Chemical Reaction Engineering - II
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Module - 12
Lecture - 59
Non-Ideal Reactors: Zero Parameter Models I

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

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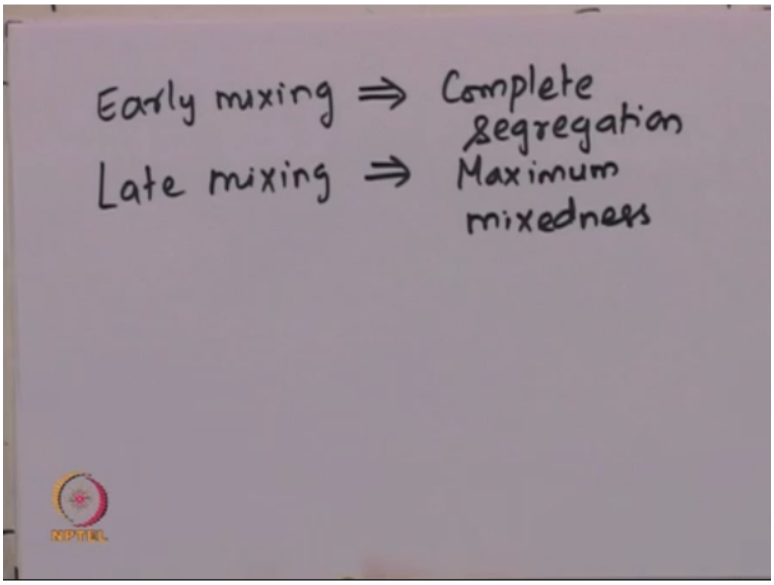

Early mixing ⇒ Complete segregation

Late mixing ⇒ Maximum mixedness

Or early mixing, 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 globules that we actually defined in the last lecture. So, let us look at the first one, the segregation model of a reactor.

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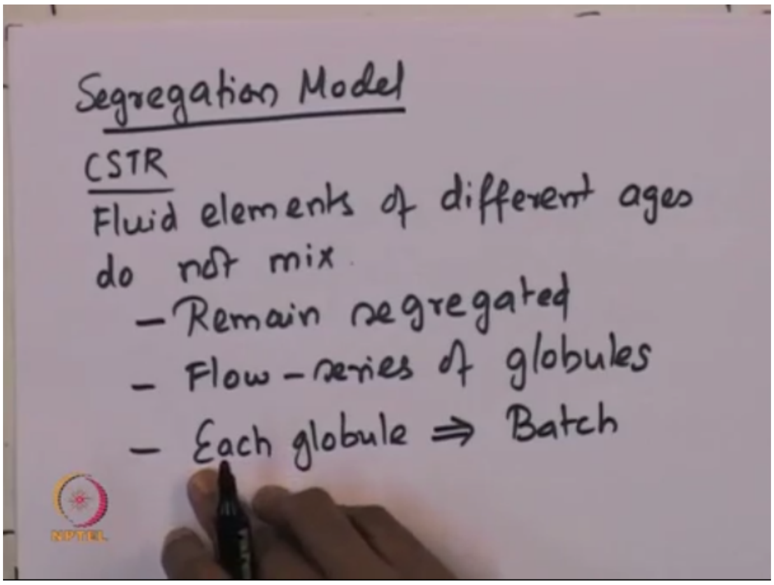

Segregation Model

CSTR

Fluid elements of different ages do not mix

- Remain segregated
- Flow - series of globules
- Each globule ⇒ Batch

Now, suppose let us consider a CSTR. So, let us consider a CSTR, a tank reactor, it could actually be any reactor. And the, let us assume that the fluid elements of different ages, they do not mix. That is the segregation model. And which will 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 gain, that 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 of 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 this globule, it continues to undergo reaction as long as all the species which is present in that globule is gradually come, going to complete conversion.

