Chemical Reaction Engineering-I
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Lecture - 14
Size Comparisn of Single and Multiple Reactors

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

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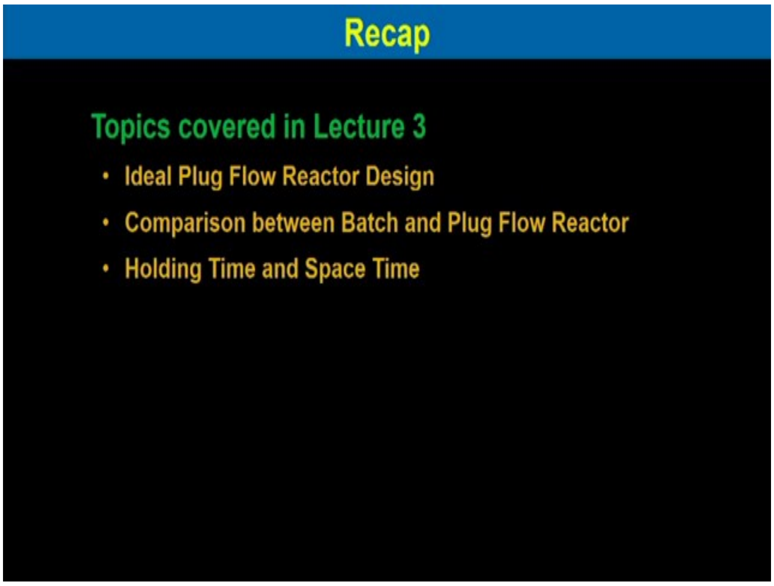

In our last lecture we have covered mostly the design of ideal plug flow reactor and then comparison between batch and plug flow reactor and we have seen that for a constant volume systems the batch reactor equations and plug flow reactor design equations can be used interchangeably. Now we have also discussed the holding time and the space time and we have seen for a variable density system the holding time and space time they are not same. Whereas for a constant density system both holding time and the space time both are same.

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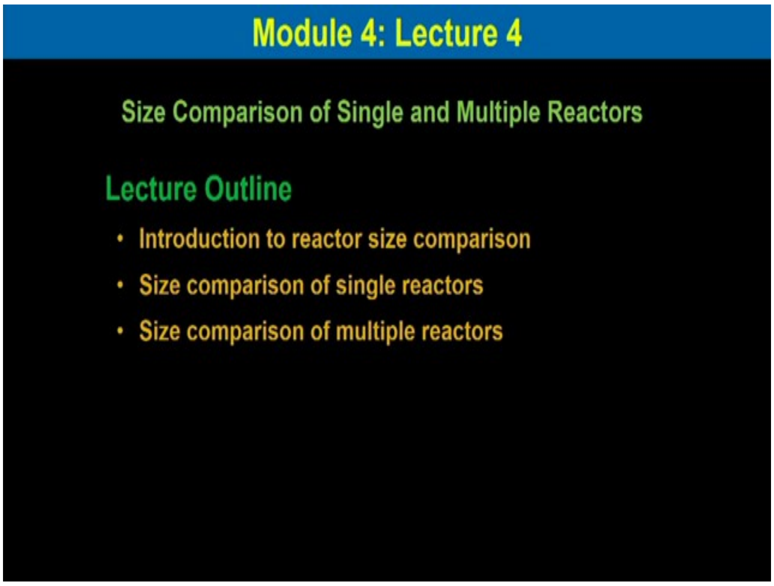

Now, in this lecture we will consider the size comparison of single and multiple reactors. So the topic which would cover in this lecture are introduction to reactor size comparison, then we will consider size comparison to single reactors and then we will compare the size of the multiple reactors.

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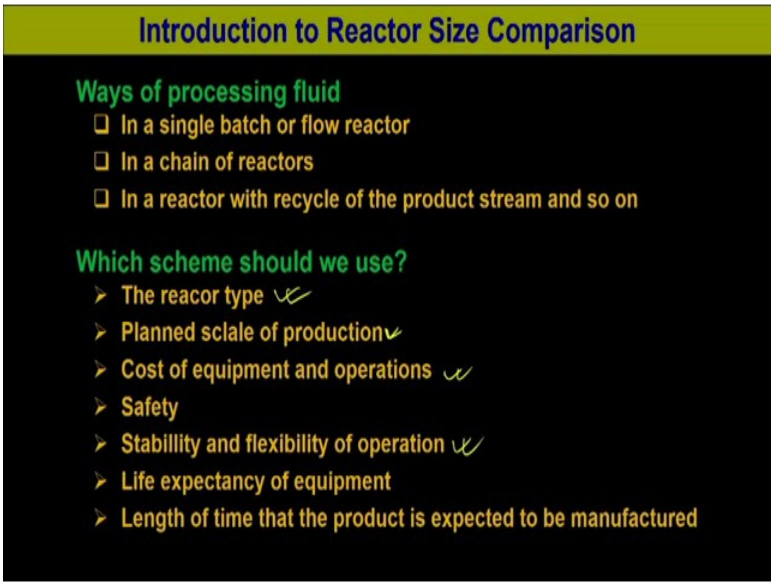

Now, let us have a brief introduction of the reactor size comparison. How many ways we can process the fluid? So there are many ways either we can use single batch reactor or we can also use single flow reactor. We can also use a chain of reactors, either chain of batch reactors, chain of different flow reactors, where the reactants from one reactor reacts and then the product which is out can be fed into the second reactors. So that way we can use particularly flow reactor in a chain of reactors.

Then in a reactor with recycle of product stream, we can also, the some product we can recycle depending on the conversion we need which we called the recycle reactor and so many other variations of it. Then which scheme should we use? This will depend on several factors, one of them is the reactor type what kind of reactor we should use for a particular job?

Then the second thing is how much is the planned scale of production? If the planned scale production is very large in that case we have to use the continues reactors, otherwise if the production is small like in case of some medicinal production. So we required small batch of the medicines, so we can use batch reactor, so planned production is also important.

The cost of equipment and operations, so whether the equipment which we need to install is the cost is very high and its operation is very complex or whether cost is minimum and also it is operation is easy. So these factors have to be consider when we consider the particular scheme. The other factor is the safety, whether the equipment is safe to operate under the conditions of the operation and stability and flexibility and operation that means if we wanted to have a very small production whether we can use it or if wanted to scale up whether it is very easy to scale up so stability and flexibility of operation.

