Chemical Reaction Engineering-I
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Lecture - 15
Size Comaprison Multiple Reactors

Welcome to the fifth lecture of module 4. In this module we are discussing reactor design. Let us have brief recap on our previous lecture before going to this lecture.

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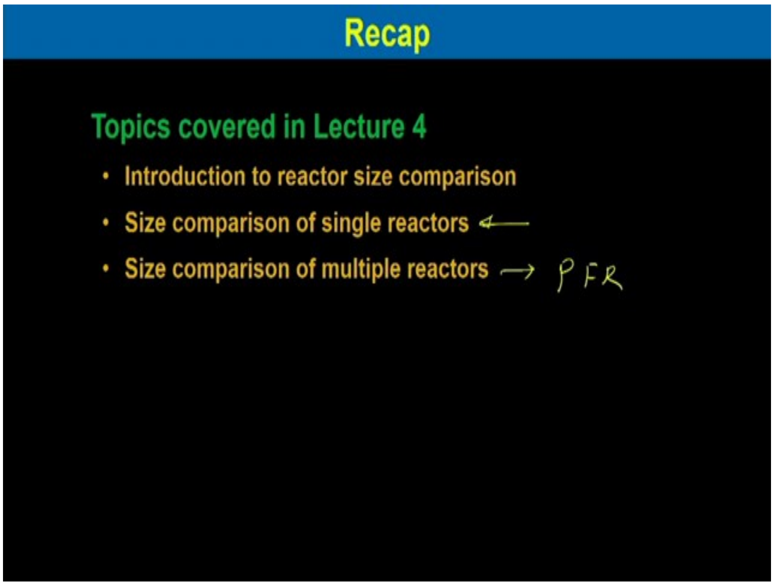

Recap

Topics covered in Lecture 4

- Introduction to reactor size comparison
- Size comparison of single reactors ←
- Size comparison of multiple reactors → PFR

In the last lecture we have covered, introduction to reactor size comparison. And then we have started with size comparison of single reactors. And then we have introduced to the size comparison of multiple reactors. So in case of single reactors we have considered batch and flow reactors. And we have seen that the performance equation for the batch reactor is similar to the plug flow reactors. And then based on this consideration the size requirements for the batch reactor is equal to the plug flow reactor for constant volume system.

And we have continued to compare between the plug flow reactor and the other flow reactor that is the mixed flow rector or continuous stirred tank reactor. Then we have tried to compare the size of the reactor. When we have same reactor of multiple numbers that means more than one reactor if we have how they, how the size requirements varies. In doing so we have considered in the last lecture the plug flow reactor. And we compared the size requirement for a given job.

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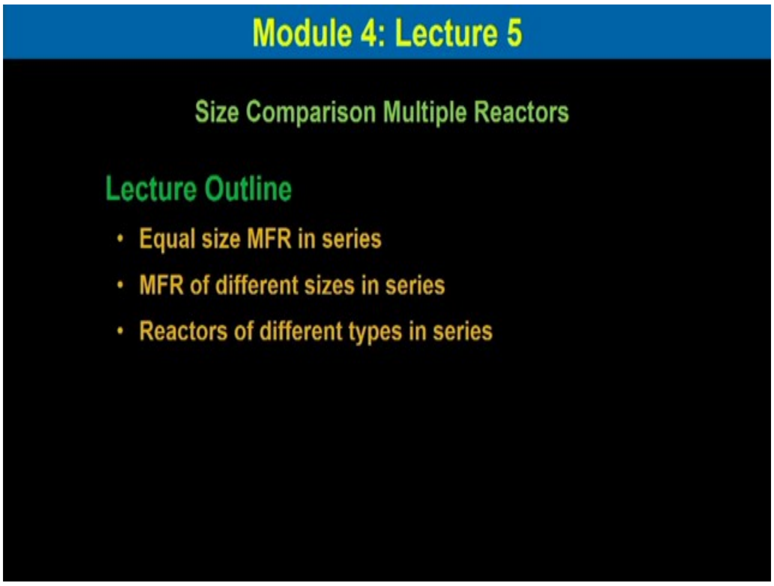

Module 4: Lecture 5

Size Comparison Multiple Reactors

Lecture Outline

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

Now, in this lecture we will continue our discussion for multiple reactor design. And the brief out line of this lecture would be equal size mixed flow reactor in series. Then we will considered mix flow reactor of different sizes in series. And if we have different type of reactors they are connected in series, how they influence the overall size requirement for a particular job.

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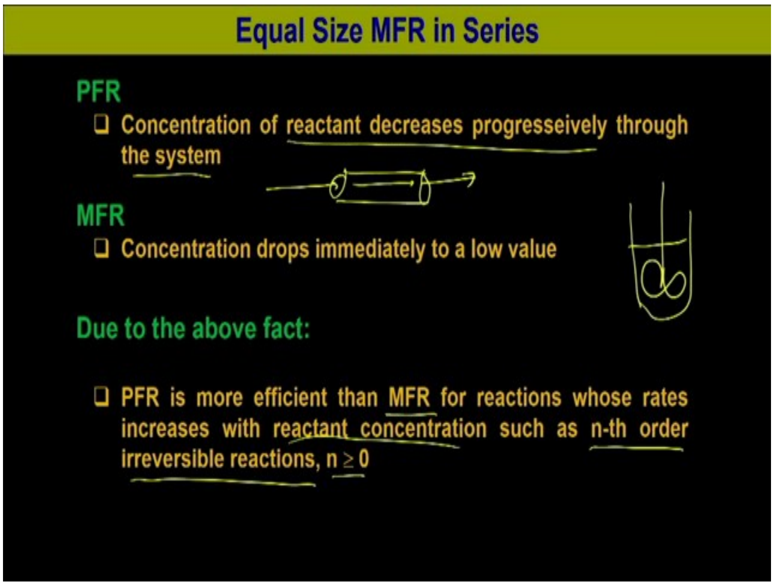

Equal Size MFR in Series

PFR

- ❑ Concentration of reactant decreases progresseively through the system

MFR

- ❑ Concentration drops immediately to a low value

Due to the above fact:

- ❑ PFR is more efficient than MFR for reactions whose rates increases with reactant concentration such as n-th order irreversible reactions, $n \geq 0$

So, let us start with the equal size mix flow reactor in series. So in case of PFR we have seen that plug flow reactor. The concentration of reactant decreases progressively through the system. So that means in ideal plug flow reactor we have considered there is no back mixing. So the concentration drop from the reactor entrance to the reactor exit would be progressive.

That means a drop in concentration will occur gradually, whereas in case of mixed flow reactor or continuous stirred tank reactor.

The concentration drops immediately at very low level because the content of the mixture in a CSTR is continuously stirred. Whereas, in case of plug flow reactor we considered the reactants which enters its progressively flows through and there is no back mixing and it exits. So due to this fact PFR is considered to be more efficient than MFR for the reaction whose rates increases with reactant concentrations such that nth order irreversible reactions, where n greater than equal to zero.

So, if the order of reaction is greater than equal to zero. And for any nth reaction and the reaction rate increases with the reactant concentration. In that case PFR is considered to be more efficient than the CSTR or mixed flow reactor.

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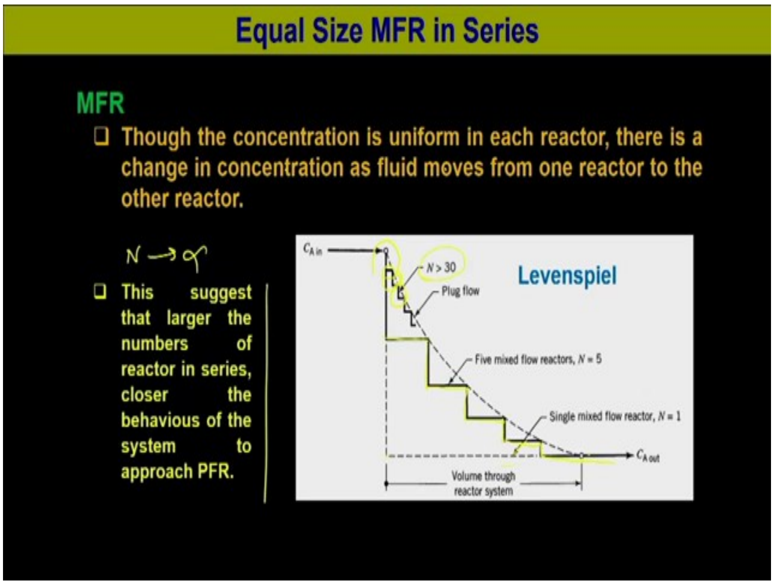

Equal Size MFR in Series

MFR

- ❑ Though the concentration is uniform in each reactor, there is a change in concentration as fluid moves from one reactor to the other reactor.

$N \to \infty$

- ❑ This suggest that larger the numbers of reactor in series, closer the behavious of the system to approach PFR.

Now, if we consider N number of plug flow reactor connected in series, N number of CSTR connected in series or MFR connected in series. So, if we connect N number of CSTR in series although the concentration drops in a particular reactor is uniform at a particular reactor. But, if we connect the several CSTR in series there would be a progressive change of concentration from one reactor to the other. So, we will find a change in concentration from one reactor to the other. The step wise drop of the concentration we can, the step wise drop in concentration we can see from this figure.

So, as we can see when the number of reactor or if it is a CSTR. Then the concentration change drop is this much. So for single CSTR the concentration drop is from this level to this level, up to this when we use single CSTR. But, when we increase the number of CSTR the change in volume you can see it is the drop in concentration is like this. So we will have if there are 5 number of CSTR connected in series. The drop will concentration will happen in a progressive manner or from one reactor to the other reactor.

Now, if we increase more number of reactor connected in series. As you can see the N greater than 30. So, in that case you can see the drop in concentration from one rector to the other reactor is less. So, this is for 1, 2 and so on, so the change in concentration which is happening keeping the total reactor volume constant. If we increase the number of reactor the drop in concentration will be less. And as long as the number of reactor increases to infinite it will behave like a plug flow reactor, so if N tends to infinite then we can see it behaves like a plug flow reactor.

So, this suggest that larger the number of reactor in series, closer the behavior of the system to approach plug flow reactor. So this is very important for the designing of mixed flow reactor connected in series. So this is the Levenspiel plot, which is shown over here.