So, therefore each globule is considered as a, we may consider that as a batch reactor. So now, how do we model this? So, we can actually it depict this, the, depict the segregation, depict this particular aspect in a CSTR;

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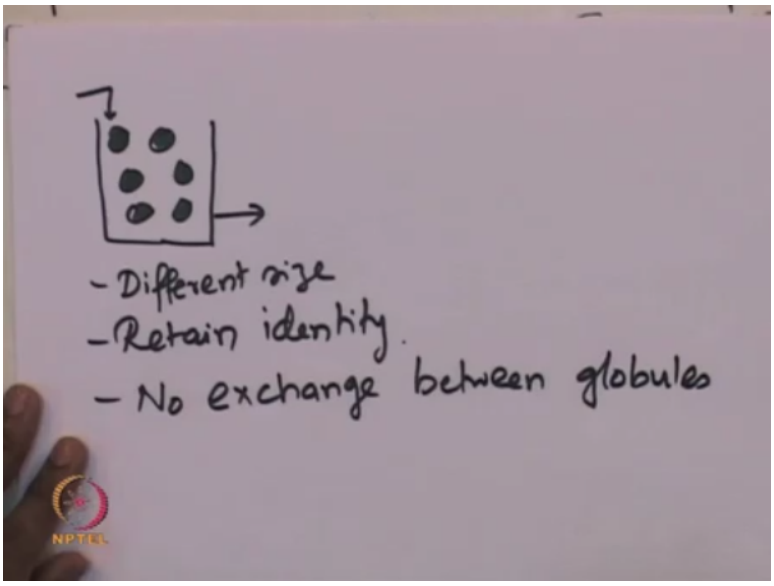

As basically a tank which contains several globules. And each of these globules are now going to have different ages. So, that is going to have a different age, this is going to have a different age and this is going to have different age. And each of these globules can actually in principle be of different sizes as well. Properties that are of these globules will be that, they will be of different sizes.

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

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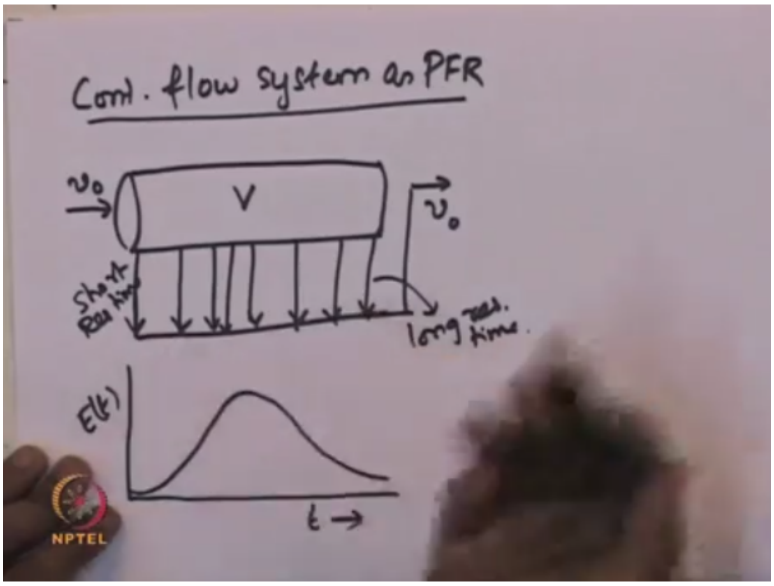

Suppose we have a continuous flow plug flow reactor. So, suppose if we model a continuous flow system of which is a continuous flow system of the non-ideal reactor as a plug flow reactor. Suppose if we model this as a plug flow reactor. Then, if you want to incorporate a segregated model for this non-ideal 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 nought into this 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 taken out from the side of this tube, at different locations along the side of the reactor. And they can all be joined together. And together they actually leave the reactor. So now, so each of these streams, if because they are withdrawn at 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 based on this RTD function, such kind of a withdrawing of the fluid from the reactor can actually be designed.

So, the fluid which is actually withdrawn from the reactor right at the entry location is going to have the shortest residence time. And the one which is actually withdrawn at the 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 we have done is, we have removed batches of fluid from different locations inside the reactor.

And the location from where it is withdrawal is actually specified by the residence time distribution function E of t which may be measured experimentally for a non-ideal reactor. And we, because we are withdrawing from the side, there is no interchange of molecules between each of these globules when they are actually present inside the reactor, when the reaction actually happens.