Then life expectancy of equipments, how long this equipment can serve for on doing successive jobs and length of time that the product is expected to be manufactured. So if we need production for a very short period we may not go for the continuous reactor, we may go for a batch reactor.

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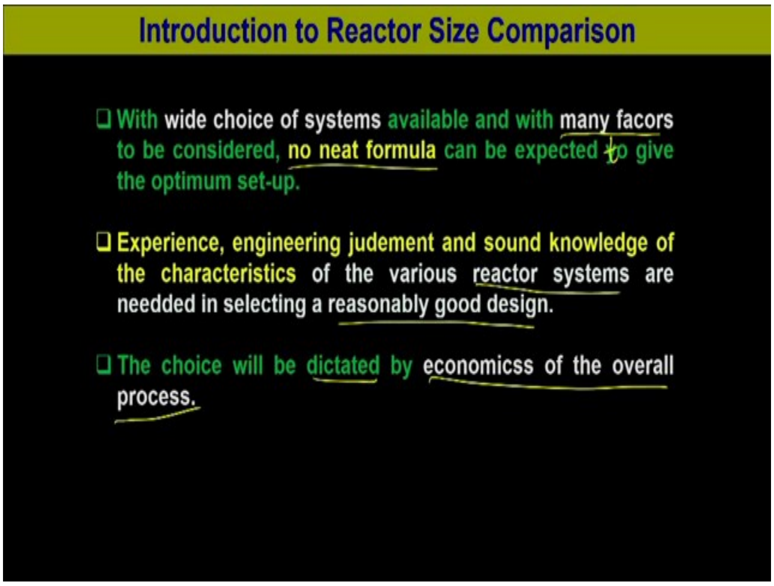

So with wide choice of systems available and with many factors to be considered no neat formula can be expected to give the optimum set-up. What we need to do? Experience, engineering judgements and sound knowledge of the characteristics of the various reactor systems are needed while selecting a reasonably good design. So if we need to select a reasonably good design we must have a strong experience and we should have a strong engineering judgement with the knowledge of the characteristics of the reactors how it behaves.

Considering all these factors we can reasonably decide a good design. But overall for doing any optimum design we need to get, we must have to consider the economics, so economics will finally tell whether that should be acceptable or not. So the choice will be dictated by the economics of the overall process. So economics of the overall process will decide whether the design which we have selected is acceptable for operation.

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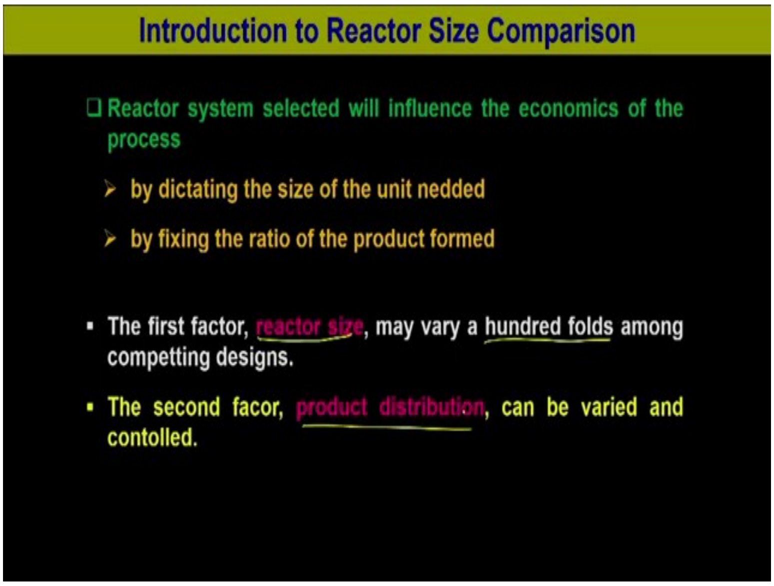

Now reactor system which we selected will influence the economics of the process by dictating the size of the unit needed. So the economics will influence the size of the unit which we need and also by fixing the ratio of the product found. So these two things size and the product distribution, these two will influence the economics of the process. Now, which one to choose? The first factor which is the reactor size may vary a 100 folds among the competing design.

So if we have several competing designs in hand the reactor size may vary several folds, several times from one design to the other, the second factor which is the product distribution which can be varied and controlled so that we can vary and control.

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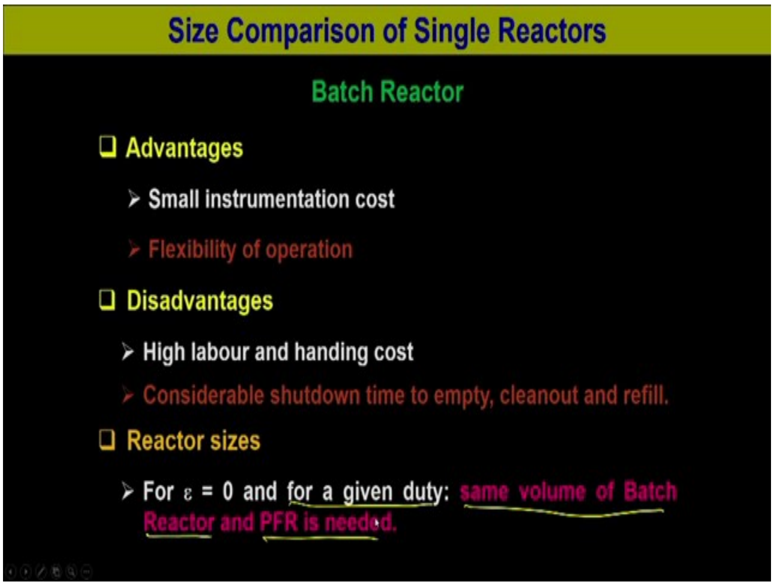

Now, if we consider batch reactor before going to the flow reactor let us consider batch reactor. The advantage of batch reactor is it is very small instrumentation cost. We really need a very high cost instruments or large number of accessories. So the instrumentation cost for the batch reactor is minimum and it is very flexible for operations, we can go for small scale to the medium scale so we can, whenever we want we can run, whenever we do not want we can stop it.