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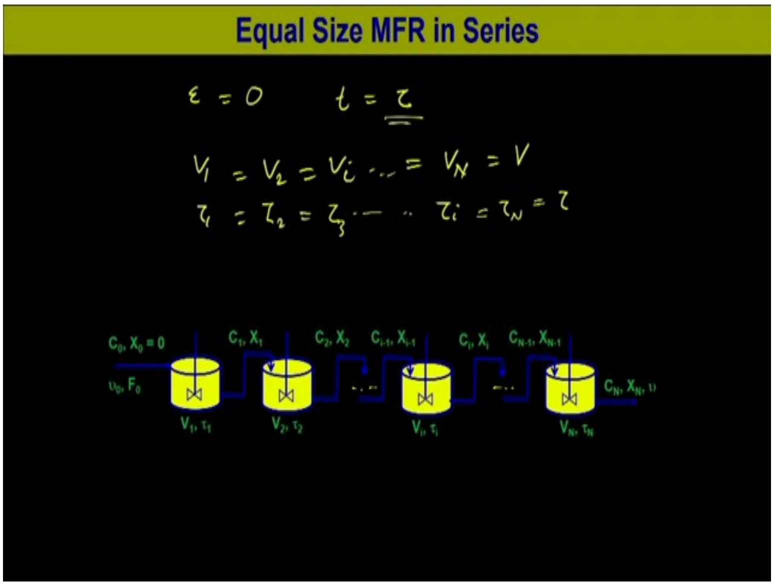

Equal Size MFR in Series

$\varepsilon = 0 \qquad t = \underline{\underline{\tau}}$

$V_1 = V_2 = V_i \cdots = V_N = V$

$\tau_1 = \tau_2 = \tau_3 \cdots \cdots \tau_i = \tau_N = \tau$

Now, if we consider equal size MFR in series. Say let N number of equal size CSTR connected in series. And, so we assume that the density of the system that is ε is equal to 0 that is constant density system or constant volume system. So in this case the t, the residence time would be equal to τ as we have discussed before. Now, if the inlet conditions is defined as C_0, X_0, v_0 and F_0. C_0 is the concentration of the inlet stream to the first reactor, X_0 is the conversion of the particular species entering to the reactor 1.

So, as it is considered to be 0 because there is now conversion, before it is going to the reactor. v_0 is the volumetric flow rate, F_0 is the Molar flow rate. Similarly, the exit stream from the first reactor is C_1, X_1 and exit from reactor 1 is going to the reactor 2, so inlet to the reactor 2 would be C_1, X_1. Similarly, this will go for ith reactor. The inlet to that would be C_{i-1}, X_{i-1} and exit to this would be C_i, X_i. Similarly, for reactor n it should be C_{n-1}, X_{n-1} and exit to this would be C_n, X_n and v.

So, v is the volumetric flow rate and reactor this is volume V_1 and its residence time is τ_1, for reactor 2 it is V_2 and residence time is τ_2. Similarly, for ith reactor V_i, τ_i and for nth reactor it is V_n and τ_n. Now, this for constant density system we have an equal size volume later on we will consider this V_1, V_2, V_3 and V_i all would be same. So

$$V_1 = V_2 = V_i = \ldots\ldots\ldots\ldots V_n = \mathrm{V}$$

or we can write V. Similarly,

$$\tau_1 = \tau_2 = \tau_3 \ldots\ldots\ldots \tau_i = \tau_n = \tau$$

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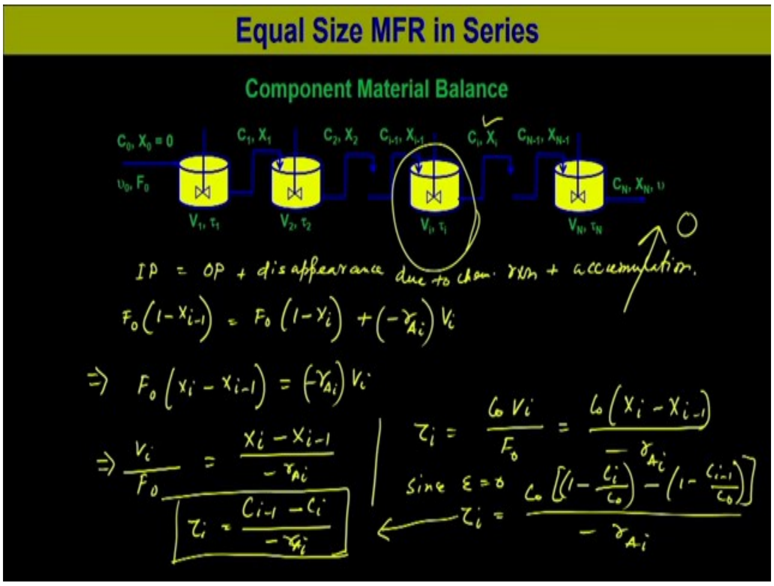

Equal Size MFR in Series

Component Material Balance

IP = OP + disappearance due to chem. rxn + accumulation. 0

$$F_0(1-X_{i-1}) = F_0(1-X_i) + (-r_{Ai})V_i$$

$$\Rightarrow F_0(X_i - X_{i-1}) = (-r_{Ai})V_i$$

$$\Rightarrow \frac{V_i}{F_0} = \frac{X_i - X_{i-1}}{-r_{Ai}}$$

$$\boxed{\tau_i = \frac{C_{i-1} - C_i}{-r_{Ai}}}$$

$$\tau_i = \frac{C_0 V_i}{F_0} = \frac{C_0(X_i - X_{i-1})}{-r_{Ai}}$$

Since $\varepsilon = 0$

$$\tau_i = \frac{C_0\left[\left(1-\frac{C_i}{C_0}\right) - \left(1-\frac{C_{i-1}}{C_0}\right)\right]}{-r_{Ai}}$$

So, now let us do the material balance for this system in reactor in series. Let us consider the ith vessel so this one and do the material balance. So as you have done before the

$$input = output + disappearance\ due\ to\ chemical\ reaction + accumulation$$

As this is a steady straight process and continuous flow reactor this accumulation term would be 0. So then input is

$$F_0(1-X_{i-1}) = F_0(1-X_i) + (-r_{Ai})V_i$$

If we simplify this, this would be

$$F_0(X_i - X_{i-1}) = (-r_{Ai})V_i$$

Now, from this we can write

$$\frac{V_i}{F_0} = \frac{X_i - X_{i-1}}{-r_{Ai}}$$

Now, form the definition of τ we know

$$\tau = \frac{C_0 V_i}{F_0}$$

So if you substitute,

$$= \frac{\mathrm{C}_0(X_i - X_{i-1})}{-r_{Ai}}$$

Now, since ε = 0, this we can write τ_i in terms of concentration. So τ , this is τ_i so,

$$\tau_i = \frac{C_0\left[\left(1-\frac{C_i}{C_0}\right)-\left(1-\frac{C_{i-1}}{C_0}\right)\right]}{-r_{Ai}}$$

So, if we simplify this. This would be

$$\tau_i = \frac{C_{i-1} - C_i}{-r_{Ai}}$$

Now this is our τ_i equation.

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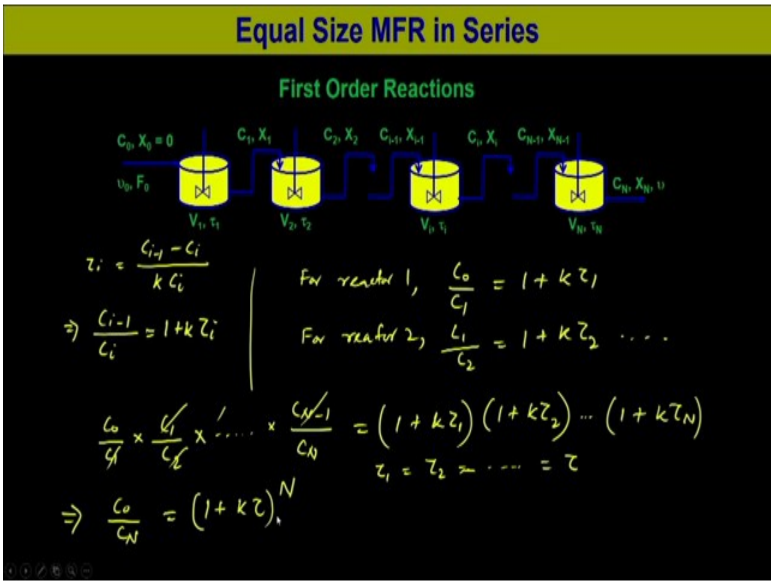

Equal Size MFR in Series

First Order Reactions

$$\tau_i = \frac{C_{i-1} - C_i}{k C_i}$$

$$\Rightarrow \frac{C_{i-1}}{C_i} = 1 + k\tau_i$$

For reactor 1, $\frac{C_0}{C_1} = 1 + k\tau_1$

For reactor 2, $\frac{C_1}{C_2} = 1 + k\tau_2$ ....

$$\frac{C_0}{\cancel{C_1}} \times \frac{\cancel{C_1}}{\cancel{C_2}} \times \ldots \times \frac{\cancel{C_{N-1}}}{C_N} = (1 + k\tau_1)(1 + k\tau_2) \cdots (1 + k\tau_N)$$

$$\tau_1 = \tau_2 = \cdots = \tau$$

$$\Rightarrow \frac{C_0}{C_N} = (1 + k\tau)^N$$

Now, if write for the first order reaction, for first order reaction this would be so we have

$$\tau_i = \frac{C_{i-1} - C_i}{kC_i}$$

This is for first order reaction. So from here we can write

$$\frac{C_{i-1}}{C_i} = 1 + k\tau_i$$

Now, let us write for reactor i or reactor 1 so if we write for reactor 1. So, it would be

$$\frac{C_0}{C_1} = 1 + k\tau_1$$

For reactor 2 it would be

$$\frac{C_1}{C_2} = 1 + k\tau_2$$

And so on for other reactors.

So, if we multiply all this reactor equations it would be

$$\frac{C_0}{C_1} * \frac{C_1}{C_2} * \ldots\ldots * \frac{C_{n-1}}{C_n} = (1 + k\tau_1) * (1 + k\tau_1) * \ldots..(1 + k\tau_n)$$

As we said before all the τ are same, if write

$$\tau_1 = \tau_2 = \ldots\ldots\ldots.\tau$$

So in that case we can write from here, if we multiply this will cancel out and finally we will have all this will cancel out. We will have

$$\frac{C_0}{C_n} = (1 + k\tau)^n$$

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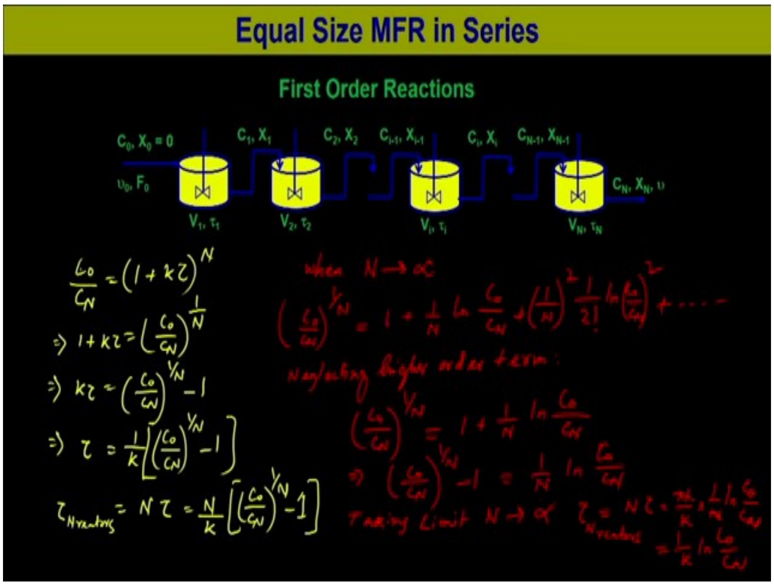