And each of these can actually be considered as actually a batch reactor. So, what it suggests is that the mixing for this kind of a system has actually, the fluid appears as a well-mixed system when it enters reactor but when it leaves, the globules are actually completely segregated. So, therefore the reaction time in batch, in each of the batch reactors, that is each of the globules, which maybe, which is basically withdrawn from different locations along the side of the reactor;

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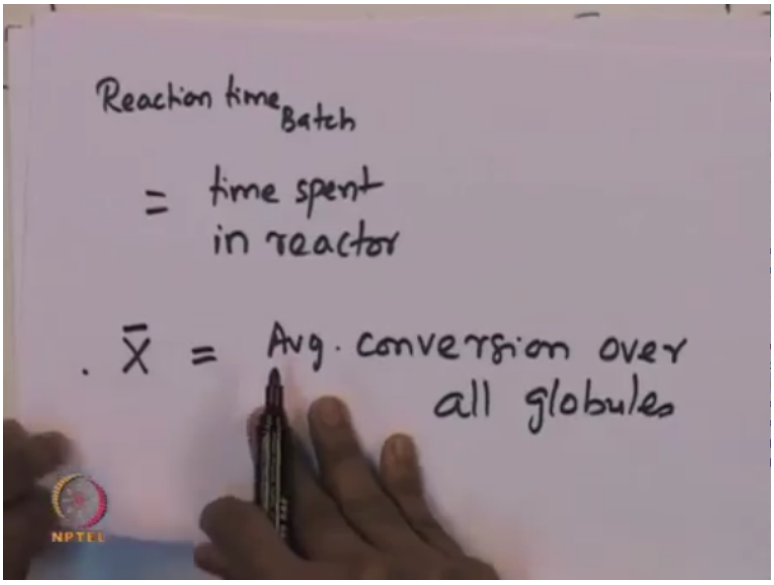

Reaction $\text{time}_{\text{Batch}}$

= time spent in reactor

. $\bar{X}$ = Avg. conversion over all globules

That time, the reaction time of batch reactor, of each of the batch reactor, is = 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 is spent by, the reaction time of each of these globules, that is each of these batch reactor is = the time that it actually spends in the reactor itself.

So, therefore the mean conversion, if X bar is the mean conversion, that is = 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 we essentially require 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 d t.

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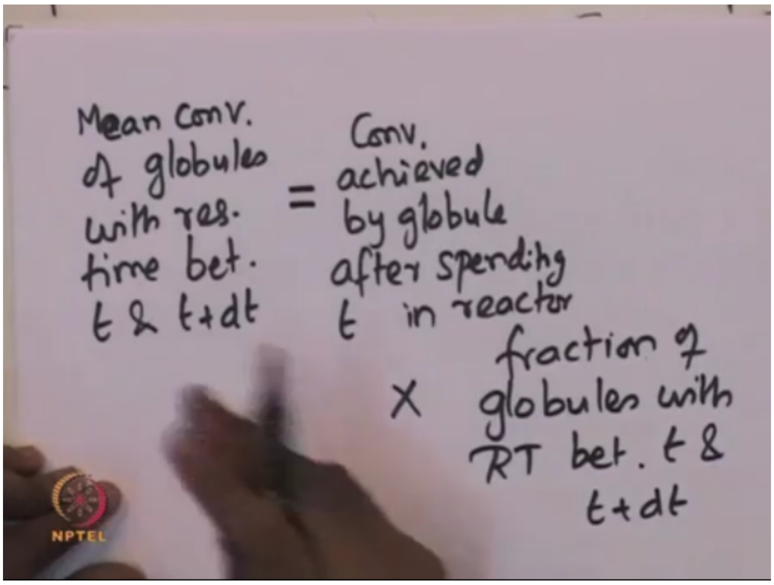

Mean conv.
of globules
with res.
time bet.
t & t+dt

=

Conv.
achieved
by globule
after spending
t in reactor

×

fraction of
globules with
RT bet. t &
t+dt

So, let us say that the mean conversion of globules with residence time between t and t + d t; 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 + delta t.

