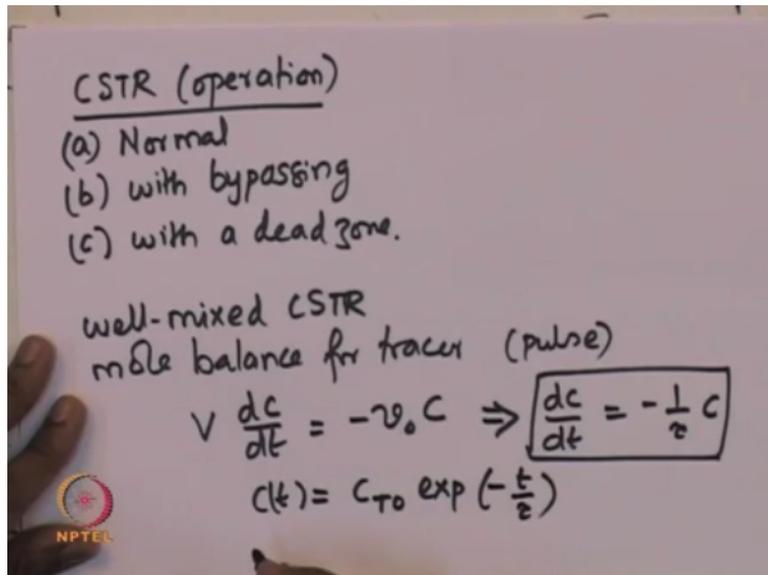


Chemical Reaction Engineering - II
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Module - 12
Lecture - 56
Reactor Diagnostics and Troubleshooting II

So, let us now look at the operation of a CSTR.

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So, let us consider a CSTR and let us look at what are all the various types of operations of CSTR, how it can be operated and what are the distribution curves for each of these situations. Now, this is very important to understand because, if there is a problem with the CSTR and if it falls in one of these operation modes, it helps in diagnosing what is the problem with the actual reactor, what is the problem with the functioning of the actual reactor.

And then the methods to correct it can actually be implemented or actually can be deciphered later. Or can actually be thought of and strategies can actually be improvised later. So, there are 3 modes of operation. Suppose if it is a, there is a real reactor whose volume is known. And let us say a volumetric flow rate with which the fluid is flowing through the reactor is known. Then, one could actually look at what is called the normal operation.

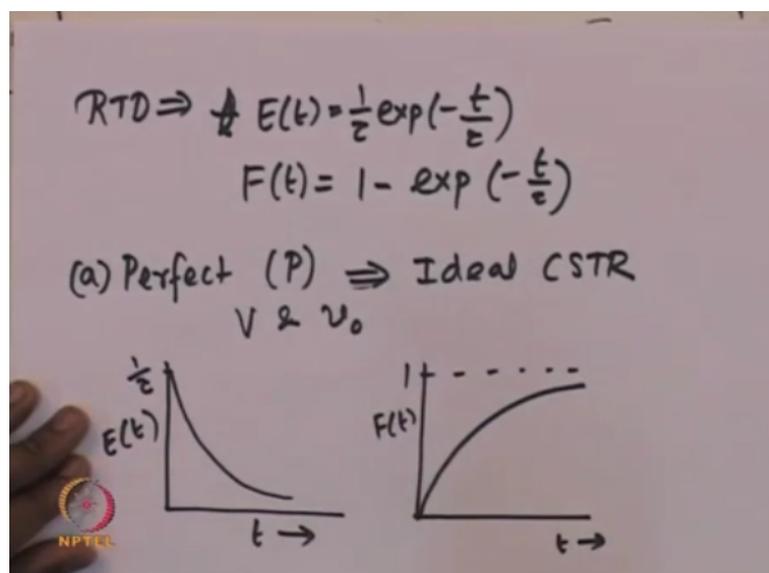
Where it behaves like an ideal CSTR, where the all locations in the reactor is actually available for the reaction. Which means there are no dead zones where the reactor is, where the reaction does not happen. And also the, it is assumed that there is perfect mixing in the reactor and there is no bypass of fluid. Which means that all fluid that comes in actually undergoes reaction, spends the sufficient amount of time inside the reactor and then they leave the reactor.

