Chemical Reaction Engineering - II
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Module - 11
Lecture - 55
Reactor Diagnostics and Troubleshooting I

Friends, in the last lecture we initiated discussion on the estimation of the residence time distribution for a laminar flow reactor. Let us continue with that.

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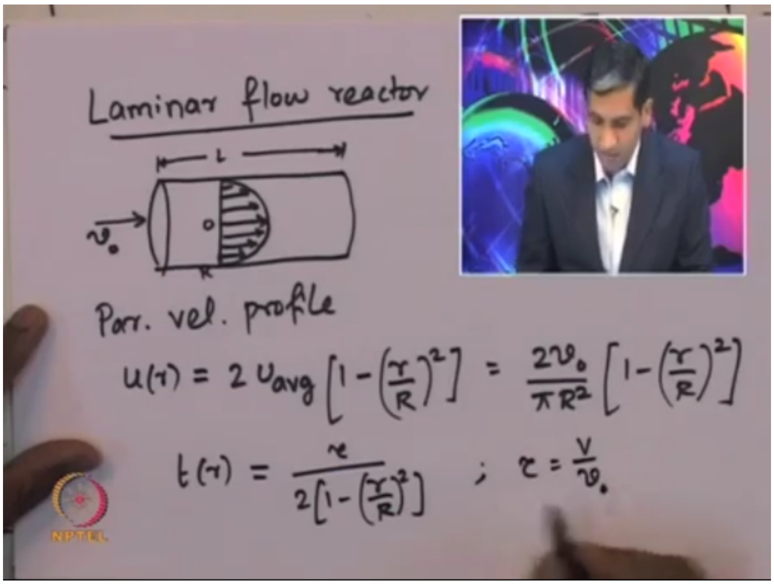

So, laminar flow reactor is essentially a tube through which a fluid is flowing. And let us say that the volumetric flow rate with which the fluid is actually flowing through the reactor is v nought. And if the length of the reactor is L. Then the velocity profile of the fluid in the radial direction will be parabolic with maximum velocity at the centre and all the other fluid streams which is flowing at any other r location will be smaller than the maximum.

So, this is r = 0 and this is R = capital R which is the radius of the cylindrical tube. So, the maximum velocity will be at the centre. So. the parabolic velocity profile as we saw in the last lecture is actually given by u at any r location is 2 times the average velocity in a cross section or the cup mixing velocity in a cross section multiplied by 1 – r by R the whole square. And that is = 2 into v nought which is the volumetric flow rate with which the fluid is actually flowing through the reactor divided by the cross-sectional area pi R square into 1 – r by capital R the whole square.

So, that is the dependence of the velocity in any radial position with respect to the position. Now, we said that the time that is actually taken by different fluid streams in different r location is going to be different because the velocity with which they are moving through the reactor is different. So, therefore the time that they would take, different fluid elements at different r location would take in order to traverse from the entry to the exit of the reactor will be tau divided by 2 into 1 – r by capital R the whole square.

Where tau is actually given by v, volume of the reactor divided by the volumetric flow rate which is essentially the space time of the reactor. So now, let us look at a particular cross section.

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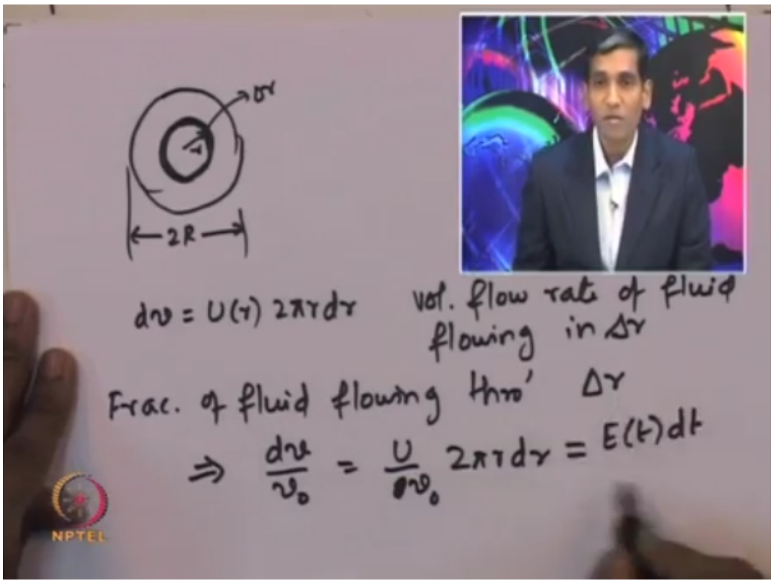

So, if at any radial location if we identify a small thickness of delta r. So, suppose if the thickness is delta r. And this thickness is located at some r location. So, the inner radius will be r of this element and the outer radius will actually be r + delta r and the diameter is given by two R where R is the radius of the tube. So now, the volumetric flow rate of the fluid that actually flows through that small element delta r is essentially given by d v.

