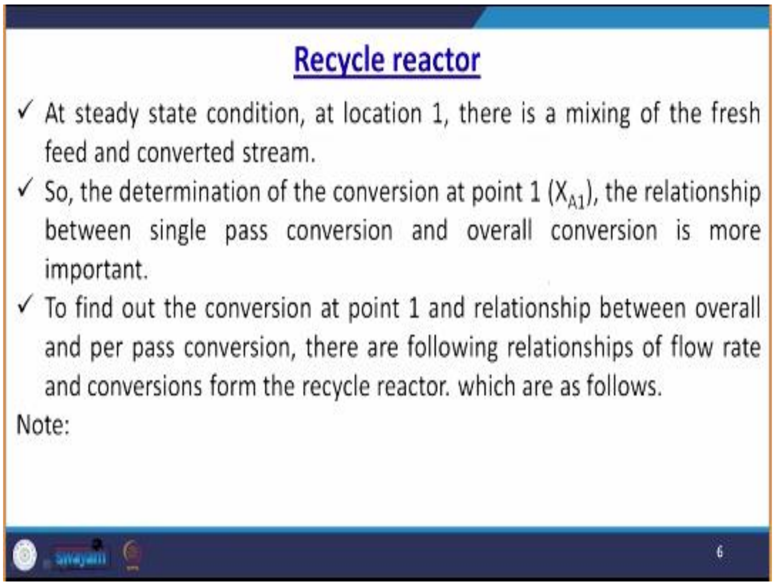

Recycle reactor

- ✓ At steady state condition, at location 1, there is a mixing of the fresh feed and converted stream.
- ✓ So, the determination of the conversion at point 1 (X_{A1}), the relationship between single pass conversion and overall conversion is more important.
- ✓ To find out the conversion at point 1 and relationship between overall and per pass conversion, there are following relationships of flow rate and conversions form the recycle reactor. which are as follows.

Note:

Now, sometimes people may look into the steady state conversion during the concept of recycle reactor. So, at a steady state condition the location 1 that is the inlet of the reactor, there is a mixing of a fresh feed and converted stream. So, these 2 streams are being mixed therefore, the determination of the conversion at point 1 after say time t that X_{A1} the relationship between the single past conversion and overall conversion is more important.

Now, to find out the conversion at point 1 and the relationship between the overall and per pass conversion and there is a requirement of several relationship of flow rate and conversion from the recycle reactor which we can develop like this.

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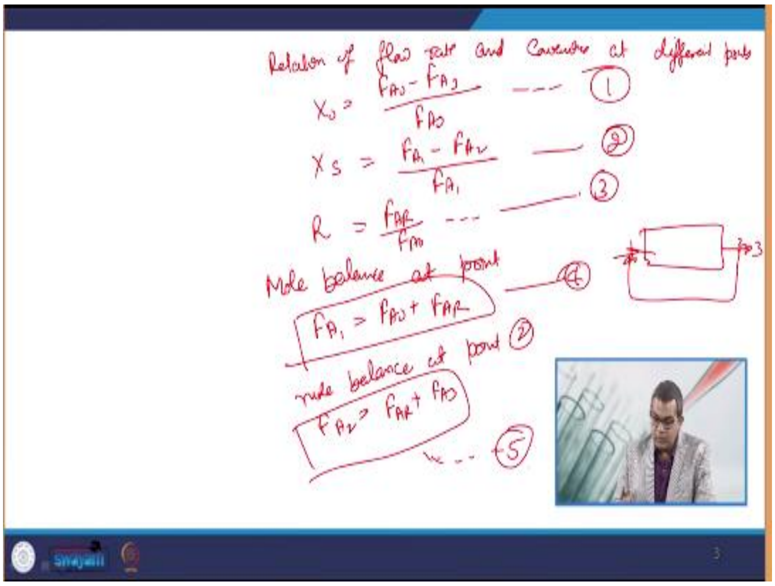

Relation of flow rate and Conversion at different points

$X_0 = \frac{F_{A0} - F_{A3}}{F_{A0}}$ --- ①

$X_S = \frac{F_{A1} - F_{A2}}{F_{A1}}$ — ②

$R = \frac{F_{AR}}{F_{A0}}$ --- ③

Mole balance at point

$\boxed{F_{A1} = F_{A0} + F_{AR}}$ — ④

mole balance at point ②

$\boxed{F_{A2} = F_{AR} + F_{A3}}$ --- ⑤

When we try to develop that is the relation of flow rate and conversion at different point. So, we can write X_0 is equal to $F_{A0} – F_{A3}$ upon F_{A0} that you can represent like equation number 1. It is different with the previous one. Now, X_S is equal to $F_{A1} – F_{A2}$ upon F_{A1}, 2. And then we talk about this recycle ratio F_{AR} upon F_{A3} that is represented as equation number 3.

$$\text{Overall conversion } (X_O) = \frac{F_{A_O} - F_{A_3}}{F_{A_O}} \ldots\ldots\ldots(1)$$

$$\text{Single pass conversion } (X_S) = \frac{F_{A_1} - F_{A_2}}{F_{A_1}} \ldots\ldots\ldots(2)$$

$$Recycle\ ratio\ (R) = \frac{F_{AR}}{F_{A_O}} \ldots\ldots\ldots(3)$$

Now, if we try to write the mole balance at point 1, then we can write the mole balance equation with respect to this fulid $F_{A1} = F_{A0} + F_{AR}$, that may be equation number 4. So, mole balance at point 2 that is this point 2 that can be written as $F_{A2} = F_{AR} + F_{A3}$. So, that we can say that this is my equation number 5.

Mole balance at point ‘1’

$$F_{A1} = F_{A0} + F_{AR} \ldots\ldots\ldots(4)$$

Mole balance at point ‘2’

$$F_{A2} = F_{AR} + F_{A3} \ldots\ldots\ldots(5)$$

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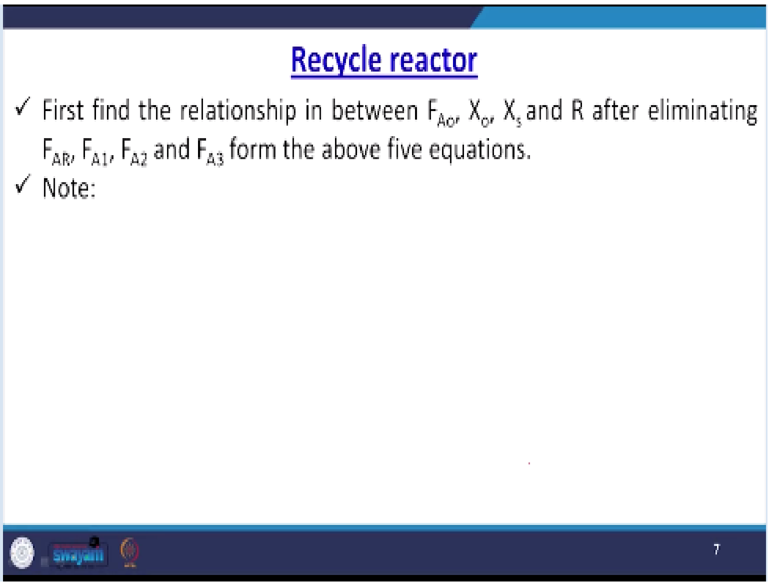

Recycle reactor

- ✓ First find the relationship in between F_{Ao}, X_o, X_s and R after eliminating F_{AR}, F_{A1}, F_{A2} and F_{A3} form the above five equations.
- ✓ Note:

So, in this in this case, we need to find the relationship in between F_{A0}, X_0, X_S and R after eliminating F_{AR}, F_{A1}, F_{A2} and F_{A3}. So, how we can eliminate these things from these 5 equations.