So, the second mode of operation is CSTR with bypassing. So, if you understand how the residence time curve of a CSTR with bypassing is going to occur, how it is going to appear, the shape of the curve can actually provide a clue as to, if you understand what it is then that can actually be used as a diagnostic tool to find out if there is bypassing in the reactor. And then the third operation is the, with the dead zone.

So now, for a well-mixed CSTR, suppose if I put a tracer. Suppose if I actually insert a tracer into the CSTR, then one can write a mole balance for the tracer. And the mole balance will be; suppose there is a tracer, the mole balance for the tracer will be $V \frac{dc}{dt}$. That is = $-Vc$. Suppose if it is a pulse tracer, $-v_0 C_0$. And that should be = $\frac{dC}{dt} - \frac{1}{\tau} C$. So, that is the mole balance for the tracer.

And by integrating this expression one would find that C of t is = the initial total concentration of the tracer $C_0 \exp(-t/\tau)$. And we know that the RTD function for this reactor is actually given by;

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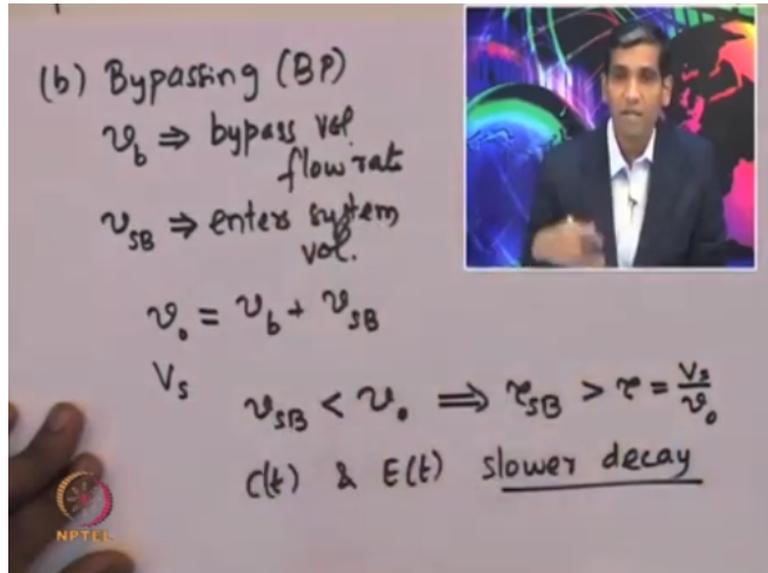
The RTD function is given by $1 - e^{-t/\tau}$. That is the RTD function. And then the F-t curve, which is the F-curve is actually given by $1 - \text{exponential of } -t \text{ by } \tau$. So, this we have already seen. Now, suppose if you want to compare these 3 cases, that is the 3 modes of operation, then we can now slowly try, we can now attempt to find the RTD curve for these 3 operations. So, suppose let us start with the perfect, so, let us start with the first case of perfect CSTR.

So, we tag, we use the symbol P for the perfect CSTR or operation of the CSTR under perfect mode. That is, there is no bypass and there is no dead zone. Which means that the CSTR is actually an ideal CSTR. And the volume and the volumetric flow rate are basically the measurable quantities of a real reactor. Let us say we know the volume and the volumetric flow rate with which the fluid is actually flowing inside the CSTR.

So, we know the residence time distribution curve and E of t versus t. And so, this starts at $1/\tau$. And then, it actually decreases with time. And then, we know the corresponding F-curve. That is an exponential increasing function. And then, it goes all the way up to 1. So, this is the F-curve and the E-curve for a CSTR. So, now if the residence of the space time of the reactor τ , if that is very large, then the decay of this exponential curve and the corresponding concentration curve is actually going to be extremely slow.