So, that is the abstraction of how to get a mean conversion of globules with a certain residence time between t and t + delta t, 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 + delta t. So, now if you put some, if you put the corresponding expressions, expressions corresponding to each of these terms in the mean conversion.

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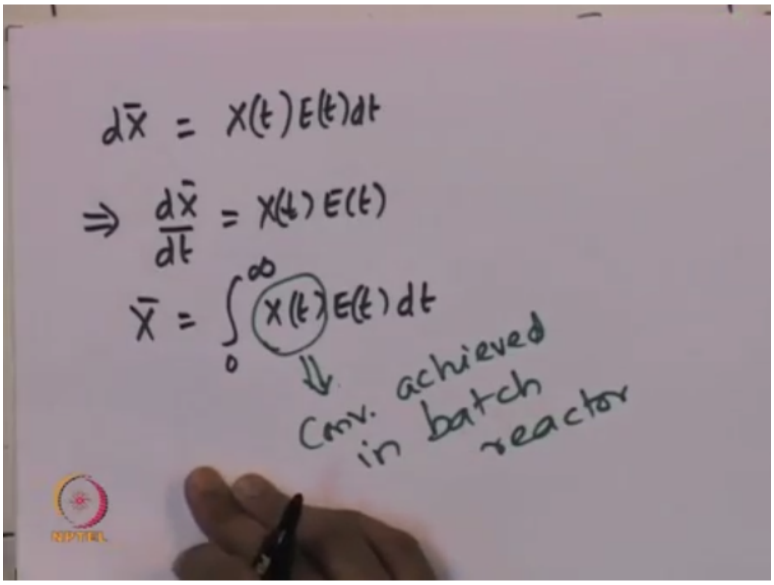

$$d\bar{X} = X(t)E(t)dt$$

$$\Rightarrow \frac{d\bar{X}}{dt} = X(t)E(t)$$

$$\bar{X} = \int_0^\infty \underbrace{\boxed{X(t)}}_{\Downarrow} E(t)\,dt$$

Conv. achieved in batch reactor

We will find that d X bar which is the mean conversion of the globules whose residence time is between t and t + delta t. So, that should be = the conversion achieved by a globule after spending that time in the reactor multiplied by the fraction that has a age of, age between t and t + delta t. So, therefore from here, we can write that d X bar by d t which is the mean conversion, that is = X t into E of t.

And therefore, X is = integral 0 to infinity, X of t, E of t d t. So, remember that the, the X of t which is actually present inside the integrand, that is essentially the conversion in batch reactor. Because we consider each of these globule 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.

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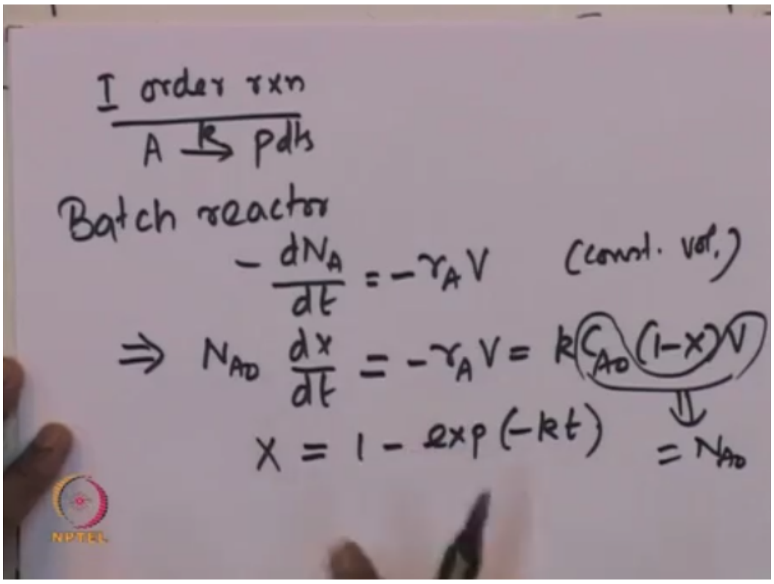

