Chemical Reaction Engineering - II
Prof. Ganesh A Viswanathan
Department of Chemical Engineering
Indian Institute of Technology - Bombay

Module - 12
Lecture - 60
Non-Ideal Reactors: Zero Parameter Models II

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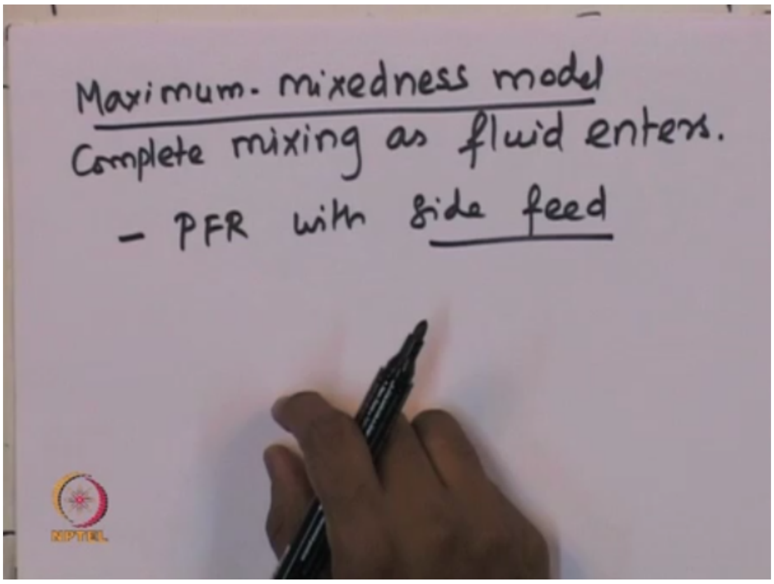

Maximum-mixedness model
Complete mixing as fluid enters.
- PFR with side feed

So now, let us move to the next model which is the maximum mixedness model. Let us look at the maximum mixedness model. So, the segregated fluid is one 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 actually flowing through the reactor.

On the other hand, on that is called the minimum segregation, minimum mixedness model, where the globules do not actually interact with each other. And each of the globules behave like a batch reactor. On the other extreme is a maximum mixedness model where the globules, the matter which is present in different globules, they are allowed to actually mix and interact with each other.

And therefore, the molecules which are of different ages they all mix with each other and that is, that kind of a representation or that can 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 this 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, the maximum mixedness is the complete mixing of the fluid right at the entry point of the reactor. 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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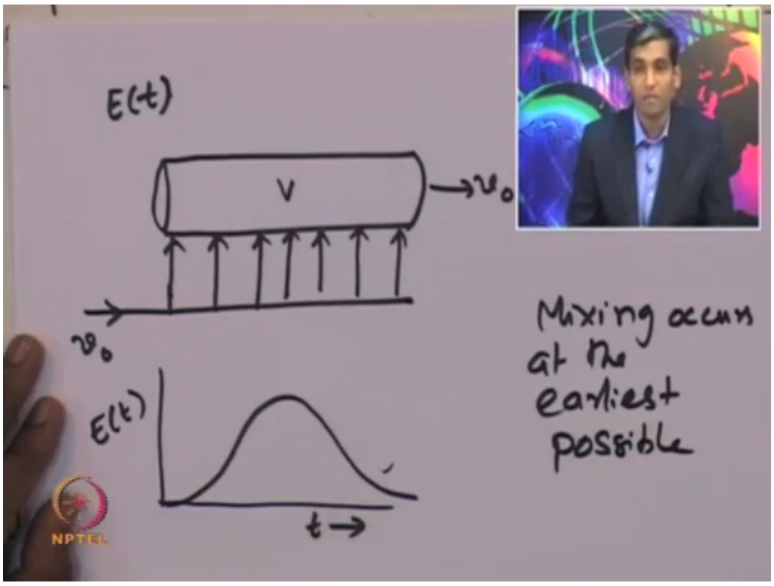

So, if we know the E of t of a real reactor, then we can actually mimic the reactor by using a plug flow reactor. And instead of providing a feed at the entry to the plug flow reactor whose volume is V, we can actually split the, we can actually feed them through the sides. We can feed them through the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

And the 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 reactor. So, mixing earliest possible which corresponds to the maximum mixedness situation in the reactor.

