

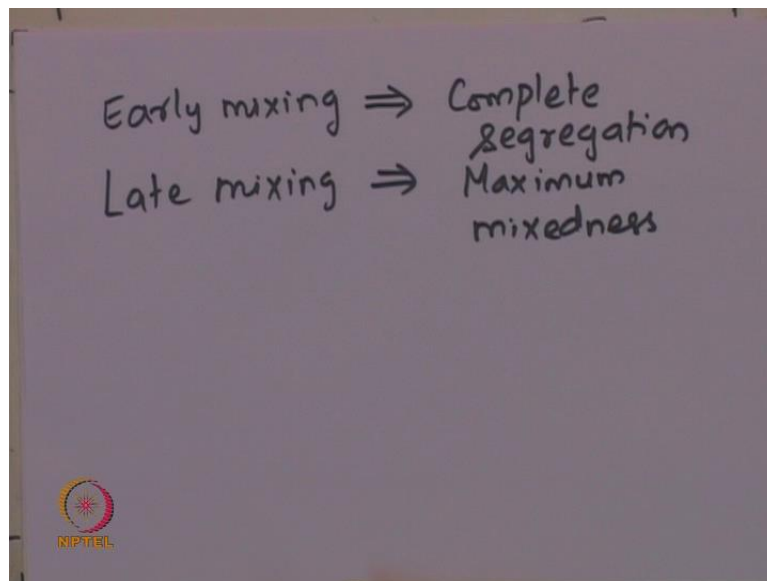
Chemical Reaction Engineering II
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Lecture - 35

Residence time distribution: Performance of non-ideal reactors

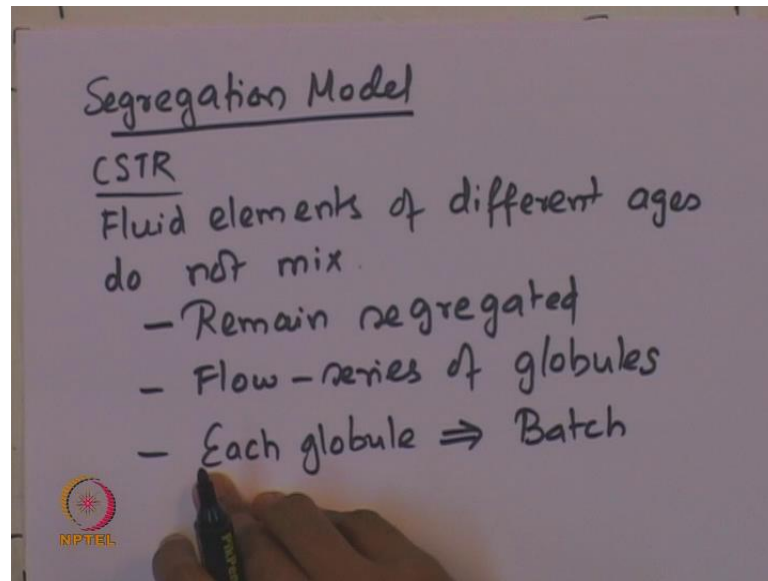
Friends, we have been looking at predicting the conversion in a non ideal reactor, provided the RTD function at function is known. So, there are 2 types of models that we going to discuss, one is the segregation model, the other one is the maximum on mixedness model. And these 2 extremes which actually provide a bound for the conversion, depending upon; which is the, what is the order of the action and the kinetics of the reaction which is conducted in the reactor.

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So, these 2 extremes are the early mixing regime, that is 1 extreme and the model that represents early mixing is the complete segregation model. While the late mixing which is; the other extreme that represents the maximum mixedness model. So, these 2 extremes essentially represent the 2 levels of mixing, where the 2 levels of mixing of the macro fluid global, that we actually defined in the last lecture. So, let us look at the first one desegregation model of a reactor.

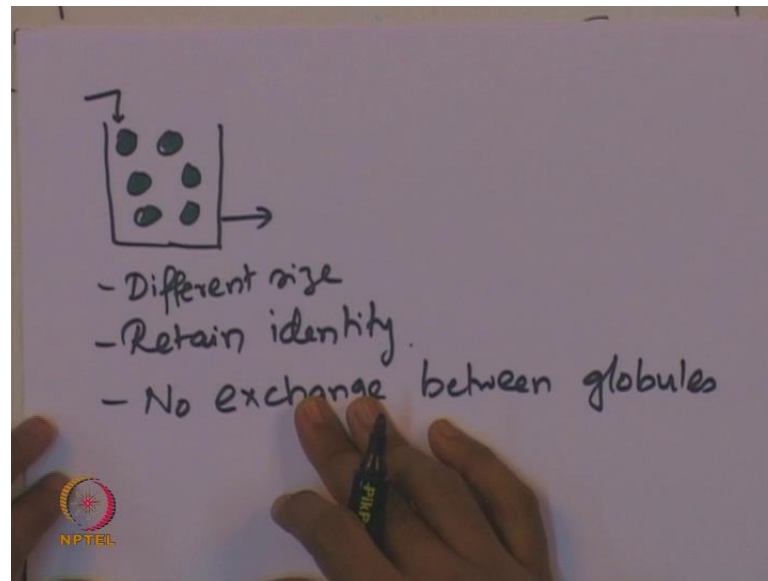
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Now suppose let us consider the CSTR. So, let us consider a CSTR or tank reactor, it could actually be any reactor. And let us assume, that the fluid elements of different ages; they do not mix that is the, that is the segregation model. And which we also which means that, they remain segregated all through. And the flow is essentially like a series of globules, where 1 globule enters the reactor at a certain time and that globule spends some time. Another globule which enters at a different time, the age of that particular globule is going to be different and which means that, the globules are different ages they do not mix with each other.

So, flow is essentially a series of globules. And we may assume, each globule as a batch reactor because, it does not mix. So, whatever reactant which is present in a globule, it continues to undergo reaction, as long as all the species which is present in that globule is gradually going to complete conversion. So, therefore, each globule is considered as, it may be considered as a batch reactor. So, now how do we model this?

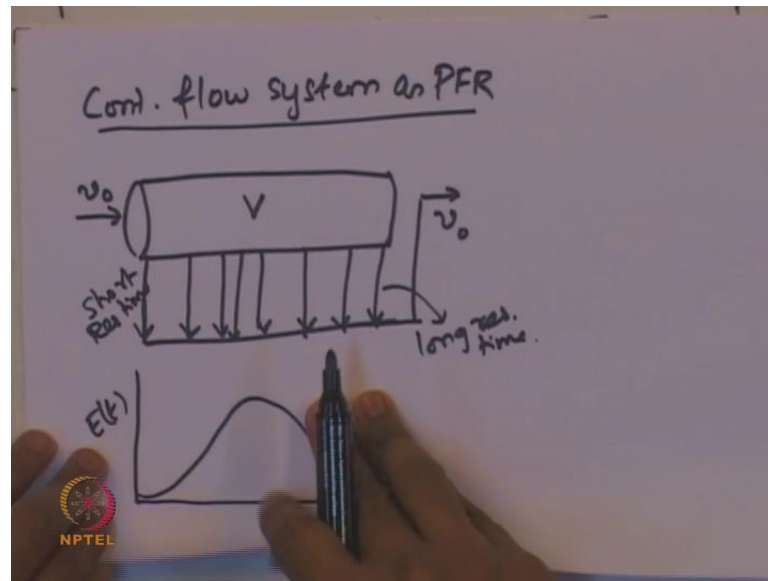
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So, we can actually depict this; depict this particular aspect in a CSTR as basically a tank which contains several globules. And each of these globules, are now going to have different ages. So, that is going to have a different age, this is going to have a different age and this is going to have different age. And each of these globules can actually in principle be are different sizes as well.

Properties that are of these globules will be that, will be of different sizes. And then more importantly, because they do not mix each of these globule as actually going to retain their identity and there is no exchange or exchange between globules. So, there is no exchange of molecules or matter between different globules and each of these globules will continue to have maintained its 1 identity. Now, I may also depict the same picture, a similar a model in a plug flow reactor.

