Chemical Reaction Engineering - II
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Module - 11
Lecture - 53
RTD Function

Friends, it is a good time to summarise what we have learnt in residence time distribution so far. So, you have looked at what is a non-ideal reactor and what is the residence time distribution function, what are its definitions. And we had looked at what are the ways to measure it experimentally. That is looking at the pulse and the step input. And we have also came, we also looked at what are the RTD or the residence time distribution functions E-curve and the cumulative distribution function F-curve in the last lecture.

So, today let us start with, in this lecture, let us start with looking at the properties of different functions and also proceed further. So, suppose, if I look at the, an important property of the residence time distribution is the mean residence time.

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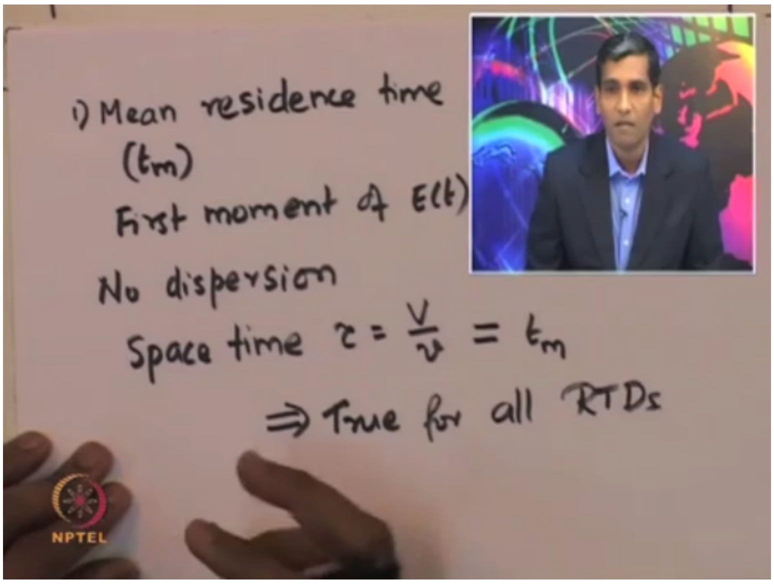

So, the mean residence time is actually given by the first moment. So, if I, t m is the symbol that I have used for mean residence time, it is actually given by the first moment of the, of E of t, that is the RTD function. So, E of t is actually a distribution and that distribution can actually be used to decipher some of the properties of the distribution itself and some of the properties of the reactor system.

For example, mean residence time is an important property that is actually used to control various things in the system. When there is no dispersion across boundaries that is between the point of injection and the entrance of the reactor. Then, in these situations the space time, that is tau which is = V by the volumetric flow rate with which fluid is actually flowing through the reactor. That is = the mean residence time itself.

Now, this is independent of any RTD function that is actually representing the non-ideal behaviour of the reactor under no dispersion conditions. Irrespective of the RTD function, the mean residence time that we obtain would be exactly = the space time of the reactor itself. So, this is true for all RTDs, all residence time distributions irrespective of what type of reactor, as long as the dispersion is actually absent. So now, let us look at how to calculate the mean residence time from the residence time distribution function E of t.

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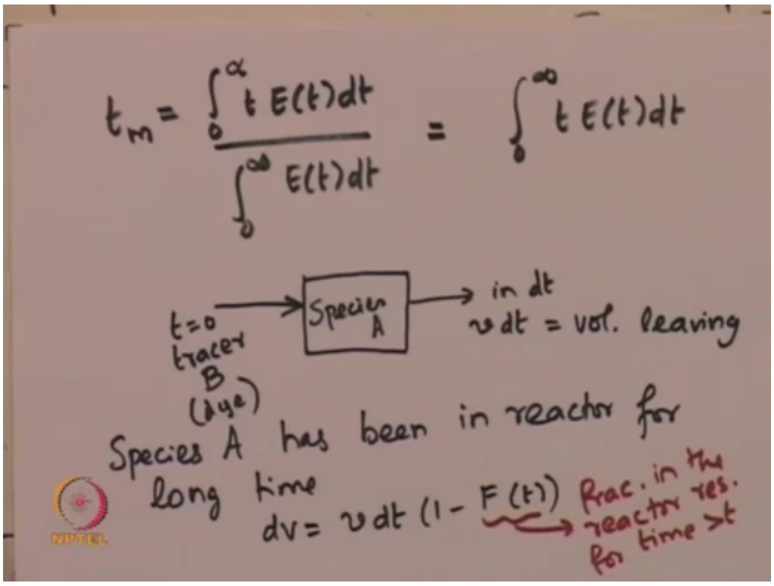