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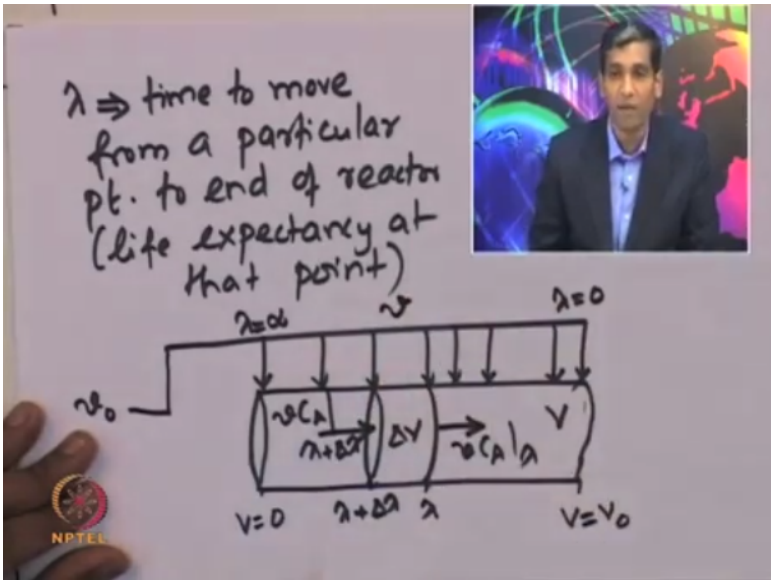

$\lambda \Rightarrow$ time to move from a particular pt. to end of reactor (life expectancy at that point)

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

So now, this also reflects the life expectancy at that point. That is, 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 in the site. So now, we can now draw a schematic of this reactor. So, suppose if 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 = 0. Because the time that is actually spent by the fluid that is pumped into the reactor near the exit of the reactor is almost = 0. So, therefore lambda = 0, the life expectancy of the fluid that enters the reactor in this location is going to be 0. So, lambda = 0 starts from here. And then, and lambda = infinity which is the maximum time that is taken inside the reactor, is at the entry of the reactor.

And if the volumetric flow rate of the fluid is V. And V = 0 is this location. And V = V nought, that is the full volume of the reactor. Now, if we now identify a small element and if the volume of that element is delta V. 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 + delta lambda. So, that is the difference in the life expectancy from this point to this point. So, this is will be v to C A at lambda + 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 flow rate with which the fluid is actually going to enter is let us 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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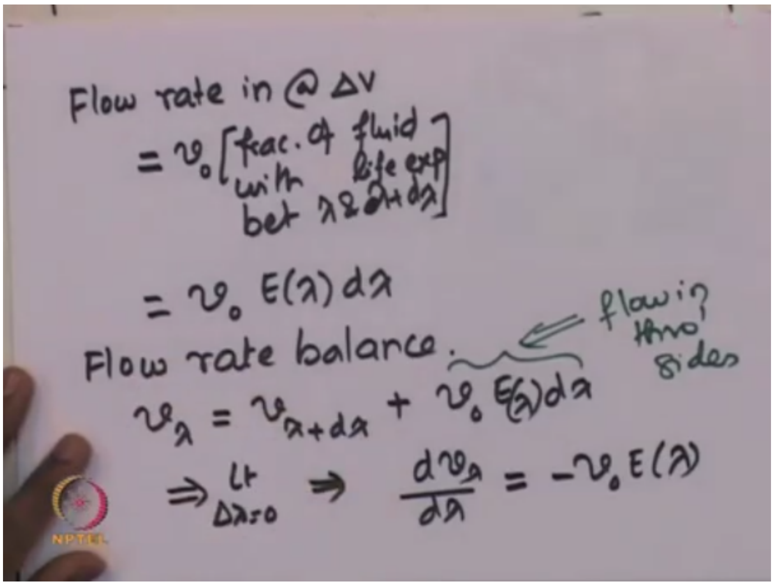

Flow rate in @ ΔV

$= v_0$ [frac. of fluid with life exp bet λ & $\lambda + d\lambda$]

$= v_0 \, E(\lambda) \, d\lambda$

Flow rate balance.

$v_\lambda = v_{\lambda+d\lambda} + v_0 E(\lambda) d\lambda$

flow in thro' sides

$\Rightarrow \lim_{\Delta\lambda \to 0} \Rightarrow \frac{dv_\lambda}{d\lambda} = -v_0 E(\lambda)$

So, the flow rate in at delta V. So, that is = the volumetric flow rate v nought, 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 fluid is actually entering in this small element delta V. So, flow rate in at delta V should be = v nought 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 lambda and lambda + d lambda. So, that is = v nought multiplied by the corresponding E lambda times d lambda where E lambda 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 a flow rate balance.