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Suppose we have a continuous flow plug flow reactor. So, suppose if we model a continuous flow system, of which is a continuous flow system of the a non ideal reactor as a plug flow reactor, suppose if we model this as a plug flow reactor. Then if you want to incorporate a segregated model for this non ideal reactor, this may be depicted as follows.

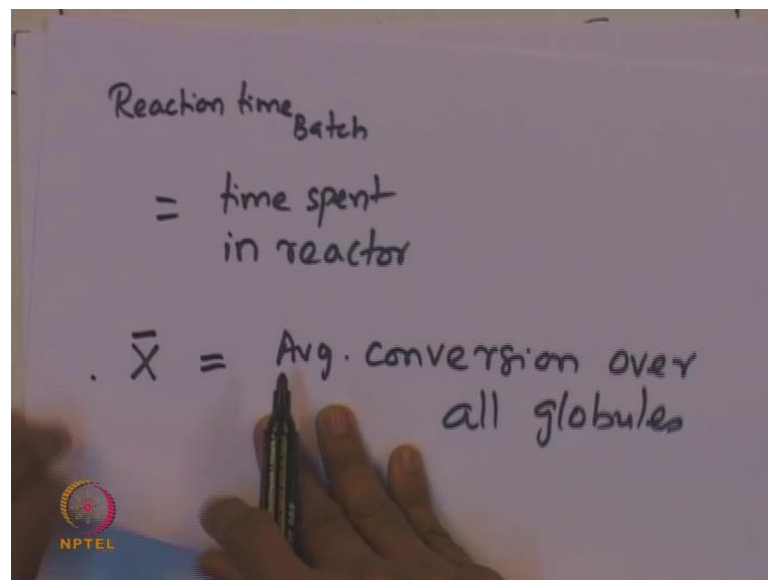
Suppose, if there is a tube and if there is a fluid which is flowing at a certain volumetric flow rate v naught into this to tube and if the volume of the tube is v . Now, instead of the fluid leaving from the other end of the reactor directly, the fluid can actually be x taken out from the side of this tube, different locations along the side of the reactor. And they can all be joined together and together they actually leave the reactor.

So, now, each of the streams, if because they are withdrawn a different locations, each of the globules will actually have different residence time. So, the location where the fluid is actually withdrawn from the reactor can actually be decided, based on the residence time distribution of the actual non ideal reactor. So, suppose if this is the residence time distribution. If that is the residence time distribution and that is the E curve which is the RTD function which is actually measured experimentally of a real reactor, then the based on this RTD function, such kind of a withdrawing of the a fluid from the reactor can actually be decide.

So, there the fluid which is actually withdrawn from the reactor right at the entry location, which going to have the shortest residence time. And the 1 which is actually withdrawn at other end of the reactor is going to have the longest residence time. So, that is going to have a long residence time. So, therefore, what you have done is, we have removed batches of fluid from different locations inside the reactor. And the location from where it is withdrawn, is actually specified by the residence time distribution function E of t , which may be measured experimentally for an non ideal reactor. And we because, we have withdrawing from the side, there is no interchange of molecules between each of these globules, and they are actually present inside the reactor, where the reaction actually occurs. And each of these can actually be considered as actually a batch reactor.

So, what its suggest is that, the mixing for this kind of a system as actually the fluid appears as a well mixed system, when it enters a reactor, but when it leaves, the globules are actually completely segregated. So, therefore, the reaction time in batch in each of the batch reactor, that is, each of the globules, which may be which is basically withdrawn from different locations along the side of the reactor.

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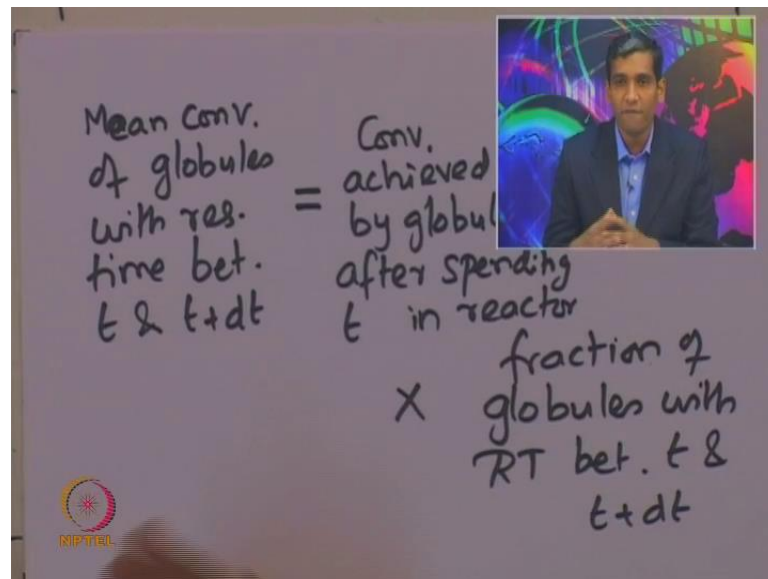


That time, the reaction time of batch reactor, of each of the batch reactor is equal to the time spent in the reactor. So, this is the reaction time spent by each of the batch reactors. Remember that, every location from where the fluid is actually withdrawn from the side

of the reactor, that globule can actually be considered as a batch reactor. And the time that the spent by the reaction time of each of these globules, that is, of these batch reactor is equal to the time that would actually spends in the reactor itself.

So, therefore, the mean conversion; if \bar{x} is the mean conversion, that is equal to the average conversion over all globules. So, what is of interest is essentially this mean conversion. So, we want to predict the conversion of the reactor and what the essentially required to need to predict is; this mean conversion from the reactor. So, how do we find this mean conversion? So, the mean conversion of globules with residence time of a certain time interval dt .

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So, let us say that the mean conversion of globules, with residence time between t and t plus dt , in that small interval of time, if that globule has a residence time in this small time interval, then that is essentially given by the conversion achieved by a globule after spending t amount of time in the reactor. And that multiplied by the fraction of globules with residence time between t and t plus dt .

So, that is the obstruction of how to get a mean conversion of globules, with a certain residence time between t and t plus dt , which is essentially the conversion achieved by the globule, after spending that time t amount of time inside the reactor multiplied by the fraction of the globules with that residence time between t and t plus dt . So, now

if we put some; if we put the corresponding expressions, expressions corresponding to each of these terms; in the mean conversion.

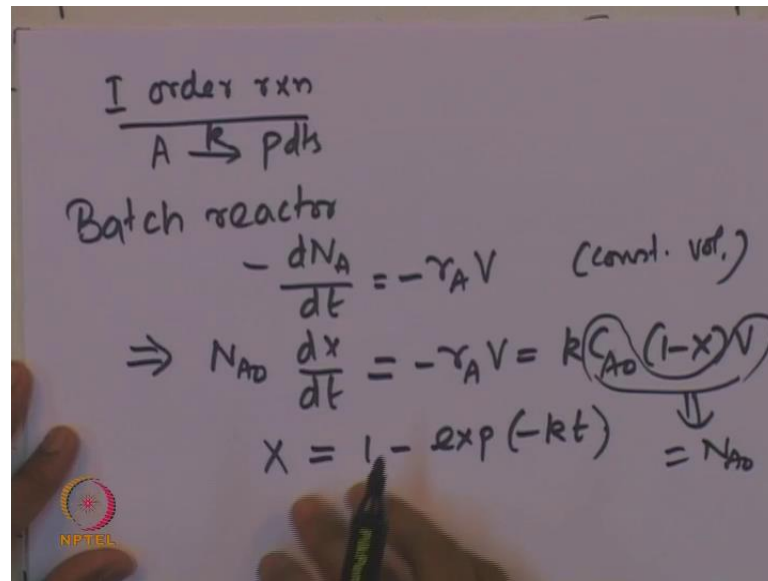
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The image shows a whiteboard with handwritten mathematical equations. At the top, it says $d\bar{X} = X(t)E(t)dt$. Below that, it says $\Rightarrow \frac{d\bar{X}}{dt} = X(t)E(t)$. Then, it shows $\bar{X} = \int_0^{\infty} X(t)E(t)dt$. The term $X(t)$ in the integral is circled, and an arrow points from it to the text "Conv. achieved in batch reactor". In the bottom left corner of the whiteboard, there is a small circular logo with a star and the text "NIPITEL" below it.