Equal Size MFR in Series

First Order Reactions

$$\frac{C_0}{C_N} = (1 + k\tau)^N$$

$$\Rightarrow 1 + k\tau = \left(\frac{C_0}{C_N}\right)^{\frac{1}{N}}$$

$$\Rightarrow k\tau = \left(\frac{C_0}{C_N}\right)^{1/N} - 1$$

$$\Rightarrow \tau = \frac{1}{k}\left[\left(\frac{C_0}{C_N}\right)^{1/N} - 1\right]$$

$$\tau_{N\,\text{reactors}} = N\tau = \frac{N}{k}\left[\left(\frac{C_0}{C_N}\right)^{1/N} - 1\right]$$

when $N \to \infty$

$$\left(\frac{C_0}{C_N}\right)^{1/N} = 1 + \frac{1}{N}\ln\frac{C_0}{C_N} + \left(\frac{1}{N}\right)^2 \frac{1}{2!}\ln\left(\frac{C_0}{C_N}\right)^2 + \cdots$$

Neglecting higher order term:

$$\left(\frac{C_0}{C_N}\right)^{1/N} = 1 + \frac{1}{N}\ln\frac{C_0}{C_N}$$

$$\Rightarrow \left(\frac{C_0}{C_N}\right)^{1/N} - 1 = \frac{1}{N}\ln\frac{C_0}{C_N}$$

Taking Limit $N \to \infty$ $\tau_{N\,\text{reactors}} = N\tau = \frac{N}{k} \times \frac{1}{N}\ln\frac{C_0}{C_N}$

$$= \frac{1}{k}\ln\frac{C_0}{C_N}$$

So we have

$$\frac{C_0}{C_n} = (1 + k\tau)^n$$

And if we simplify this we can write

$$1 + k\tau = \left(\frac{C_0}{C_n}\right)^{\frac{1}{n}}$$

So from here we can write

$$k\tau = \left(\frac{C_0}{C_n}\right)^{\frac{1}{n}} - 1$$

So

$$\tau = \frac{1}{k}\left[\left(\frac{C_0}{C_n}\right)^{\frac{1}{n}} - 1\right]$$

So, we have this equations of τ that is for a particular reactor. So τ this is for N number of reactors. We can write

$$\tau_{n,reactors} = n\tau$$

which is

$$= \frac{n}{k}\left[\left(\frac{C_0}{C_n}\right)^{\frac{1}{n}} - 1\right]$$

Now, when N tends to infinite we can expand this in this equation that is $\left(\frac{C_0}{C_n}\right)^{\frac{1}{n}}$ as infinite series. So we can write this is

$$\left(\frac{C_0}{C_n}\right)^{\frac{1}{n}} = 1 + \frac{1}{n}\ln\frac{C_0}{C_n} + \left(\frac{1}{n}\right)^2 \frac{1}{2!}\ln\left(\frac{C_0}{C_n}\right)^2 + \ldots..$$

So this is infinite series. Now, if we neglect the higher order term, so neglecting higher order term we can write

$$\left(\frac{C_0}{C_n}\right)^{\frac{1}{n}} = 1 + \frac{1}{n}\ln\frac{C_0}{C_n}$$

So from here if we rearrange we can write

$$\left(\frac{C_0}{C_n}\right)^{\frac{1}{n}} - 1 = \frac{1}{n}\ln\frac{C_0}{C_n}$$

So, if we take limit $n \to \infty$,taking limit in N tends to infinite. We can write

$$\tau_{n,reactors} = n\tau = \frac{n}{k} * \frac{1}{n}\ln\frac{C_0}{C_n}$$

So then N will cancelled out, so we will have

$$= \frac{1}{k}\ln\frac{C_0}{C_n}$$

So this is essentially the equation for the plug flow reactor. So that means when we connect N number of equal size CSTR in series it behaves when N tends to infinite it behaves like a plug flow reactor.

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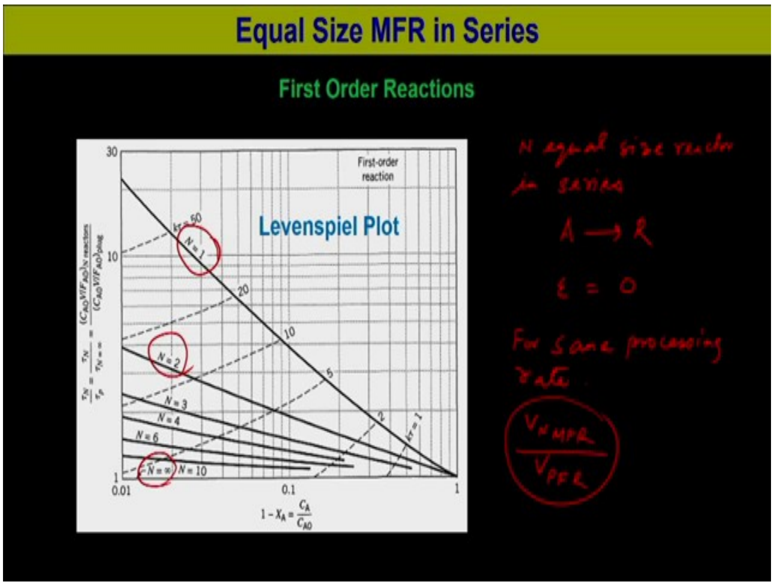

Equal Size MFR in Series

First Order Reactions

N equal size reactor in series

$A \longrightarrow R$

$\varepsilon = 0$

For same processing rate.

$\frac{V_{N\,MFR}}{V_{PFR}}$

So, let us look into this by for the first order reaction, the graphical representation is given by Levenspiel. So, this is Levenspiel plot and this is for first order reaction. So this is for N equal size reactor in series and for the reaction first reactions A → R irreversible reaction and the density change is constant. So ε is equal to zero and for constant or identical feed ratio if we use the same processing rate. For same processing rate we can see this is nothing but V_{nMFR}/V_{PFR}.

So it directly gives the volume ratio the Y axis on this plot. And then on the X axis it gives the conversion and this is a log log plot. And as you can see for first order reaction for N equal to 1 the volume requirement for CSTR is higher compared to the plug flow reactor, as the number of reactor increases from 1 to 2. And, then infinite the volume requirement or there is no difference between the plug flow reactor and CSTR size requirement. If N number of CSTR connected in series and N is very large.

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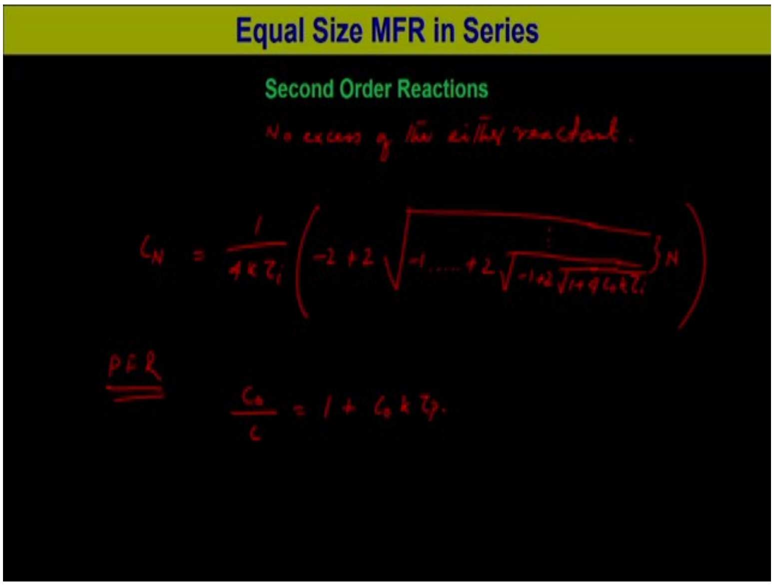

Equal Size MFR in Series

Second Order Reactions

No excess of the either reactant.

$$C_N = \frac{1}{4k\tau_i}\left(-2+2\underbrace{\sqrt{-1 \ldots\ldots +2\sqrt{-1+2\sqrt{1+4C_0k\tau_i}}}}_{N}\right)$$

PFR

$$\frac{C_0}{C} = 1 + C_0 k \tau_p.$$

Now, let us consider second order reaction for N number of reactor connected in series and we can consider second order bimolecular type reaction. No excess of either reactant similar to the first order reaction. If N number of reactors are connected in series we can find

$$C_n = \frac{1}{4k\tau_i}\left(-2+2\sqrt{-1+2\sqrt{-1+2\sqrt{1+4C_0k\tau_i}}}\right)$$

And this would be with other values into N, this is for second order reaction for N number of reactors connected in series.

The same thing for the same volume the PFR equation is

$$\frac{C_0}{C} = 1 + C_0 k \tau_p$$

So the comparison between the second order reactions is also shown in figure.

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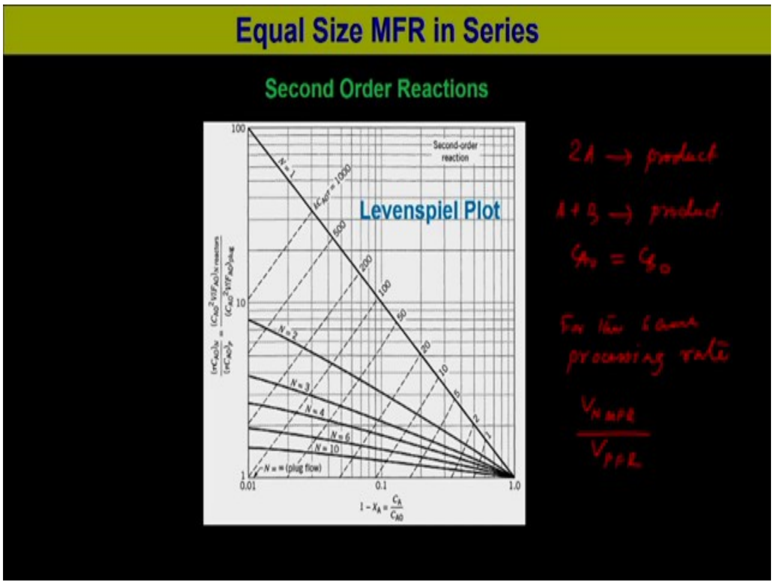

Equal Size MFR in Series

Second Order Reactions

2A → product

A + B → product

$C_{A_0} = C_{B_0}$

For the same processing rate

$\frac{V_{N\,MFR}}{V_{PFR}}$

This as we can see this is also the similar to the first order reaction and this is also the Levenspiel plot. And this is valid for the reaction

$$2A \rightarrow product$$
$$A + B \rightarrow product$$

with CA naught is equal to CB naught that is equimolar of A and B. And for the same processing rate this Y axis is give the volume ratio that is V_{nMFR}/V_{PFR}, so it directly gives the comparison of their volume ratio and as we can see when the number of reactors in this case also increases to infinite it behaves like a plug flow reactor.