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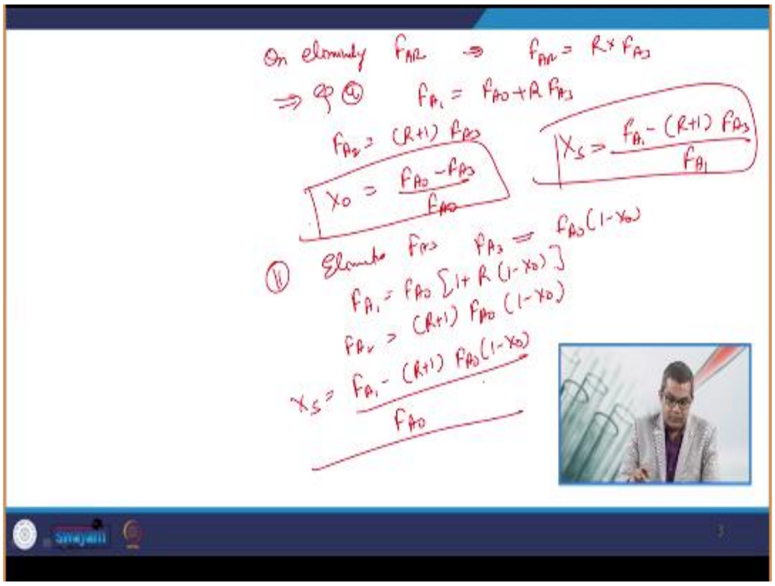

On elimunly $F_{AR} \Rightarrow F_{AR} = R \times F_{A3}$

$\Rightarrow$ eq ④ $F_{A1} = F_{A0} + R\,F_{A3}$

$F_{A2} = (R+1)\,F_{A3}$

$\boxed{X_0 = \frac{F_{A0} - F_{A3}}{F_{A0}}}$

$\boxed{X_S = \frac{F_{A1} - (R+1)\,F_{A3}}{F_{A1}}}$

⑪ Elimate F_{A3} $F_{A3} = F_{A0}(1-X_0)$

$F_{A1} = F_{A0}\left[1 + R(1-X_0)\right]$

$F_{A2} = (R+1)\,F_{A0}\,(1-X_0)$

$X_S = \frac{F_{A1} - (R+1)\,F_{A0}(1-X_0)}{F_{A0}}$

So, if we try to write the eliminating F_{AR}, this can be given as F_{AR} is equal to R x F_{A3}. That is from equation if we talk about the equation 4, then F_{A1} is equal to F_{A0} + R F_{A3}. And if we take the help of equation 5, then $F_{A2} = (R + 1)F_{A3}$. So, X_0 will become $F_{A0} – F_{A3}$ upon F_{A0}. Similarly, X_S this will become F_{A1} – (R + 1) F_{A3} upon F_{A1}. This is again.

Now if in the second step, if we try to eliminate F_{A3}, so, F_{A3} can be given as $F_{A0}(1 – X_0)$ or F_{A1} is equal to F_{A0} (1 + R(1 – X_0) and F_{A2} is equal to (R + 1) $F_{A0}(1 – X_0)$ and this is F_{A1} – (R + 1) F_{A0} (1 – X_0) upon F_{A0}. So, this is again the important equation.

On eliminating F_{AR}

$$F_{A_R} = R \times F_{A_3}$$

$$F_{A_1} = F_{A_o} + R \times F_{A_3}$$

$$F_{A_2} = (R+1) \times F_{A_3}$$

$$\text{Overall conversion } (X_O) = \frac{F_{A_o} - F_{A_3}}{F_{A_o}}$$

$$\text{Single pass conversion } (X_S) = \frac{F_{A_1} - (R+1)F_{A_3}}{F_{A_1}}$$

Now eliminating F_{A3} from the above equation, we have

$$F_{A3} = F_{A0}(1 - X_0)$$

$$F_{A_1} = F_{A_o} + R \times F_{A_o}(1 - X_o)$$

$$F_{A_2} = (R+1) \times F_{A_o}(1 - X_o)$$

$$(X_S) = \frac{F_{A_1} - (R+1)F_{Ao}(1 - X_o)}{F_{A_1}}$$

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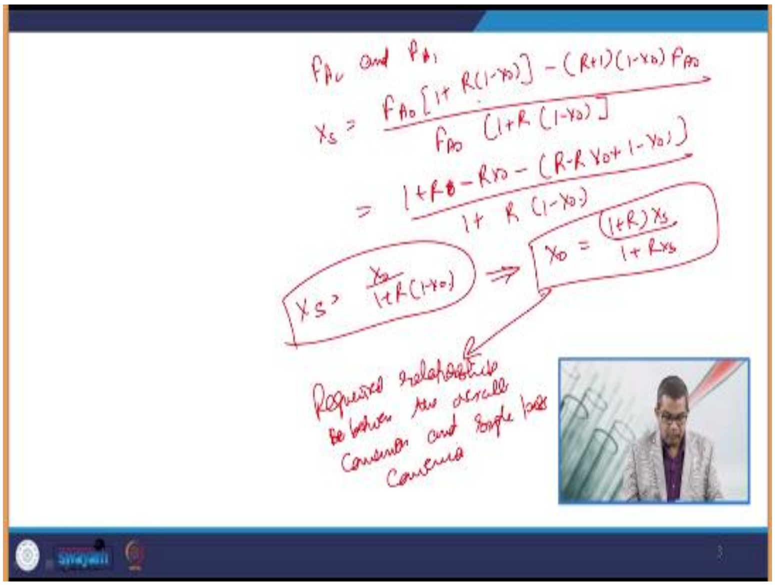

F_{A_2} and F_{A_1}

$$X_s = \frac{F_{A0}[1 + R(1-X_0)] - (R+1)(1-X_0)F_{A0}}{F_{A0}(1+R(1-X_0)]}$$

$$= \frac{1 + R - RX_0 - (R - RX_0 + 1 - X_0)}{1 + R(1-X_0)}$$

$$\boxed{X_s = \frac{X_0}{1+R(1-X_0)}} \Rightarrow \boxed{X_0 = \frac{(1+R)X_s}{1+RX_s}}$$

Required relationship between the overall conversion and single pass conversion

Now, if we eliminate F_{A2} and F_{A1}, so, X_S is equal to F_{A0} (1 + R into (1 – X_0) – (R + 1) (1 – X_0) F_{A0} divided by F_{A0} [1 + R into (1 – X_0). Or after rearrangement, it can be given as 1 + R – R X_0 from this equation, – (R – R X_0 + 1 – X_0). This is divided by 1 + R (1 – X_0). So, at last, we can write X_S is equal to X_0 upon 1 + R (1 – X_0) and if we rearrange this, then it can become X_0 is equal to 1 + R X_S upon 1 + R X_S.

On putting the value of F_{A1} in the conversion per pass and rearranging we have

$$(X_S) = \frac{F_{A_o}[1 + R \times (1 - X_o)] - (R+1)F_{Ao}(1 - X_o)}{F_{A_o}[1 + R \times (1 - X_o)]}$$

$$(X_S) = \frac{[1 + R \times (1 - X_o)] - (R + 1)(1 - X_o)}{F_{A_o}\,[1 + R \times (1 - X_o)]}$$

$$(X_S) = \frac{1 + R + (-RX_o) - R + RX_o + 1 + X_o)}{[1 + R \times (1 - X_o)]}$$

On simplifying we have

$$(X_S) = \frac{X_o}{[1 + R \times (1 - X_o)]}$$

$$(X_o) = \frac{X_S(1 + R)}{[1 + RX_S]}$$

Now, this is the required relationship between the overall conversion and single pass conversion.

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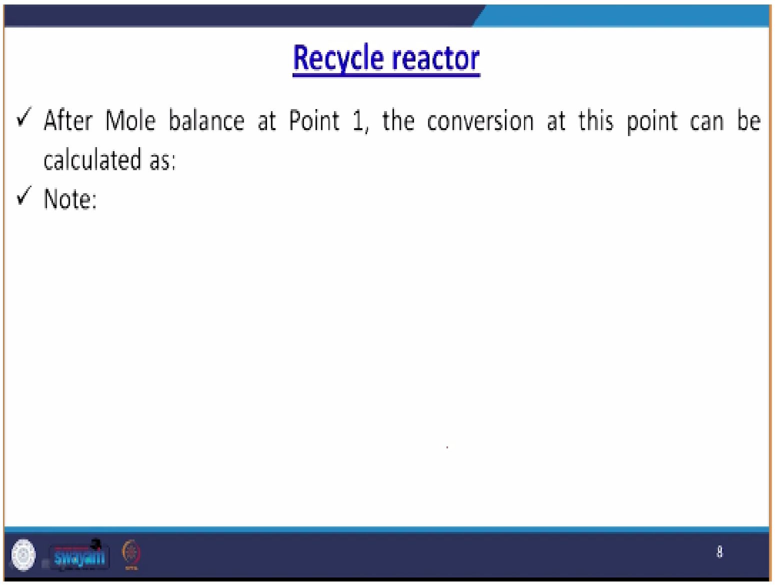

Recycle reactor

- ✓ After Mole balance at Point 1, the conversion at this point can be calculated as:
- ✓ Note:

Now, after mole balance at point 1 the conversion at this point can be calculated with this particular approach.