We will find that $d\bar{X}$ which is the mean conversion of the globules, whose residence time is between t and t plus Δt . So, that should be equal to the conversion achieved by a globule, after spending that time in the reactor multiplied by the fraction that has an age between t and t plus Δt . So, therefore, from here we can write that $d\bar{X}$ by dt which is the mean conversion, that is equal to $X(t)E(t)$. And therefore, \bar{X} is equal to the integral from 0 to infinity of $X(t)E(t)dt$.

So, remember that $X(t)$ which is actually percent inside the integrand; that is essentially the conversion in a batch reactor because, we consider each of these globules as actually a batch reactor. So, that is the conversion as though it were a batch reactor. And that multiplied by the corresponding residence time distribution, integrated over all residence times will give the mean conversion. So, let us consider a first order reaction.

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Let us consider a first order reaction, where A goes to products with a rate with a specific reaction rate k. And for a batch reactor, the performance equation is dN_A by dt that is, equal to minus r_A into V , where V is the volume of the reactor and let us assume that it is a constant volume system. So, now, we can use the relationship between the number of moles with the corresponding conversion and we can rewrite this equation as $N_{A0} dx$ by dt , that is equal to minus r_A into V which is equal to $k C_{A0} (1-x) V$.

So, from here, we can easily decipher that, the conversion is equal to exponential of minus k into t . And remember that $C_{A0} V$ is essentially equal to that is equal to N_{A0} . So, therefore, the conversion as though, conversion in each of these globule is given by $1 - \exp(-kt)$. And so from here we can now find out what is the mean conversion. We know the mean conversion equal to integral 0 to infinity; that is overall residence time of the product of the conversion in the batch reactor multiplied by the corresponding residence time.

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The image shows a whiteboard with handwritten mathematical derivations. At the top, the mean conversion \bar{X} is defined as the integral of $X(t)E(t)$ from 0 to infinity. This is then simplified to $\int_0^\infty (1 - \exp(-kt))E(t) dt$. Below this, for a Plug Flow Reactor (PFR), the residence time distribution $E(t)$ is given as a delta function $\delta(t - \tau)$. Substituting this into the integral for \bar{X} yields $\bar{X} = 1 - \int_0^\infty \exp(-kt) \delta(t - \tau) dt$. The final result is $\bar{X} = 1 - \exp(-k\tau)$, where $k\tau$ is identified as the Damköhler number Da .

$$\bar{X} = \int_0^\infty X(t) E(t) dt$$
$$= \int_0^\infty (1 - \exp(-kt)) E(t) dt$$

PFR: $E(t) = \delta(t - \tau)$

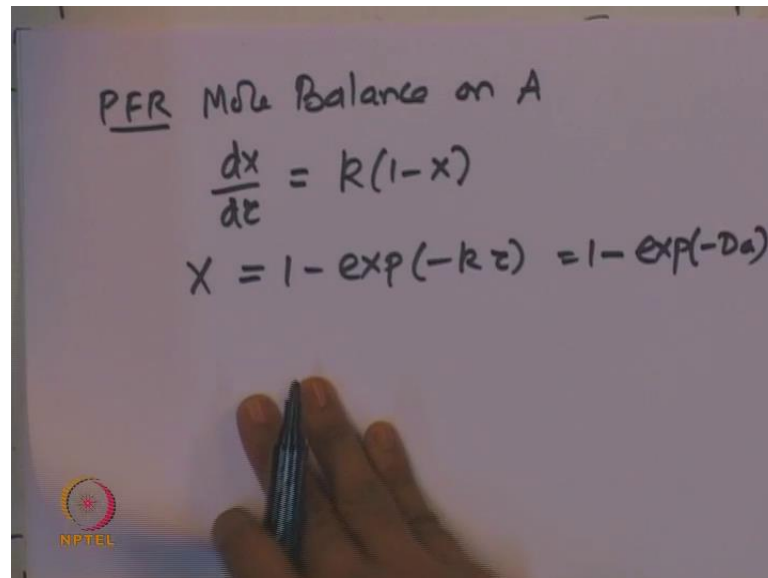
$$\bar{X} = 1 - \int_0^\infty \exp(-kt) \delta(t - \tau) dt$$
$$= 1 - \exp(-k\tau) = 1 - \exp(-Da)$$

So, therefore, \bar{X} is equal to 0 to infinity X of t E of t dt and so that is equal to integral to infinity $1 - \exp(-kt) E$ of t dt . Now, suppose if it were suppose if the reactor is actually a plug flow reactor. So, suppose if it is a plug flow reactor, then the residence time distribution E of t is simply given by the delta function of t minus τ where τ is the space time of the reactor, which is the ratio of the volume to the volumetric flow rate of the reactor.

So, now, from for a plug flow reactor, it will simply be $1 - \int_0^\infty \exp(-kt) \delta(t - \tau) dt$. And that is nothing $1 - \exp(-k\tau)$. And $k\tau$ is essentially the dimensionless quantity called the Damköhler number; this is the Damköhler number which is the ratio of the space time to the reaction time. So, we can write this as exponential of minus Da .

So, that is the mean conversion that would be achieved, if it were to be a an ideal plug flow reactor. And what is interesting is that, the model that we actually obtained from the segregated model is actually same as that of the mole balance of the plug flow reactor. We know that, from the mole balance of the plug flow reactor, the performance is actually, performance equation suggest that the conversion is actually equal to $1 - \exp(-Da)$. And let us see how that is the case.

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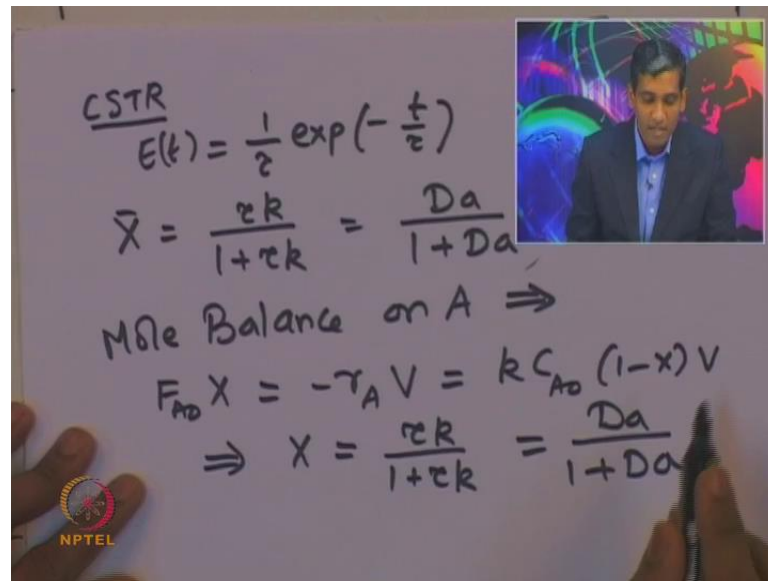


The image shows a whiteboard with handwritten text and equations. At the top, it says "PFR Mole Balance on A". Below that, the differential equation is written as $\frac{dx}{d\tau} = k(1-x)$. The integrated form of the equation is written as $X = 1 - \exp(-k\tau) = 1 - \exp(-Da)$. A hand holding a pen is visible at the bottom of the whiteboard. In the bottom left corner, there is a small logo for NPTEL.

So, the mole balance of a plug flow reactor on species A is nothing, but dX by $d\tau$, that is equal to k into 1 minus X . And therefore, X is equal to 1 minus exponential of minus k into τ which is equal to 1 minus exponential of minus Da . So, therefore, the conversion that is actually achieved by using a completely segregated model is actually exactly equal to the conversion that is achieved by an ideal plug flow reactor, if it were to be a first order reaction.