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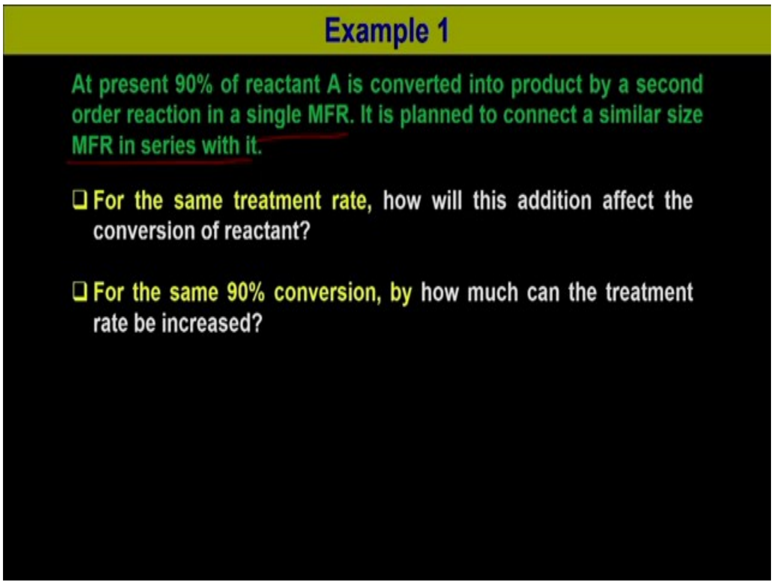

Example 1

At present 90% of reactant A is converted into product by a second order reaction in a single MFR. It is planned to connect a similar size MFR in series with it.

- ❑ For the same treatment rate, how will this addition affect the conversion of reactant?
- ❑ For the same 90% conversion, by how much can the treatment rate be increased?

Let us take an example to see how we can see the performance when we add you know additional reactor in series with 1 reactor. So at present 90 present of A is converted into product by second order reactions in a MFR. It is planned to connect a similar size MFR in series with it. Now, the problem is for the same treatment rate, how this addition affect the conversion of reactant? And second thing is that for the same 90 percent conversion, by how much can the treatment rate be increased?

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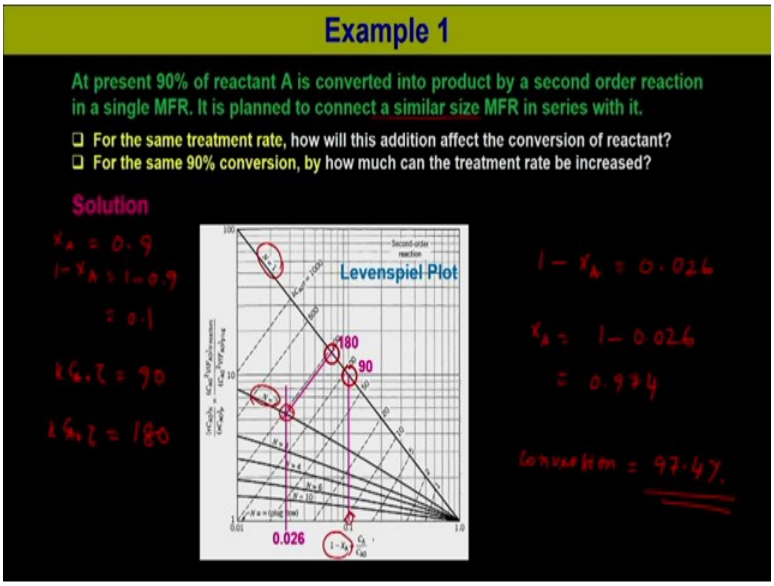

Example 1

At present 90% of reactant A is converted into product by a second order reaction in a single MFR. It is planned to connect a similar size MFR in series with it.

- ☐ For the same treatment rate, how will this addition affect the conversion of reactant?
- ☐ For the same 90% conversion, by how much can the treatment rate be increased?

Solution

$X_A = 0.9$

$1-X_A = 1-0.9$

$= 0.1$

$kC_{A0}\tau = 90$

$kC_{A0}\tau = 180$

$1-X_A = 0.026$

$X_A = 1-0.026$

$= 0.974$

Conversion = 97.4%

Now, let us solve it. So this is the Levenspiel plot as we have discussed before. And this is only for the second order reaction and as per the problem it is for 90 percent conversion. So 90 percent conversion means $1-X_A$ if you look into over here $1-X_A$,so

$$X_A = 0.9$$
$$1-X_A = 1-0.9 = 0.1$$

So, this is the point where the conversion is given. Now, from this point if we go this straight for a single reactor first reactor we can obtain the values here which is for N = 1. We can obtained the $kC_{A0}\tau$ values. So $kC_{A0}\tau$ value at this location is 90.

Now the thing is given the same treatment rate you are increasing the 1 more reactor so $kC_{A0}\tau$ would be double which is similar size. So if it is double so it would be $kC_{A0}\tau$ so we had 90 and it is double so $kC_{A0}\tau$ is becoming 180. Now, for 180 we have to locate the point at 180. So this is at 180 and draw a parallel line with this $kC_{A0}\tau$. And which will cut the second reactor, which is connected N is equal to 2 in this line at this location.

Now from this if you go down or go vertically to the X axis, you will find the values 0.026. So $1 - X_A$ is equal to 0.026. So then we can write

$$1 - X_A = 0.026$$
$$X_A = 1 - 0.026 = 0.974$$

That means the conversion is equal to 97.4 percent. So in addition of one more reactor increases the conversion from 90 percent to 97.4 percent. Now the second problem which is given for the 90 percent conversion, how much can the treatment rate be increased?

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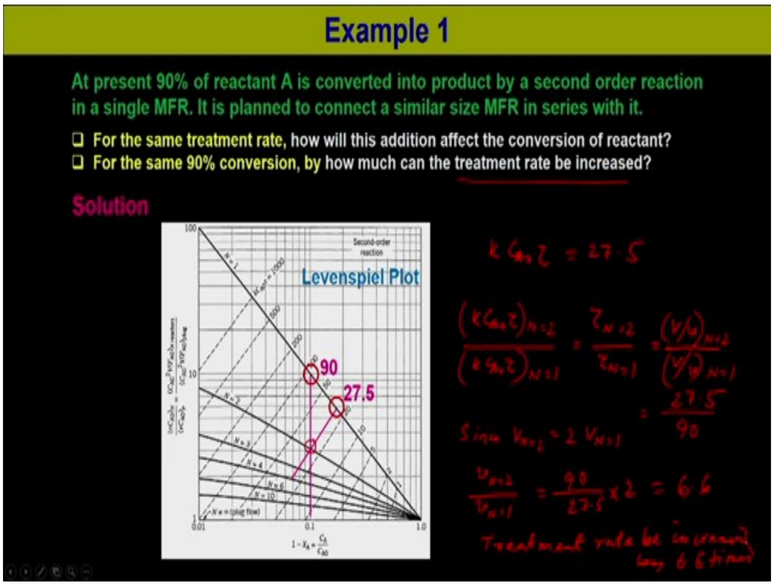

Example 1

At present 90% of reactant A is converted into product by a second order reaction in a single MFR. It is planned to connect a similar size MFR in series with it.

- ☐ For the same treatment rate, how will this addition affect the conversion of reactant?
- ☐ For the same 90% conversion, by how much can the treatment rate be increased?

Solution

$k C_{A0}\tau = 27.5$

$$\frac{(kC_{A0}\tau)_{N=2}}{(kC_{A0}\tau)_{N=1}} = \frac{\tau_{N=2}}{\tau_{N=1}} = \frac{(V/v_0)_{N=2}}{(V/v_0)_{N=1}} = \frac{27.5}{90}$$

Since $V_{N=2} = 2 V_{N=1}$

$$\frac{v_{N=2}}{v_{N=1}} = \frac{90}{27.5} \times 2 = 6.6$$

Treatment rate be increased by 6.6 times

So this is for 90 percent conversion and we have added one more reactor to it. Keeping the same, the treatment rate has to be increased so that the conversion level remains same by addition of the second reactor. That means when we add keep the conversion level $kC_{A0}\tau$ S 90. So, we have to come down to reactor 2. And we have to find out the values of $kC_{A0}\tau$ if we increase the no treatment rate. So, this would be equal to 27.5, so by addition of the second reactor $kC_{A0}\tau$ is 27.5.

Now, for N is equal to 1 and N is equal to 2 if we write this group. This group y axis that is

$$\frac{(kC_{A0}\tau)_{n=2}}{(kC_{A0}\tau)_{n=1}} = \frac{\tau_{n=2}}{\tau_{n=1}}$$

And then we can write this is

$$= \frac{(V/v)_{n=2}}{(V/v)_{n=1}}$$

And then this would be equal to, so for when it was single reactor that is 90 by addition of the second reactor it becomes 27.5.

So from this we can calculate, since

$$V_{n=2} = 2V_{n=1}$$

The ratio of the flow rate, if we write this would be

$$\frac{v_{n=2}}{v_{n=1}} = \frac{90}{27.5} * 2 = 6.6$$

That means the treatment rate should be increased by 6.6 times, so the treatment rate.

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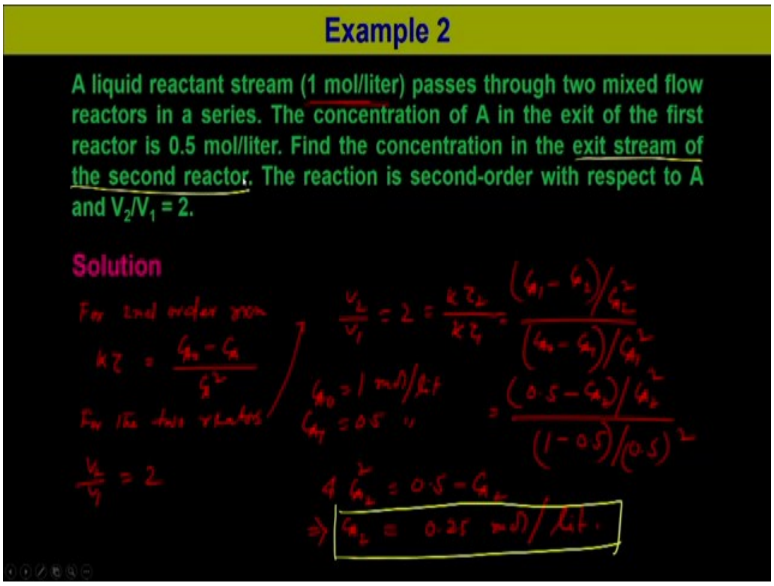

Example 2

A liquid reactant stream (1 mol/liter) passes through two mixed flow reactors in a series. The concentration of A in the exit of the first reactor is 0.5 mol/liter. Find the concentration in the exit stream of the second reactor. The reaction is second-order with respect to A and $V_2/V_1 = 2$.