If U is the velocity with which the fluid is actually flowing in that r location multiplied by 2 pi r d r. So, that is the volumetric flow rate of fluid flowing in delta r. So, that is the volumetric flow rate. Now, what is the fraction of the total fluid that actually flows through that small element delta r? So, that fraction of fluid through delta r; so, that is actually given by d v by v nought where v nought is the flow rate with which the fluid actually is entering the reactor.

But that is = U by r, U by v nought into 2 pi r d r. And that is nothing but the E of t d t which is the fraction of the fluid that is actually going through this small element whose volumetric flow rate is actually between v and delta v. And also the time that is actually spending inside the reactor is given by t, is given by the time that is between t and t + delta t. So, therefore the fraction of the fluid that is flowing through should be = the corresponding residence time of that particular fluid element. So now, we know that, the time that the fluid element takes to actually traverse from 0 to L, that is along the length of the reactor is actually given by;

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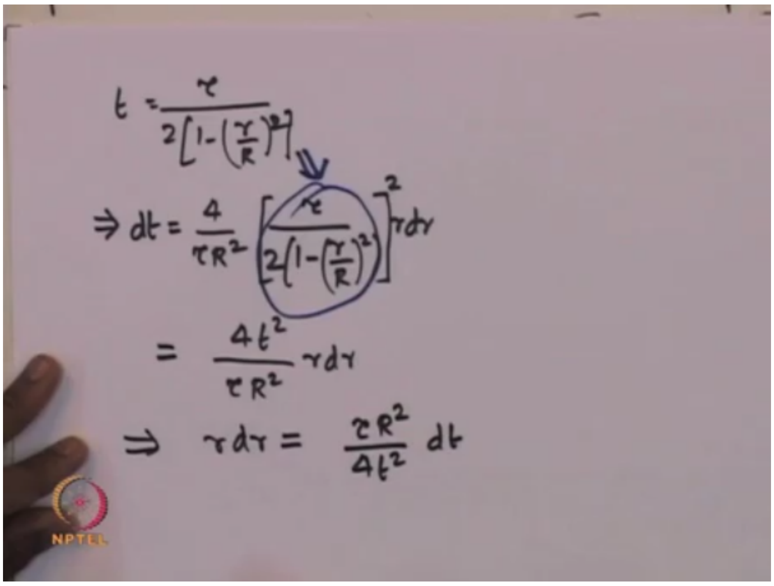

t = tau divided by 2 into 1 – r by capital R the whole square where capital R is the diameter of the tube. Now, from here, by differentiating this expression we can find out that d t = 4 by tau r square multiplied by tau divided by 2 into 1 – r by R square. So, one needs to perform a little bit of algebra to get this expression. So, into r d r. So, that is the expression for d t as a function of, so when we take the first differential of this expression, this is the expression that would get as a function of d t = r and d r.

So, we can further simplify this by substituting the expression for the time that the fluid which is present in a particular r location takes to travel from the 0, from the inlet to the exit stream of the reactor. So, that is given by 4 t square divided by tau R square into r d r. So, this is obtained simply by substituting this expression which is present inside this brackets with the corresponding time.

So, that is nothing but the time taken by the fluid at r location to travel from the inlet to the exit of the reactor. So, from here we can find out that r d r is actually given by tau R square by 4 t square into d t. So, now we can plug this in into the expression for the fraction of the fluid whose volumetric flow rate is between v and v + v nought and v and v + d v. And that the fraction that spends the time, residence time of that fraction is between t and t + d t.