In fact, we observe this in 1 of the lectures before; that we mentioned that, if it is a first order reaction, then it does not matter, only RTD function is sufficient to estimate the conversion and level of mixing actually does not play role. So, we will see in a short while as to why that is the case. Now, before we look at that, let us consider if it were to be a CSTR.

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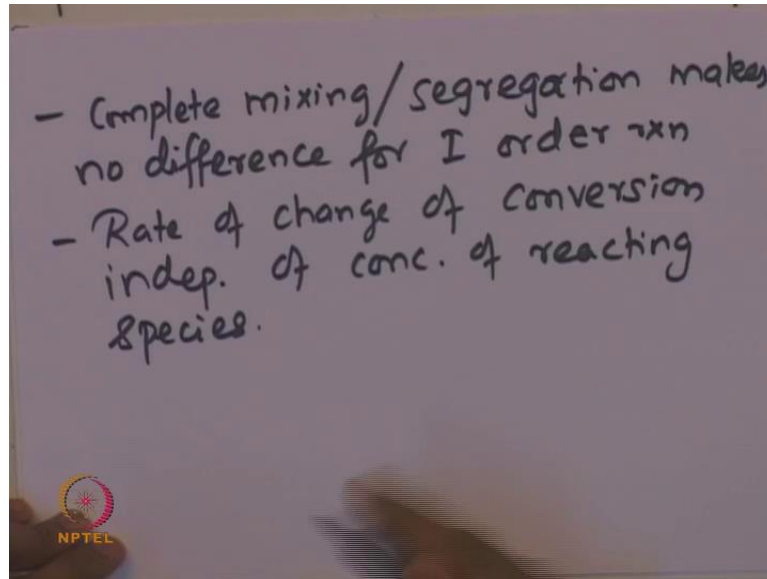

$$\begin{aligned} \text{CSTR} \\ E(t) &= \frac{1}{\tau} \exp\left(-\frac{t}{\tau}\right) \\ \bar{X} &= \frac{\tau k}{1 + \tau k} = \frac{Da}{1 + Da} \\ \text{Mole Balance on A} &\Rightarrow \\ F_{A0} X &= -r_A V = k C_{A0} (1 - X) V \\ \Rightarrow X &= \frac{\tau k}{1 + \tau k} = \frac{Da}{1 + Da} \end{aligned}$$

So, the residence time distribution function for a CSTR is given by $\frac{1}{\tau} \exp(-t/\tau)$. So, therefore, \bar{X} the mean conversion, plugging this into the integral and integrating the expression, shows that \bar{X} is equal to τk divided by $1 + \tau k$ which is equal to the Damkohler number divided by $1 + \text{Damkohler number}$.

So, now, if we write the mole balance for a CSTR, the performance equation for the CSTR is; the mole balance on A is $F_{A0} X$ which is the plug flow rate of this species at inlet that is multiplied by X is equal to $-r_A V$ that is equal to $k C_{A0} (1 - X) V$. And $-r_A$, r_A is the rate of generation, $-r_A$ is the rate at which the species is actually being consumed. So, from here we can see that X is equal to τk by $1 + \tau k$, where τ is the space time of the reactor $1 + Da$.

So, clearly you can see, that the conversion is achieved through a segregation model is actually exactly same as the conversion, that is achieved from the performance equation of the ideal CSTR. So, this suggests that, for a first order reaction, the information of RTD function there is actually sufficient. And the degree of mixing this not going to add any additional information and the RTD function itself can be used to predict the conversion mean conversion of the reactor.

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Now, the question is why is that the case? So, reason is the complete mixing or segregation, actually makes no difference for first order reaction. This is because; the rate of change of conversion actually does not depend upon the concentration of the reacting molecule. So, the rate of change of conversion is independent of concentration of the reaction reacting molecule. So, this is the reason, why for a first order reaction, the RTD function alone is sufficient to predict the conversion that is achieved by the non ideal reactor.

So, the rate of change of conversion is independent of the concentration of the reacting species. That explains why for a first order reaction, RTD function is sufficient to estimate the conversion of the reactor. So, now let us extend this to a laminar flow reactor.

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The image shows a hand-drawn slide with the following content:

$$\text{L.F.R. } E(t) = \begin{cases} 0 & t < \tau/2 \\ \frac{\tau^2}{2t^3} & t \geq \tau/2 \end{cases}$$
$$E(\theta) = \begin{cases} 0 & \theta < 0.5 \\ \frac{1}{2\theta^3} & \theta \geq 0.5 \end{cases}$$
$$\bar{X} = 1 - \int_0^{\infty} \exp(-kt) E(t) dt = \int_0^{\infty} \exp(-k\tau\theta) E(\theta) d\theta$$

An NPTEL logo is visible in the bottom left corner of the slide.

L F R stands for the laminar flow reactor. And the residence time distribution is given by 0 for t less than τ by 2 and τ^2 by $2t^3$ for t greater than or equal to τ by 2. So, that is the residence time distribution for a laminar flow reactor, which we have actually derived in the previous lecture. And in the normalized form E of θ is equal to 0 1 by 2 θ^3 and this is θ less than 0.5 and θ greater than or equal to 0.5 .

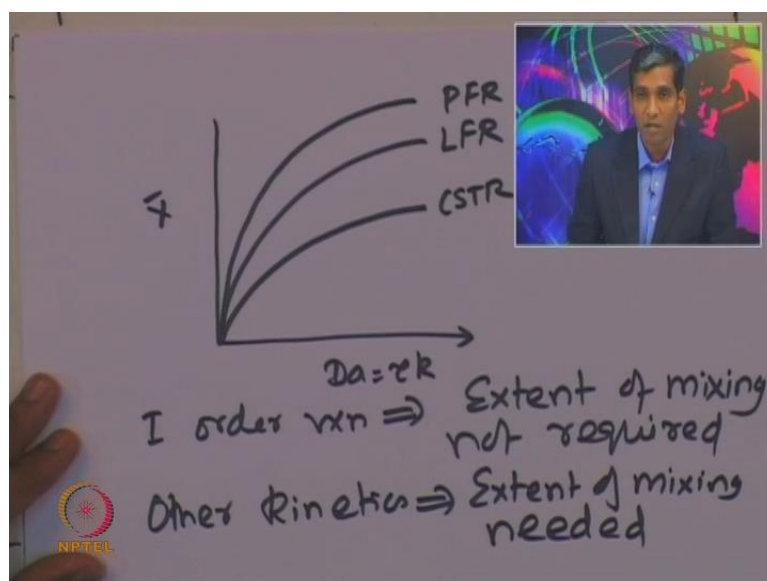
So, now, we can plug this distribution into the conversion equation, we can find that to be equal to $\int_0^{\infty} \exp(-kt) E(t) dt$. And that is equal to $1 - \int_0^{\infty} \exp(-k\tau\theta) E(\theta) d\theta$.

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$$\bar{x} = 1 - (1 - 0.5 \tau k) \exp(-0.5 k \tau) - (0.5 k \tau)^2 \int_{0.5}^{\infty} \frac{\exp(-\tau k \theta)}{\theta} d\theta.$$

So, on performing the integration, by substituting the corresponding distribution, I can find that the mean conversion in a laminar flow reactor is essentially given by 1 minus 0.5 into the space time multiplied by the specific reaction rate into exponential of minus 0.5 k tau minus 0.5 k tau the whole square integral 0.5 to infinity exponential of minus tau k theta divided by theta into d theta. So, that is the expression and I will be able to find out what is the conversion in a laminar flow reactor. So, let us now compare the mean conversion that is achieved, using these 3 different types of reactors.