Solution

For 2nd order rxn

$$k\tau = \frac{C_{A0} - C_A}{C_A^2}$$

For the two reactors

$$\frac{V_2}{V_1} = 2$$

$$\frac{V_2}{V_1} = 2 = \frac{k\tau_2}{k\tau_1} = \frac{(C_{A1} - C_{A2})/C_{A2}^2}{(C_{A0} - C_{A1})/C_{A1}^2}$$

$C_{A0} = 1$ mol/lit

$C_{A1} = 0.5$ "

$$= \frac{(0.5 - C_{A2})/C_{A2}^2}{(1-0.5)/(0.5)^2}$$

$$4C_{A2}^2 = 0.5 - C_{A2}$$

$$\Rightarrow \boxed{C_{A2} = 0.25 \text{ mol/lit.}}$$

Now, let us considered another example. A liquid reactant stream, which is 1 mole per liter passes through two mixed flow reactors in a series. The concentration of A in the exit of the first reactor is 0.5 mole per liter. Find the concentration of the exit stream of the second reactor. The reaction is second order with respect to A and $\frac{V_2}{V_1} = 2$. So, let us solve it for second order reaction. We know

$$k\tau = \frac{C_{A0} - C_A}{C_A^2}$$

Now, for the two reactors $\frac{V_2}{V_1} = 2$.

So this is given, so then we can write $\frac{V_2}{V_1} = 2 \; = \frac{k\tau_2}{k\tau_1}$, which is

$$= \frac{C_{A0} - C_{A2} / C_{A2}^2}{C_{A0} - C_{A1} / C_{A1}^2}$$

Now, if we substitute the values this would be

$$= \frac{(0.5 - C_{A2}) / C_{A2}^2}{(1 - 0.5) / (0.5)^2}$$

Now, so the stream which is entering is given that is C_{A0} which is 1 mole per liter. And C_{A1} exit is 0.5 mole per liter.

So we have substituted over here and from this we can write

$$4C_{A2}^2 = 0.5 - C_{A2}$$

And, if we solve it this will give C_{A2} would be equal to 0.25 mole per liter. So, this is the concentration at the exit of the second reactor.

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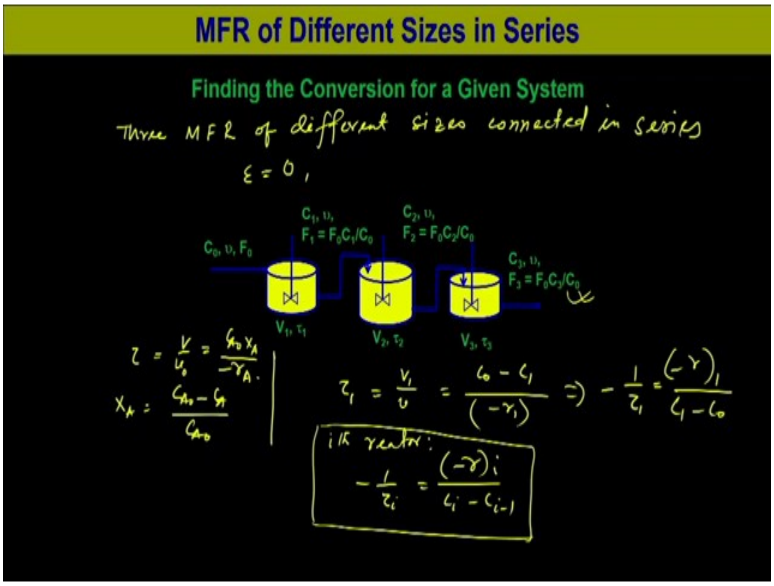

MFR of Different Sizes in Series

Finding the Conversion for a Given System

Three MFR of different sizes connected in series

$\varepsilon = 0$,

$\tau = \frac{V}{v_0} = \frac{C_{A0}X_A}{-r_A}$.

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

$\tau_1 = \frac{V_1}{v} = \frac{C_0 - C_1}{(-r_1)} \Rightarrow -\frac{1}{\tau_1} = \frac{(-r)_1}{C_1 - C_0}$

ith reactor:

$\boxed{-\frac{1}{\tau_i} = \frac{(-r)_i}{C_i - C_{i-1}}}$

Now, if we consider different size CSTR connected series. So, let us consider there are three reactors which are connected in series. And their concentrations, the volume for reactor 1 is

V_1 and the precedence time is τ_1, for reactor 2 is V_2 and τ_2, for reactor 3 is V_3 and τ_3. The concentration which is coming to reactor 1 is C_0 with volumetric flow rate v. And the Molar flow rate is F_0 the exit to reactor 1 is C_1 which is going to reactor 2. Volumetric flow rate remains constant and the Molar flow rate to tank 2 is $\mathrm{F}_1 = \frac{\mathrm{C}_1}{C_0}$.

Similarly, for rector 2 exit and entrance to the reactor 3 is C_2 volumetric flow rate v, $\mathrm{F}_2 = \frac{\mathrm{C}_2}{C_0}$. And the exit for reactor 3 is C_3 volumetric flow rate V and $\mathrm{F}_3 = \frac{\mathrm{C}_3}{C_0}$. So this is for 3 MFR of different sizes connected in series. Here ε is equal to 0 so constant density system. If we write the component balance for the first reactor as we have done before that is

$$\tau = \frac{V}{v_0} = \frac{C_{A0}X_A}{-r_A},$$
$$X_A = \frac{C_{A0} - C_A}{C_{A0}}$$

So similar way if do for reactor 1 we can write

$$\tau_1 = \frac{V_1}{v} = \frac{C_0 - C_1}{-r_1}$$

For reactor 2 if we write, so form here we can write

$$-\frac{1}{\tau_1} = \frac{(-r_1)}{C_0 - C_1}$$

Similarly, for any ith reactor we can write

$$-\frac{1}{\tau_i} = \frac{(-r_i)}{C_i - C_{i-1}}$$

So with this balance equation we can write for any reactors and we can find out the values of $-\frac{1}{\tau_i}$.

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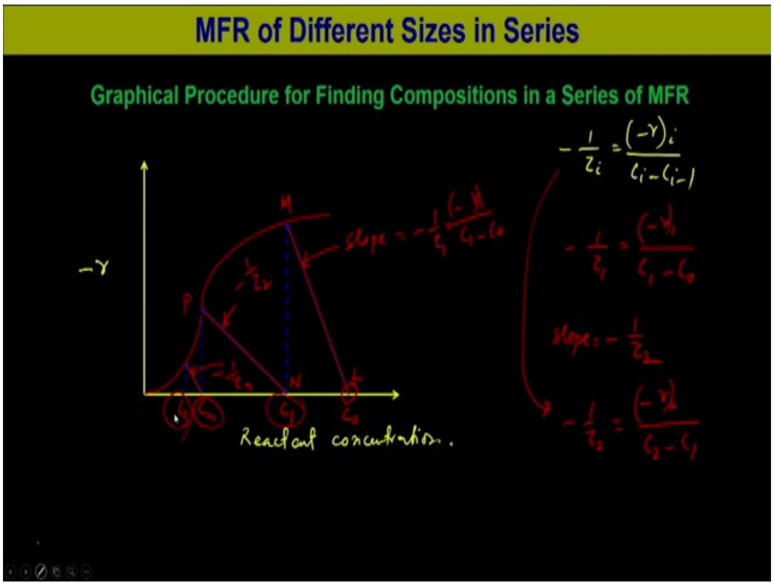

MFR of Different Sizes in Series

Graphical Procedure for Finding Compositions in a Series of MFR

Now, let us see the graphical procedure for finding the compositions in a CSTR. For doing so we need to plot the concentration versus rate curve. So we have general relations

$$-\frac{1}{\tau_i} = \frac{(-r_i)}{C_i - C_{i-1}}$$

Now, if we plot -r versus reactant concentration, so this is -r and this is reactant concentration. Now, plot any arbitrary curve say rate versus reactant concentration and we can calculate the slope of the curve which is $-\frac{1}{\tau_i}$.

So, if we calculate slope would be $\frac{(-r_i)}{C_i - C_{i-1}}$. So for reactor 1 we know the initial concentration, so this is say initial concentration this is C_0 at point L. Now, if we know the residence time we can calculate

$$-\frac{1}{\tau_1} = \frac{(-r_1)}{C_1 - C_0}$$

So, if we calculate with a slope $-\frac{1}{\tau_1}$ so we can plot this line say this slope is $-\frac{1}{\tau_1}$ which is equal to $\frac{(-r_1)}{C_1 - C_0}$.

So, say its meets the point M and to calculate the exit concentration of reactor 1 we can come down vertically from this point, which will meet on the X axis at say N and the concentration over here would be C_1. Now, if we can calculate the slope which is for the second reactor. That would be slope would be $-\frac{1}{\tau_2}$, with this slope if we plot. Say this is, slope is $-\frac{1}{\tau_2}$ so that means τ_2 this would be, this relation would be

$$-\frac{1}{\tau_2} = \frac{(-r_2)}{C_2 - C_1}$$

So, if we come down from this location say this is location P and if we come down vertically. We will meet at X axis at so we will obtain C_2 and then if we plot with $-\frac{1}{\tau_3}$ say slope is $-\frac{1}{\tau_3}$. So then we can come down vertically and we obtain the concentration C_3. So this way we can follow the graphical procedure to find out the exit concentration for each reactor.

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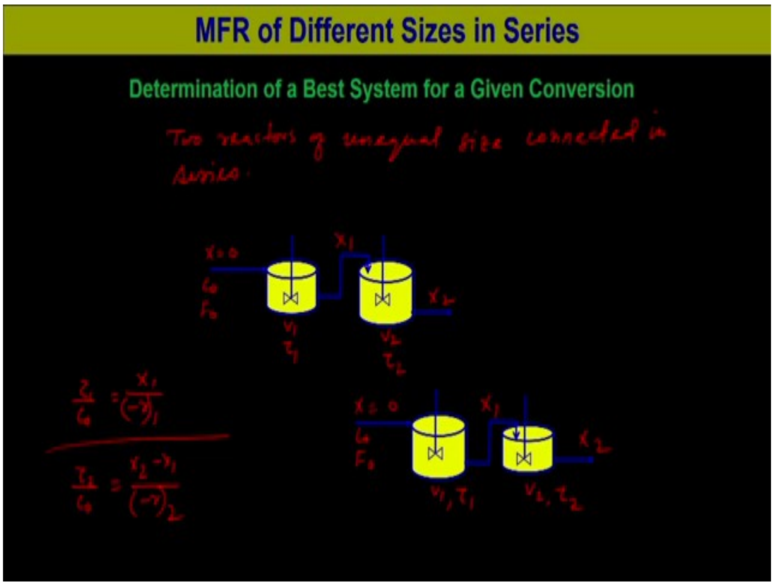

MFR of Different Sizes in Series

Determination of a Best System for a Given Conversion

Two reactors of unequal size connected in series.

$$\frac{\tau_1}{C_0} = \frac{X_1}{(-r)_1}$$

$$\frac{\tau_2}{C_0} = \frac{X_2 - X_1}{(-r)_2}$$

Now, we will consider determination of the best system for a given conversion. So, let us consider two reactor connected in series and they are of different sizes. Say the first series is connected like this, so we can calculate so this is the conversion is for the reactor 1 is 0 and C_0 is the concentration of the reactant, F_0 is the molar flow rate, this is for reactor 1. That is volume V_1 and τ_1. This is volume V_2 and residence time τ_2, exit is X_2 from here and this is X_1.