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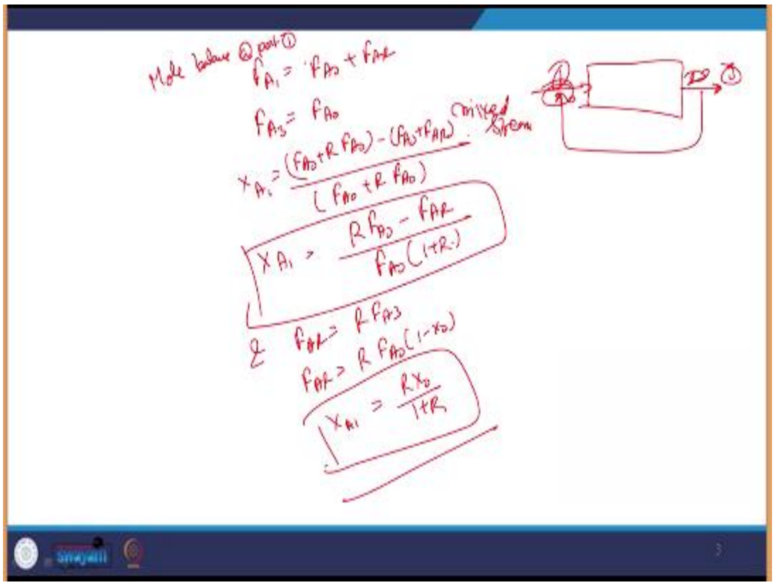

Mole balance @ point ①

$F_{A_1} = F_{A_0} + F_{AR}$

$F_{A_3} = F_{A_0}$

$X_{A_1} = \frac{(F_{A_0} + R F_{A_0}) - (F_{A_0} + F_{AR})}{(F_{A_0} + R F_{A_0})}$ mixed stream

$\boxed{X_{A_1} = \frac{R F_{A_0} - F_{AR}}{F_{A_0}(1+R)}}$

& $F_{AR} = R F_{A_3}$

$F_{AR} = R F_{A_0}(1 - X_0)$

$\boxed{X_{A_1} = \frac{R X_0}{1+R}}$

Again, we need to draw this reactor just for the ease of understanding. So, this is point 1, 2 and 3. So, F_{A1} that is mole balance at point 1, so, F_{A1}, F_{A0} + F_{AR}. It is the mixed stream because here this is the mixed stream. So, if there were no reaction the concentration of A would be higher because of the reason quite obvious. So, F_{A3} is equal to F_{A0} let us say, then X_{A1} is equal to F_{A0} + R F_{A0} – F_{A0} + F_{AR} upon F_{A0} + R F_{A0}.

Now here, we can write X_{A1} is equal to R. If we try to rearrange the things R F_{A0} – F_{AR} upon F_{A0} 1 + R. So, and F_{AR} is equal to R F_{A3} and F_{AR} is equal to R F_{A0} 1 – X_0 or X_{A1} is equal to R X_0 upon 1 + R. So, this is the required equation which is sometimes very useful for assessing the things. Now, we can use the recycling in the plug flow reactor because sometimes it is quite useful in the industrial approach.

Therefore, to write the differential form of performance equation for plug flow reactor and putting the initial value of a molar flow rate at the entrance of the reactor (R + 1)F_{A0} with the conversion X_{A1} it can be given as such.

Mole balance at point 1 we have

$$F_{A_1} = F_{A_o} + F_{A_R}$$

$$F_{A_3} = F_{A_o}$$

$$X_{A_1} = \frac{(F_{A_o} + RF_{A_o}) - (F_{A_o} + F_{A_R})}{F_{A_o} + RF_{A_o}}$$

$$X_{A_1} = \frac{(RF_{A_o} - F_{A_R})}{F_{A_o}(1+R)}$$

$$F_{A_{R=}} R \times F_{A_3}$$

$$F_{A_R} = R \times F_{A_o}(1 - X_o)$$

$$X_{A_1} = \frac{RX_o}{1 + R}$$

This is the required conversion at point ‘1’.

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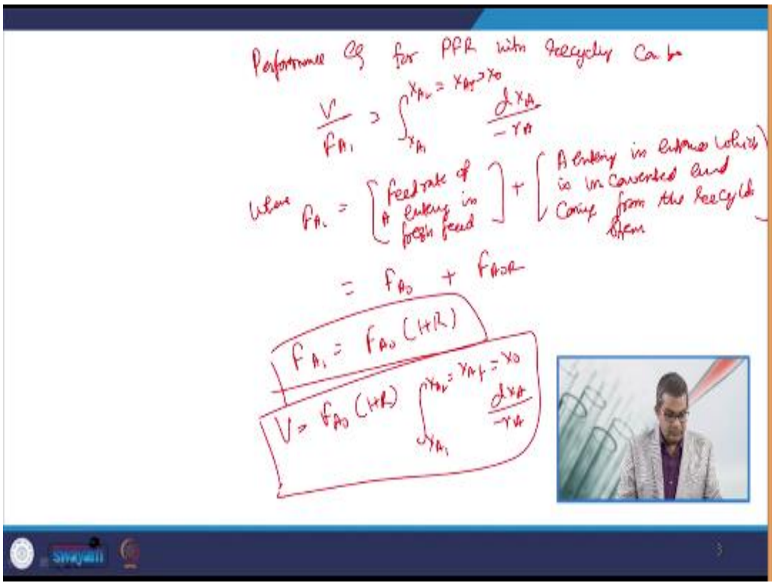

Performance eq for PFR with Recycling can be

$$\frac{V}{F_{A_1}} = \int_{X_{A_1}}^{X_{A_2} = X_{Af} = X_0} \frac{dX_A}{-r_A}$$

where $F_{A_1} = \left[\begin{array}{l}\text{feed rate of} \\ \text{A entering in} \\ \text{fresh feed}\end{array}\right] + \left[\begin{array}{l}\text{A entering in entrance which} \\ \text{is unconverted and} \\ \text{coming from the recycle stream}\end{array}\right]$

$$= F_{A_0} + F_{A_0}R$$

$$\boxed{F_{A_1} = F_{A_0}(1+R)}$$

$$\boxed{V = F_{A_0}(1+R)\int_{X_{A_1}}^{X_{A_2} = X_{Af} = X_0} \frac{dX_A}{-r_A}}$$

So, the performance equation, equation for PFR with the recycling can be V upon F_{A1} X_{A1}, X_{A2} sometimes referred as X_{Af}, X_0, etcetera, dX_A upon – r_A. Now, where F_{A1} that is equal to the feed rate of A entering in fresh feed plus A entering in entrance, which is unconverted and coming from the recycle string. So, mathematically if we try to write this thing that is that will become F_{A0} + F_{A0} R or F_{A1} will become $F_{A0}(1 + R)$. That is the recycle ratio.

Now, V can be represented as V is equal to F_{A0} (1 + R), X_{A1}, X_{A2}, X_{AF} is equal to X_0, dX_A upon – r_A.