So flexibility of operation is there so these are the advantages of batch reactor, whereas the major disadvantages for the batch reactor are high labour and handling cost. So because it requires for its operation there would be shutdown cleaning and refilling. So the number of labours required is high compare to the continous reactor and its handling of the materials is also no costly appears.

And the time, considerable shut down time to empty, clean out and refill these are the disadvantages of the batch reactor. So when we consider reactor size which we need for a constant density system ε is equal to 0 and for a given duty if we compare the design equations between the plug flow reactor and the batch reactor the design equation for both of them are same.

So they require for a given duty, same duty, same volume of batch reactor and the PFR is needed. However, in case of batch reactor it requires the shutdown, cleaning and empty, the time and the handling cost and the labour cost that are the disadvantages, otherwise volume wise for a particular job at constant volume system both require same volume of the batch or same volume of the reactor.

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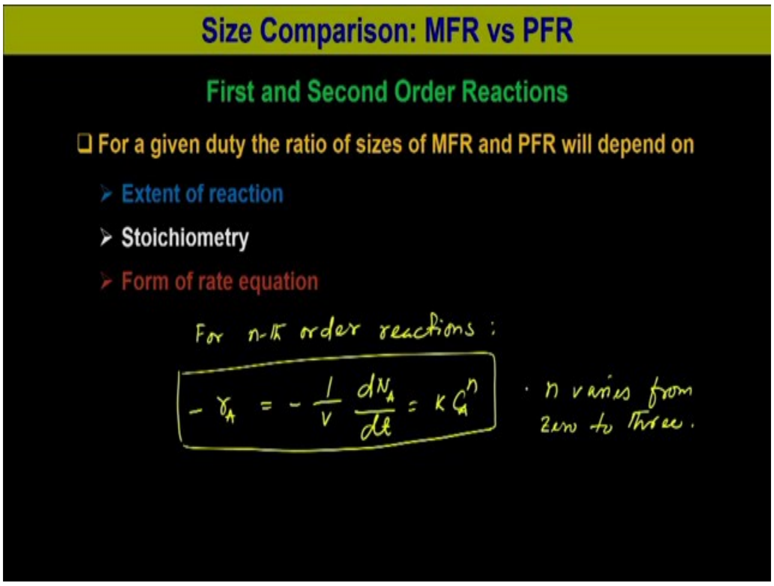

Now, if we compare size among the MFR and the PFR, mixed flow reactor and the plug flow reactor. So for a first order and second order reactions we will see the comparison between these two. So for a given duty the ratio of the sizes MFR and PFR will depend on the following factor is the extent of reaction, then the stoichiometry and the form of rate equation.

Now if we consider the general rate expression say for a single reaction. For nth order reactions we can write

$$-r_A = -\frac{1}{V}\frac{dN_A}{dt} = kC_A^2$$

That is for nth order reaction as we have discussed earlier in last few lectures and here n varies from 0 to 3.

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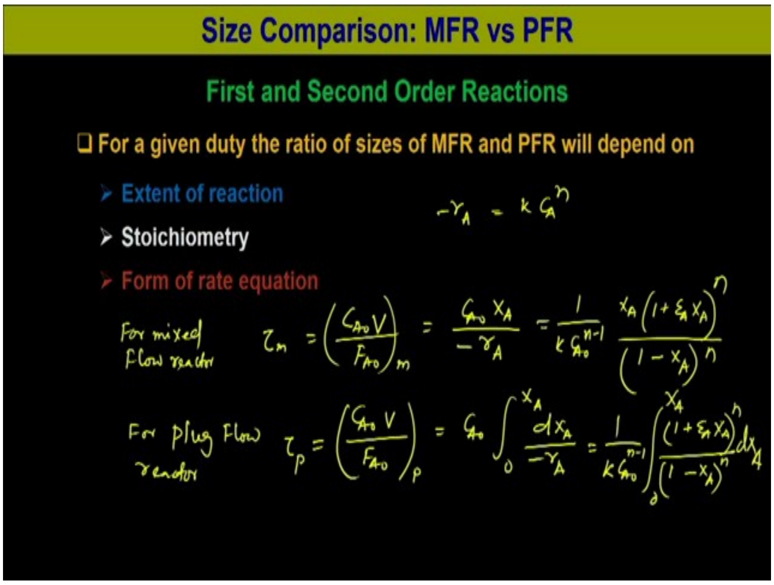

Now, if we consider for the two reactors, the same equation for nth order reaction the tau m that is for mixed flow reactor,

$$\tau_m = \left(\frac{C_{A0}V}{F_{A0}}\right)_m = \frac{C_{A0}X_A}{-r_A}$$

Which we can write for nth order reaction, if we substitute,

$$-r_A = kC_A^n$$

if we substitute this would be

$$= \frac{1}{kC_{A0}^{n-1}}\frac{X_A(1+\varepsilon_A X_A)^n}{(1-X_A)^n}$$

Now, if we consider Plug Flow Reactor, this space time we can write tau p would be equal to

$$\tau_P = \left(\frac{C_{A0}V}{F_{A0}}\right)_P = C_{A0}\int_0^{X_A}\frac{dX_A}{-r_A} = \frac{1}{kC_{A0}^{n-1}}\int_0^{X_A}\frac{X_A(1+\varepsilon_A X_A)^n}{(1-X_A)^n}$$

So this is for, τ_M is for the mixed flow reactor or CSTR and τ_P is for the plug flow reactor.

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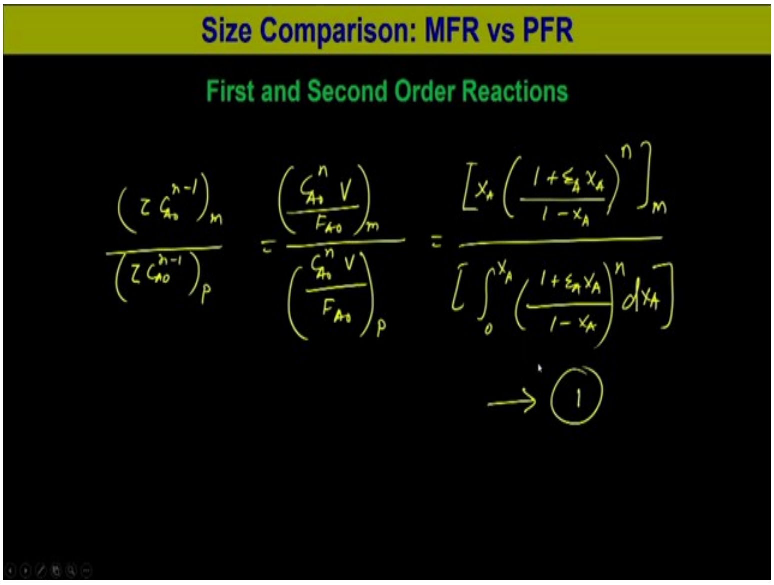