And the flow rate balance is volumetric flow rate at lambda should be = the volumetric flow rate of the fluid at lambda + d lambda + whatever is actually added through the side. So, the, that will be = v nought into E lambda d lambda. So, this is the flow rate in through the side. So, this is the, that is the flow in through the side of the plug flow reactor. And, so now we know, so now we can actually take the limits of delta lambda going 0.

So, limit delta lambda going 0, this essentially becomes d v lambda by d lambda. That is = – v nought into E lambda. So, that is the differential equation which captures what is the flow rate with flow rate at a certain life expectancy lambda. So now, v nought is the flow rate with which the fluid is actually flowing at the entrance of the reactor.

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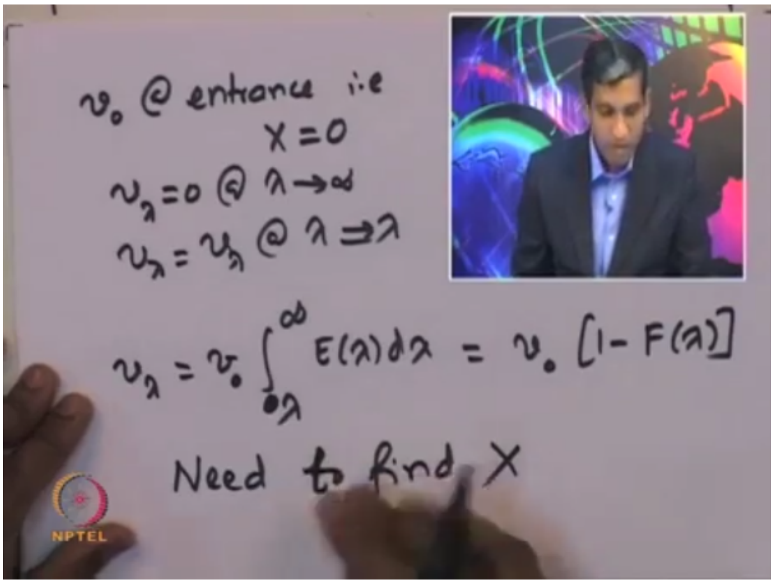

v_0 @ entrance i.e $X = 0$

$v_\lambda = 0$ @ $\lambda \to \infty$

$v_\lambda = v_\lambda$ @ $\lambda \Rightarrow \lambda$

$$v_\lambda = v_0 \int_{\lambda}^{\infty} E(\lambda)\, d\lambda = v_0 \left[1 - F(\lambda)\right]$$

Need to find X

So, which means at entrance, that is, when conversion is actually = 0. So, before at, v nought 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 = 0 at as lambda tends to infinity. So, the flow rate of the fluid that is actually at the entrance is v nought and the conversion at that location is = 0.

And so, therefore, the amount of fluid that is actually right at the 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 = infinity, is = 0 and v lambda is = v lambda at some lambda = lambda. That is, at certain age, let us assume that v lambda is the corresponding volumetric flow rate.

And so, using these 2 as limits, we can now integrate to find that v lambda = v nought into integral 0 to, integral lambda to infinity E lambda d lambda which is = v nought into 1 – F of lambda. So, that is the volumetric flow rate with which the fluid is actually flowing at any location lambda. So now, in the 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 mole balance of the species in order to find the conversion of the species in the reactor. So, before we write a mole balance, we need to know certain aspects of the reactor, a certain aspects before we write the mole balance.