Which means that the, if the space time is large, then the tracer actually spends a lot more time inside the reactor. And therefore, the decay of this E-curve as a function of time is going to be very slow. On the other hand, if the if the space time is very small then the amount of time that the tracer spends inside the reactor is going to be very small. And therefore, the E of t and the time curve is going to have a sharp slope at a small times. And which means that it is going to decay faster. So now, let us look at the second case of bypassing, CSTR operation under bypassing conditions.

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So, suppose we look at the, suppose we consider a CSTR where bypassing is known that bypassing is present. We refer to that as BP. If v_b is the volumetric flow rate of the fluid which is actually bypassing the reactor. So, that is the bypass volumetric flow rate. So, v_b is the bypass volumetric flow rate. And let us assume that v_{SB} is the volumetric flow rate which is actually going through the system volume.

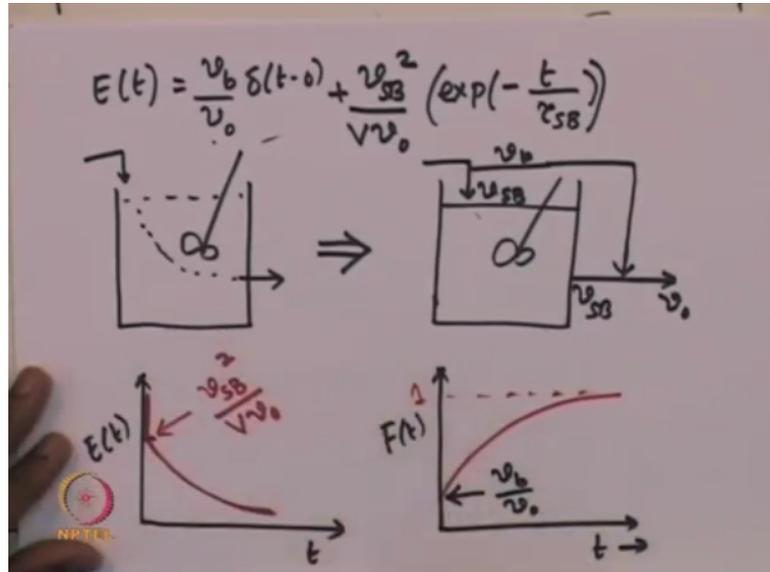
So, that is the, that enters the system volume. So therefore, v_0 which is the volumetric flow rate with which the fluid is actually entering the reactor should be $= v_b + v_{SB}$. Now, if you assume that V is the is the volume of the tank, then we know that v_{SB} is actually $< v_0$ because it is only a fraction of the total volumetric flow rate with which the fluid is actually being pumped that goes into the reactor.

So, therefore clearly, τ_{SB} should actually be $>$ the space time of the reactor. Which means that the amount of time that this fraction of the fluid which is not being bypassed, the amount of time that it spends inside the reactor is actually larger than the actual space time of the reactor itself, based on the overall volumetric flow rate. So, remember that τ is actually defined as V by v_0 , where V is the volume of the reactor and v_0 is the volumetric flow rate with which the fluid is actually flowing through the reactor.

So therefore, because this τ_{SB} is $>$ τ , the $C(t)$, the concentration curve and the $E(t)$ curve, they are going to decay very slowly. So, as we observed a few moments ago, as we actually discussed a few moments ago. Because the residence time of the fluid stream which is actually going through the system volume is actually larger than the space time. The decay

of the concentration and the E-curve is going to be slower when compared with the case of a perfect operation, that is there is no bypassing. So, in a similar fashion, now we can actually look at what is the possible residence time distribution under this condition.

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So, what is the possible, so, the various possible residence time distributions have been considered. And one of the possible distribution is that, it will be v_b divided by v_0 into $\delta(t-0)$. That means, this is the component or a fraction which is actually bypassing the reactor and leaving the fluid stream very soon after it actually enters the reactor. That + v_{SB}^2 divided by V into v_0 . That multiplied by exponential of $-t$ by τ_{SP} .