So, t m which is the mean residence time is actually given by the first moment as we observed, as I mentioned in the previous note, a few moments ago. That is, 0 to infinity, t into E of t d t divided by integral 0 to infinity E of t d t. So, that is the residence time distribution. And because the integral of the E-curve which is the RTD function between 0 to infinity. That is = 1, the, this expression can further be simplified as integral between 0 to infinity t into E of t d t.

So, that is the expression for the mean residence time if the RTD function E of t is known. So, if the residence time distribution function is known, one can simply plug it in, in this expression and find out what is the mean residence time. Now, suppose let us look at a, suppose let us consider the reactor. And let us assume that it is filled with species A. And let us say that at time $t = 0$, a tracer molecule, tracer species B is injected into the reactor.

Let us say it is a dye. And then, in some time d t, so let us say that the amount of tracer which is actually leaving the reactor in this time delta t, whose age is actually, lies between that time. Is actually given by v times d t where v is the volumetric flow rate with which the fluid actually leaves the reactor. And that is = the volume of the tracer which is actually leaving the, that is actually the volume of the effluent stream which is actually leaving the reactor, not the tracer,

So now, suppose if we want to know that the species has been there for a long time. So, species A has been in the reactor for a long time. So, remember v d t is the volume of the effluent which is actually leaving the reactor in this time d t. And if you want to know what is the volume of species A which is actually leaving in that time delta t. So, then, that will be given by, d v which is = the total volume of the fluid that is actually leaving the reactor, multiplied by 1 – F of t.

So, F of t is basically the fraction that has been in the reactor for time which is > t. So, this is the fraction which is actually, so that is the fraction in the reactor residing for time larger than t. So, 1 – F t multiplied by the volume of the effluent stream will actually tell us what is the amount of species A which is actually leaving the reactor in that small time d t. So now, if we sum this over, all the molecules of A, then that will tell us what is the net volume of the species which is actually leaving the reactor. So, if we sum over all A molecules.

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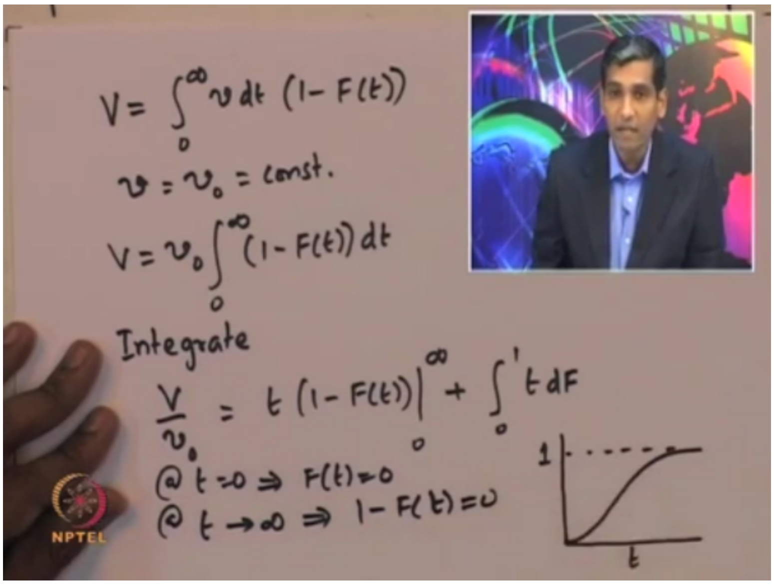

Say, the total volume that is leaving is given by 0 to infinity v d t into 1 – F of t. So, from here, if you assume that the volumetric flow rate with which the fluid stream leaves the reactor, if that remains constant. And this is generally not true for gas stream, but it is normally true for liquid streams that is actually leaving the reactor. If it is a gas stream, suppose if it is operated under constant pressure and at isothermal conditions, that is constant temperature.