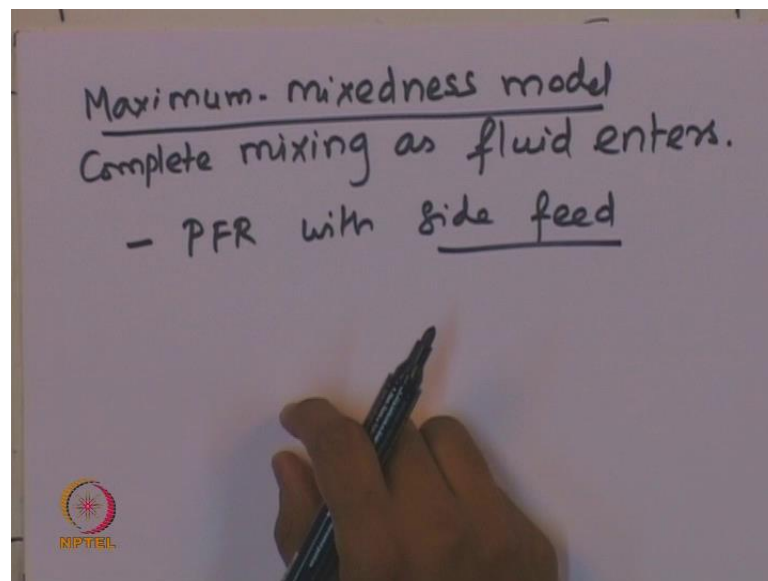
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So, if we plot as a function of the Damkohler number, which is the ratio of the space time to the reaction time \bar{X} . So, CSTR would actually be like this and the plug flow reactor actually predict a much higher conversion, for a first order reaction, this is for a first order. And the laminar flow reactor would be somewhere in between. So, the plug flow and the CSTR, they sort of provide a bound for the predict conversion of the first order reaction, in a non ideal reactor. And such kind of graphs actually can be generated for such kind of plots can be generated for reactions of other orders and other types of kinetics.

So, what it suggests is that, for a first order reaction, the extent of mixing not required. While for other reactions, other kinetics extent of mixing place an important role, extent of mixing actually plays an important role. And it is required in order to predict the conversion of the non idea reactor. So, now let us moved to the next model, which is the maximum mixedness model.

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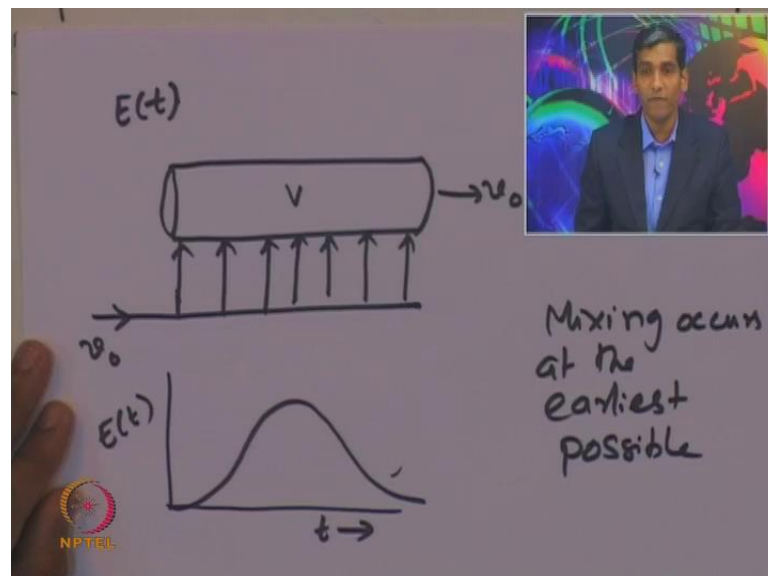
Let us look at the maximum mixedness model. So, the segregated fluid is 1, where the mixing between the fluid globules actually does not occur. So, there is no exchange of material between the globules which are present inside the reactor. So, the flow is essentially like a series of globules which are flowing through the reactor. On the other hand, on that is called the minimum segregation minimum mixedness model, where the

where the globules do not actually interact with each other. And each of the globule behave like a batch reactor.

On the other extreme is a maximum mixedness model, where the globules the matter which is present in different globule, they are allow to actually mix and interact with each other. And therefore, the molecules which are different ages, they all mix with each other and that is that kind of representation or that kind of a situation is called the maximum mixedness model. So, let us look at how to estimate the conversion for that kind of a situation.

So, maximum mixedness is achieved, when there is complete mixing as fluid enters. So, as soon as they get into the reactor, all the globules can actually exchange matter with each of them. And so, therefore, there is complete mixing. So, there are maximum mixedness is the complete mixing of the fluid right at the entry point of the reactor. So, so how do we depict such kind of a situation is; we can consider a plug flow reactor with side feed. So, where the feed is actually fed through the sides of the plug flow reactor at different locations and that can be used to depict the situation of maximum mixedness in a non ideal reactor. So, suppose if we know the residence time distribution function.

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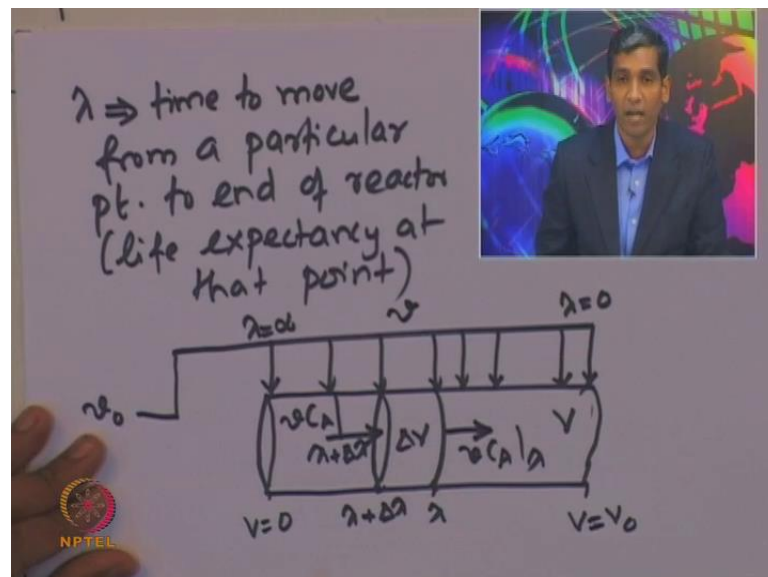


So, if we know the E of t of a real reactor. Then, we can actually mimic reactor by using a plug flow reactor. And instead of providing a feed at the entry to the plug flow reactor whose volume is V , we can actually split the ... we can actually feed them through the

sides and the feed through the side can actually be according to the ... we can split the feed and feed them to the side and this feed could be according to a certain distribution function, which is the residence time function of the real reactor.

So, the residence time distribution function could be something like this, where the side entrance is actually according to this distribution function. So, which suggest that, the mixing actually occurs as early as possible and then they actually go into the reactors. So, mixing earliest possible which corresponds to the maximum mixedness situation in the reactor.

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So, now, suppose we define lambda as the time name to move from a particular point to end of the reactor. So, that is the time taken by a fluid element, to move from a particular location inside the reactor at the end of the reactor. Remember that, we have now that present the non ideal reactor, using a plug flow with the sides stream in different locations in the side of the plug flow reactor.

So, now this also reflects the life expectancy at that point, at this the amount of time that actually the fluid particles are going to spend inside the reactor, which is actually fed into the reactor at that point the side. So, now, we can now draw schematic of this reactor. So, suppose this is the plug flow reactor with a volume V. And then, we now make a feed, we feed the fluid; we feed the reactor with fluid along the sides and according to a certain residence time distribution function. Now if we assume that, this is lambda equal

to 0 because, the time that is actually spent by the fluid that is bumped into the reactor, it near the exit of the reactor is almost equal to 0.

So, therefore, lambda equal to 0, the life expectancy of the fluid that enters the reactor in this location is going to be 0. So, lambda equal to 0 starts from here and then lambda equal to infinity which is the maximum time that is taken in the inside the reactor, is at the entry of the reactor. And if the volumetric flow rate of the fluid V and V equal to 0 is this location and V equal to V naught; that is the full volume of the reactor.

Now, if we now identify a small element and if the volume of that element is ΔV . And the flux with which the fluid actually enters that element, is given by v into $C A$ that is the volumetric flow rate at that location and if this point is lambda in the life expectancy dimension. And this is lambda plus delta lambda. So, that is the difference in the life expectancy from this point at this point. So, this is the v into $C A$ at lambda plus delta lambda. And whatever is leaving from here will be $v C A$ at lambda.