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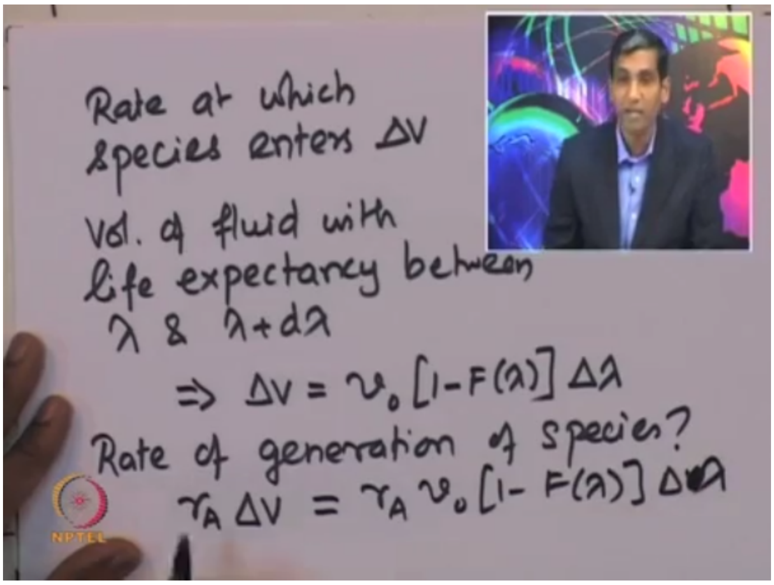

Rate at which
species enters ΔV

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?

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

For example, the what is the amount of species; what is the rate at which enters the small element delta V. So, this can actually be found by using what is the volume of the fluid whose life expectancy is actually between the, between lambda and lambda + d lambda. So, the volume of the fluid with life expectancy between lambda 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 delta V.

So, that is =, so delta V will be = v nought into 1 – F of 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 a certain life expectancy that is =, that is somewhere between lambda and lambda + d lambda. So now, what is the rate of generation of the species? 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 delta V. So, that is = r A into v nought into 1 – F lambda into delta lambda. So, we now have all information that we need to write the mole balance. So, let us now write the mole balance for this particular species.

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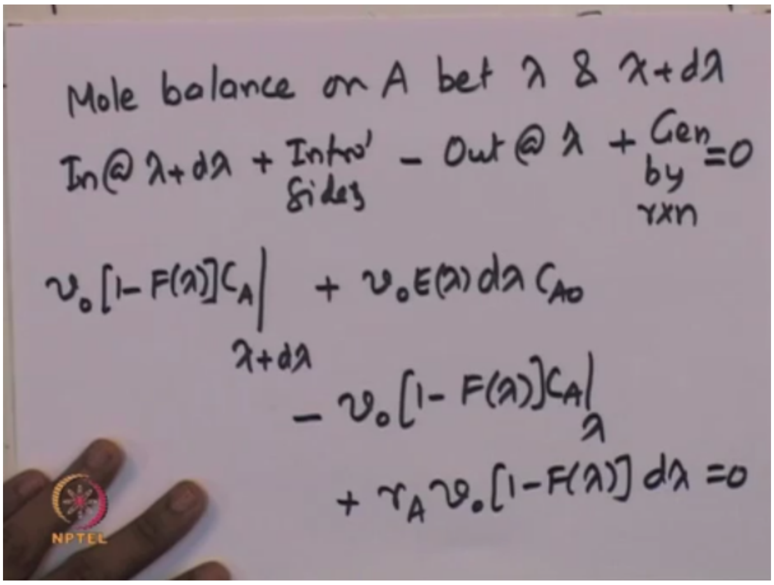

Mole balance on A bet λ & $\lambda+d\lambda$

In@ $\lambda+d\lambda$ + Intro' Sides − Out @ λ + Gen by rxn $=0$

$$v_0[1-F(\lambda)]C_A\Big|_{\lambda+d\lambda} + v_0E(\lambda)d\lambda\, C_{A0} - v_0[1-F(\lambda)]C_A\Big|_{\lambda} + r_A v_0[1-F(\lambda)]d\lambda = 0$$

So, the mole balance for the species is, so mole balance on A between with life expectancy of lambda and lambda + d lambda. So, let us write a mole balance for this. So, what is the rate at which things are coming inside at lambda + 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 volume from the entry of the reactor to the exit of the reactor.

So, in at lambda + d lambda + the introduction through the side. What is rate at which things are actually introduced into the reactor through the sides – what leaves reactor, what leaves that element at lambda + whatever is generated by reaction. So, that should be = 0. So, that is the mole balance on A for age between lambda and lambda + d lambda. So, we know all these quantities. So, v nought into 1 – F lambda.

So, that is the volumetric flow rate at lambda, lambda + d lambda into C A at evaluated at lambda + d lambda will tell us what is the rate at which the species is actually getting into that element + the whatever is introduced through the sides. That is given by v nought into E lambda d lambda multiplied by C A nought where C A nought is the concentration of the species in the feed stream – v nought into 1 – F lambda into C A evaluated at lambda + r A into v nought which is the volumetric flow rate of the feed into 1 – F lambda multiplied by d lambda = 0. So, that is the mole balance on A between the age lambda and lambda + d lambda.