I order rxn

$A \xrightarrow{k} \text{pdts}$

Batch reactor

$$-\frac{dN_A}{dt} = -r_A V \quad \text{(const. vol.)}$$

$$\Rightarrow N_{A0}\frac{dx}{dt} = -r_A V = k\underbrace{C_{A0}(1-x)V}_{\Downarrow\; = N_{A0}}$$

$$X = 1 - \exp(-kt)$$

So, let us consider a first order reaction where A goes to products with the rate, with the specific reaction rate k. And for a batch reactor the performance equation is d – d N A by d t. That is = – r A into V, where V is the volume of the reactor. And let us assume that it is a constant volume system. And so, now we can use the relationship between the number of moles with the corresponding conversion and we can rewrite this equation as N A nought into d X by d t.

That is = – r A into V which is = k C A nought into 1 – X into V. And so, from here we can easily decipher that the conversion is = exponential of – k into t. And remember that the C A nought into V is essentially =, that is = N A nought. So, therefore the conversion as though, conversion in each of these globule is given by 1 – exponential of – k t. And so, from here, we can now find out what is the mean conversion.

We know the mean conversion is = integral 0 to infinity. That is the overall residence time of the product of the conversion in the batch reactor multiplied by the corresponding residence time.

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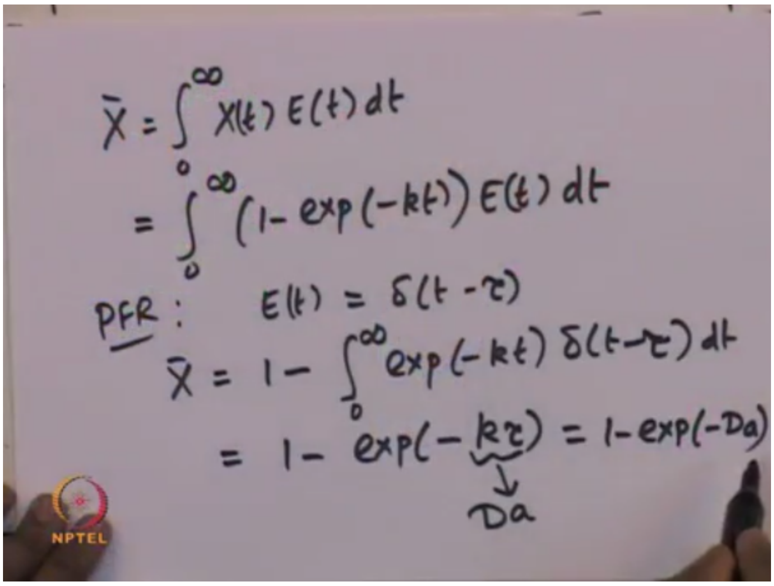

$$\bar{X} = \int_0^\infty X(t)\, E(t)\, dt$$

$$= \int_0^\infty (1-\exp(-kt))\, E(t)\, dt$$

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

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

$$= 1 - \exp(-\underbrace{k\tau}_{Da}) = 1-\exp(-Da)$$

So, therefore X bar is = 0 to infinity X of t E of t d t. And so, that is = integral 0 to infinity, 1 – exponential – k t E of t d t. 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 – tau, where tau 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 – integral 0 to infinity, exponential of – k t into delta function t – tau d t. And that is nothing but 1 – exponential of – k into tau. And k into tau is essentially the dimensionless quantity called the Damkohler number. This is the Damkohler number which is the ratio of the space time to the reaction time. And so, we can write this as exponential of – D a.

So, that is the mean conversion that would be achieved if it were to be 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 suggests that the conversion is actually = 1 – exponential of – D a. And let us see how that is the case.