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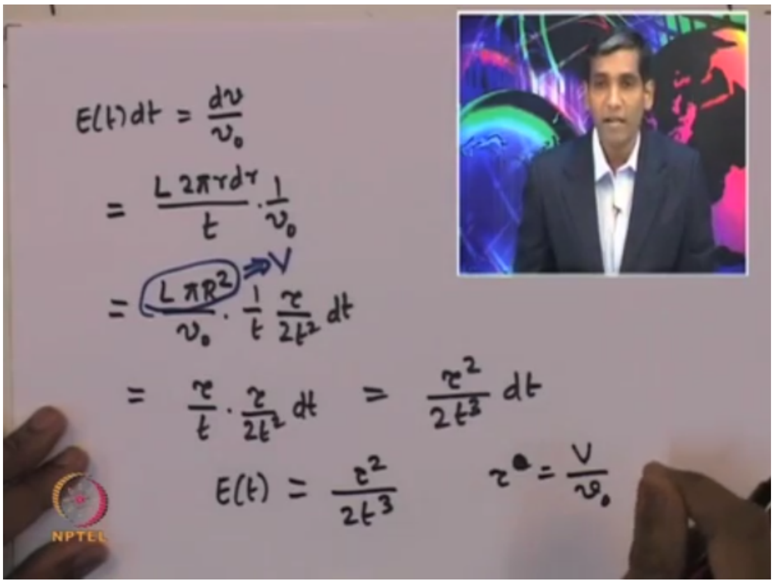

So, that is given by E of t d t. And that is = d v by v nought. And that is given by L, d v is nothing but length of the reactor into the area of that small element. That is 2 pi r d r divided by the time that is actually taken by the fluid in that particular element to travel from the inlet to the outlet of that particular reactor, of that particular shell. And that ratio will give what is this differential volumetric flow rate multiplied by 1 by v nought.

So, that is the expression for d v by v nought. So, now from here we can now substitute r d r using the time that it actually, differential time that the fluid actually takes to travel from 1 end to the other end of the reactor. So, that can actually be related. And so, would get that L into pi R square divided by v nought into 1 by t into tau by 2 t square into d t. So, all that has been done is, we have substituted r d r with the corresponding expression we just derived in a short while ago.

Now, L into pi R square is nothing but the volume of the reactor itself. So, L into pi R square is the, that is the volume of the reactor. And so, therefore v by v nought is nothing but the space time of the reactor. So, that is given by, so that is = tau by t into tau by 2 t square into d t. So, that is nothing but tau square by 2 t cube into d t. So, E t d t which is the residence time of the fluid in the fractional time that is actually spent, fraction of the fluid that spends, that time t whose residence time is between t and t + d t is actually given by E t d t.

And for a laminar flow reactor, that is = tau square which is the square of the space time divided by 2 into t cube where t is the time that is spent by a particular fluid element at a particular location from the entry to the exit of the reactor. So, therefore by simply comparing, simply by observation we can deduct, deduce that E of t should be = tau square by t t cube. Where tau square is, where tau is given by volume of the reactor divided by volumetric flow rate if we assume that the flow rate is actually constant.

So, now the question is, when is this particular expression valid, what is the validity of this expression? Or, the question is, when will the fluid start leaving. Suppose I put a tracer at the entry of reactor, how much time will it take for this tracer to first appear at the exit stream of the reactor. That is, if I put tracer, let us say pulse tracer at X = or at the entry of the reactor, how much time will that pulse take to travel through the reactor and what will be the first time at which the fluid will actually leave the reactor at L.

And this is important because E of t is essentially the age distribution of the effluent stream. So therefore, the E of t d t is actually valid only from the time at which the fluid is actually, at which the tracer is actually seen at the exit stream of the or effluent stream of the reactor. So, how do we find this? So, we can find this by observing that for a laminar flow parabolic profile the fluid elements which is actually present at r = 0, it travels at a maximum speed.

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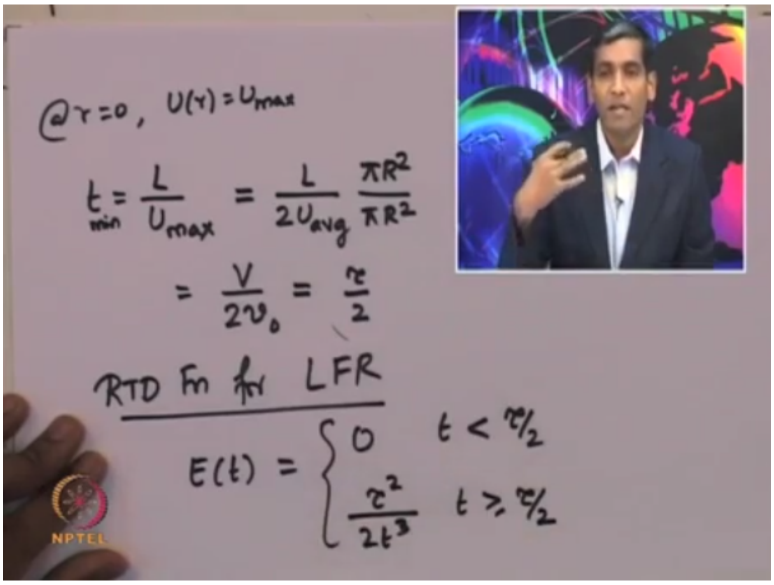