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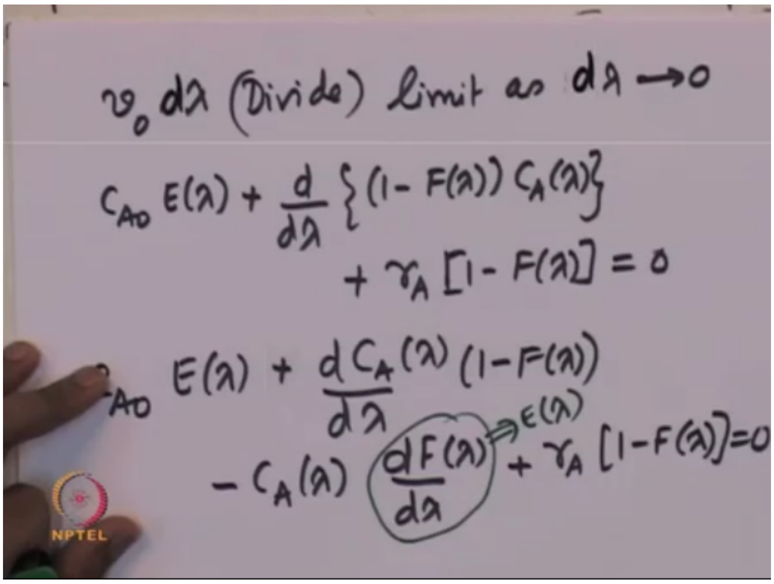

$v_0 \, d\lambda$ (Divide) limit as $d\lambda \to 0$

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

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

So, now we can actually divide this expression by v nought into delta lambda. We can divide this expression by v nought and d lambda and take limit as d lambda goes to 0. So, that will be C A nought into E lambda + d by d lambda into 1 – F of lambda into C A lambda + r A into 1 – F of lambda = 0. So, that is the expression for, that is the mole balance. And so now, we can open up this differential here.

And we can rewrite the expression as C A nought into E lambda E of lambda + d C A lambda by d lambda into 1 – F lambda – C A lambda into d F lambda by d lambda + r A into 1 – F lambda = 0. Now, if we stare at this expression, this d F by d 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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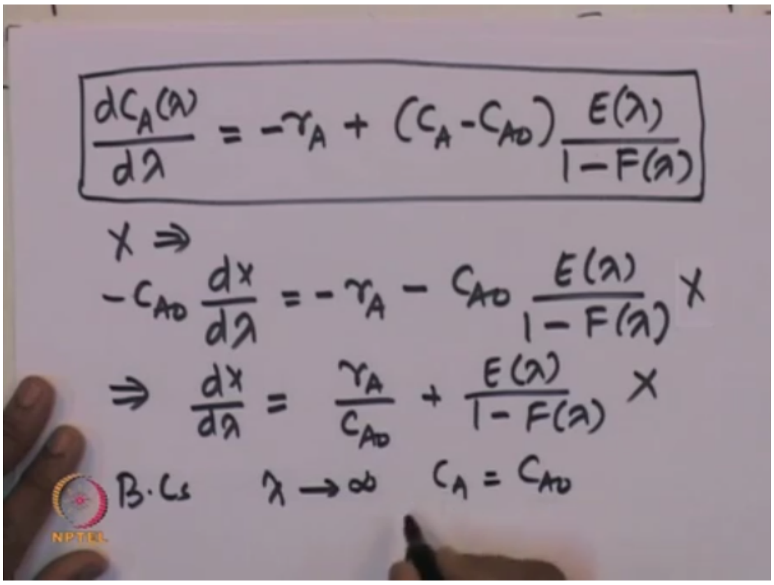

$$\boxed{\frac{dC_A(\lambda)}{d\lambda} = -r_A + (C_A - C_{A0})\frac{E(\lambda)}{1-F(\lambda)}}$$

$X \Rightarrow$

$$-C_{A0}\frac{dX}{d\lambda} = -r_A - C_{A0}\frac{E(\lambda)}{1-F(\lambda)}X$$

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

B.Cs $\lambda \to \infty \quad C_A = C_{A0}$

So, the final mole balance essentially is d C A of lambda by d lambda. That is = – r A + C A – C A nought into E lambda by 1 – F lambda. So, that is the mole balance for the species for a maximum mixedness model. And so, in terms of conversion, we can actually write this expression as – C A nought d X by d lambda. That is = – r A – C A nought into E lambda by 1 – F of lambda.