So, that is a possible residence time distribution function that actually describes the residence time distribution of a CSTR which is actually operator along with a bypassing of some part of the fluid stream that enters the reactor. So now, the system can actually be depicted in the following way. So, suppose if this is the CSTR and this is the inlet stream. And if there is a bypassing of the fluid stream in the CSTR, then this can actually be depicted as a, in the following cartoon.

So, suppose if here is a tank and if let us say that the inlet fluid stream is actually split into 2 parts where there is a bypassing component v_b which actually goes and directly joins the exit stream and only a fraction of the fluid stream, fraction of the inlet fluid stream actually which is v_{SB} , the volumetric flow rate v_{SB} actually enters the CSTR and participates in the same volume which is available otherwise and leaves the reactor.

So, this is the S_B and it leaves the reactor. In otherwise same volume the amount of, the volumetric flow rate of the tracer that actually enters the reactor is $v S_B$. And then, $v S_B$ is what is actually leaves. If we assume that bypass is essentially taking some of the volumetric flow rate and directly joining it with the effluence stream. So, this kind of a distribution curve essentially captures this representation.

So, now if I attempt to sketch the E-curve. So, right at $t = 0$, there is going to be a fall in the E-curve. And this is because, some fraction actually gets bypassed and directly goes and joins the effluent stream. And therefore, there is going to be a sharp fall in the E-curve. That is the fraction that is actually leaving. And then, after which there is going to be an exponential fall in the E-curve.

So, this first part corresponds to the bypass and the second part corresponds to this exponential term. And this location here is essentially given by $v S_B^2$ divided by V into v nought. So, that is this location from where the exponential fall in the E-curve actually starts. Now, the corresponding F-curve will be, if this is the corresponding F-curve, then we will see that the F-curve actually has a jump, right at $t = 0$.

So, this is 1. This is the F-curve. So, there is a jump right at the, at $t = 0$ and the jump actually occurs up to $v b$ divided by v nought which corresponds to the bypass, the fraction of the inlet volumetric flow rates, the fraction of the inlet stream which actually gets bypassed and leaves effluent stream immediately. And that is reflected in the F-curve and also in the E-curve. So, the important message from here is that, an E-curve and F-curve is actually detect, is actually measured experimentally, can indicate whether there is a bypass in such kind of a system.

So, the third mode of operation is the, is what happens if there is dead volume which is present inside the tank reactor, in the inside the CSTR.

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(c) Dead volume (DV)

- ~~Ideal~~ CSTR
- No bypassing
- Dead vol. (V_D)

$$V = V_D + V_{SD}$$

The image shows a hand-drawn diagram of a CSTR with a dead volume. The tank is represented as a rectangular vessel with a stirrer. A shaded region at the bottom represents the dead volume. To the right, there are two graphs. The first graph plots $\frac{1}{\tau_{SD}}$ on the y-axis against $E(t)$ on the x-axis, showing an exponential decay curve. The second graph plots $F(t)$ on the y-axis against t on the x-axis, showing a curve that rises and levels off at 1. The text above the graphs states $V = V_D + V_{SD}$ and $\tau_{SD} < \tau$.

If there is a dead volume inside. So, let us assume that it is a CSTR. There is no bypassing, let us assume that there is no bypassing inside the reactor. And then, there is some dead volume. Let us say that the volume of this dead zone is essentially V_D . And this dead volume essentially is one where, is the volume where the fluid stream does not reach that location. And so, it is the presence of this location is of no use for the performance of the reactor.