The performance equation for PFR with recycling can be written as;

$$\frac{V}{F_{A_1}} = \int_{X_{A_1}}^{X_{A_f} = X_{A_2} = X_o} \frac{d_{X_A}}{-r_A}$$

$$F_{A_1} = F_{A_o}(1 + R)$$

$$V = F_{A_o}(1 + R) \int_{X_{A_1}}^{X_{A_f} = X_{A_2} = X_o} \frac{d_{X_A}}{-r_A}$$

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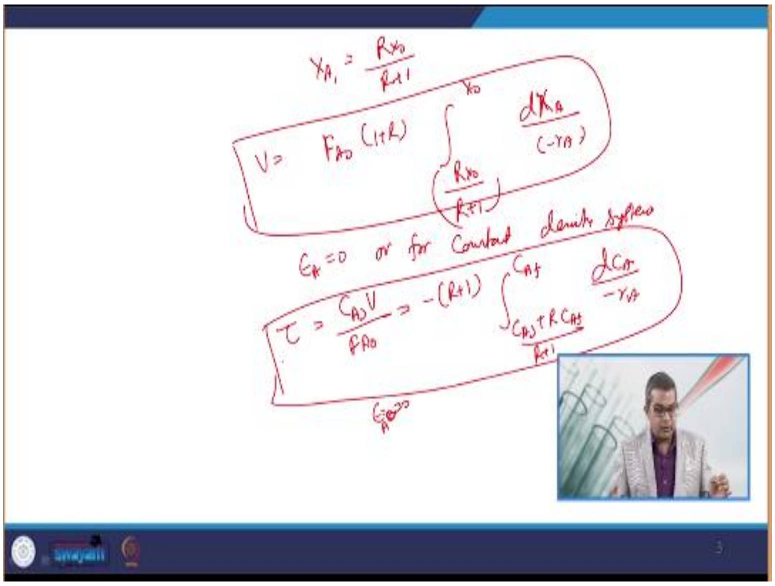

$$X_{A_1} = \frac{RX_0}{R+1}$$

$$V = F_{A0}(1+R)\int_{\frac{RX_0}{R+1}}^{X_0} \frac{dX_A}{(-r_A)}$$

$\epsilon_A = 0$ or for constant density system

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

$\epsilon_A \neq 0$

Now, this form of equation in terms of conversion this can be used for any (( )) (16:52), that is for the varying volume system. So, if we say that X_{A1} is equal to R X_0 upon (R + 1), then V is equal to F_{A0} (1 + R) RX_0 upon (R + 1) X_0 dX_A upon – r_A. Now, for a special case when epsilon A is equal to 0 or for constant density system, it can be represented with respect to the concentration term. So, tau may become C_{A0} V upon F_{A0}.

This is equal to – R + 1 C_{A0} + R C_{AF} upon R + 1 C_{AF} dC_A upon – r_A. That is for the epsilon A is equal to 0. So, this is you can say, now, suppose sometimes people may opt for graphical representation.

$$X_{A_1} = \frac{RX_o}{1+R}$$

$$V = F_{A_o}(1+R)\int_{\frac{RX_o}{1+R}}^{X_{A_f}=X_{A_2}=X_o} \frac{d_{X_A}}{-r_A}$$

For constant density system

$$\tau = \frac{VC_{A_o}}{F_{A_o}} = -(1+R)\int_{\frac{RC_{A_f}+C_{A_o}}{1+R}}^{C_{A_f}} \frac{d_{X_A}}{-r_A}$$

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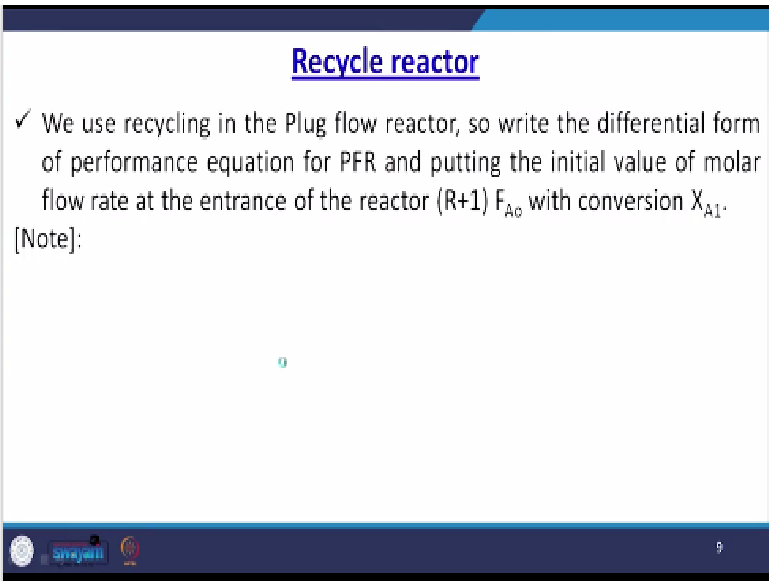

Recycle reactor

- ✓ We use recycling in the Plug flow reactor, so write the differential form of performance equation for PFR and putting the initial value of molar flow rate at the entrance of the reactor (R+1) F_{Ao} with conversion X_{A1}.

[Note]:

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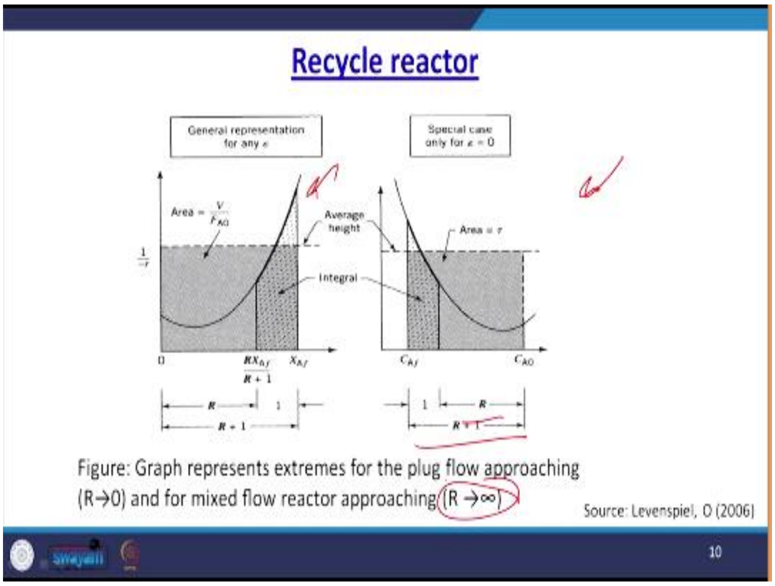

Recycle reactor

Figure: Graph represents extremes for the plug flow approaching (R→0) and for mixed flow reactor approaching (R →∞)

Source: Levenspiel, O (2006)

Now, before we go into the graphical representation, here you see that there are various type of epsilon. This is the general representation and that is for the special case when which we discussed that is epsilon is equal to 0. In that case, you can see that this one is the recycle ratio here and these extremes of the plug flow reactor sometimes approaching to R tends to 0 and the mixed flow reactor approaching to R tends to infinity.

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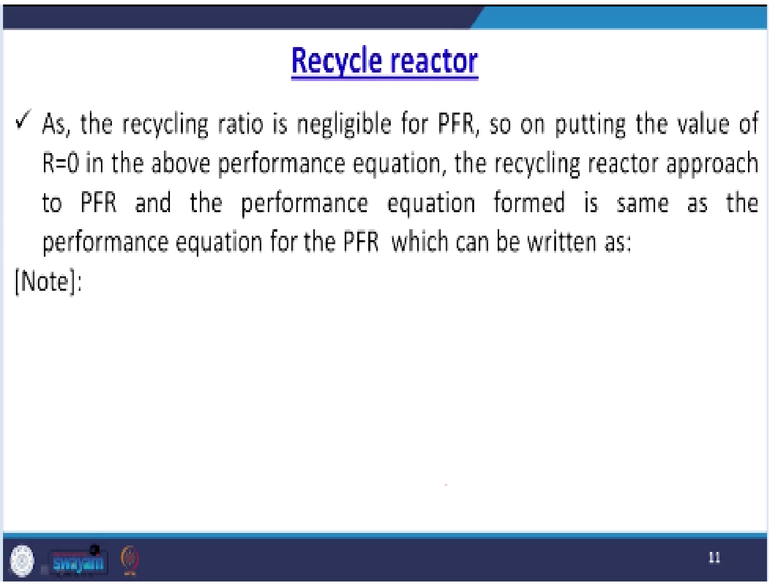

Recycle reactor

- ✓ As, the recycling ratio is negligible for PFR, so on putting the value of R=0 in the above performance equation, the recycling reactor approach to PFR and the performance equation formed is same as the performance equation for the PFR which can be written as:

[Note]:

Now, sometimes when we see that the recycling ratio is negligible for PFR. So, on putting the values of R, that is the recycle ratio the R is equal to 0 in the performance equation which we discussed the recycle link reactor approach to PFR and the performance equation is found same as the performance equation for the PFR. Now, we can write these equations in the following form.