Now, if we divide

$$\frac{(\tau C_{A0}^{n-1})_m}{(\tau C_{A0}^{n-1})_p} = \frac{\left(\dfrac{C_{A0}V}{F_{A0}}\right)_m}{\left(\dfrac{C_{A0}V}{F_{A0}}\right)_P} = \frac{\left[\dfrac{X_A(1+\varepsilon_A X_A)^n}{(1-X_A)^n}\right]_m}{\left[\displaystyle\int_0^{X_A} \frac{X_A(1+\varepsilon_A X_A)^n}{(1-X_A)^n}\right]_p}$$

So say this is equation 1.

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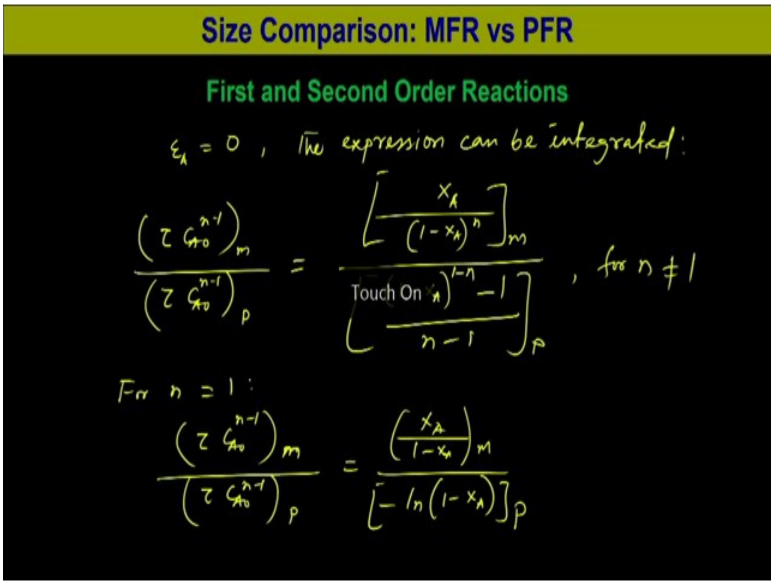

Now, if we consider the constant density system that means ε_A would be naught and the expression can be integrated and we would obtain

$$\frac{(\tau C_{A0}^{n-1})_m}{(\tau C_{A0}^{n-1})_p} = \frac{\left[\dfrac{X_A}{(1-X_A)^n}\right]_m}{\left[\dfrac{(1-X_A)^{1-n}-1}{n-1}\right]_p}$$

So this is valid for n $\neq$ 1. So for n = 1, we can get

$$\frac{(\tau C_{A0}^{n-1})_m}{(\tau C_{A0}^{n-1})_p} = \frac{\left[\dfrac{X_A}{1-X_A}\right]_m}{\left[-\ln(1-X_A)\right]_p}$$

This is for the first order.

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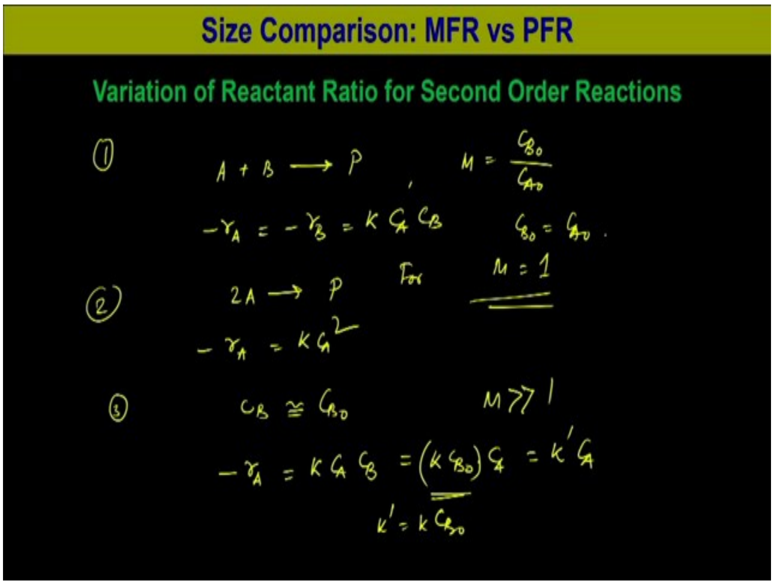

Now, if we consider second order the variation of the reactant ratio for second order reactions we can write say two component systems

$$A + B \rightarrow P$$

and if we consider $M = \dfrac{C_{B0}}{C_{A0}}$

$$-r_A = -r_B = kC_AC_B$$

This is the rate expression. This will behave second order when the reactant ratio is unity that means C_{B0} is equal to C_{A0}.

So M is equal to 1, so in that case the reactions can behave like second order that is twice A to product.

$$2A \rightarrow P$$

So we can write

$$-r_A = kC_A^2$$

that is for M = 1. Now, if we have one of the reactants in large excess whose concentration change with respect to the other is negligible, then this second order reactions can behave like a pseudo first order reactions.

So if we consider the change in concentration for B is very less that means for third case $C_B \cong C_{B0}$. So in that case

$$-r_A = (kC_{B0})C_A = k^{'}C_A$$

So which we can write $k^{'}$, which is $k^{'} = kC_{B0}$ which is approximately. So this will behave for a second order reaction when $M >> 1$. So these are the cases which we will see for the second order reaction when they behave different order relative ratio of the components in the mixture.