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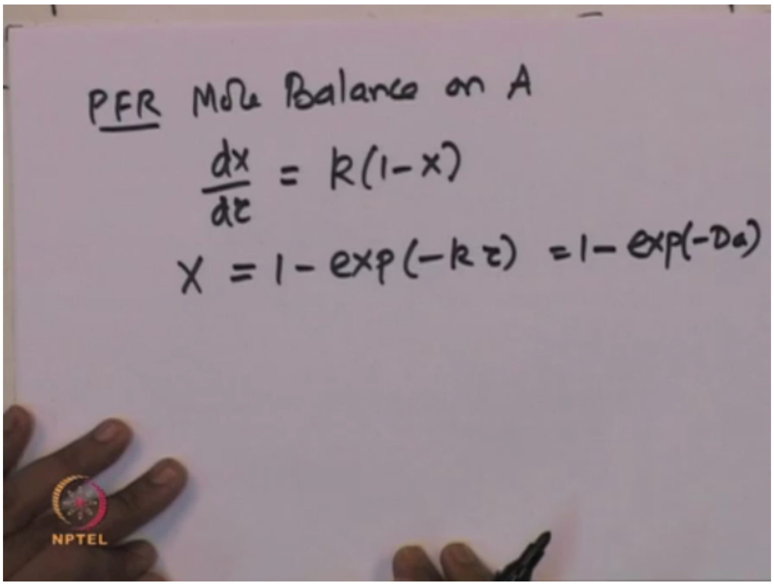

PFR Mole Balance on A

$$\frac{dx}{d\tau} = k(1-x)$$

$$X = 1 - \exp(-k\tau) = 1 - \exp(-Da)$$

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

In fact, we observed this in one of the lectures before that we mentioned that, if it is a first order reaction, then it does not, only RTD function is sufficient to estimate the conversion. And the level of mixing actually does not play any 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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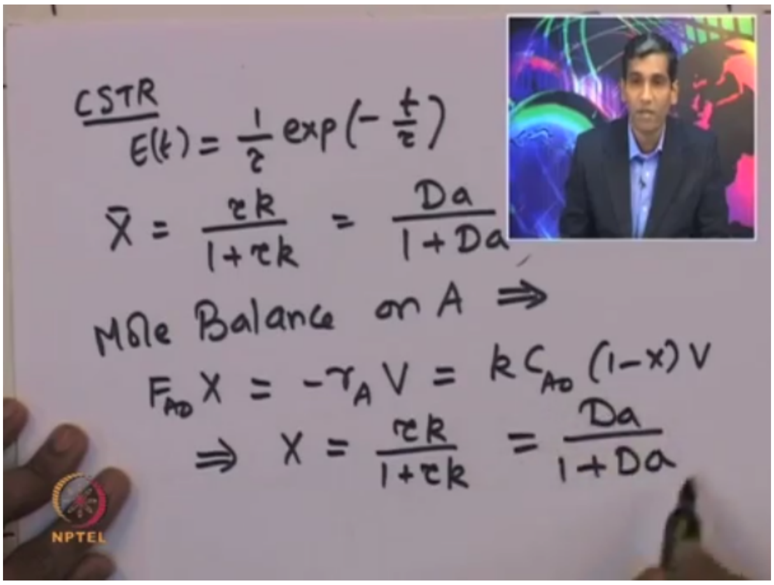

CSTR

$$E(t) = \frac{1}{\tau}\exp\left(-\frac{t}{\tau}\right)$$

$$\bar{X} = \frac{\tau k}{1+\tau k} = \frac{Da}{1+Da}$$

Mole Balance on A $\Rightarrow$

$$F_{A0} X = -r_A V = k C_{A0} (1-X) V$$

$$\Rightarrow X = \frac{\tau k}{1+\tau k} = \frac{Da}{1+Da}$$

So, the residence time distribution function for a CSTR is given by 1 by tau into exponential of – t by tau. So, therefore X bar, the mean conversion, plugging this into the integral and integrating the expressions shows that X bar is = tau into k divided by 1 + tau into k which is = the Damkohler number divided by 1 + Damkohler number. So, now if we write the mole balance for a CSTR.

So, the performance equation for the CSTR is, the mole balance on A is F A nought which is the molar flow rate of the species at inlet. That is, multiplied by X is = – r A multiplied by V. That is = k into C A nought into 1 – X into V. And – r A is, 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 = tau into k by 1 + tau k where tau is the space time of the reactor, 1 + D a.