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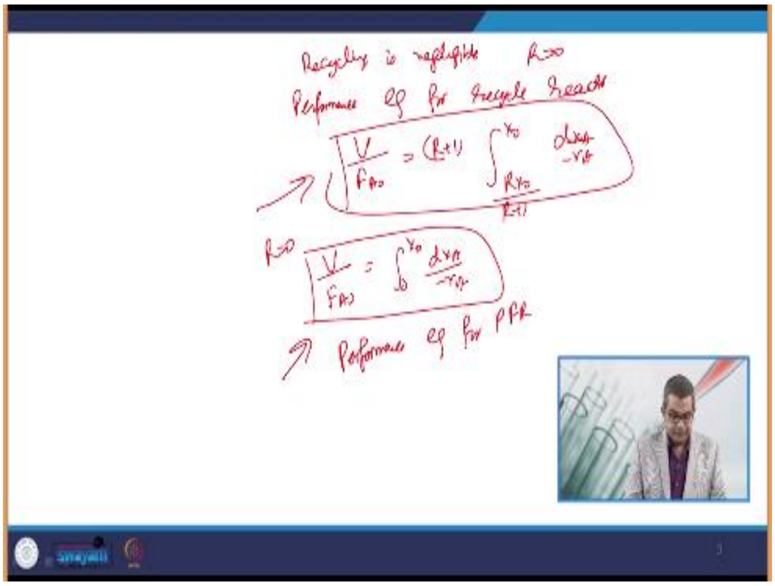

Recycling is negligible $R \to 0$

Performance eq for recycle reactor

$$\frac{V}{F_{A0}} = (R+1) \int_{\frac{RX_0}{R+1}}^{X_0} \frac{dX_A}{-r_A}$$

$R \to 0$

$$\frac{V}{F_{A0}} = \int_0^{X_0} \frac{dX_A}{-r_A}$$

Performance eq for PFR

Let us take the example that when the recycling is negligible. That is R, sometimes you may take the R is equal to 0. And the performance equation for recycle reactor that is V upon F_{A0}, R + 1, R X_0 upon R + 1, X_0 dX A upon – r_A. Now, if we put R is equal to 0 in this equation, then it may become V upon F_{A0} is equal to 0. Now, this is the performance equation for PFR.

$$\frac{V}{F_{A_o}} = (1+R) \int_{\frac{RX_o}{1+R}}^{X_o} \frac{d_{X_A}}{-r_A}$$

If $R \rightarrow 0$ i.e., negligible recycling ratio then

$$\frac{V}{F_{A_o}} = \int_0^{X_A} \frac{d_{X_A}}{-r_A}$$

The required performance equation for a PFR for constant density system.

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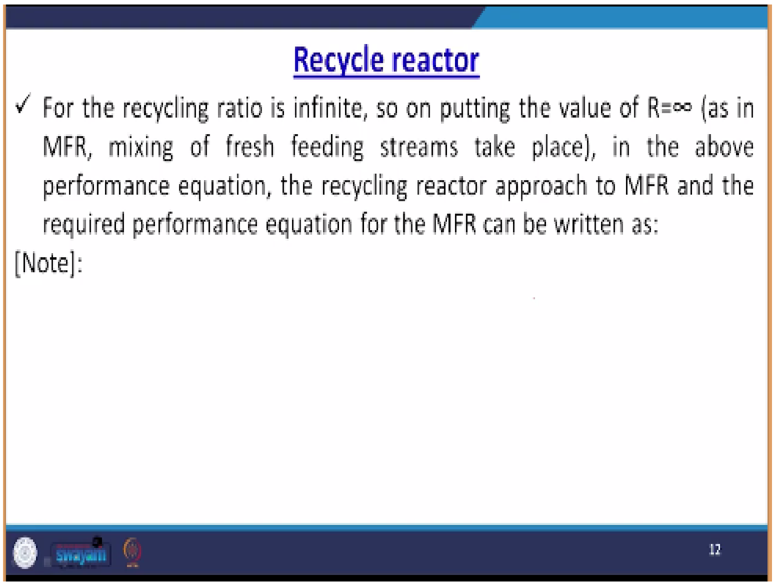

Recycle reactor

✓ For the recycling ratio is infinite, so on putting the value of R=∞ (as in MFR, mixing of fresh feeding streams take place), in the above performance equation, the recycling reactor approach to MFR and the required performance equation for the MFR can be written as:

[Note]:

Now, if we talk about the recycling ratio is infinite, so, in putting the value of R tends to infinity, sometimes we use this equation, this particular condition in mixed flow reactor for mixing a fresh feeding system sometimes will take place. So, in that case the performance equation for recycling reactor approach to mixed flow reactor the required performance equation can be modified like this when R is equal to infinite.

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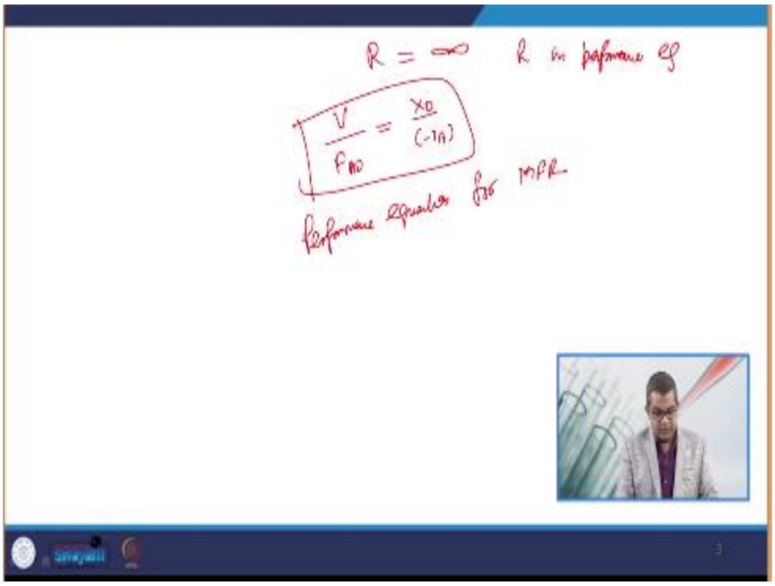

$R = \infty$ R in performance eq

$$\boxed{\frac{V}{F_{A0}} = \frac{X_A}{(-r_A)}}$$

Performance equation for MFR

So, putting the value of R in performance equation in the for the recycle reactor we have 1 upon F_{A0}, sorry, V upon F_{A0} is equal to X_0 upon – r_A. So, this is my final equation. This is the performance equation for mixed flow reactor system.

For mixed flow reactor ($R \rightarrow \infty$) i.e.,

$$\frac{V}{F_{A_o}} = \frac{X_o}{-r_A}$$

This is the required performance equation for the MFR.

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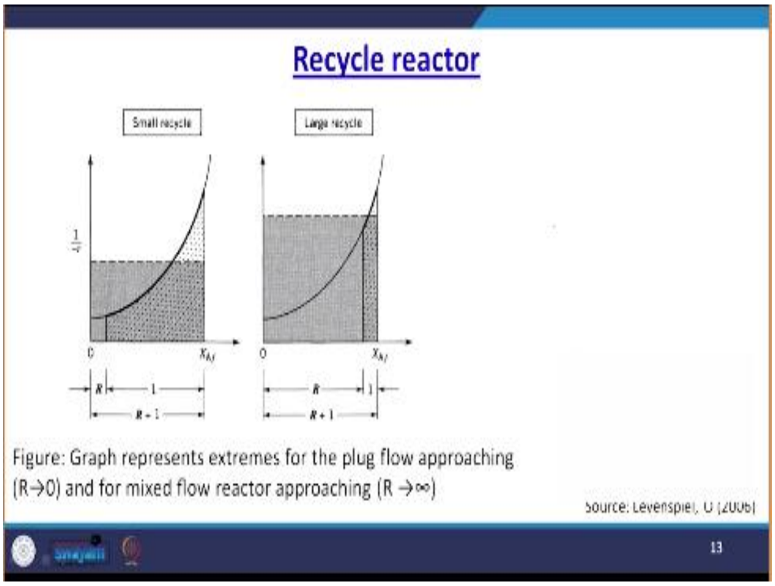

Recycle reactor

Figure: Graph represents extremes for the plug flow approaching (R→0) and for mixed flow reactor approaching (R →∞)

Source: Levenspiel, O (2006)

Now, this you can draw, we can draw with X plots and you can see that for small reactors and large reactor there is a wide variation in the particular approach.