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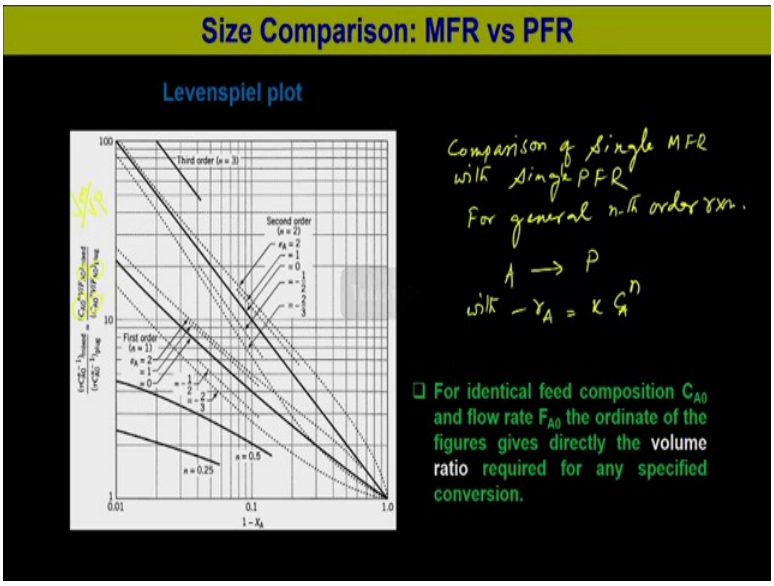

Now, the comparison between the mixed flow reactor with the plug flow reactor is shown in this Levenspiel plot, you can see that it is plotted with $(\tau C_{A0}^{n-1})_m$ for mixed flow reactor divided by $(\tau C_{A0}^{n-1})_p$ for plug flow reactor and if we consider this would be equal to $\left(\frac{C_{A0}^{n}V}{F_{A0}}\right)_m$ for the mixed flow reactor divided by $\left(\frac{C_{A0}^{n}V}{F_{A0}}\right)_p$ for plug flow reactor.

So this is the comparison of single plug flow reactor with the single CSTR, their volume requirement and this is for general nth order reactions. So comparison of single MFR with single PFR for general nth order reaction. That means

$$A \rightarrow products \text{ ; with } -r_A = kC_A^n$$

Now for identical fit composition that is C_{A0} and flow rate F_{A0}. So if C_{A0} and F_{A0} if they are same for both the reactors in that case this plots directly now give the volume ratio required for any specified conversion. So this gives the volume of mixed flow reactor V_{mixed}/V_{plug} . So it gives the volume ratio between the two reactors.

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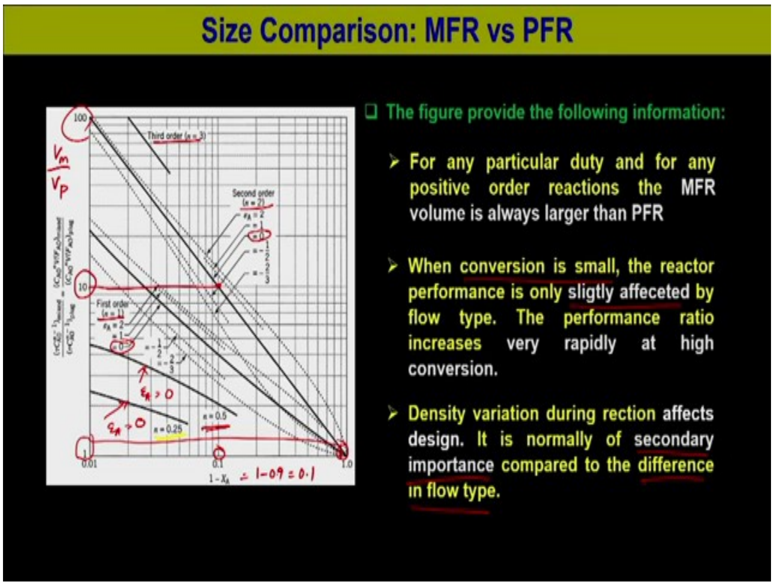

Now, from this figure what we can draw or what we can understand that for any particular duty and for any positive order reaction, so if we look over here this is for all the lines shown over here are for n positive n > 0. So this is for n is equal to 0.25, this is for n is equal to 0.5 and this is n is equal to 1, this is n is equal to 2 and this is n is equal to 3. So all the bold line you can see over here is for or solid line plotted in this figure is basically the positive order reactions.

So we can see for any particular duty and for any positive order reactions the MFR volume is always larger than PFR. So the volume require for a particular duty the volume require for mixed flow reactor is higher than the plug flow reactor as you can see this is a log log plot and y-axis starts with 1 their volume ratio that is V_{mixed}/V_{plug} and this is 10, the volume ratio is 10 and this volume ratio is 100.

So for all the positive order reactions the volume required for mixed flow reactor is always higher than the plug flow reactor for a given duty and positive order reaction. Now another thing we can understand when conversion is small the reactor performance is only slightly effected by the flow type. So we can see that if we come closer to this point this x-axis shows $1-X_A$.

That means when conversion is very low say 0.1 it would be $1-X_A$ would be 0.9. So which is close to here at this location. So for all the order so positive order reaction we can see their ratio is hardly close to 1.1 or so. So that means the, all though the volume requirement for mixed flow reactor is higher than the plug flow reactor, but that volume change or their ratio is very negligible very small which is close to unity.

So that is why for, when the conversion is small the reactor performance only slightly effected by the flow type, but the performance ratio increases very rapidly at high conversion. If we consider say conversion is 90 percent. So $1-X_A$ would be 0.1, 1-0.9 90 percent conversion. So it would be 0.1 so if you consider over here for 90 percent conversion and if we go to the second order reaction say here.

So their volume ratio would be 10. So similarly for all positive order reactions their performance ratio increases very rapidly at high conversion. Now this plot also shows the variation of the density for the system as you can see the solid line which is shown for all positive order reaction is for ε_A is equal to 0 this is for 0 and this is also for 0. So for this also ε_A is equal to 0 and ε_A is equal to 0.

So the solid line represents the at constant density system, but if there is a change in density we can see it shifts either when ε_A is positive then it goes to the upper side, when it is negative it goes to the downwards, but it effects the design obviously but it is of secondary importance compared to the difference of their flow type. So all though the ratio of the volume requirements is changes, but that change is marginal compared to the change or the influence of the different flow types.