And if the number of molecules or number of moles does not change because of the reaction, then one may also assume that the volumetric flow rate with which the fluid leaves the reactor, the effluent stream volumetric flow rate is, probably perhaps remains constant. So, by using this we can say that V = v nought into integral 1 – F t d t. So, now we can integrate this by parts. So, if we integrate, we will find that V by v nought, that is = t into 1 – F of t limits 0 to infinity + integral 0 to 1 t d F.

So, that is the integral. This is basically when we do an integration by parts we can see that, we can split the integral into 2 sections. It is t into 1 – F t evaluated between 0 and infinity and 0 to 1 t times d F. Now, if I look at the F-curve, the F-curve typically looks like this. So, this is with respect to time. And this is 1. So, at time t = 0, F of t is 0 and when t goes to infinity, 1 – F of t is 0. So, that can actually be easily seen from the F t curve or the F-curve.

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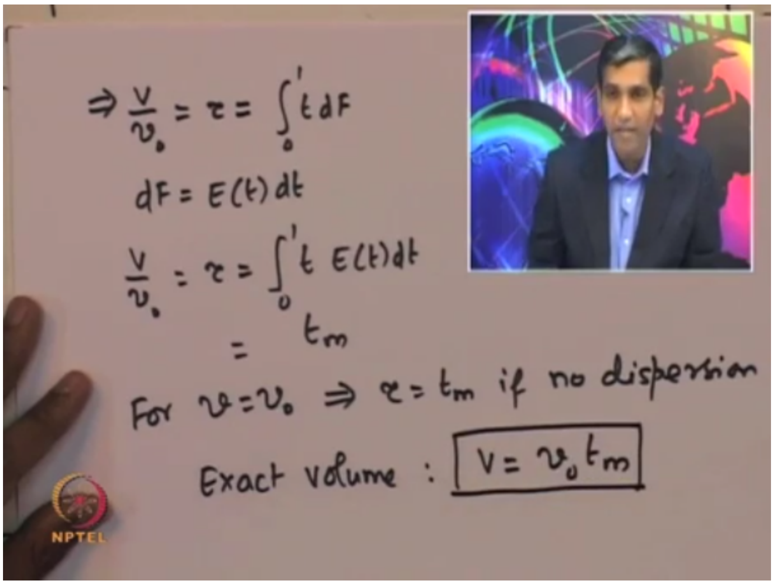

So now, substituting these expressions, we will find that V by v nought, that is = tau which is the space time of the reactor. And that is 0 to 1 t times d F. What is d F? d F is nothing but the residence time distribution itself, E t into d t gives the first differential of the F-curve. And therefore, V by v nought, that is = tau. And that is = integral 0 to 1 t times E of t d t. And that is nothing but the mean residence time itself.

So, this shows that for any RTD if there is no dispersion between the point of injection and the entrance of the reactor, one can show that the mean residence time is actually = the space time of the reactor itself irrespective of what is the RTD function E of t. So, clearly, for v = v nought, for constant volumetric flow rate, then, tau = t m if no dispersion. And remember that this v = v nought is true for gases only if the reactor is operated under constant pressure drop and the temperature is maintained constant.

That is at isothermal conditions and if the number of moles does not change because of the reaction, only under those conditions, the effluent stream volumetric flow rate may be assumed as a constant. So therefore, the exact volume of the reactor, if there is no dispersion is actually given by v nought multiplied by the average residence time. So, if the average residence time is known, then we can actually calculate what is the exact volume of the reactor in which the fluid is actually flowing.

So, are there other properties? So, we looked at mean residence time and we also showed that the mean residence time should be = the space time irrespective of the RTD function, as long as the dispersion is negligible or 0. And also if the volumetric flow rate with which the fluid stream leaves remains nearly constant. So, are there other properties? And the answer is yes, there are other properties.