So for this, if write for the first rector if we do the balance equation. So we have considered two reactors of unequal size connected in series. And now if we write for this

$$\frac{\tau_1}{C_0} = \frac{X_1}{-r_1}$$

And for the second reactor we can write

$$\frac{\tau_2}{C_0} = \frac{X_2 - X_1}{-r_2}$$

Now, if we take first the larger reactors and second the smaller reactors with the same nomenclature this would be V_1 and τ_1. This would be V_2 and τ_2 and this would, X would be 0, C_0, F_0, this is X_1 this is X_2. So, for the first and the second reactor we will have the similar balance equation. Now, let us see graphically how to get a best system.

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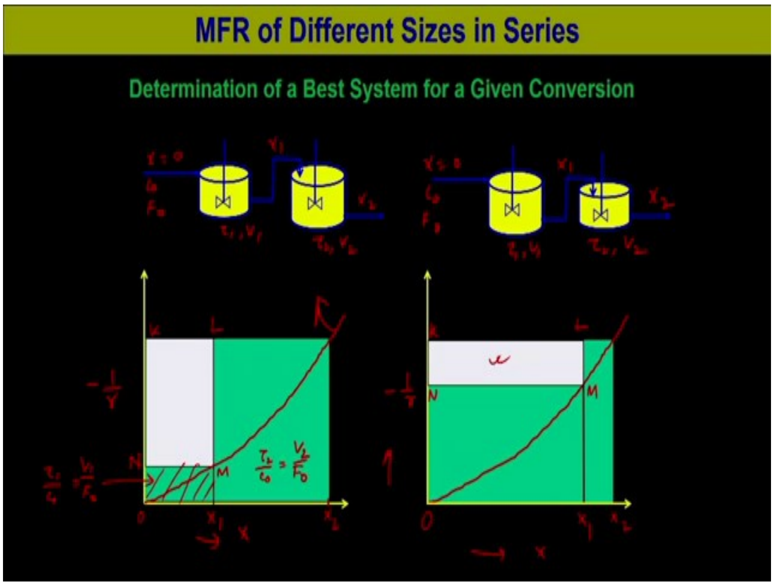

MFR of Different Sizes in Series

Determination of a Best System for a Given Conversion

So, if we plot the any arbitrary kinetics so this is the nomenclature we have given X is equal to 0, C_0, F_0, τ_1, V_1, τ_2, V_2 this is τ_1, V_1, τ_2, V_2. Here this is X_1 and this is X_2 so this is X_1, this is X_2 and X is equal to 0, C naught, F naught. Now, if we plot $-\frac{1}{r}$ versus conversion. So if we do that for a single reactor this is the conversion if we want it to achieve X_2 up to this, if want it to achieve the reactor volume requirement is this. So the area under the curve is nothing but, $\frac{V_2}{F_0}$.

Now, if we add smaller CSTR first, so this is the smaller CSTR volume requirement. So this is the volume requirement for smaller CSTR. And then if we add so it will give conversion from 0 to X_1. And this area under this curve would be

$$\frac{\tau_1}{C_0} = \frac{V_1}{\mathrm{F}_0}$$

Now, for this reactor 2 it will give the conversion X_1 to X_2 and this is the area under this curve is $\frac{\tau_2}{C_0} = \frac{V_2}{\mathrm{F}_0}$. So, this is any arbitrary curve rate $-\frac{1}{r}$ versus conversion curve.

Now, this is the area which is located on the shaded part is M, L, K, N. So this is the area which is, we have to optimize this rectangles. Now, if we consider the second case, second case what we have done, we have incorporated bigger reactor first and then the smaller reactor second. So, this is $-\frac{1}{r}$, this is X so if the bigger reactor first, then the volume requirement for the bigger reactor is this is one. So first reactor if bigger then it will take up to X_1 and then the second reactor will convert from X_1 to X_2.

So what we can see the total volume requirement if the reactor, if they are connected in series of unequal size. Their arrangement which should come first? Will depend on the optimization of the total volume required that means we have to optimize this rectangle that is M, N, K, L. So, if this area of this rectangle is this rectangle is bigger, then the total volume requirement by arranging that two CSTR in series would be minimum.

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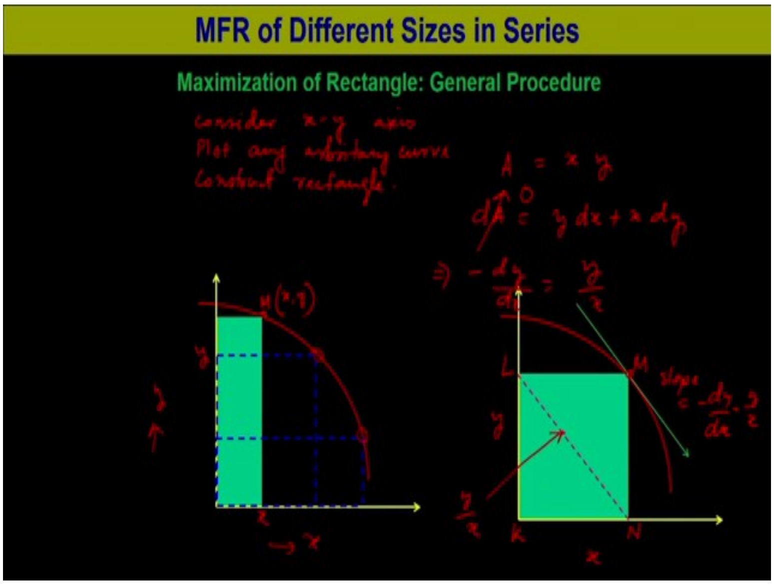

MFR of Different Sizes in Series

Maximization of Rectangle: General Procedure

consider x-y axis
Plot any arbitrary curve
Construct rectangle.

Now, let us consider maximization of the rectangle a general procedure. Let us consider X, Y axis. And we can plot any arbitrary curve so Y and X and then plot any arbitrary curve. We can construct a rectangle on which, so then we construct rectangle which touches the point M which is XY at this location. The area under this curve is A is equal to x, y and how we can maximize this area? If we differentiate this would be

$$dA = ydx + xdy$$

And at maximum d A would be 0, so we can write

$$\Rightarrow -\frac{dy}{dx} = \frac{y}{x}$$

So we plot the rectangle and see whether at different points it is touching and we plot the tangent and see whether that is with the diagonal. So this curve is say initially we had at Y and this is X. And then this point we have shifted to here, here and we see whether this diagonal matches with point touches at the curve point, whether the tangent is the equal to the diagonal of this rectangle.

So, if we plot again and if we plot the diagonals of this rectangle and then the tangent we could see that if both of them are parallel, diagonal of this rectangle that is M, where the tangent is drawn N, K, L. So the slope of this line, this is Y and this is X. So slope of this line is the diagonal is Y/X and slope of this tangent over here at we have drawn a tangent at a particular point. So that would be slope which is equal to $-\frac{dy}{dx} = \frac{y}{x}$. So the area of this rectangle we can maximize when the diagonal is parallel with the tangent to the curve.

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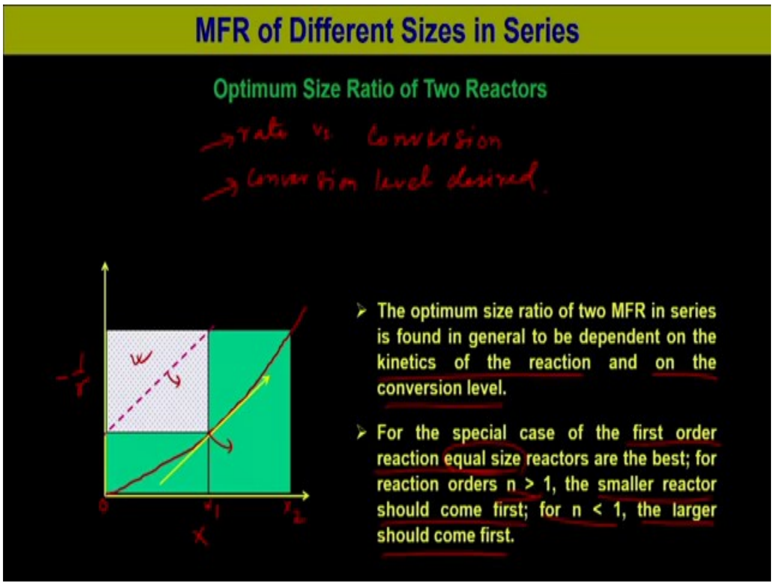

MFR of Different Sizes in Series

Optimum Size Ratio of Two Reactors

→ rate vs conversion

→ conversion level desired

- The optimum size ratio of two MFR in series is found in general to be dependent on the kinetics of the reaction and on the conversion level.
- For the special case of the first order reaction equal size reactors are the best; for reaction orders n > 1, the smaller reactor should come first; for n < 1, the larger should come first.

Now the return to our problem to the optimization of the size ratio of the two reactors, if we plot any arbitrary curve and then we plot the rectangle and then we find out the tangent to this rate curve to diagonal. So this is basically we can plot $-\frac{1}{r}$ versus conversion. So for the first reactor conversion is 0 to X_1. And for the second reactor the conversion is X_1 to X_2.

Now to optimize this we need to find out the volume of the first reactor requires. So the rectangle corresponding to this, this rectangle is the diagonal slope and the slope of this curve should be same. So this way we can calculate the optimum unit required for the particular operation. Now, the optimum size ratio of two MFR in series is found to be in general to be dependent on the kinetics of the reaction and the conversion level desired. So basically we have to look into the rate versus conversion curve that is one. And second point is the conversion level desired.

So these two factors are important to optimize the size requirement of the two MFR which is connected in series. For special case of the first order reaction of equal size reactor are the best show if the reaction is the first order in kind, then equal size reactors are the best one. But for order greater than 1 the smaller reactor should come first and for n less than 1 the larger should be at the beginning. So if reaction order is more than 1 so then smaller reactor should be at the beginning. And then we connect the larger reactor in series. And if the order is less than 1, then the larger reactor should be connected first and then the smaller one. But for the order which is equal to 1 equal size reactor are the best.