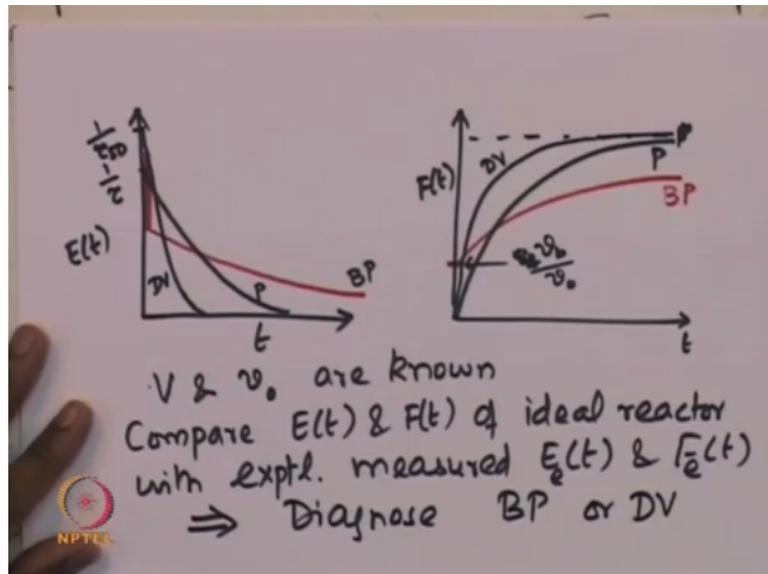
So, the overall volume is actually $= V_D + V_{SD}$ where $S D$ is the available volume for the, available volume which is actually accessible by the fluid stream which is flowing into the reactor. So now, this can actually be depicted as. So, there may be some zone below which is actually a dead zone where the fluid stream actually does not access this location. And then the, there may be an exit stream through which, effluent stream through which the fluid that enters actually leaves the reactor.

So, the E-curve for this particular situation would actually look like; it starts at 1 by τ_{SD} . So, remember that the accessible volume is V_{SD} which is smaller than the actual volume of the reactor. And for the same flow rate, if it was conducted and under perfect conditions where there is no dead volume. Then the τ_{SD} which is the space time of the reactor for the fluid stream which is actually accessing the non-dead volume space in the reactor.

So, that will actually be smaller than that of the actual space time of the reactor V by v nought. And as a result, the exponential curve, the C-curve and the E-curve is going to decay faster than, if it were to be conducted under normal perfect operation. And the corresponding F-curve would be. So, the F-curve also will be correspondingly steeper. And, it will actually

slowly increase and go to 1. So, now if you put all these 3 together, let us make a comparison of the RTD functions for these 3 modes of operation.

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So, suppose let us draw the E-curve. Now, for a perfect operation, the E-curve starts at $1/\tau$ which is the, τ is the space time of the reactor. And then, there is an exponential decay as a function of time. This is the E-curve. Now, if there was bypassing in the reactor, then the curve starts right at $t = 0$. Then, there will be a sharp fall in the E-curve. And then, followed by an exponential decay with respect to time.

Now, supposing if there was dead volume inside the reactor. Supposing if this is, this corresponds to the perfect operation. This corresponds to bypassing. Now, if there were to be dead volume inside the reactor, we just observed, we just noted a few moments ago, that the decay of the E-curve is going to be significantly faster. And therefore, the curve starts above $1/\tau$ because $\tau < \tau + S D$; so this starts at $1/(\tau + S D)$.

And we said that $\tau + S D$ is actually smaller than that of τ . And therefore, $1/(\tau + S D)$ is going to be larger than $1/\tau$. And then, it starts from here and decay is actually faster than the, than that of the perfect operation because $\tau + S D$ is actually smaller than the space time of the reactor. So now, if there is a real data for a tank reactor, then one can actually look at, one can compare the actual RTD function measured experimentally with the RTD functions present in this graph.