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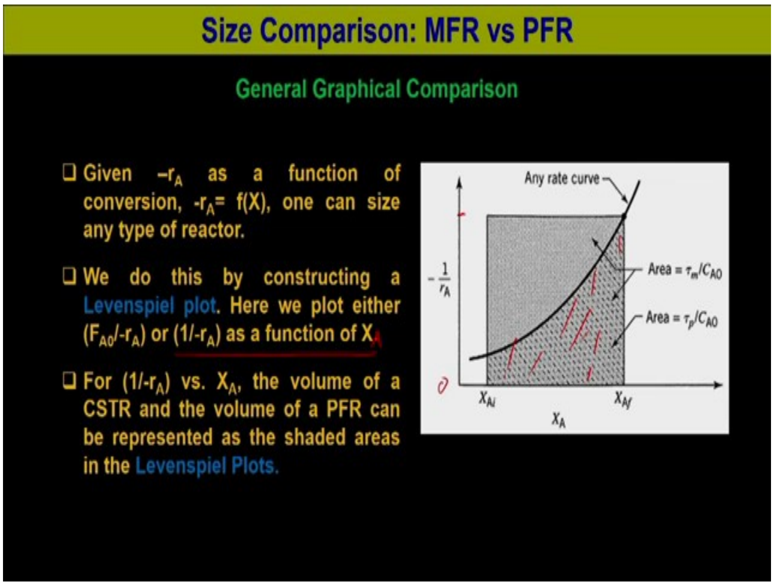

Now, we can graphically compare between the mixed flow reactor and plug flow reactor, their volume. So from their performance equation we can graphically compare them. To graphically compare given a rate as a function of conversion that is $-r_A = f(X)$, one can size any type of reactor, whatever type of reactor you take if you have minus rA versus no conversion, relation, you can see their size from graphical comparison.

We can do this by constructing a Levenspiel plot. Here we plot either $\frac{F_A}{-r_A}$ or $\frac{1}{-r_A}$ as a function of X. So if we plot from the Levenspiel, if we have seen that $\frac{1}{-r_A}$ versus conversion X_A if we plot you can see the area under this shaded portion over here below this curve is basically is a plug flow area $\frac{\tau_P}{C_{A0}}$. As we know the design equation for plug flow reactor is the integral form which is $\frac{\tau_P}{C_{A0}}$.

So, for $\frac{1}{-r_A}$ versus X_A plot the volume of a CSTR and the volume of a PFR can be represented as the shaded areas in the Levenspiel Plot. So for CSTR it is not the integral form of the equation so the CSTR volume will be this rectangle where conversion varies from X_{Ai} to X_{Af} and $-r_A$ varies from $-\frac{1}{r_A}$ varies from 0 to up to this location. So this area is both the shaded portion of the areas is the volume required for CSTR which is or mixed flow reactor it is $\frac{\tau_m}{C_{A0}}$.

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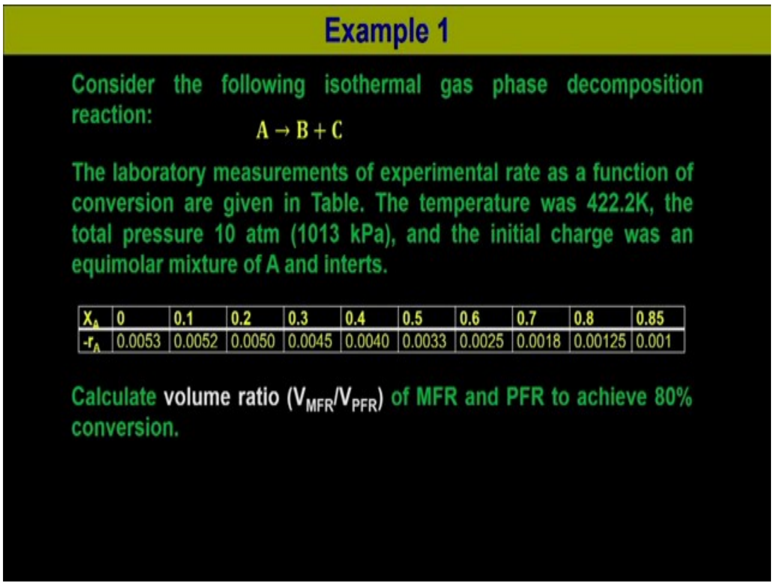

Now, let us take an example to see the volume requirement between the plug flow reactor and the mixed flow reactor for a given duty. Consider the following isothermal gas phase decomposition reaction that is $A \rightarrow B + C$. The laboratory measurements of the (experiments) experimental rate as a function of conversion are given in the table. So this is the table conversion and rate.

The temperature was 422.2 kelvin, the total pressure of the system is 10 atmosphere which is 1013 kilo Pascal and the initial charge was an equimolar mixture of A and inert. Calculate the volume ratio V_{MFR}/V_{PFR} of mixed flow reactor and plug flow reactor to achieve 80 percent conversion.

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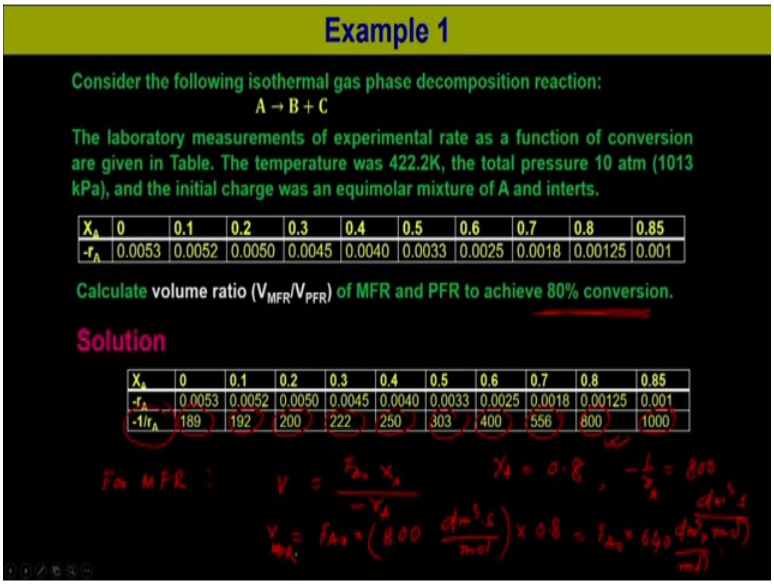

Now, let us solve it. So from this X_A versus $-r_A$ data which are given in the table we can calculate the $-\frac{1}{r_A}$. So if we calculate these values we can obtain $-\frac{1}{r_A}$ at different conversion.