And so, that can actually be written as d X by d lambda = r A which is the rate of generation of the species divided by C A nought which is the concentration of the species in the inlet stream into E lambda by 1 – F lambda into the conversion X. So, while solving this equation, we 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. The boundary conditions are very simple. So, lambda goes to infinity when C A = C A nought. That is, at the entry point into the reactor, 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 a very large lambda.

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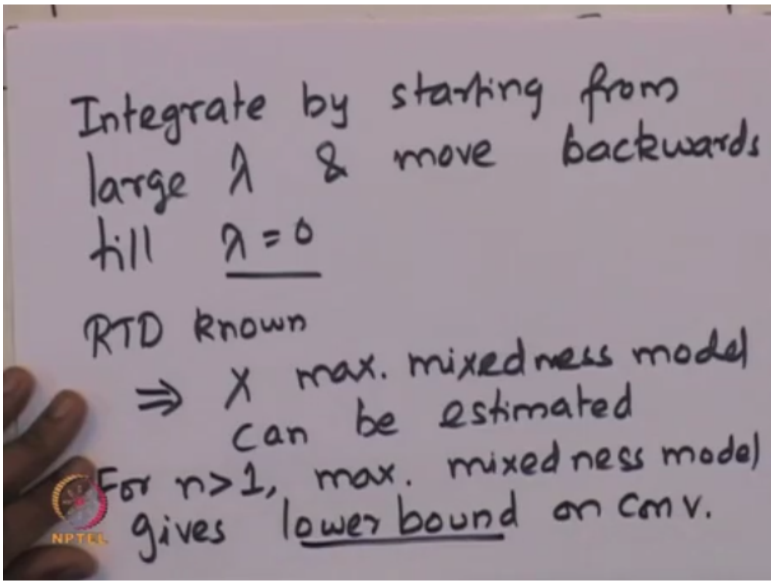

Integrate by starting from
large λ & move backwards
till $\lambda = 0$

RTD known
$\Rightarrow$ X max. mixedness model
can be estimated
For $n>1$, max. mixedness model
gives lower bound on conv.

So, we have to integrate this equation by starting from large lambda and move backwards till lambda = 0. So, that is the method to integrate this equation and once we integrate the equation, we will be able to find out what is the conversion in under the situation of maximum mixedness. So now, so if RTD is known, then the conversion for the maximum mixedness situation can actually be, model can be estimated.

So, this conversion provides a bound for the conversion of the species in the non-ideal reactor. And so, for n equal, n > 1, it has been observed that for n > 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. Now, is it possible to extend it to multiple reactions? In reality, many reactions are, can actually occur simultaneously in parallel. So, there can be sequence reactions, there can be sequential parallel reactions and etcetera. So, several reactions can actually happen simultaneously in a reactor. So, is it possible to predict conversion when there are multiple reactions happening inside the reactor. And the answer is yes, it is possible.

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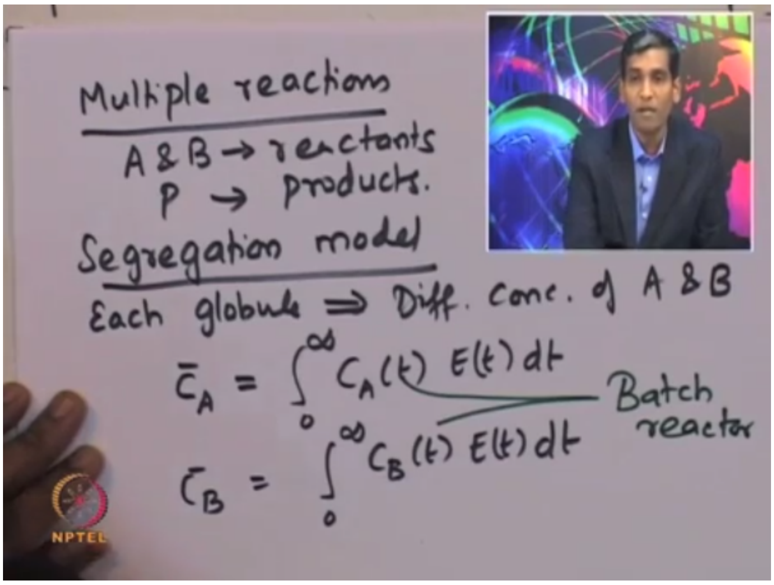

Multiple reactions

A & B → reactants

P → products.