So, at r = 0 the fluid travels, the U of r = U max. So, that is the maximum velocity. So now, therefore, the residence time of the fluid elements which is actually sitting at r = 0 or entering the reactor at the centre of the reactor, would actually spend the least time to travel from the inlet to the exit of the reactor. So, therefore the minimum residence time should actually be = the residence time of the fluid stream which is actually entering at this location r = 0.

So, how do we find this? So, we know that the time that is actually taken to, for the fluid elements to travel from 1 end of a reactor to the other end of the reactor is simply given by L by U. And the minimum time is actually given by L by U max. That is the maximum velocity and that is at the centre of the reactor. So, from here, by simply plugging in the corresponding expression we can find that minimum time that is actually taken for the tracer to be seen at the exit of the reactor is given by L by 2 U average.

That is the cup mixing average into pi R square divided by pi R square. And that is nothing but v by 2 v nought. And that is = half of the space time. So, the fluid elements that is actually entering the reactor at the centre of the tube, would actually take half the space time before it actually reaches the other end of the reactor. And in fact, the residence time distribution actually starts from that particular time tau by 2, the minimum time.

So, therefore the RTD function for the laminar flow reactor is actually given by E of t. That is = 0 if time is < tau by 2. Which means that, there is no fluid stream which is actually leaving the reactor if the time at which it is monitor is < tau by 2. Whereas at, for any time > tau by 2 the residence time distribution is actually given by tau square by 2 t cube, for t greater than or = tau by 2.

So, this is a nice example of how to find the residence time distribution function for a reactor, for a real reactor. So, such kind of a method can actually be employed to find the residence time distribution of any reactor where the dispersion is not present. So now, what about F of t?

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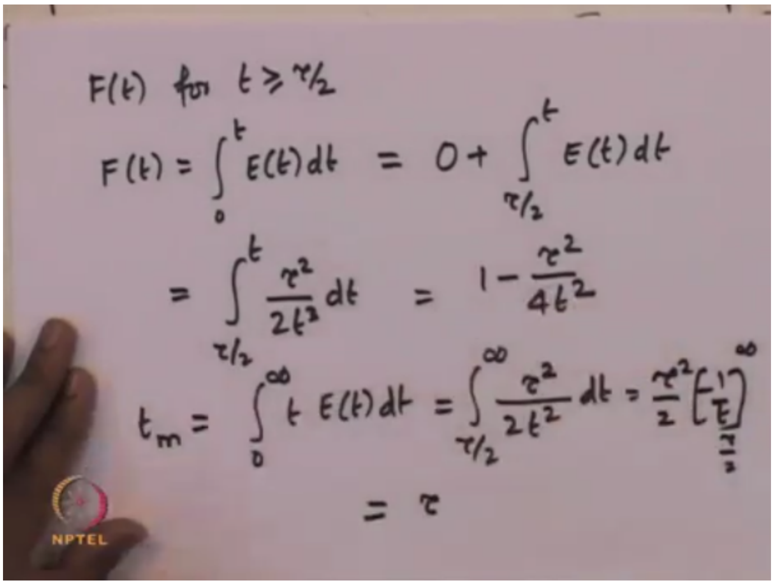

The F-curve for the laminar flow reactor. So, for t greater than or = tau by 2, that is the time for which E of t is actually valid. And F of t is given by integral 0 to t E of t d t. And that is = 0 + integral tau by 2 to t E of t d t. And now plugging in the expression for E of t, we can find that this is = integral tau by 2 to t tau square by 2 t cube d t. And on integration one would find that this will be = 1 – tau square by 4 t square.