Now what is the amount of fluid that actually enters through the side, so that, amount of the volumetric a flow rate with which the fluid is actually going to enter is; let say is given by v at that location and we will be calculating that in a short while. So, what is the flow rate with which the fluid actually enters a small element delta v ?

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Flow rate in @ Δv
 $= v_0$ [frac. of fluid with life exp bet λ & $\lambda + \Delta\lambda$]
 $= v_0 E(\lambda) d\lambda$
 Flow rate balance.
 $v_\lambda = v_{\lambda + \Delta\lambda} + v_0 E(\lambda) d\lambda$
 $\Rightarrow \lim_{\Delta\lambda \rightarrow 0} \Rightarrow \frac{dv_\lambda}{d\lambda} = -v_0 E(\lambda)$

flowing thro' sides

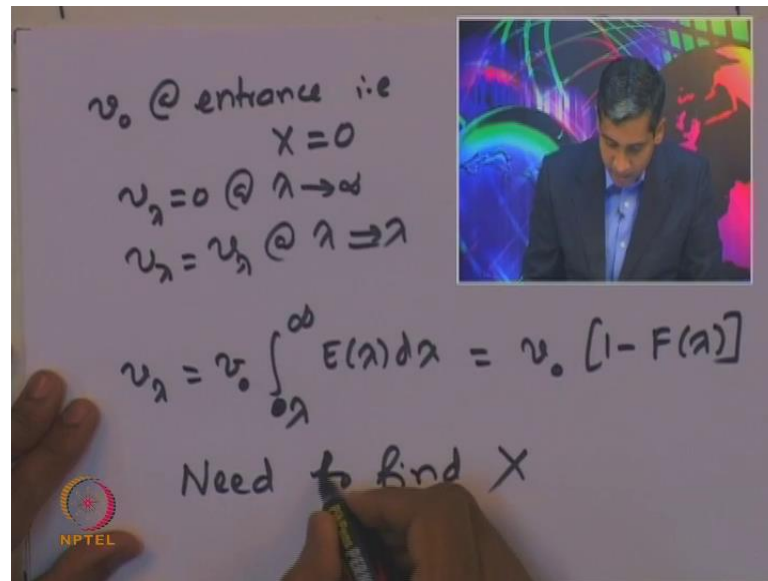
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So, the flow rate in at Δv . So, that is equal to the volumetric flow rate v_{naught} , that is the overall volumetric flow rate of the reactor. So, we are essentially trying to calculate; what is the volumetric flow rate with which the volumetric fluid is actually entering in this small element Δv . So, fluid rate at in Δv should be equal to v_{naught} which is the volumetric flow rate with which the fluid is being pumped into multiplied by the fraction of fluid with between with life expectancy.

So, let us call this life expectancy, life expectancy between λ and $\lambda + d\lambda$. So, that is equal to v_{naught} multiplied by the corresponding $E_{\lambda} d\lambda$ where, E_{λ} is the essentially the RTD function which says; what is the residence time distribution of the fluid element inside the reactor. So, now once we know this, the we can now write a flow rate balance. We can now formulate flow rate and the fluid balance is; volumetric flow rate at λ should be equal to the volumetric flow rate of the fluid at $\lambda + d\lambda$ plus whatever is actually added through the side. So, that will be equal to v_{naught} into $E_{\lambda} d\lambda$. So, this is the flow rate in though the side. So, this is the flow in through the side of the plug flow reactor.

So, now, we know. So, now, we can actually take the limits of $\Delta \lambda$ going to 0. So, limit $\Delta \lambda$ going to 0, this essentially becomes $d v_{\lambda}$ by $d\lambda$, that is equal to minus v_{naught} into v_{λ} . So, that is the differential equation, which captures what is the flow rate with flow rate at a certain life expectancy λ . So, now v_{naught} is the flow rate with which the fluid is actually flowing at the entrance of the reactor.

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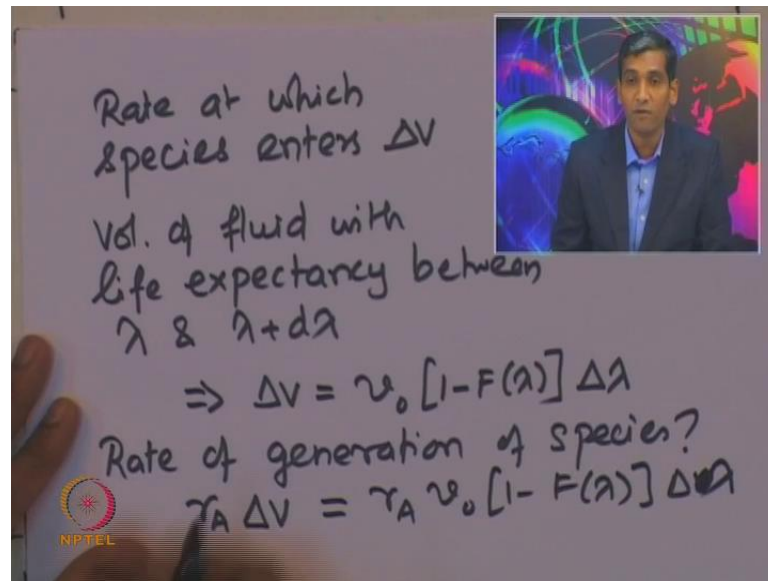


So, which means; at entrance, that is, when conversion is actually equal to 0. So, before at the v naught is the overall volumetric flow rate of the fluid that is actually flowing through the reactor. So, now, we can actually integrate this expression as v lambda equal to 0 at as lambda tends to infinity. So, the flow rate of the fluid that is actually at the entrance is v naught and the conversion at that location is equal to 0.

So, therefore, the amount of fluid that is actually right at the no entry point of the reactor, remember that it is a feed that is coming at different locations in the side. So, at the volumetric flow rate of the fluid whose age is almost equal to infinity is equal to 0. And v lambda is equal to v lambda at some lambda equal to 0 lambdas, that is, at certain age let us assume that v lambda is the corresponding volumetric flow rate. So, using these 2 as limits we can now integrate to find that, v lambda equal to v naught into integral 0 to integral lambda to infinity E lambda d lambda which is equal to v naught into 1 minus F of lambda. So, that is the volumetric flow rate with which the fluid is actually flowing at any location lambda.

So, now, we objective is to find the overall conversion, need to find X . So, that is the objective. So, how do we find X ? We need to write a we need to write a mole balance of the species, in order to find the a conversion of the species in the reactor. So, before we write a mole balance, we need to know certain aspects of the reactor, certain aspects before we write the mol e balance.

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Rate at which species enters ΔV

Vol. of fluid with life expectancy between λ & $\lambda + d\lambda$

$$\Rightarrow \Delta V = v_0 [1 - F(\lambda)] \Delta \lambda$$

Rate of generation of species?

$$r_A \Delta V = r_A v_0 [1 - F(\lambda)] \Delta \lambda$$

The image shows a whiteboard with handwritten text and equations. In the top right corner, there is a small video inset showing a man in a dark suit and light blue shirt speaking. The whiteboard text is written in black marker. At the bottom left of the whiteboard, there is a small logo for NPTEL (National Programme on Technology Enhanced Learning).

For example: what is the, what is the amount of species, what is the rate at which enters the small element Δv . So, this can actually be found, by using what is the volume of the fluid, whose life expectancy is actually between the between λ and $\lambda + d\lambda$. So, the volume of the fluid with life expectancy between λ and $\lambda + d\lambda$. So, if we know this volume, this volume multiplied by the concentration will tell us; what is the number of moles that is actually entering that particular element Δv .

So, that is equal to. So, ΔV will be equal to $v_0 [1 - F(\lambda)] \Delta \lambda$. So, that is the volumetric flow rate multiplied by the corresponding age $\Delta \lambda$ will tell us; what is the volume of the fluid with at certain life expectancy, that is equal to that is somewhere between λ and $\lambda + d\lambda$.