Segregation model

Each globule ⇒ Diff. conc. of A & B

$$\bar{C}_A = \int_0^\infty \underbrace{C_A(t)}_{\text{Batch reactor}} E(t)\,dt$$

$$\bar{C}_B = \int_0^\infty C_B(t)\,E(t)\,dt$$

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 say A and B are the reactants. And P is let us say the products which is formed. And if it is a segregation model, if it is a complete segregation model, then if you assume that each globule has different concentrations of A and B.

And if you assume that each of them behave like a batch reactor which is one of the assumptions of the segregation model, each of these globules. Then C A bar 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 A will simply be 0, integral 0 to infinity C A of t, E of t d t where E of t d t is the residence time function distribution function of that reactor. And similarly, 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 of, 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 you write the, a batch reactor performance equation for each of these species.

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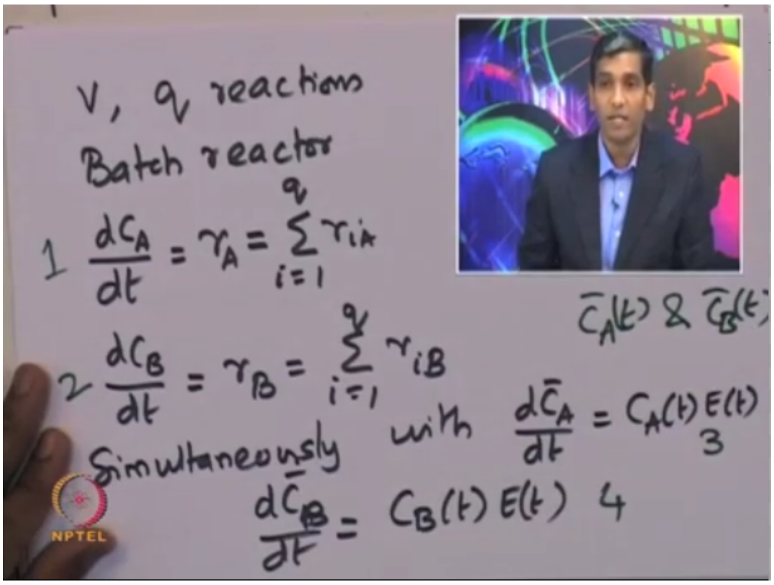

V, q reactions

Batch reactor

1 $\frac{dC_A}{dt} = r_A = \sum_{i=1}^{q} r_{iA}$

$\bar{C}_A(t)$ & $\bar{C}_B(t)$

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

So, if there are a q reactions occurring simultaneously. So, if the reactor volume is V and q reactions are occurring, and there are q reactions which are occurring simultaneously. Then for batch reactor we can write the performance equation as d C A by d t. That is = the rate of generation of r A. So, that is = sigma 1 to q. That is, some over all the reactions and the reaction rate of the individual reactions which is leading to the formation of species A.

And similarly, we can write for the species B, d C B by d t = r B which is = sum 1 to q r i B. Now this actually has to, in order to find the concentration of the species as A and B in this model in this reactor following the segregation model. So, these 2 batch reactor rate expressions has 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 d t, that is = C A t into E of t. So, 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 = of t into E of t. So, by solving these 4 equations simultaneously this 1 equation 1, equation 2, equations 3 and 4, so, these 4 equations have to be solved simultaneously and we need to find C A of t and C B of t.