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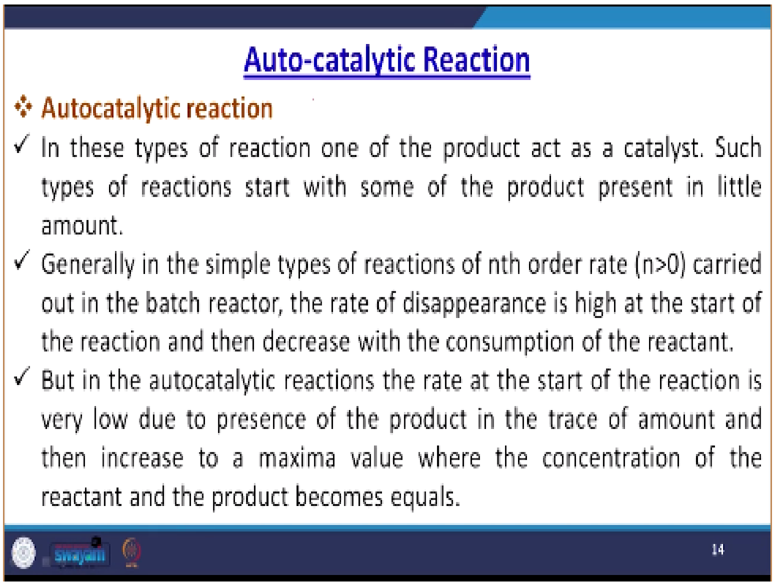

Auto-catalytic Reaction

- Autocatalytic reaction
  - ✓ In these types of reaction one of the product act as a catalyst. Such types of reactions start with some of the product present in little amount.
  - ✓ Generally in the simple types of reactions of nth order rate (n>0) carried out in the batch reactor, the rate of disappearance is high at the start of the reaction and then decrease with the consumption of the reactant.
  - ✓ But in the autocatalytic reactions the rate at the start of the reaction is very low due to presence of the product in the trace of amount and then increase to a maxima value where the concentration of the reactant and the product becomes equals.

Now, let us have a look about the autocatalytic reaction. Now, before we go for the performance equation of these autocatalytic reaction system, let us have a look about what are these reaction systems. So, in this type of reaction, one of the product act as a catalyst that is quite obvious. And it says (( )) (22:04) from the catalytic autocatalytic concept. Now, such type of reaction start with some of the product present in the little amount and then they can approach and then they can start the things exponentially.

Now, the generally when we talk in terms of a mathematical approach the simple type of reaction of nth order that is the n is greater than 0 that means the positive order reaction that is carried out in the batch reactors. The rate of disappearance is usually high at the start of the reaction and then decrease with the consumption of the reactor and that is quite obvious.

But, in autocatalytic type of reaction, the rate at the start of the reaction is very low due to the presence of the product in the trace amount and then increases because the product acts like the catalyst. So, then they have the tendency to increase to the maximum value where the concentration of the reactants and the products they sometimes become equal.

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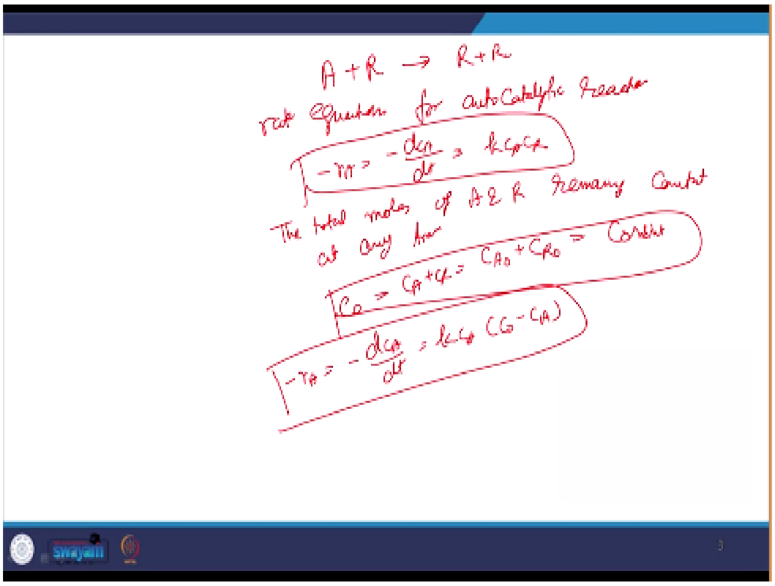

$A + R \rightarrow R + R$

rate equation for autocatalytic reaction

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

The total moles of A & R remaining constant at any time

$$\boxed{C_0 = C_A + C_R = C_{A0} + C_{R0} = \text{Constant}}$$

$$\boxed{-r_A = -\frac{dC_A}{dt} = kC_A(C_0 - C_A)}$$

So, when we say that the mathematical approach, so, this can be represented as the autocatalytic reaction. They can be represented at A + R is equal to R and the rate equation for autocatalytic reaction $-r_A = kC_AC_R$. So, the total moles of A and R remaining constant at any time, C_0 is equal to $C_A + C_R$ or $C_{A0} + C_{R0}$ that is that become the constant.

Now, the rate equation you can write the rate equation. That is quite easy-r_A is equal to –dC_A upon dt, k C_AC_0 – C_A. So, this is the start of this autocatalytic reaction.

An autocatalytic reaction can be written as;

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

The rate equation for the autocatalyst reaction can be written as

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

The total moles of A and R remaining constant at any time so,

$$C_o = C_A + C_R = C_{A_o} + C_{R_o} = constant$$

$$-r_A = -\frac{dC_A}{dt} = kC_A(C_o - C_A)$$

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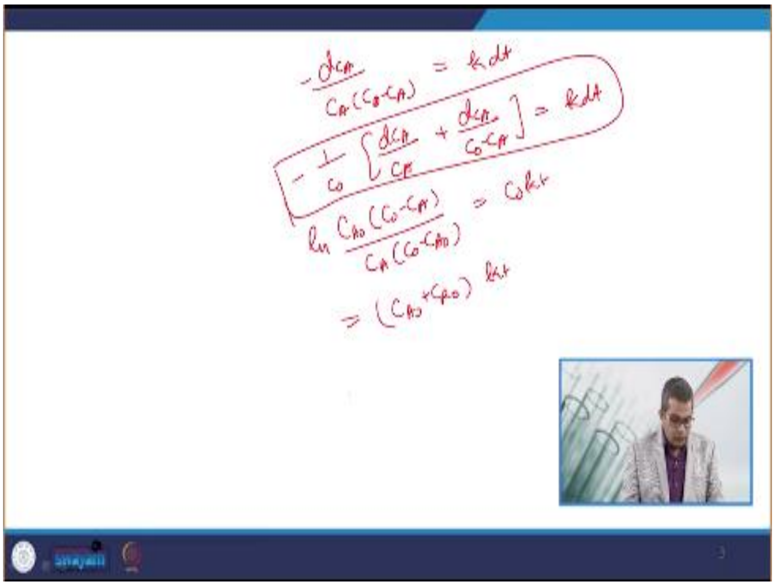

$$-\frac{dC_A}{C_A(C_0-C_A)} = k\,dt$$

$$\boxed{-\frac{1}{C_0}\left[\frac{dC_A}{C_A} + \frac{dC_A}{C_0-C_A}\right] = k\,dt}$$

$$\ln\frac{C_{A0}(C_0-C_A)}{C_A(C_0-C_{A0})} = C_0kt$$

$$= (C_{A0}+C_{R0})\,kt$$

Now, if we try to rearrange this equation, then it becomes – dC_A upon C_A upon C_0, k dt. So, if we break into the partial fractions, in that case, it becomes – 1 upon C_0 dC_A upon C_A + dC_A upon C_0 – C_A, k dt. Now, if we integrate the things, then we may have ln C_{A0} C_0 – C_A upon C_A C_0 – C_{A0} is equal to C_0kt and C_{A0} + Ckt. Now, if we try to represent these things into the graphical representation, it is quite simple.