So therefore, the mean residence time which is one of the properties of the residence time function is actually given by 0 to infinity t of E t d t. So, this is the F-curve. This is the relationship between F-curve, F and the time. And the mean residence time is actually given by integral 0 to infinity t E t d t. And that is because between 0 and tau by 2 E t is 0. So, this integral simply becomes tau by 2 to infinity. The limits will change.

And that, and the integral will be tau square by 2 t square into d t. Which is = tau square by 2 into – 1 by t. And the limits are tau by 2 and infinity. So, those are the, that is the limits. And substituting the limits, we will find that, that will be exactly = tau which is what we intuited before, that if there is no dispersion then the mean residence time would be = the space time itself irrespective of the RTD function. And in fact, we have shown this for 3 different types of reactors, the plug flow reactor, CSTR and that of the laminar flow reactor. Now let us now look at the normalised residence time distribution function.

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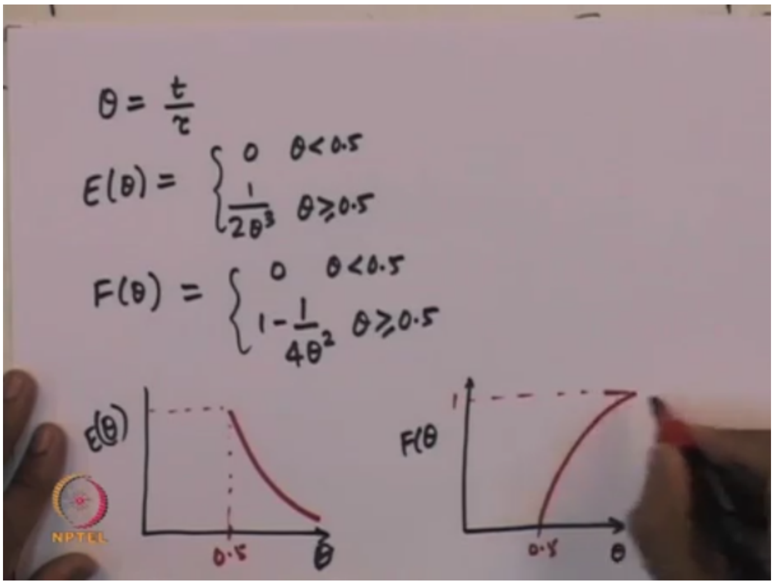

So, suppose if we define theta as t by tau. Tau is the space time or the mean residence time for this particular case. And so, E of theta would be 0 for theta < 0.5 and it will be 1 by 2 theta cube for theta greater than or = 0.5. And similarly, F theta will be 0 for theta < 0.5 and it will be 1 – 1 by 4 theta square for theta greater than or = 0.5. So now, if you look at the E-curve and the F-curve.

Suppose if I sketch the E-curve of the normalised residence time distribution function, then we can observe that the E-curve is going to start at 0.5, because before 0.5 it is not valid. So, at 0.5 it will start. And so, it will start, it will look something like this. And the F-curve can actually be, again F-curve will also start at 0.5. This is the F-curve and it will start at 0.5. And then, it will actually, it will slowly increase and go to 1. So, that is the F-curve.

So, now we have looked at the residence time distribution functions of 3 different reactors. So, let us now attempt to put them all together and compare how the residence time distribution functions are actually different for these 3 reactors.

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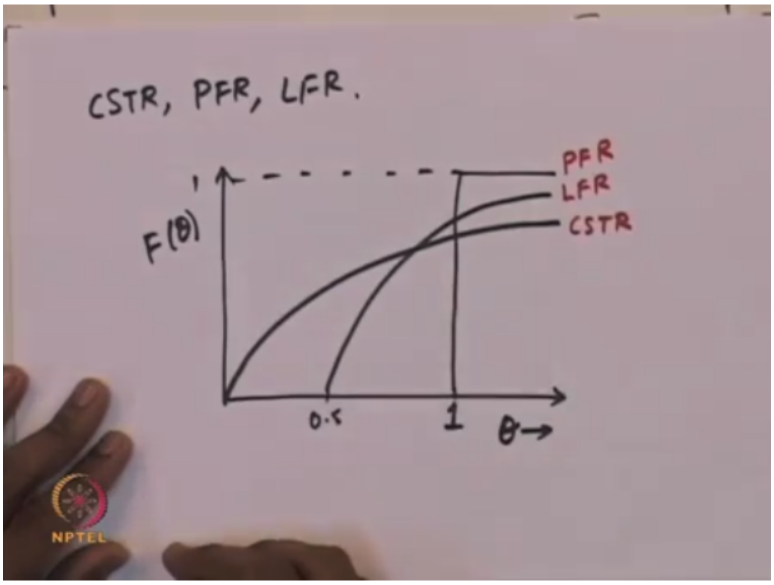