So, that gives us 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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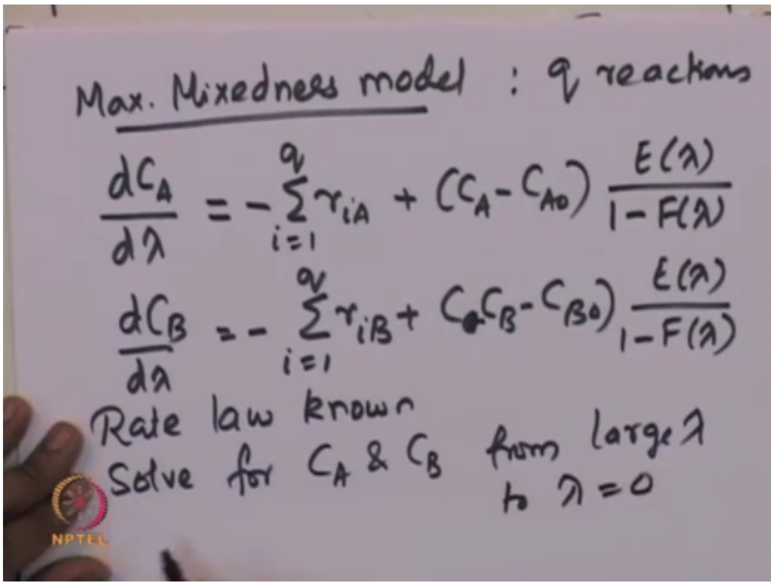

Max. Mixedness model : q reactions

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

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

Rate law known

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

So, for a maximum mixedness case, so, if 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 d C A by d lambda is just an extension of the single reaction case. So, d C A by d lambda is – summation of reaction rate over all reactions which is actually happening simultaneously + C A – C A nought where C A nought 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 d C B by d lambda, that is = – sum i = 1 to q r i B + C B – C B nought 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 rate law and then solve for the concentration.

So, solve for C A and C B from large value of lambda to lambda = 0. So, once we solve this equation, we will be able to find out what is the concentration of C A and C B as a function of different age. So, this is the set of equations and this can actually be extended for many other species. Even if n species are participating, one can actually write the maximum mixedness model for all n species and similarly for the segregation model. So, let us summarise what we have actually discussed in the last several lectures in the residence time distribution problems.

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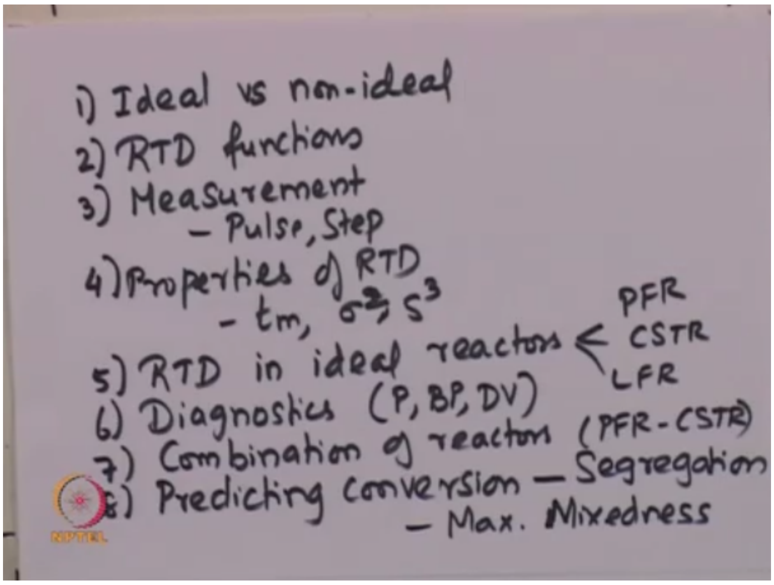

1) Ideal vs non-ideal
2) RTD functions
3) Measurement
   - Pulse, Step
4) Properties of RTD
   - t_m, σ^2, s^3
5) RTD in ideal reactors ← PFR, CSTR, LFR
6) Diagnostics (P, BP, DV)
7) Combination of reactors (PFR-CSTR)
8) Predicting conversion — Segregation
   — Max. Mixedness

So, first we looked at the ideal versus non-ideal reactors. And then we looked at the RTD 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 to actually estimate the RTD function, what to measure, etcetera, etcetera.

And then, we looked at RTD properties of distribution, properties of RTD function. So, particularly we looked at 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 at single CSTR and then we looked at the laminar flow reactor. These are the 3 cases that we looked at for RTD in ideal reactors. And 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 is perfect but how close is it to a perfect operation.

Whether there is bypassing of the fluids that is actually entering the reactor or 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 for PFR followed by CSTR and CSTR followed by PFR is actually same.

However, the sequence actually dictates us to what is going to be the performance of the combination of reactor. So, which we 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 marched 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. And then, we extended, we looked at these models for first order reaction and we also extended this to multiple reactions. Thank you.