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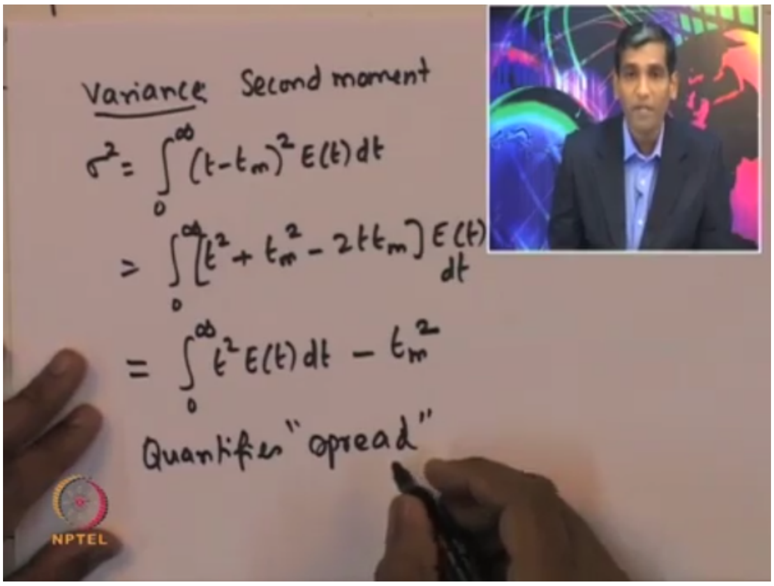

So, the other properties is, we can also estimate what is the variance of the distribution. And that can be obtained using the second moment. So, the sigma square which is the variance is given by 0 to infinity t – t m square into E of t d t. And so now, if we expand this square term, quadratic, this product here. So, we can expand this as 0 to infinity t square + t m square – 2 into d, t into t m into E of t d t. So, that is the integral.

And this is nothing but 0 to infinity t square E of t d t – t m square. So, this essentially, the variance, it is essentially quantifies the, it quantifies the spread in the distribution of the RTD function. So, that is another property that is actually very commonly used in the real systems. And the third property is not very commonly used is the skewness property. It is called the skewness.

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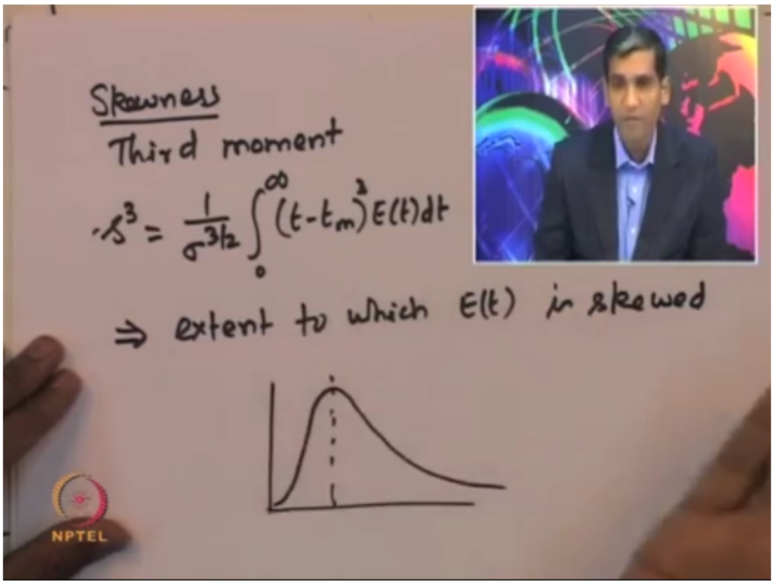

And that is obtained using the third moment of the distribution. And that is given by, if s q s is the skewness parameter, there will be 1 by sigma to the power of 3 by 2 where sigma is the standard deviation. That is square root of the variance 0 to infinity. t – t m the whole cube into E of t d t. So, that is the skewness. And this is basically, reflects the extent to which the distribution, residence time distribution function is skewed.

So, remember that it may be skewed in either directions. So, for example if the residence time distribution looks like this, then it is sort of skewed to the right-hand side of the mean. So, the s cube essentially says how skewed is the distribution with respect to the mean of the distribution itself. So, now once we know these properties, next the question is from real reactor data. Suppose if there is a tracer that goes inside. And from the real data, is it possible to estimate some of these parameters and what are the steps that is involved.