So, now let us compare the residence time distribution function, the F-curve for CSTR, plug flow reactor and the laminar flow reactor. So, if we plot the normalised F-curve, then, if for a plug flow reactor, the F-curve would start exactly at the space time of the reactor. So, therefore it is exactly at 1 because it is a delta function. And so, the F-curve will actually be, so that will be 1. Then, for a CSTR, that is the F-curve that one would get for a CSTR.

Now, if we plot for laminar flow reactor. So, it starts at 0.5 and it appears somewhere in-between the CSTR and the plug flow reactor. So, this is CSTR, this is the F-curve for CSTR. And this is F-curve for plug flow reactor. And this is the F-curve for laminar flow reactor. So, one can actually, experimentally, if one performs the, one estimates the F-curve and the E-curve experimentally from the methods that we described earlier.

That is, if we use a pulse or a step input and one finds out what is the F-curve for the reactor, then by simply making a comparison of this chart, one can actually estimate whether the real reactor is close to what type of these 3 reactors that we have actually looked at so far. That is CSTR, the laminar flow reactor and the plug flow reactor. So, such kind of a comparison provides a method for actually diagnosis of the nature of the RTD function for a given real-world reactor.

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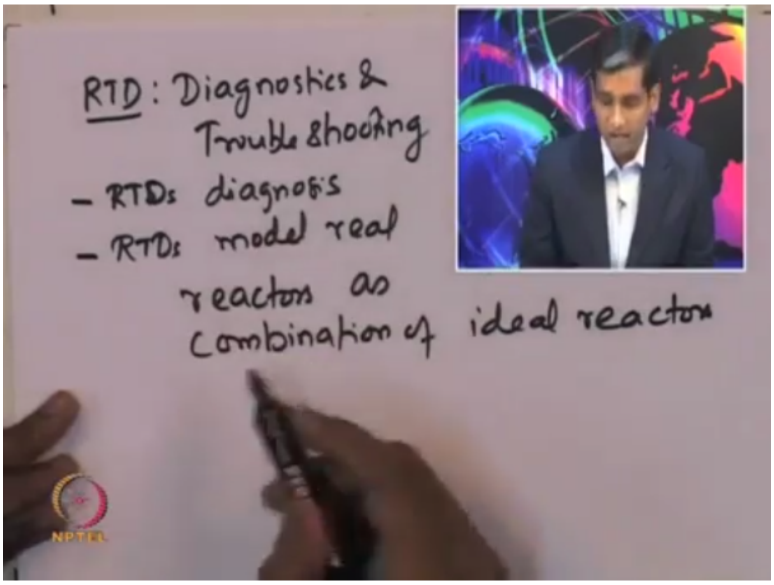

So, that brings us to the next topic where we want to see how to use RTD function for diagnosis, diagnostics and troubleshooting. So, RTD functions can actually be used for diagnosis of certain properties of the reactor or certain aspects of the reactor and also to troubleshoot if something undesirable is actually happening inside the reactor. So, how do we do this? So, the RTDs are actually used for diagnosis.

So, by comparing the RTDs that are actually theoretically estimated for some, for certain type of reactors and comparing that with the RTD of the real-world reactor which may be estimated using experimental methods. By comparing that, one can actually find out what is the class of the real-world reactor based on the RTD function. So, RTD function can actually be used for diagnosis.

And not just that, it can also be used, RTD functions can also be used in order to model the real reactor as a combination of ideal reactors. So, RTDs play a huge role in actually modelling, model real reactors as combination of ideal reactors. So, the RTDs, the residence time distribution function, they play a crucial role in this process as well, in order to model the real reactors as a combination of ideal reactors. So, before we get into the how to do the diagnostics, let us look at what are all the common residence time distribution functions.