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

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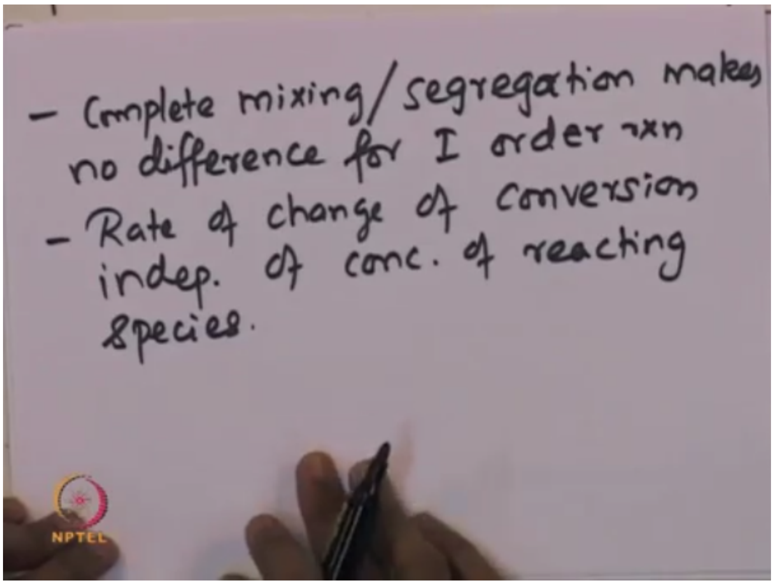

- Complete mixing/segregation makes no difference for I order rxn
- Rate of change of conversion indep. of conc. of reacting species.

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 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 reactant 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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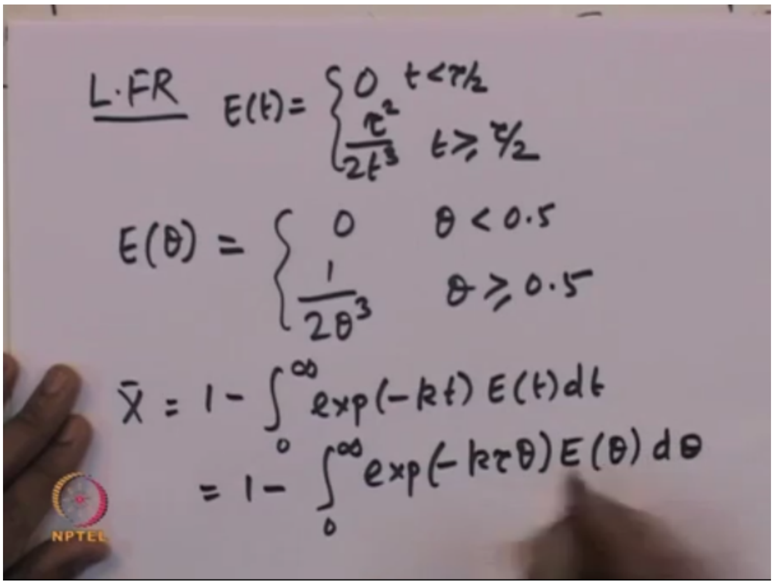

L.FR

$$E(t) = \begin{cases} 0 & t < \tau/2 \\ \dfrac{\tau^2}{2t^3} & t \geq \tau/2 \end{cases}$$

$$E(\theta) = \begin{cases} 0 & \theta < 0.5 \\ \dfrac{1}{2\theta^3} & \theta \geq 0.5 \end{cases}$$

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

$$= 1 - \int_0^\infty \exp(-k\tau\theta)\, E(\theta)\, d\theta$$

LFR stands for the laminar flow reactor. And the residence time distribution is given by 0 for t < tau by 2 and tau square by 2 t cube for t greater than or = tau by 2. So, that is the residence time distribution for a laminar flow reactor which we have actually derived in the previous lecture. In the normalised form, E of theta is = 0 1 by 2 theta cube. And this is theta < 0.5. And theta greater than or = 0.5.