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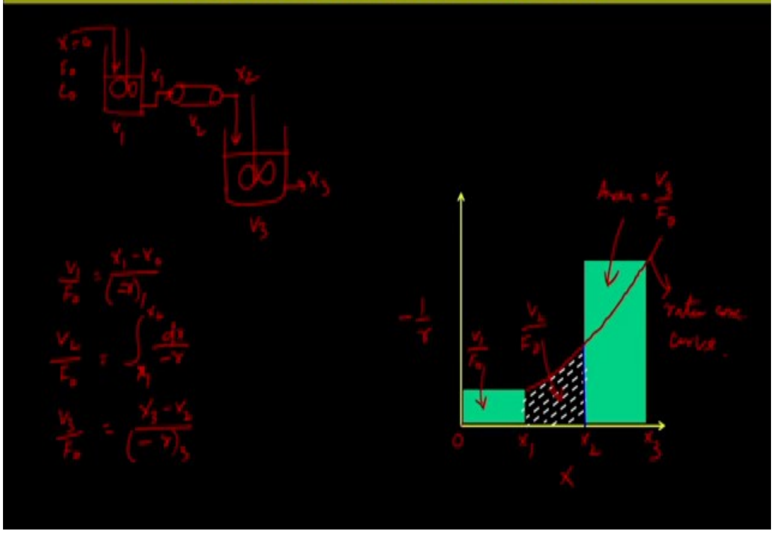
Reactors of Different Sizes in Series



Now, if we have reactors of different size. So say, we have three reactors, one is small CSTR, another is PFR and then bigger CSTR. So, if they connected, so inlet to this each conversion is 0, F_0 and C_0, this is volume V_1, this is volume V_2 and this is V_3 and exit to this is X_3. So exit to reactor 1 will go to PFR which is X_1 and exit to this will go the reactor 3. Plug flow reactor exit would be in reactor 3, so this would be X_2 and if this is connected in series of different sizes, how to order them, how to optimize their series?

So, if we write the performance equation for CSTR for the first reactor we can write

$$\frac{V_1}{F_0} = \frac{X_1 - X_0}{-r_1}$$

$$\frac{V_2}{F_0} = \int_{X_1}^{X_2} \frac{dX}{-r}$$

And

$$\frac{V_3}{F_0} = \frac{X_3 - X_2}{-r_3}$$

The relationship all this three reactor are shown graphically. If we plot the arbitrary curve which is $-\frac{1}{r}$ versus conversion. So then this is arbitrary curve and this is the first which CSTR which is connected.

And this is here the conversion is 0 and this is the conversion X_1. So, the area under this is $\frac{V_1}{F_0}$. Now, we connected the PFR, so the PFR volume will be this is much so area under this curve so this the PFR volume. So this is basically $\frac{V_2}{F_0}$ and finally if connect the larger CSTR, the volume requirement is under this curve. So this is X_2 and this is X_3 so this is for larger CSTR and the volume required area under this curve is $\frac{V_3}{F_0}$. And this is the rate concentration curve.

So this way we can see the volume requirement for different conversion level required when they are connected in series. Now, how to get the best arrangement of the three different ideal reactors connected in series?

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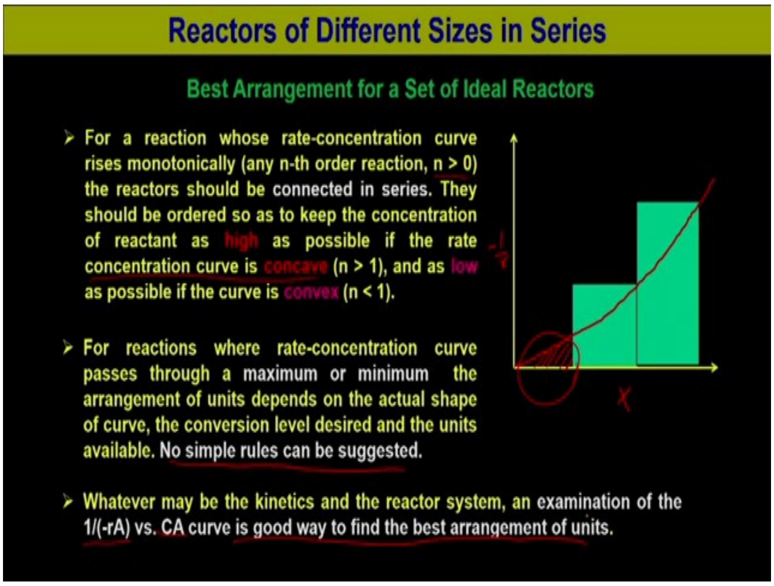

Reactors of Different Sizes in Series

Best Arrangement for a Set of Ideal Reactors

- For a reaction whose rate-concentration curve rises monotonically (any n-th order reaction, $n > 0$) the reactors should be connected in series. They should be ordered so as to keep the concentration of reactant as high as possible if the rate concentration curve is concave ($n > 1$), and as low as possible if the curve is convex ($n < 1$).
- For reactions where rate-concentration curve passes through a maximum or minimum the arrangement of units depends on the actual shape of curve, the conversion level desired and the units available. No simple rules can be suggested.
- Whatever may be the kinetics and the reactor system, an examination of the 1/(-rA) vs. CA curve is good way to find the best arrangement of units.

So the best arrangement we can get for a reaction whose rate concentration curve rises monotonically that is for nth order reaction. So, if we plot $-\frac{1}{r}$ versus conversion, and versus concentration. So, if we plot $-\frac{1}{r}$ versus conversion so this is the requirement of the area this is for PFR first one. Then we have small CSTR, then large CSTR. So for a reaction which rate concentration curve rises monotonically that is for the reaction order greater than 0 the reactor should be connected in series.

They should be ordered, so as to keep the concentration of the reactant as high as possible if the rate concentration curve is concave that is for n greater than 1. And as low as possible that is convex for n less than 1. Now, for reactions where rate concentration curve passes through a maximum or minimum the arrangement of the units depends on the actual shape of the curve, and the conversion level desired. The units available and no simple rules can be suggested.

So, what we can see only when the order is positive that is N greater than 0. And the rate concentration curves rises monotonically. We can have two different ways to arrange the reactor connected in series. And when the rate concentration curve is concave, that is for n greater than 1. We have to keep the concentration as high as possible that means we have to connect first the PFR. Then small CSTR and then larger CSTR. And this trend or ordering of the reactor would be reverse if we have the convex curve that is for L less than 1. So, in that case the larger CSTR should be connected first and then small CSTR and then PFR.

But, where the rate concentration curve is such the maxima or minima simple rule can be suggested. And we have to look into the shape of the curve and optimize the area. Whatever may be the kinetics and the reactor system and examination of the $\frac{1}{r_A}$ versus C_A, the rate versus concentration curve is good way to find the best arrangement of the units.

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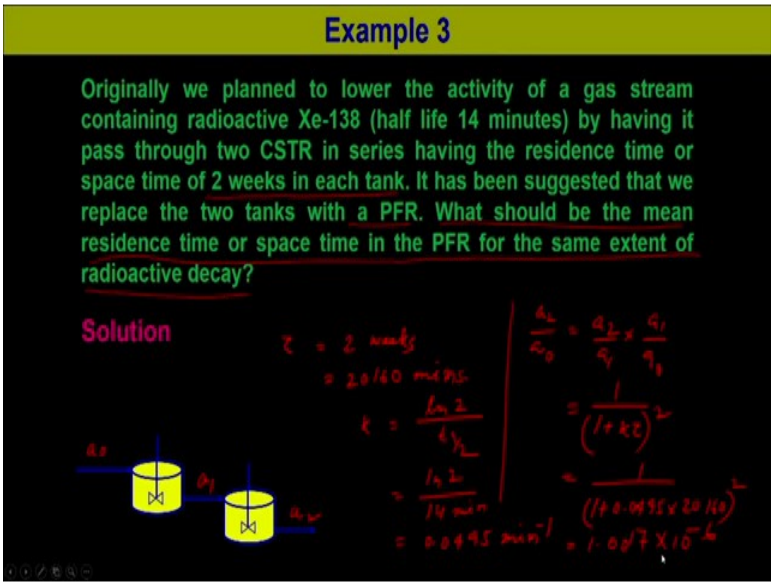

Example 3

Originally we planned to lower the activity of a gas stream containing radioactive Xe-138 (half life 14 minutes) by having it pass through two CSTR in series having the residence time or space time of 2 weeks in each tank. It has been suggested that we replace the two tanks with a PFR. What should be the mean residence time or space time in the PFR for the same extent of radioactive decay?

Solution

$\tau = 2$ weeks

$= 20160$ mins

$k = \frac{\ln 2}{t_{1/2}}$

$= \frac{\ln 2}{14 \text{ min}}$

$= 0.0495 \text{ min}^{-1}$

$\frac{a_2}{a_0} = \frac{a_2}{a_1} \times \frac{a_1}{a_0}$

$= \frac{1}{(1+k\tau)^2}$

$= \frac{1}{(1+0.0495 \times 20160)^2}$

$= 1.0017 \times 10^{-6}$

Now, let us see one example. Originally we planned to lower the activity of a gas streams containing radioactive materials xenon 138, half line is 14 minutes by having it pass through the two CSTR connected in series. And they are having the residence time or the space time 2 weeks in each tank. It has been suggested that we replace the two tanks with a PFR. What should be the mean residence time or space time of PFR for the same extent of radioactive decay?

So, now consider two CSTR connected in series and this is a naught and this is a_1 and this is a_2. Now τ is given, τ is equal to 2 weeks so which is 20160 minute. So radioactive decay of the first order reaction we can write K first order kinetics

$$k = \frac{\ln 2}{t_{1/2}}$$

So which is equal to (ln 2)/14 minute and this is about 0.0495 minute inverse. Now, if write for the exit or for tank two we can write

$$\frac{a_2}{a_0} = \frac{a_2}{a_1} = \frac{a_1}{a_0}$$

So then we can write for two tank connected in series this would be $\frac{1}{(1+k\tau)^2}$. Now, if we substitute the values this would be

$$= \frac{1}{(1+0.0495*20160)^2}$$

So this would be equal to $1.0017*10^{-6}$.

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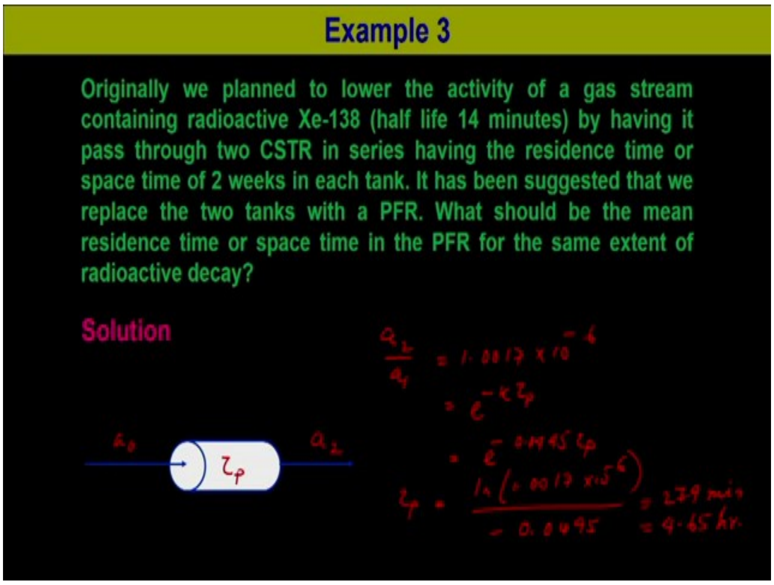

Example 3

Originally we planned to lower the activity of a gas stream containing radioactive Xe-138 (half life 14 minutes) by having it pass through two CSTR in series having the residence time or space time of 2 weeks in each tank. It has been suggested that we replace the two tanks with a PFR. What should be the mean residence time or space time in the PFR for the same extent of radioactive decay?