Now, for CSTR or mixed flow reactor the equations of volume is equal to

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

Given that X_A is 0.8, 80 percent conversion. So, and at 80 percent conversion our rate $-\frac{1}{r_A}$ these values are given is 800.

So $-\frac{1}{r_A}$ at 80 percent conversion is 800 these are in units of decimetre cube second per mole.

So we can calculate from here

$$V = F_{A0} * \left(800 \frac{dm^3.s}{mol}\right) * 0.8 = F_{A0} * 640 \frac{dm^3.s}{mol}$$

So this is volume for MFR mixed flow reactor volume.

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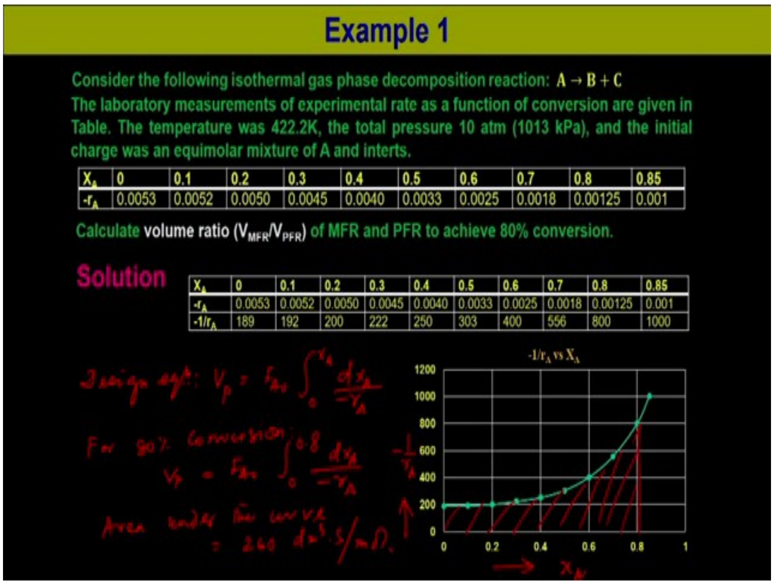

Now, for PFR we know the design equation

$$V_p = F_{A0} \int_0^{X_A} \frac{dX_A}{-r_A}$$

So for 80 percent conversion we can write

$$V_p = F_{A0} \int_0^{0.8} \frac{dX_A}{-r_A}$$

So the data which are given this is the data and we have calculated $-\frac{1}{r_A}$. Now if we plot $-\frac{1}{r_A}$ versus X_A so the plot will show this is $-\frac{1}{r_A}$, this is X_A.

So, the area under the curve up to 0.8 so that would be the area under the integral that is for plug flow reactor. So this area we can calculate using any of the method either Simpson one third method or trapezoidal rule whatever we can use and calculate the area under the curve. So the area would be is about 260 decimetre cube second per mole. So now, if we substitute over here

$$V_p = F_{A0} * 260 \frac{dm^3.s}{mol}$$

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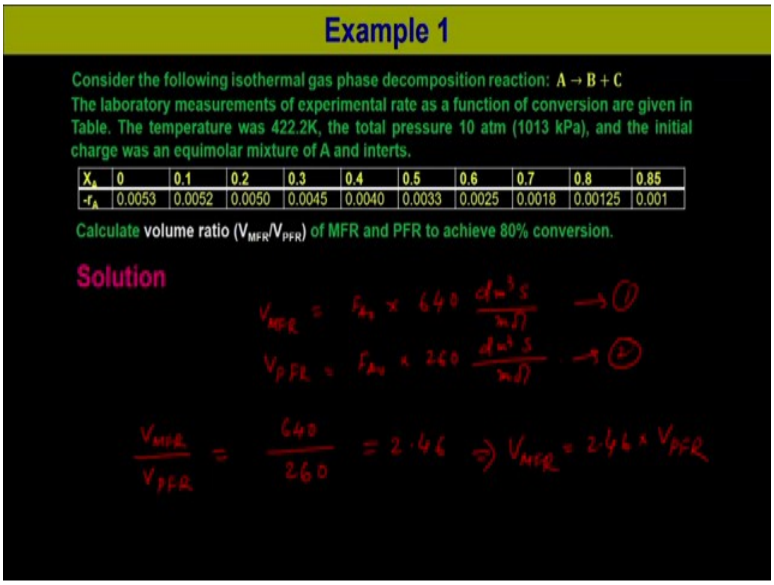

Now, we have calculated

$$V_m = F_{A0} * 640 \frac{dm^3.s}{mol} \text{ ....(1)}$$

$$V_p = F_{A0} * 260 \frac{dm^3.s}{mol} \text{ ....(2)}$$

Now, if we substitute if we divide these two relations, so divide two, equation 2, divide equation 1 by equation 2 we can get V_{MFR}/V_{PFR} would be equal to 640 divided by 260 which is equal to 2.46 that means $V_{MFR} = 2.46\ V_{PFR}$. So the MFR volume requirement for 80 percent conversion is about 2.46 times higher compared to the plug flow reactor volume requirement to perform the same job.

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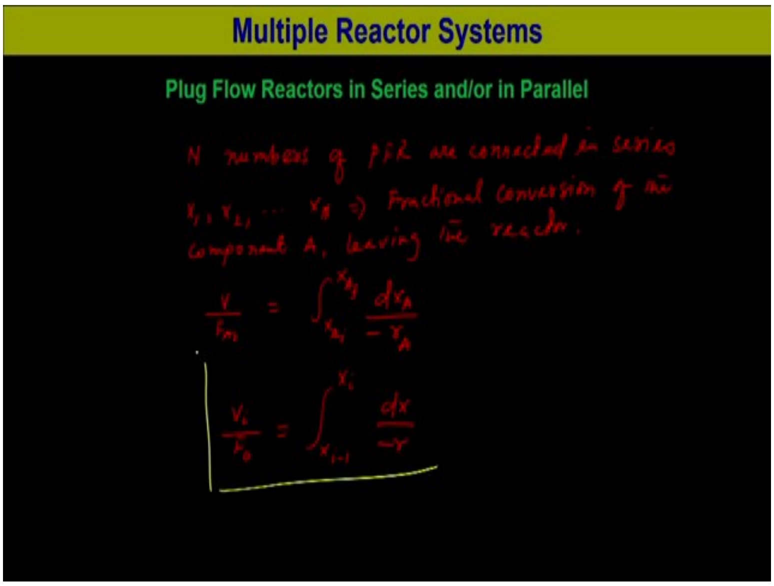