So, now we can plug this distribution into the conversion equation and we can find that it will be = 1 – 0 to infinity exponential of – k into t into E of t d t. And that is = 1 – integral 0 to infinity exponential of – k tau theta into E of theta into d theta. So, on performing the integration by substituting the corresponding distribution, one can find that the mean conversion in a laminar flow reactor is essentially given by:

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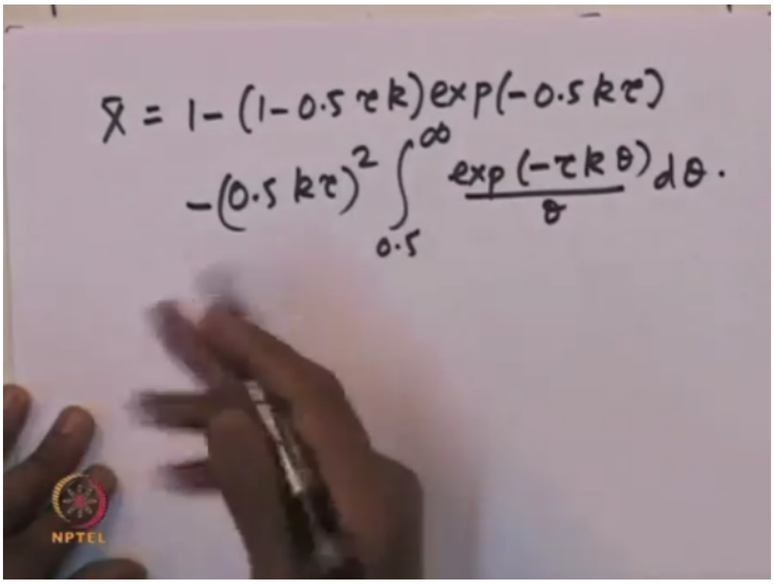

$$\bar{X} = 1-(1-0.5\tau k)\exp(-0.5k\tau) - (0.5k\tau)^2\int_{0.5}^{\infty}\frac{\exp(-\tau k\theta)}{\theta}\,d\theta .$$

1 – 1 – 0.5 into the space time multiplied by the specific reaction rate into exponential of – 0.5 k tau – 0.5 k tau the whole square, integral 0.5 to infinity exponential of – tau k theta divided by theta into d theta. So, that is the expression and one, if one solves this integral, one 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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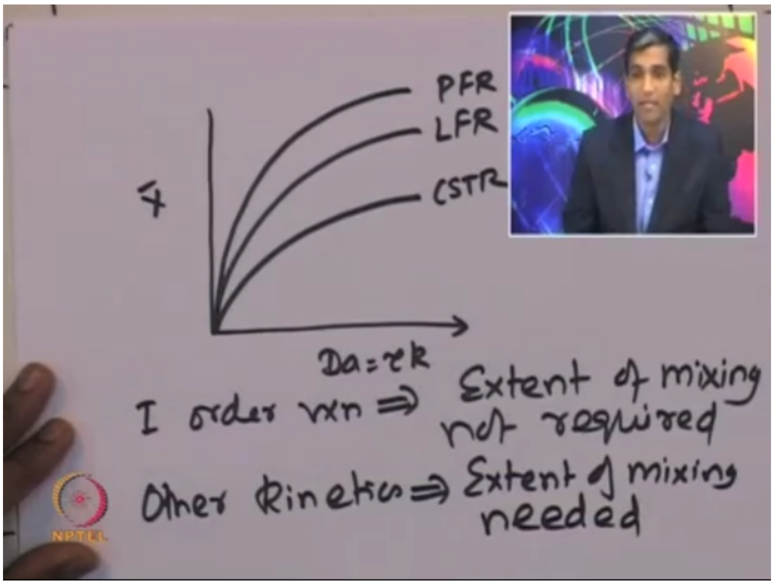

So, if we plot as a function of the Damkohler number which is the ratio of the space time to the reaction time X bar. So, the CSTR would actually be like this and the plug flow reactor would actually predict a much higher conversion for a first order reaction. Remember this is for a first order. And the laminar flow reactor would be somewhere in between. So, the plug flow and the CSTR, they sort of provide a bound for the 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 that, for a first order reaction the extent of mixing not required, while for other reactions, other kinetics, extent of mixing plays an important role. So, extent of mixing actually plays an important role and it is required in order to predict the conversion of the non-ideal reactor.