Solution

$$\frac{a_2}{a_1} = 1.0017 \times 10^{-6} = e^{-k\tau_p} = e^{-0.1445\tau_p}$$

$$\tau_p = \frac{\ln(1.0017 \times 10^{-6})}{-0.0495} = 279 \text{ min} = 4.65 \text{ hr.}$$

Now, for PFR this is a naught and outlet would be a_2 and we have calculate τ_p. So

$$\frac{a_2}{a_1} = 1.0017 * 10^{-6}$$

$$= e^{-k\tau_p}$$

$$= e^{-0.1445\tau_p}$$

So if we solve this we will get

τ_p = ln 1.0017*10^{-6}/-0.0495.

So, which is about 279 minute or 4.65 hour.

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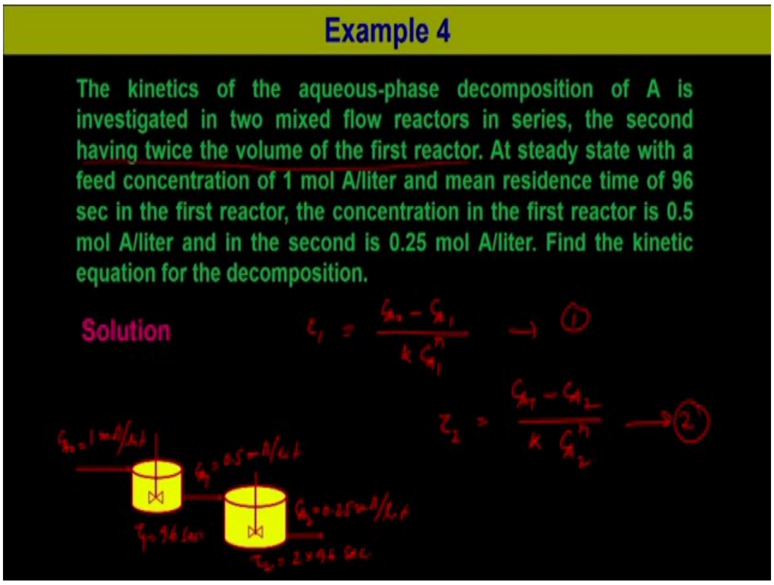

Example 4

The kinetics of the aqueous-phase decomposition of A is investigated in two mixed flow reactors in series, the second having twice the volume of the first reactor. At steady state with a feed concentration of 1 mol A/liter and mean residence time of 96 sec in the first reactor, the concentration in the first reactor is 0.5 mol A/liter and in the second is 0.25 mol A/liter. Find the kinetic equation for the decomposition.

Solution

$$\tau_1 = \frac{C_{A0} - C_{A1}}{k C_{A1}^n} \rightarrow ①$$

$$\tau_2 = \frac{C_{A1} - C_{A2}}{k C_{A2}^n} \rightarrow ②$$

Now, if we take another examples, where the kinetics of non-aqueous phase decomposition of A is investigated in two mixed flow reactors connected in series, the second reactor is having twice the volume of the first reactor. So, the volume of the reactor is increased at steady state with a feed concentration of 1 mole of A per liter and mean residence time is 96 second in the first reactor. The concentration in the first reactor is 0.5 mole A per liter. And in the second reactor is 0.25 mole per liter, find the kinetic equation for the decomposition.

So, if we take two reactor which are connected in series and there it is given that at the inlet we have 1 mole per liter feed concentration. So, C_{A0} = 1 mole per liter and C_{A1} = 0.5 mole per liter, and C_{A2} = 0.25 mole per liter, τ for the first reactor is given is τ_1 = 96 second. Whereas, for the second reactor it should be double so τ_2 = 2*96 second.

Now, for the first reactor for any nth order kinetics we can write

$$\tau_1 = \frac{C_{A0} - C_{A1}}{kC_{A1}^n} \quad \text{......................}(1)$$

And for the second reactor that is

$$\tau_2 = \frac{C_{A0} - C_{A2}}{kC_{A2}^n} \quad \text{....................}(2)$$

So this is equation 2, so tau 1 and tau2.

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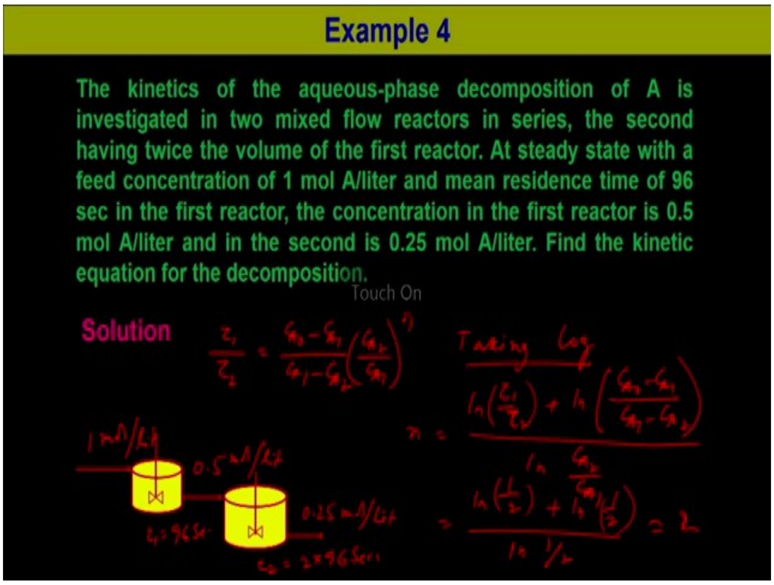

Example 4

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Solution

$$\frac{\tau_1}{\tau_2} = \frac{C_{A0}-C_{A1}}{C_{A0}-C_{A2}}\left(\frac{C_{A2}}{C_{A1}}\right)^n$$

Taking Log

$$n = \frac{\ln\left(\frac{\tau_1}{\tau_2}\right) + \ln\left(\frac{C_{A0}-C_{A1}}{C_{A0}-C_{A2}}\right)}{\ln\frac{C_{A2}}{C_{A1}}} = \frac{\ln\left(\frac{1}{2}\right) + \ln\left(\frac{1}{2}\right)}{\ln 1/2} = 2$$

Now, if we divide equation 1 by equation 2 the ratio would be, we can write. This is

$$\frac{\tau_1}{\tau_2} = \frac{C_{A0}-C_{A1}}{C_{A0}-C_{A2}}\left(\frac{C_{A2}}{C_{A1}}\right)^n$$

So taking log both sides, taking log we obtain

$$n = \frac{\ln\left(\frac{\tau_1}{\tau_2}\right) + \ln\left(\frac{C_{A0}-C_{A1}}{C_{A0}-C_{A2}}\right)}{\ln\left(\frac{C_{A2}}{C_{A1}}\right)}$$

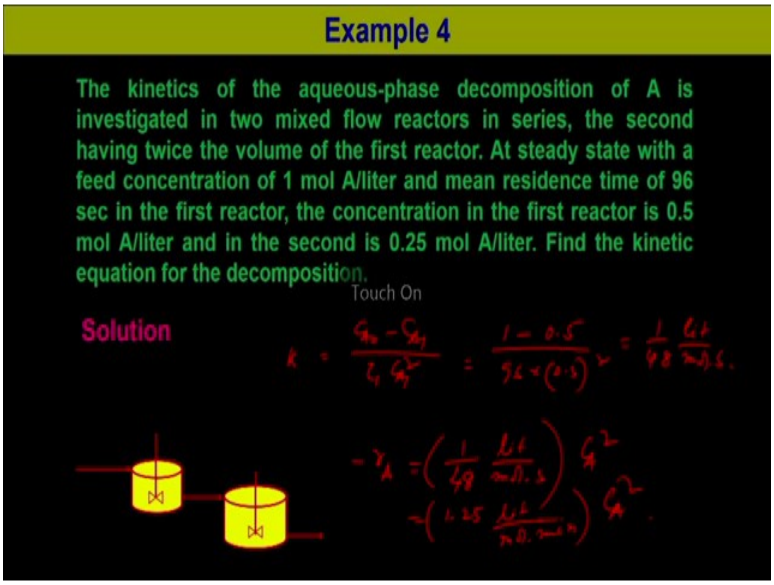
And if we substitute by values then this is 1 this is 0.5 and this 0.25 mole per liter.

Now, if you substitute the values this is τ_1 is 96 second and τ_2 is 2*96 second. So if we substitute here this would be

$$n = \frac{\ln\left(\frac{1}{2}\right) + \ln\left(\frac{1}{2}\right)}{\ln\left(\frac{1}{2}\right)}$$

So this would give n = 2. So this is second order reaction.

(Refer Slide Time: 87:18)



Example 4

The kinetics of the aqueous-phase decomposition of A is investigated in two mixed flow reactors in series, the second having twice the volume of the first reactor. At steady state with a feed concentration of 1 mol A/liter and mean residence time of 96 sec in the first reactor, the concentration in the first reactor is 0.5 mol A/liter and in the second is 0.25 mol A/liter. Find the kinetic equation for the decomposition.

Touch On

Solution

$$k = \frac{C_{A0}-C_{A1}}{\tau_1 C_{A1}^2} = \frac{1-0.5}{96\times(0.5)^2} = \frac{1}{48}\frac{lit}{mol.s}$$

$$-r_A = \left(\frac{1}{48}\frac{lit}{mol.s}\right)C_A^2 = \left(1.25\frac{lit}{mol.min}\right)C_A^2$$

So now, if we replace this order in the first reactor τ equation τ_1, so

$$k = \frac{C_{A0} - C_{A1}}{\tau_1 C_{A1}^2} = \frac{1-0.5}{96*(0.5)^2} = \frac{1}{48}\frac{lit}{mol.s}$$

And hence, we can calculate the rate equation is

$$-r_A = \left(\frac{1}{48}\frac{lit}{mol.s}\right)C_A^2$$

or

$$= 1.25\frac{lit}{mol.\text{min}}C_A^2$$

So this is how we can obtain the kinetics of the decomposition reactions in the aqueous phase. So thank you very much for attending this lecture and we will continue our reactor design in the next lecture as well.