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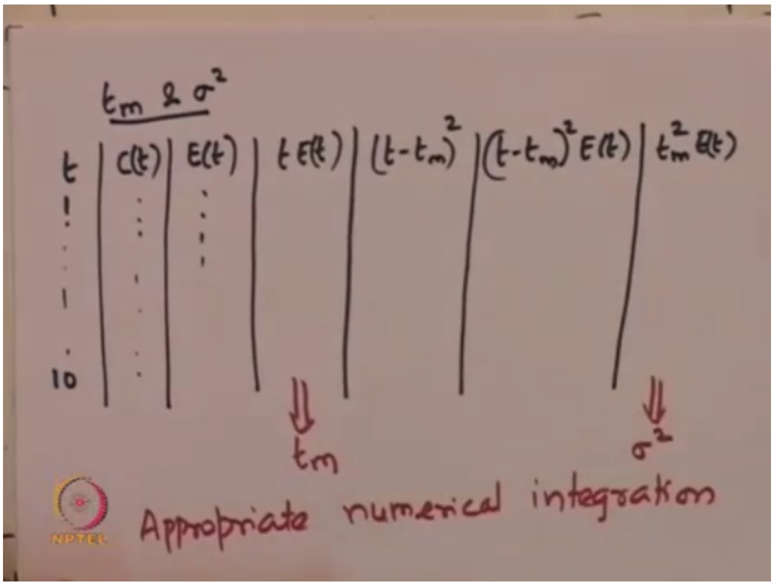

So, let us look at how to calculate the mean residence time and sigma square from the actual data. So, normally the actual data that one would get is basically the measurement of concentration as a function of time. So, let us say that there are several concentrations that has been measured. Let us say from time 1 to 10. And there has been concentration C t that has been measured.

So, then one needs to create a table, where as a first step one calculates E of t. So, we know the formula for E of t which is essentially given by C t divided by the integral of C over the whole time domain. And then the next thing one needs to estimate is t into E of t. So, this provides a, this column provides an estimate of the first moment which is the mean residence time, can be used to find the mean residence time. And the next step is to estimate t – t m the whole square.

And then, find out t – t m the whole square into E of t. And then from here one can actually find out what is t m square into E of t. So, one can make such a table moment the experimental data of time versus concentration is available, of the tracer is available. Then, one can actually fill up this table. And from this column, one can estimate the mean residence time. And from this column one can actually estimate what is the sigma square.

So, and one needs to use an appropriate numerical integration scheme. Remember that the concentration is actually discreet values at different time points. And so, one has to use appropriate numerical integration in order to complete this table. Once this table is complete, we will actually be able to estimate what is the mean residence time and the variance for the distribution that represents the RTD function for the reactor. Now, the, suppose if we change the, suppose if there is a reactor, and we know the RTD function.

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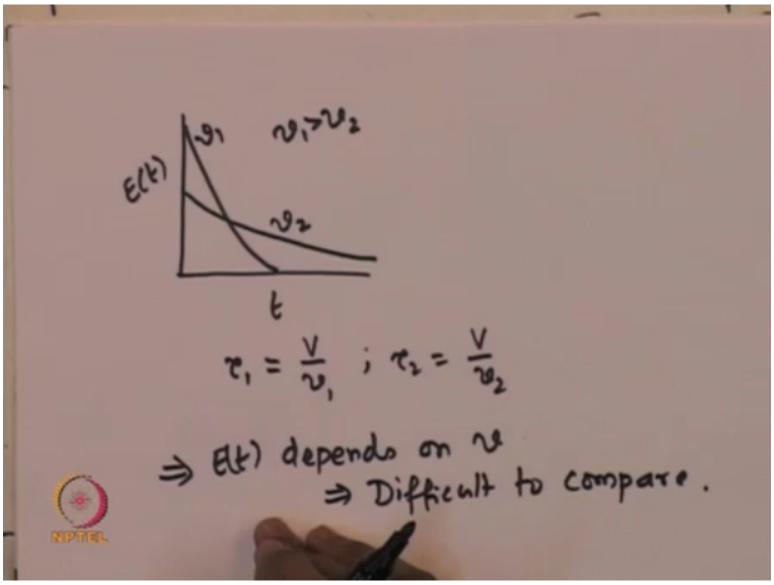

Suppose we know the RTD function, suppose we know the E-curve for a given volumetric flow rate v 1. Now, if we want to find out what is the E-curve or the RTD function for a different volumetric flow rate. So now, let us consider the situation where we are actually feeding the reactor with a fluid of volumetric flow rate which is less than v 1. So, then the amount of time that the fluid stream spends inside the reactor is going to be larger because the volumetric flow rate is actually lesser than v 1.