On rearranging we have

$$-\frac{dC_A}{(C_o - C_A)} = kC_Adt$$

$$-\int_{C_{A_o}}^{C_A} \frac{1}{C_o}\left[\frac{dC_A}{(C_o - C_A)} + \frac{dC_A}{(C_o - C_A)}\right] = kC_o\int_0^t dt$$

$$\ln\left(\frac{C_{A_o}(C_o - C_A)}{C_A(C_o - C_{A_o})}\right) = kC_o t = (C_{A_o} - C_{R_o})kt$$

This is the required performance equation for autocatalytic reaction.

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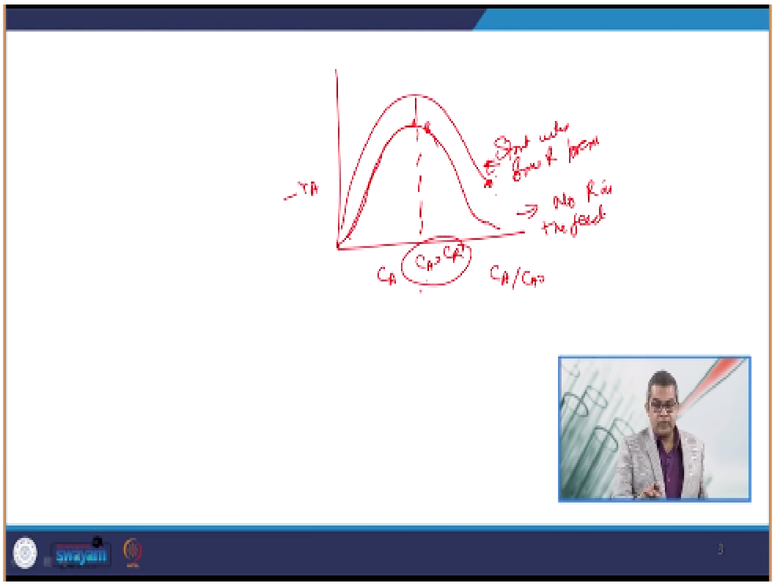

Now, see here, you are having this thing at the start. Now, this is C_A, now, here you see that at the start we are when you are having negligible product and as long as if it goes on increasing, then the product which is being formed during the course of the reaction, it acts like a catalyst to the reaction mass. Then this may become go up to the maxima. Now, when it approaches to this particular maximum at that particular point of time, it may go down.

The reason is that because the reactant, maximum amount of reactants in the reaction mass may get consumed over the period of time. So, this is the progress of time and if we talk about the sometimes you may talk about this the start with some R present. In that case, you may have this type of a curve and if there is no R in the field, then you may have like this. So, you can calculate the C_A, in that C_A is equal to C_R and C_{A0} C_A upon C_{A0}.

So, when we conceptualise this thing here, in an autocatalytic reactor reaction a batch reactor, some R must be present. Starting with a very small concentration of R at this start, we can see that the rate will rise as R is formed. Now, at the outer stream when A is just about to used up through the rate must drop at the to the zero.

Now, this also shows that the the rate follows a parabolic approach and the maxima where the concentration of A and R both are equal. So, you can see that here, the maxima the concentration of both are equal.

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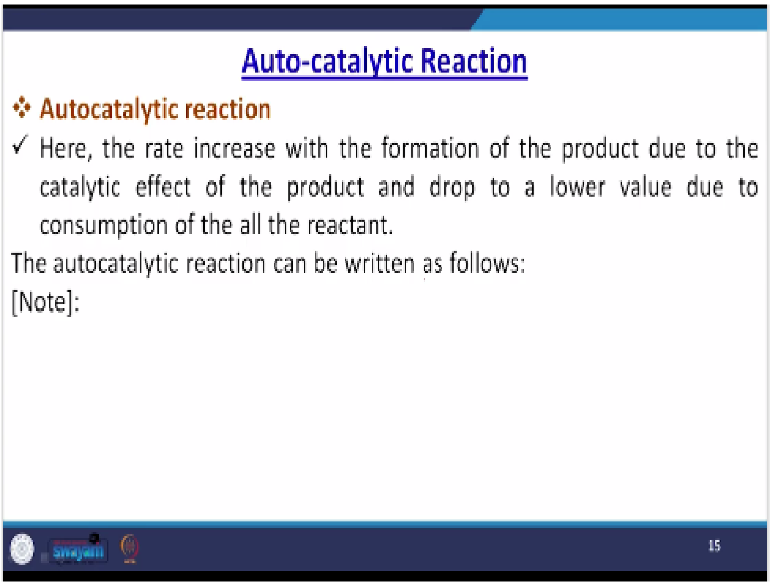

Auto-catalytic Reaction

❖ Autocatalytic reaction

✓ Here, the rate increase with the formation of the product due to the catalytic effect of the product and drop to a lower value due to consumption of the all the reactant.

The autocatalytic reaction can be written as follows:

[Note]:

Now, usually when we try to write the mathematical approach for the optimization purpose of these autocatalytic reaction.

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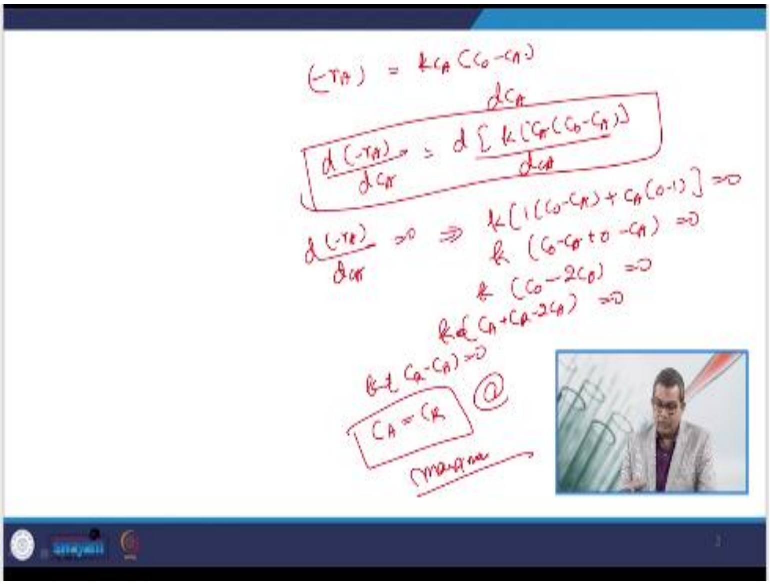

$$(-r_A) = kC_A(C_0 - C_A)$$

$$\boxed{\frac{d(-r_A)}{dC_A} = \frac{d[k(C_A(C_0 - C_A))]}{dC_A}}$$

$$\frac{d(-r_A)}{dC_A} = 0 \Rightarrow k[1(C_0 - C_A) + C_A(0-1)] = 0$$

$$k(C_0 - C_A + 0 - C_A) = 0$$

$$k(C_0 - 2C_A) = 0$$

$$k(C_A + C_R - 2C_A) = 0$$

$$k(C_R - C_A) = 0$$

$$\boxed{C_A = C_R} \text{ @ maxima}$$

In that case, we can write these equations like – r_A is equal to kC_A (C_0 – C_A). On differentiating this equation with respect to dC_A on both sides, then we can have d (– r_A) upon dC_A that is equal to d[kC_A(C_0 – C_A)] upon dC_A. Now, for maxima if we consider for maxima this equation from this equation, we can write that d – r_A upon dC_A be equal to 0 or sometime it implies that k into [1 (C_0 – C_A) + C_A (0 – 1).

That should be equal to 0 or k(C_0 – C_A + 0 – C_A) is equal to 0 or k (C_0 – 2C_A) is equal to 0 or k is equal to k(C_A + C_R – 2C_A) is equal to 0 or k is k(C_R - C_A) is equal to 0. Or in that case, C_A is equal to C_R that is at maxima that which we have already discussed in the previous one.