So, now what is the rate of generation of species? That is actually given by the rate at which the species is being consumed multiplied by the corresponding volume ΔV . So, that is equal to $r_A \Delta V = r_A v_0 [1 - F(\lambda)] \Delta \lambda$. So, we now have all information that we need into write the mole balance. So, let us now write the mole balance for this particular species.

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Mole balance on A bet λ & $\lambda+d\lambda$

$$\text{In @ } \lambda+d\lambda + \text{Intro Sides} - \text{Out @ } \lambda + \text{Gen by rxn} = 0$$

$$v_0 [1 - F(\lambda)] C_A \Big|_{\lambda+d\lambda} + v_0 E(\lambda) d\lambda C_{A0} - v_0 [1 - F(\lambda)] C_A \Big|_{\lambda} + r_A v_0 [1 - F(\lambda)] d\lambda = 0$$

So, mole balance on A between with life expectancy of lambda and lambda plus d lambda. So, let us write a mole balance for this. So, what is the rate at which things are coming inside at lambda plus d lambda? Remember that, the age of the fluid is actually decreasing from the exit of the increasing from the exit of the reactor, while the positive direction is actually increase of the volume from the entry of the reactor to the exit of the reactor. So, in at lambda plus d lambda plus the introduction through the side, what is rate at which things are actually introduced into the reactor through the sides minus what leaves the reactor, what leaves that element at lambda plus whatever is generated by reaction.

So, that that should be equal to 0. So, that is the mole balance on A for age between lambda and lambda plus d lambda. So, we know all this quantity. So, v_0 into $1 - F(\lambda)$. So, that is the volumetric flow rate at lambda, lambda plus d plus lambda into C_A evaluated at lambda plus d lambda will tell us; what is the rate at which the species is actually getting into that element plus the whatever is introduced to the sides that is given by $v_0 E(\lambda) d\lambda C_{A0}$, where C_{A0} is the concentration of the species in the feed stream minus v_0 into $1 - F(\lambda)$ into C_A evaluated at lambda plus r_A into v_0 which the volumetric flow rate of the feed into $1 - F(\lambda)$ multiply by $d\lambda$ equal to 0. So, that is the mole balance on A between the age lambda and lambda plus d lambda.

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$$v_0 d\lambda \text{ (Divide) Limit as } d\lambda \rightarrow 0$$

$$C_{A0} E(\lambda) + \frac{d}{d\lambda} \{ (1-F(\lambda)) C_A(\lambda) \} + r_A [1-F(\lambda)] = 0$$

$$C_{A0} E(\lambda) + \frac{d C_A(\lambda)}{d\lambda} (1-F(\lambda)) - C_A(\lambda) \frac{dF(\lambda)}{d\lambda} + r_A [1-F(\lambda)] = 0$$

So, now we can actually divide this expression by v naught into delta lambda. We can divide this expression by v naught d lambda and take limit as d lambda goes to 0. So, that will be C_A naught into E lambda plus d by d lambda into $1 - F$ of lambda into C_A lambda plus r_A into $1 - F$ of lambda equal to 0. So, that is the expression for that is the mole balance. So, now, we can open up this differential here and we can rewrite this expression as C_A naught into E lambda plus $d C_A$ lambda by d lambda into $1 - F$ lambda minus C_A lambda into $d F$ lambda by d lambda plus r_A into $1 - F$ lambda equal to 0.

Now, if we stare at this expression this $d F$ by lambda is nothing, but the RTD function E lambda, where F is the F curve or the cumulative distribution function. So, using this property we can actually write the mole balance.

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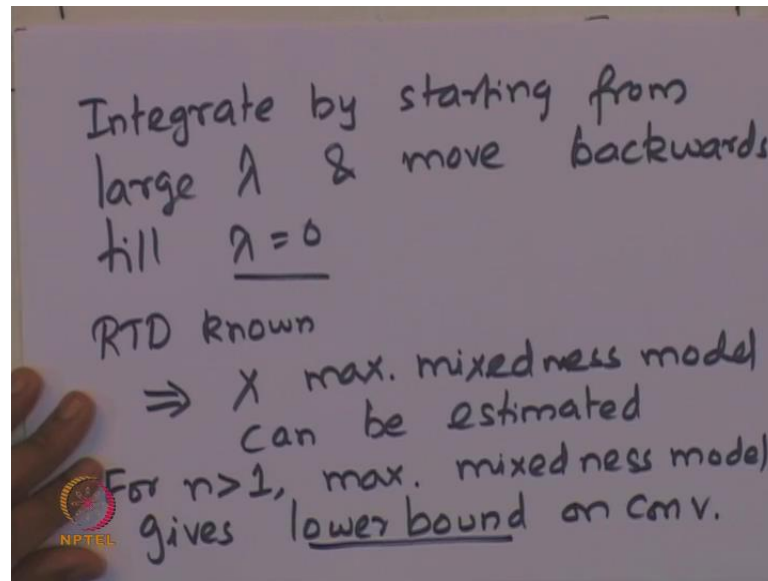
$$\frac{dC_A(\lambda)}{d\lambda} = -r_A + (C_A - C_{A0}) \frac{E(\lambda)}{1 - F(\lambda)}$$
$$X \Rightarrow$$
$$-C_{A0} \frac{dx}{d\lambda} = -r_A - C_{A0} \frac{E(\lambda)}{1 - F(\lambda)} X$$
$$\Rightarrow \frac{dx}{d\lambda} = \frac{r_A}{C_{A0}} + \frac{E(\lambda)}{1 - F(\lambda)} X$$

B.C. $\lambda \rightarrow \infty \quad C_A = C_{A0}$

So, the final mole balance essentially is dC_A of λ by $d\lambda$ that is equal to minus r_A plus C_A minus C_{A0} into $E(\lambda)$ by $1 - F(\lambda)$. So, that is the mole balance for the species for a maximum mixedness model. So, in terms of conversion, we can actually like this expression as minus C_{A0} dx by $d\lambda$, that is equal to minus r_A minus C_{A0} into $E(\lambda)$ by $1 - F(\lambda)$ into conversion X . And so, that can actually be written as dx by $d\lambda$ equal to r_A which is the rate of generation of the species divided by C_{A0} which is the concentration of the species in the inlet stream into $E(\lambda)$ by $1 - F(\lambda)$ into conversion X .

So, while solving this equation you will be able to find out what is the conversion, if we know the residence time distribution function. So, what are the boundary conditions for this equation? Boundary conditions are very simple. So, λ goes to infinity when C_A equal to C_{A0} , that is, at the entry point into the reactor with the age of the fluid is actually approximately infinity. So, how do we integrate this, we have to integrate this equation from backwards starting from very large λ .

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So, we have integrate this equation by starting from large lambda and move backwards till lambda equal to 0. So, that is the method to integrate this equation. And once we integrate the equation, you will be able to find out what is the conversion in under the situation of maximum mixedness. So, now, so if RTD is known. So, if RTD is known, then the conversion for the maximum mixedness situation can actually be model, can be estimated. So, this can conversion provides a bound for the conversion of the species in the non ideal reactor. So, far n equal to n greater than 1, it is been observed that for n greater than 1, the maximum mixedness model gives the lower bound on the conversion.

So, the maximum mixedness model actually gives the lower bound on the conversion and the complete segregation model gives the upper bound on the conversion. So, now, we have looked at the single reaction case. So, now, is it possible to extend it to multiple reactions. In reality, many reactions are actually occur simultaneously in parallel. So, there can be sequence reactions that can be sequential parallel reactions etcetera. So, several reactions can actually happen simultaneously in a reactor. So, is it possible to predict conversion, when the multiple reactions happening inside the reactor? And the answer is yes it is possible.

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Multiple reactions
 $A \& B \rightarrow \text{reactants}$
 $P \rightarrow \text{products.}$
Segregation model
Each globule \Rightarrow Diff. conc. of A & B
 $\bar{C}_A = \int_0^{\infty} C_A(t) E(t) dt$
 $\bar{C}_B = \int_0^{\infty} C_B(t) E(t) dt$ Batch reactor
NPTEL

So, it is very simple to extend the segregation and the maximum mixedness model for multiple reactions. So, if there are multiple reactions which are actually happening. And let us A and B is the reactance. And P is let us say the products which is formed, let us say the products which is formed. And if it is a segregation model, if it is a complete segregation model, then if we assume that each globule has different concentrations of A and B. And if we assume that, each of them behaves like a batch reactor, which is 1 of the assumptions of the segregation model each of the globules. Then \bar{C}_A which is the concentration of the species, the average concentration of the species.