And as a result, the E-curve would actually look like this, the slope of the E-curve will correspondingly change. So now, because of this problem, so, this corresponds to volumetric flow rate v 2. And because of this issue, it is very difficult to now compare the E-curves at different conditions, because the E-curve is now going to be dependent on the volume of the reactor and also on the volumetric flow rate with which the fluid is actually being fed into the reactor.

Even for a fixed volume, the E-curve is now going to be a function of the volumetric flow rate. because the volumetric flow rate decides the residence time of the fluid stream inside the reactor. So, therefore the tau 1 which is the space time when the volumetric flow rate is v 1 is given by V by v 1 and tau 2 is given by V by v 2. So, clearly, the amount of time that is spent by the second, in the second case, that is when the fluid is being fed at a volumetric flow rate of v 2, that is going to clearly be larger than that of the time that is actually spent by the fluid elements inside the reactor, when the volumetric flow rate is v 1 because v 2 is actually smaller than v 1.

So, because E t depends on properties such as volumetric flow rate, it is difficult to compare. So, as a result it is useful to actually define a normalised RTD function in order to facilitate to the ability to compare different RTD curves.

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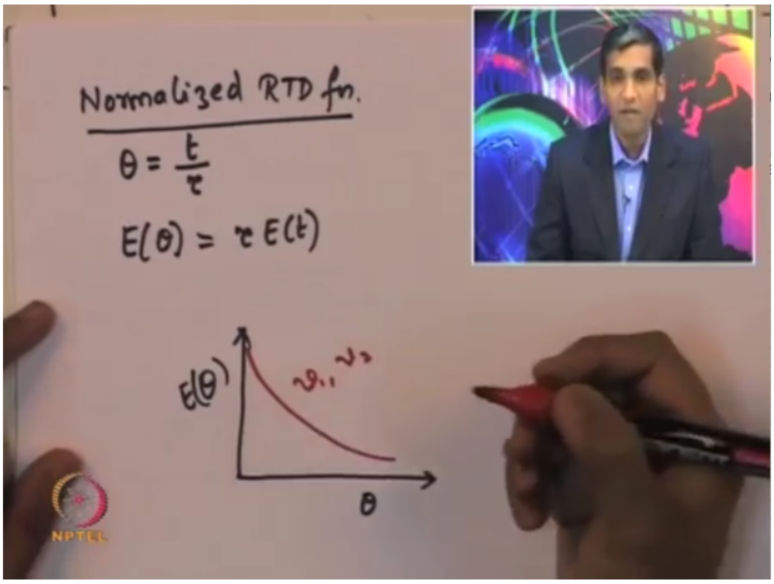

So, let us look at what is the normalised RTD function. So, suppose if we define theta as the ratio of t divided by tau where tau is the space time of the reactor. If we define theta as the ratio of time versus the space time of the reactor, then we can now rewrite the RTD function E theta, as basically tau multiplied by E t. So, that is tau is the space time. Multiplied by the corresponding RTD function, gives the normalised RTD function E of theta.

And so now, theta here which is the ratio of time into tau essentially represents the number of reactor volumes of fluid based on the entrance condition that are actually flown through the reactor in that particular time t. So, now this normalised RTD function E theta provides a facilitates a way by which the performance of the reactor or the RTD function itself can be compared when the sizes are different.

So, therefore if I, if we look at the RTD curve of the normalised RTD function, then the curve looks like this. Where, so irrespective of whatever is the volumetric flow rate for a given reactor volume, the RTD function essentially looks like this. So now, there is another definition that one needs to know is the internal age distribution.