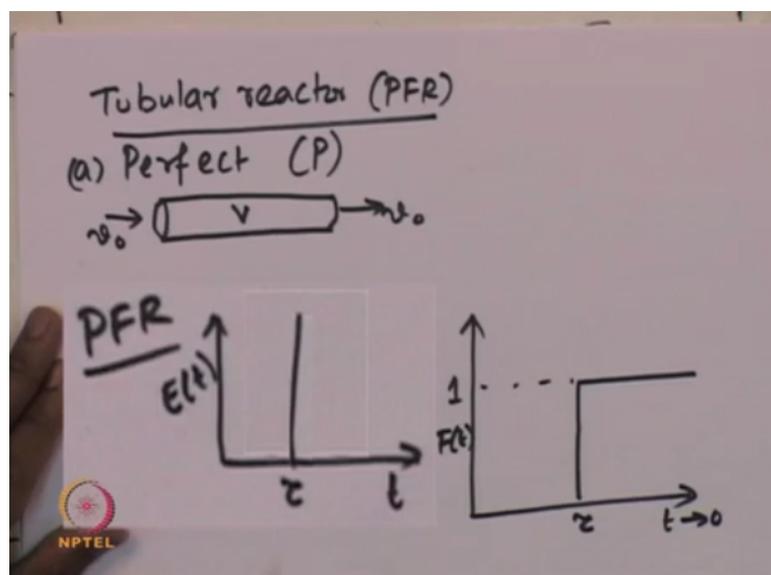
And that can actually provide a clue as to compare that with the perfect operation. That can provide a clue whether there is a bypass or if there is a dead volume present inside the reactor. Now similarly, we can actually plot the F-curve. So, for a perfect operation, that is the kind of behaviour. That is the perfect operation. And then, for a bypassing, it is, there is a jump right at $t = 0$. That is the kind of behaviour for bypassing.

And the bypassing, the curve starts exactly at V_B by v nought. And then the, for dead volume case, the curve actually increases rapidly. And then, it reaches 1. And so, this is for the dead volume case and this is for the perfect operation case. So, either E-curve or the F-curve can actually be used to detect what is the diagnose if there is any problem in the operation of that particular CSTR.

So therefore, the recipe is that if the volume of the reactor and the volumetric flow rates are known. So, volumetric flow rate can actually be measured and V is the volume of the tank. So, one can actually compare $E(t)$ and $F(t)$ F-curve of ideal reactor, so, ideal CSTR. That is the perfect operation. And you can compare that with experimentally measured E and F -curve. So, I put a subscript e for experimentally measured.

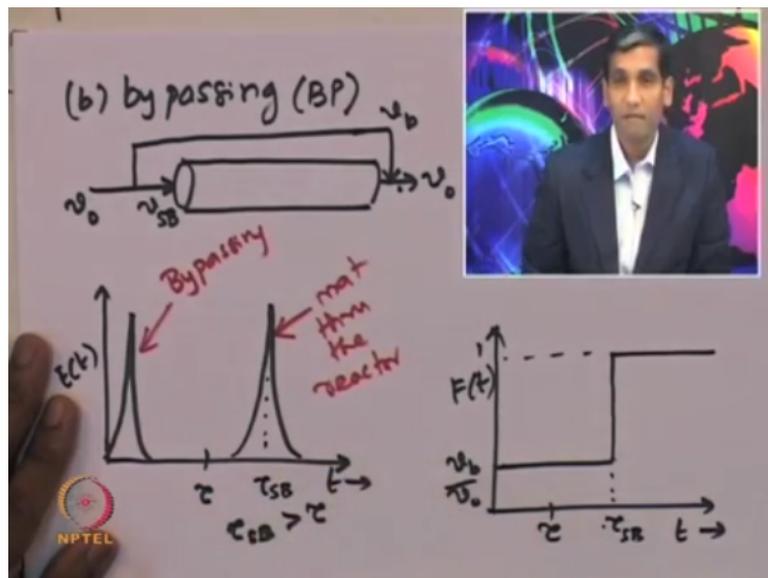
So, one can actually compare the experimentally measured RTD functions with the RTD functions of the ideal reactor. And that can be used to diagnose the presence of the bypassing or the presence of dead volume inside the CSTR. So, next let us look at the same, let us look at these 3 operations for a tubular reactor.

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So, let us assume that it is a plug flow reactor. So, the first case is perfect operation. So, let us tag that with a P. So, here is a tube. And there is a fluid which is actually flowing at a volumetric flow rate of V nought and the volume of the plug flow reactor V . So, now the RTD curve, we know that it is a delta function centred at the space time of the reactor. So, that is E of t . And then, the F -curve is essentially given by, it starts at τ and reaches 1. It is a step function in the F versus t plain. So, that we already know. Now, what happens in the bypassing case. So, suppose if there is a bypass in the reactor;

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Suppose if there is bypassing in the reactor. So, if I tag that with B P, then, that can actually be depicted as, suppose if v nought is the volumetric flow rate with which the fluid is supposed to enter the reactor. And if this is the reactor. And that is the final effluent stream volumetric flow rate. Then, a fraction of the fluid is actually bypassed. And so, we can represent that using, by actually taking some part of the feed and directly connecting into the effluent stream.