Remember that, if you are looking at multiple reactions and multiple species, it is actually better to work with concentrations rather than conversion. So, the average concentration of species, say will simply be the 0 to integral 0 to infinity C_A of $t E$ of $t dt$ where E of $t dt$ is the residence time function distribution function of that reactor. And similarly \bar{C}_B is given by integral 0 to infinity $C_B t$ into residence time of the reactor. And the $C_A t$ and $C_B t$ are essentially the concentrations up the can be achieved from a batch reactor because, this is the concentration of the species in each of the globule and we assume that each of these globule actually behave like a batch reactor. So, now if write the batch reactor performance equation for each of these species.

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V, q reactions
 Batch reactor
 1 $\frac{dC_A}{dt} = r_A = \sum_{i=1}^q r_{iA}$
 2 $\frac{dC_B}{dt} = r_B = \sum_{i=1}^q r_{iB}$
 Simultaneously with $\frac{d\bar{C}_A}{dt} = C_A(t)E(t)$ 3
 $\frac{d\bar{C}_B}{dt} = C_B(t)E(t)$ 4
 $\bar{C}_A(t)$ & $\bar{C}_B(t)$
 NPTEL

So, if there are q reactions occurring simultaneously. So, if the reactor volume is v and q reactions are occurring. If the q reactions which are occurring simultaneously, then for batch reactor, we can write the perform equation as $d C A$ by dt that is equal to the rate of generation of $r A$. So, that is equal to sigma 1 to q that is some over all the reactions and the reaction rate of the individual reactions, it is leading to the formation of species a.

Similarly, we can write for the species B; $d C B$ by dt equal to $r B$ which is equal to some 1 to q $r i B$. Now this actually has to in order to find the concentration of the species A and B in this model, in this in this reactor for following the segregation model. So, these 2 batch reactor rate expressions have to be solved simultaneously with the other 2 reactions which represent the overall concentration of the species in the reactor.

So, $d C A$ bar by dt , that is equal to $C A$ into E of t . So, that that defines how the concentration of the species, overall concentration of the species in the reactor that changes with time. And the corresponding equation for species B, that is equal to of t into E of t . So, by solving these 4 equation simultaneously this 1 equation 1, equation 2 equation 3 and 4. So, these 4 equations have be solved simultaneously and need to find $C A$ of t and $C B$ of t . So, that gives as the concentration of the species as a function of time, which actually follows the segregation model. So, next let us look at the multiple reactions for the maximum mixedness model.

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Max. Mixedness model : q reactions

$$\frac{dC_A}{d\lambda} = -\sum_{i=1}^q r_{iA} + (C_A - C_{A0}) \frac{E(\lambda)}{1 - F(\lambda)}$$
$$\frac{dC_B}{d\lambda} = -\sum_{i=1}^q r_{iB} + (C_B - C_{B0}) \frac{E(\lambda)}{1 - F(\lambda)}$$

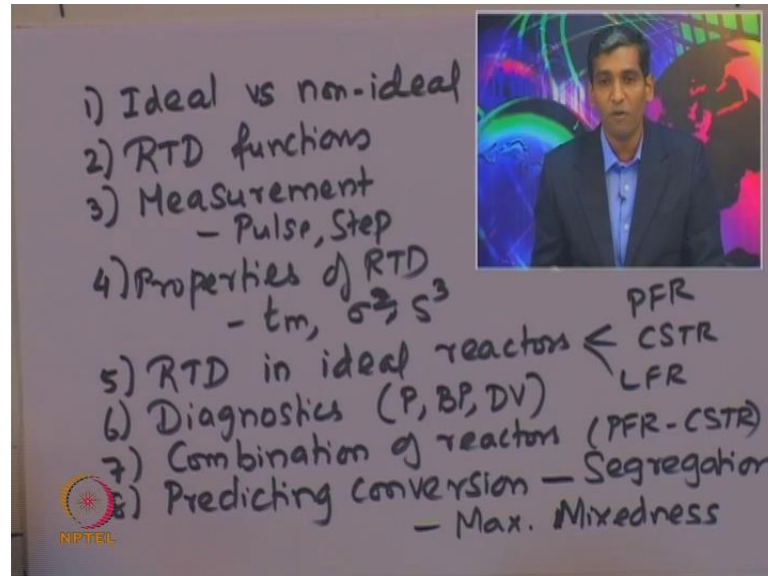
Rate law known
Solve for C_A & C_B from large λ to $\lambda = 0$

So, for a maximum mixedness case of it is the maximum mixedness model. If, once again if we assume that there are q reactions which are actually happening simultaneously, then the model equation is $dC_A/d\lambda$, is just an extension of the a single reaction case. So, $dC_A/d\lambda$ is minus summation of reaction rate over all reactions which is actually happening simultaneously, plus C_A minus C_{A0} where C_{A0} is the concentration of the species in the feed stream of the reactor multiplied by $E(\lambda)$ which is the distribution function for that particular reactor divided by $1 - F(\lambda)$. And similarly for $dC_B/d\lambda$ that is equal to minus some i equal to 1 to q r_{iB} plus C_B minus C_{B0} into $E(\lambda)$ by $1 - F(\lambda)$. So, where E is the RTD function for that particular reactor and F is the cumulative distribution function.

So, now, for once we know the rate law for all of the reactions. So, if we know the rate law. So, we can simply have to plug in this a rate law and then solve for the concentration. So, solve for C_A and C_B from large value of λ to λ equal to 0 . So, once we solve this equation, we will be able to find out what is the concentration of the C_A and C_B as a function of different age. So, this is the a set of equations and this can actually be extended for many other species. Even if n species are participating, I can actually write the maximum mixedness model, for all n species and similarly for the segregation model.

So, let us summarize what we have actually discussed in the last several lectures, in the residence time distribution problems.

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So, first we looked at the ideal versus non ideal reactors, we looked at ideal versus non ideal reactors. And then we looked at the RTD functions, we looked at the r t d functions; what is RTD function, why do we need RTD function etcetera. And then we looked at measurement of RTD functions, measurement of the RTD distribution function in real reactors, where we looked at the pulse tracer input and we looked at the step tracer input and we looked at how to perform these experiments and how actually estimate the RTD function, what to measure etcetera.

Then, we looked at RTD properties of distribution, properties of RTD function. So, particularly we looked; the mean, we looked at the variance and then we looked at the skewness of the distribution which actually tells us how skewed is the function around the mean of the distribution. And then we looked at RTD that is the residence time distribution in ideal reactors. We looked at plug flow reactor, we looked single CSTR and then we looked at the laminar flow reactor. These are the 3 cases that we looked and for RTD ideal reactors.

Then, we observed that the RTD function can actually be used for diagnostics purposes, in order to estimate whether the reactor is operating under perfect conditions. Usually it never perfect, but how close is it to a perfect operation, whether there is by passing of the

fluids that is actually entering the reactor, on and if there is a dead volume which may be present inside the reactor. And then we looked at the combination of reactors, we looked at combination of reactors particularly; we looked at the PFR-CSTR combination. And we looked at how to estimate the residence time distribution and we also observed that, if the residence time distribution a for PFR followed by CSTR and CSTR followed by PFR is actually same; however, the sequence is actually a dictate as to what is going to be the performance of the combination of reactor.

So, which is suggested that the RTD function alone is insufficient to actually predict the complete conversion or it is not the complete picture of the performance of the reactor, additional piece of information is required. And from there we marked on to the next topic of looking at the predicting the conversion. So, in this case we looked at the segregation model, and we looked at the maximum mixedness model. We looked at the maximum mixedness model, then we extended we looked at these models for first order reaction and we also extended this to multiple reactions.

Thank you.