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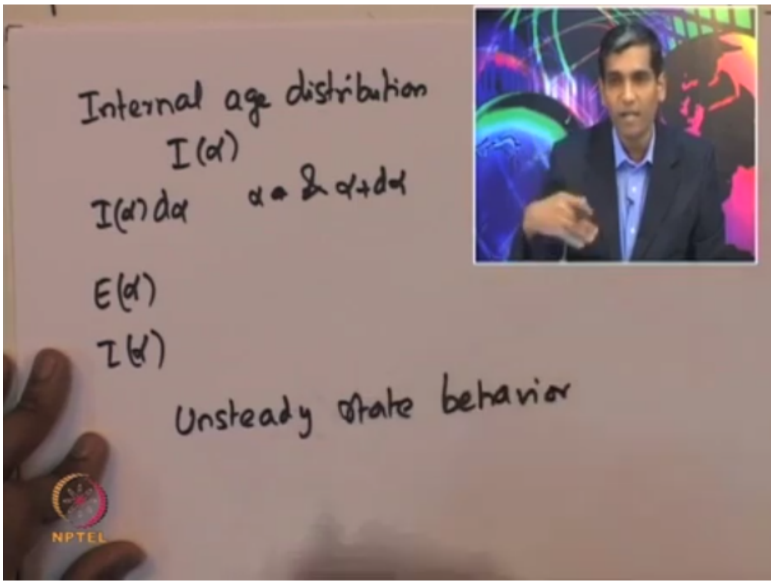

And the symbol that is commonly used is I of alpha. Where I of alpha d alpha, that essentially represents the fraction of the material that is present inside the reactor in a time span of, for a period between, that is between alpha and alpha + d alpha. So, that represents the fraction of the material that is actually residing inside the reactor whose period of residing inside lies between this, lies between alpha and alpha + d alpha in that small interval.

So, E alpha essentially represents the age of the fluid that actually is leaving the reactor and I alpha represents the age of the fluid that is actually present inside the reactor. So, these 2 have its own utility. And particularly, the internal the age of the fluid elements that is actually present inside the reactor has a significant importance when one looks at when one wants to study the unsteady state behavior of a particular reactor.

In particular, a good example of that would be that suppose if there is a catalytic reaction, and the catalyst is actually decaying with time, then it is important to know what is the internal age distribution. And it is important to actually consider the age distribution in modelling the performance of such kind of a reactor.

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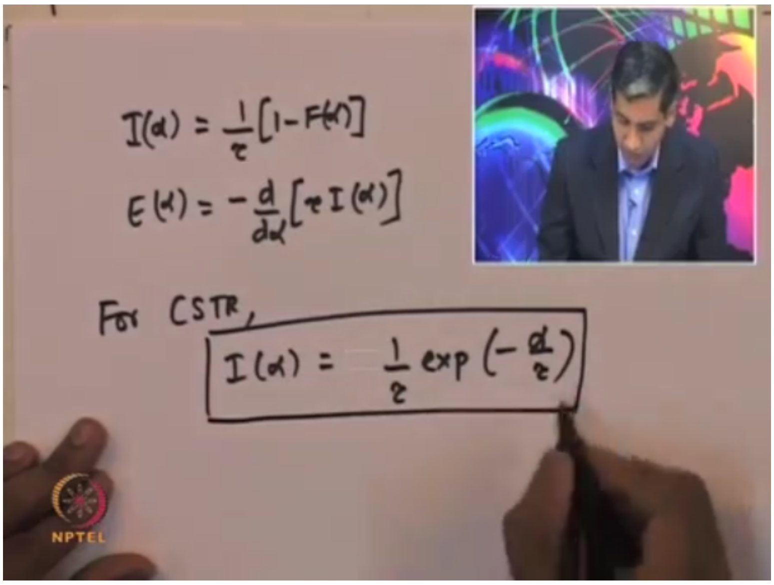

So, I alpha, the internal age distribution is essentially given by 1 by tau into 1 – F of alpha. And E of alpha as we know is actually given by – d by d alpha tau into alpha. Because of the connection between the E-curve and the F-curve. So, the relationship between the E-curve and the I-curve is nothing but E of alpha is – d by d alpha into tau into I alpha. Now, for a CSTR, for an ideal CSTR, I alpha is essentially given by 1 by tau into exponential of – alpha by tau. So, that is the internal age distribution for a CSTR.