For optimization of autocatlytic reaction

$$-r_A = -\frac{dC_A}{dt} = kC_A(C_o - C_A)$$

On differentiating w.r.t dC_A on both side we have

$$\frac{d(-r_A)}{dC_A} = \frac{d[kC_A(C_o - C_A)]}{dC_A}$$

For maxima $\frac{d(-r_A)}{dC_A} = 0$

$$k[1 + (C_o - C_A) + C_A(0+1)] = 0$$

$$k[C_o - C_A - C_A + 0] = 0$$

$$k[C_o - 2C_A] = 0$$

$$k[C_R + C_A - 2C_A] = 0$$

$$k[C_R - C_A] = 0$$

$$C_R = C_A$$

This is the optimization value of an autocatalytic reaction.

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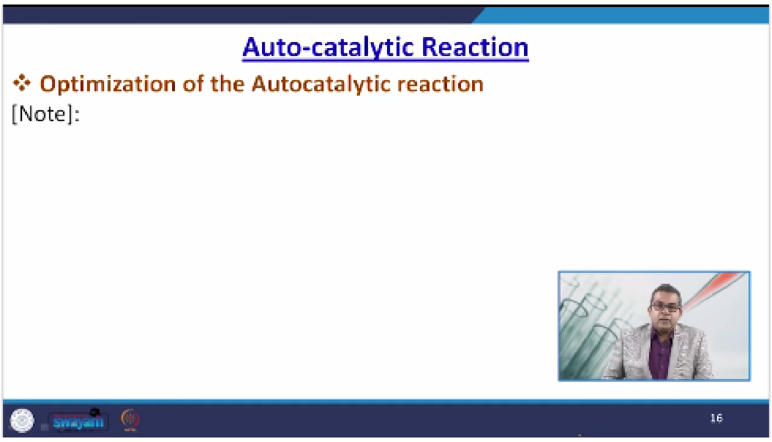

Auto-catalytic Reaction

- Optimization of the Autocatalytic reaction

[Note]:

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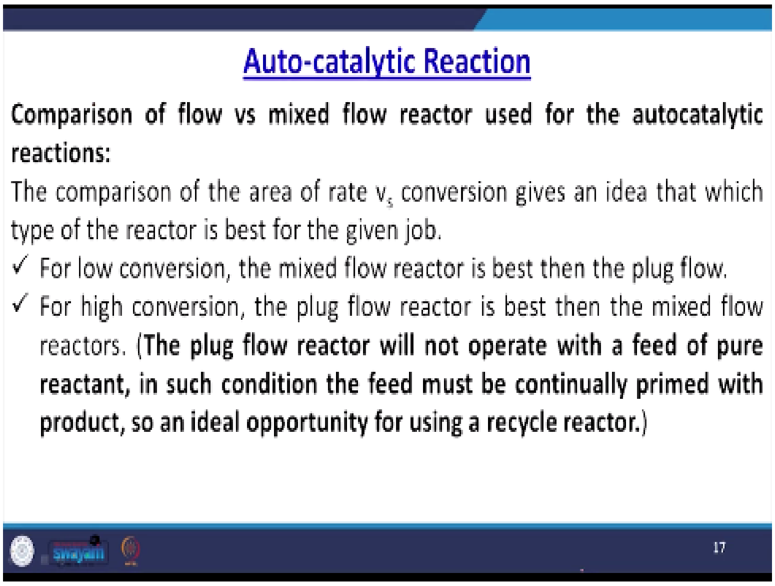

Auto-catalytic Reaction

Comparison of flow vs mixed flow reactor used for the autocatalytic reactions:

The comparison of the area of rate v_s conversion gives an idea that which type of the reactor is best for the given job.

- ✓ For low conversion, the mixed flow reactor is best then the plug flow.
- ✓ For high conversion, the plug flow reactor is best then the mixed flow reactors. (**The plug flow reactor will not operate with a feed of pure reactant, in such condition the feed must be continually primed with product, so an ideal opportunity for using a recycle reactor.**)

Now, when we talk about the comparative note of flow versus mixed flow reactor used for the autocatalytic reaction, the comparison of the area of rate v S conversion gives you an idea that which type of reactor is best suited for the given job. For low conversion, the mixed flow reactor is the best one than the plug flow reactor. For high conversion, the plug flow reactor is deemed to be the best than the mixed flow reactor.

So, the plug flow reactor will not operate with a feed of pure reactant. In such condition, the feed must be continually primed with the product so, an ideal opportunity for using a recycled reactor. You can see in this particular figure where we presented the graphical representation of MFR and a PFR reactor for autocatalytic reaction.

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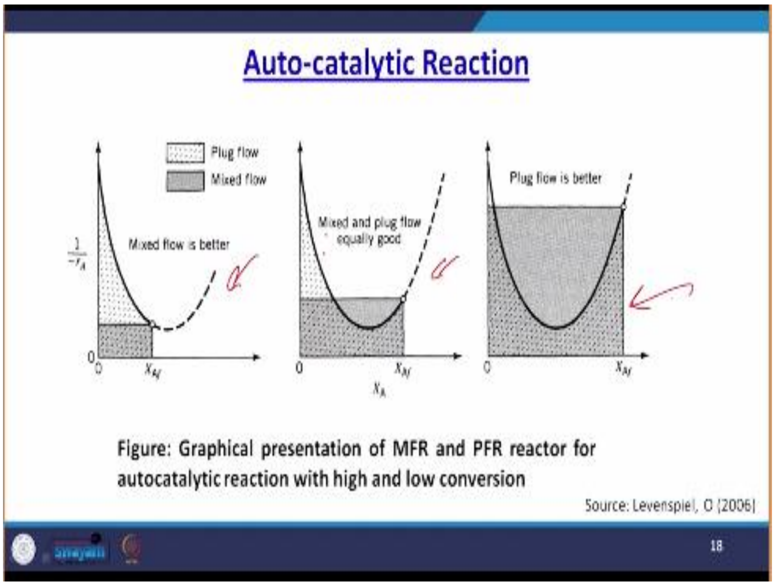

Auto-catalytic Reaction

Figure: Graphical presentation of MFR and PFR reactor for autocatalytic reaction with high and low conversion

Source: Levenspiel, O (2006)

Here you see that the mixed flow reactor is better than you can see that both mix flow flow and plug flow reactor both are good. And here you based on this conversion, you can see that the plug flow reactor is having the upper edge. So, in this particular chapter, we discussed the autocatalytic reaction, we developeed the performance equation for autocatalytic reaction reactors.

And apart from this, we discussed about various permutation and combination through which we can assess that which reactor is most optimised one for our suited purpose.

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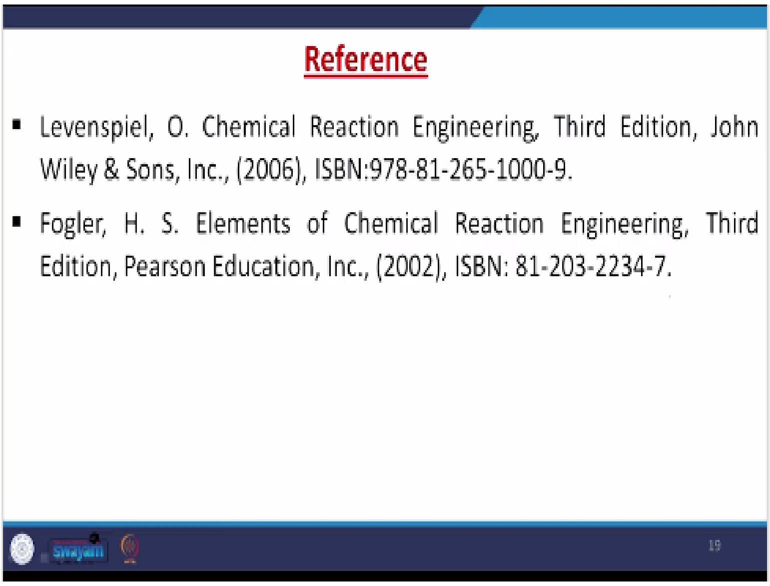

Reference

- Levenspiel, O. Chemical Reaction Engineering, Third Edition, John Wiley & Sons, Inc., (2006), ISBN:978-81-265-1000-9.
- Fogler, H. S. Elements of Chemical Reaction Engineering, Third Edition, Pearson Education, Inc., (2002), ISBN: 81-203-2234-7.

Now, in case if you wish to have a further study, you can seek the help of those differences which are enlisted in this particular slides. Thank you very much.