Now, let us consider plug flow reactor in series and or in parallel arrangements. So, if we consider, this is the multiple reactor systems. So, if we consider the n number of plug flow reactor are connected in series and if we consider the conversion for each reactor is X_1, X_2 up to X_n. These are the fractional conversion of the component A leaving the reactor. Now we know the from the earlier lectures the design equation for the plug flow reactor is

$$\frac{V}{F_{A0}} = \int_{X_{Ai}}^{X_{Af}} \frac{dX_A}{-r_A}$$

Now, if we consider the same material balance equation for each of the plug flow reactor we can write the generalised form

$$\frac{V_i}{F_0} = \int_{X_{i-1}}^{X_i} \frac{dX}{-r}$$

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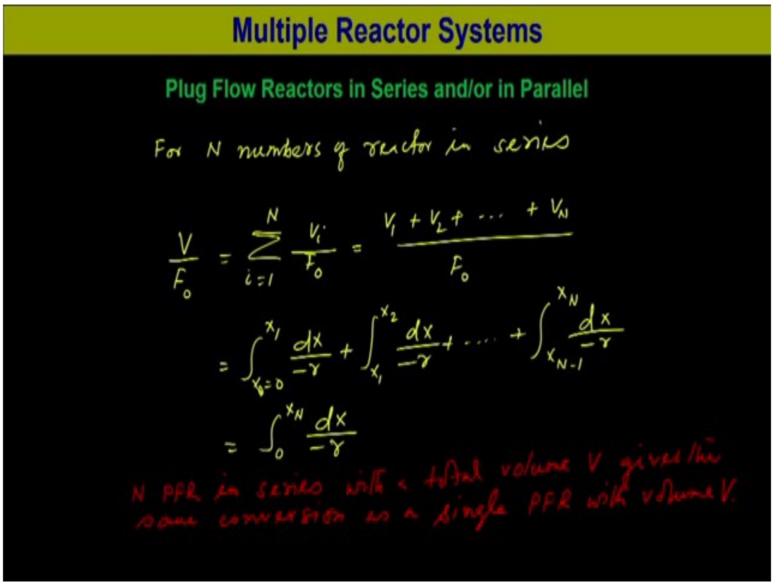

Now, for N number of reactors in series

$$\frac{V}{F_0} = \sum_{i=1}^{n} \frac{V_i}{F_0} = \frac{V_1 + V_2 + \ldots\ldots\ldots\ldots V_n}{F}$$

This we can write

$$= \int_0^{X_1} \frac{dX}{-r} + \int_{X_1}^{X_2} \frac{dX}{-r} + \ldots\ldots\ldots\ldots\ldots\ldots \int_{X_{N-1}}^{X_N} \frac{dX}{-r}$$

And this we can write

$$= \int_0^{X_N} \frac{dX}{-r}$$

So this suggest that N plug flow reactor in series, N plug flow reactor in series with the total volume V gives the same conversion as a single plug flow reactor with volume V. So for plug flow reactor whether they are connected in series or if they are connected in parallel combination we can straight the whole system as a single plug flow reactor of volume V or the total volume of the reactor equal to the sum of the volume of the individual units. So for reactors which are connected in parallel their V/F or the τ must be same for each parallel line.

If they are connected in any other ways or their τ is not same for both the parallel lines the system will not be efficient as compared to the one which is connected in parallel having the τ same for both the parallel lines.

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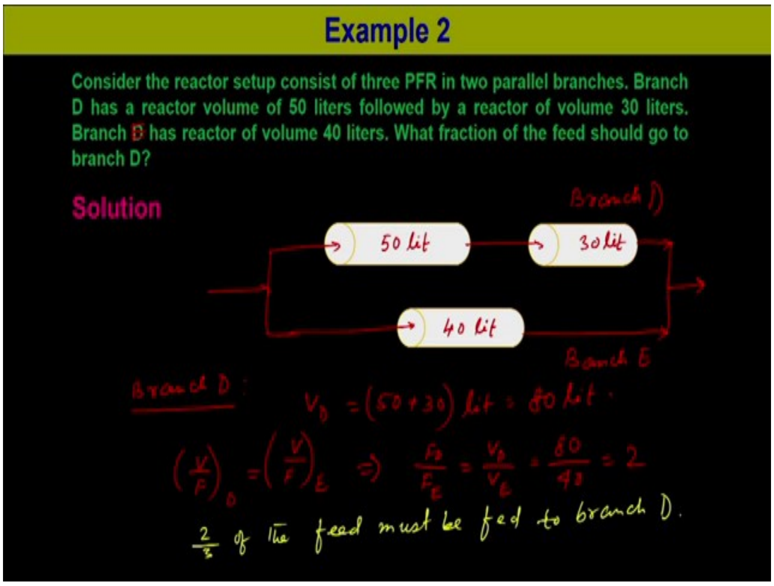

So, let us take an example which is given in Levenspiel. Consider the reactor setup consist of three PFR in two parallel branches. Branch D has a reactor volume of 50 litters followed by a reactor of volume 30 litters. Branch D has reactors of volume 40 litter. What fraction of the feed should go to branch D? So let us solve it as given over here, so in one place we have two reactors connected in series. So this is volume is 50 litters and this volume is 30 litters and they are connected.

In other branch, another reactor having volume is 40 litter. So this is connected in parallel, so this is branch E. So this is branch D and this is branch E. Now branch D it consist of two reactors in series. So we can consider from the earlier discussion V_D in this branch would be (50 + 30) litter. So total is 80 litter and the other branch is having 40 litter 1 unit of PFR. So the feed which is coming over here has to be distributed in such a way that their τ must be same.

That means V/F for branch D would be equal to V/F for branch E. So from here we can write

$$\frac{F_D}{F_E} = \frac{V_D}{V_E} = \frac{80}{40} = 2$$

So that means since $\frac{F_D}{F_E} = 2$, so two third of the feed, two third of the feed must be fed to branch D. So that V/F or τ would be same for both the branch.

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So thank you very much for attending this lecture and we will continue our discussion on the reactor sizing of multiple reactors when they are connected in series or parallel and which one is efficient in our next lecture.