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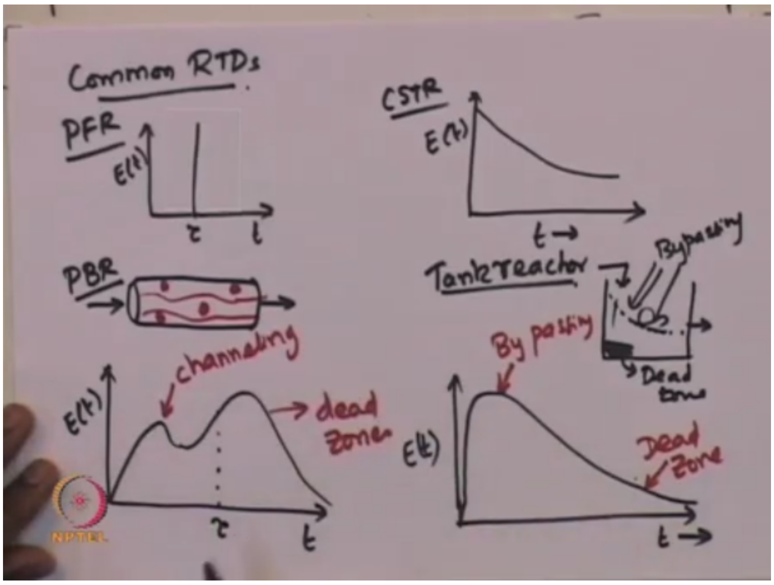

So, the commonly common RTDs. So, for a plug flow reactor, the residence time distribution is essentially a del function. So, that is the residence time distribution. And it is centred at the space time of the reactor. And that is the E-curve, E of t. And if I look at CSTR, so, the residence time distribution is actually exponential. And that is E of t and t. That is the, that is the E-curve for CSTR.

Now, if I take a packed bed reactor, now what has been observed. So, suppose if there is a reactor and there is a fluid which is actually flowing through this reactor. One of the commonly observed RTD curve for such kind of a real-world packed bed reactor is actually, it looks as below. So, 2 peaks have been observed. This is one of the commonly observed type of RTD function where 2 peaks are observed.

And typically, the first peak, if the, if there are 2 peaks and the first peak which actually appears before the space time of the reactor indicates that there may be channeling in the reactor, channeling or bypassing inside the reactor. So, that is the first peak which appears before the space time of the reactor. And the second one, the second peak which actually appears after the space time of the reactor, that is, that indicates that there may be dead zones which may be present inside the reactor which does not serve any useful purpose inside the reactor.

So now, if we attempt to depict this in the packed bed reactor. So, there may be channels which may be present inside reactor through which the fluid which is actually going through the packed bed reactor will easily escape and leave the reactor. And because there is a channel with which the fluid easily escapes, the time that they spend inside the reactor should actually be, is actually smaller than the space time of the reactor.

And that is the reason why the first peak corresponds to the channelling of the fluid stream inside reactor. On the other hand, if there are dead zones which are actually present inside, where the reactor is virtually inaccessible. Then, there will be some of these fluids which are actually present. They will spend a too longer time inside the dead zones before they leave the reactor and that is why it appears as a second peak, particularly the tail part of the distribution curve.

So, another commonly observed RTD function is that of a tank reactor, a stir tank reactor. So, suppose if we have a tank and it is well stirred. And let us say this is the inlet to the tank and this is the outlet to the tank. And then, maybe there is bypassing through this particular tank. And maybe there are some dead zones which are present here. So, this is the dead zone and this is the bypassing.

So, if such kind of a situation is there in a tank reactor that can actually be observed in the RTD curve. So, in the RTD distribution function; so, the typical, so the first peak which appears very close to the, to time $t = 0$ is because of this channelling or because of this bypassing. And this bypassing can occur because of the placement of the entry and the exit stream, exit fluid stream of the tank reactor, that these fluid streams simply quickly escapes and leaves the reactor.

And that can actually be captured, that is actually captured by this short peak which is actually present at time close to 0. That is at the initial stages. And then, the long tails which is actually; so, this corresponds to the channel bypassing. And then the long tail which is actually present here is because of the dead zone. So, the long tail indicates the presence of a dead zone inside the tank reactor.

And this long tail is because this dead zone is actually not available for the fluids to actually go and they are not exchanging material with the location inside the tank which is well mixed. And therefore, the whatever residual fluid which is present here, they will take a very long time before they actually appear at the effluent stream of the reactor. Therefore, these dead, long tail virtually corresponds to the dead zones that may be present inside the reactor.

So, this kind of an approach, this the detection of the residence time distribution curve can actually provide a lot of information about what is actually happening inside the reactor. And this common RTD that has been explained just now, is a good example of that.