So, that is a depiction of the bypassing in the reactor and v S B is the volumetric flow rate with which the fluid is actually flowing through the reactor. Now, the residence time distribution for this kind of a system can actually be written as, actually, will actually have 2 peaks. So, the first peak will actually appear very close to time $t = 0$. And this is because of the bypassing of the fluid. And then, there will be another peak which will appear much later.

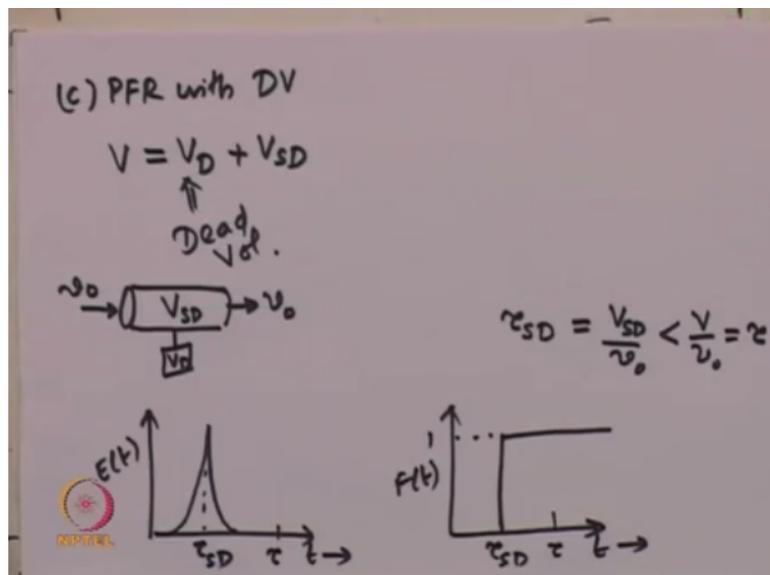
And that is because of the fluid that is actually flowing through the plug flow reactor. And the residence time, the space time of the reactor will actually appear somewhere in between. So,

this is the E-curve. And so, the first peak is due to bypassing. The first curve is actually due to bypassing and the second curve is actually due to the material through the reactor. That is because of the material that is actually flowing through the reactor.

Now, why is there a delay in these 2 peaks or why is there delay in the residence time for the material that is flowing through the reactor? The delay is because the τ_{SB} which is the space time based on the fluid that is actually flowing through the reactor, is actually larger than the space time of the reactor based on the overall volumetric flow rate that is actually expected to that is actually flowing to the reactor.

Now, one can actually sketch an F-curve for the same, F of t. So, that starts at V B by v nought. That goes to 1. And this is the, this is τ and this is τ_{SB} . So, remember that this second peak is actually centred at the space time based on the volumetric flow rate of the fluid that is actually flowing through the, that is the actual volumetric flow rate which is accessible to all parts of the reactor. So now, let us look at the third case of a plug flow reactor with a dead volume.

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We tag it with D V. And suppose if the volume of the fluid, volume of the reactor which is actually not accessible to the fluid is given by V D. Then, the total volume is V D + S D. So, this is the dead volume. So, that is the dead volume. And typically, this happens because there will be recirculation of the fluid at the entry locations in the reactor and that causes the inaccessibility of this in those regions for the fluid stream.

And that can virtually be called as the dead volume inside reactor. So, that can actually be depicted as; so, this is the volume of the reactor $V - V_D$. That is the dead volume which is removed from the reactor. And that is the volumetric flow rate with which the fluid is actually entering and leaving the stream. So, now in this case the τ_{SD} which is the space time based on the volume of the reactor which is actually accessible for the fluid stream.

That is given by τ_{SD} by $V - V_D$. And that will be $< V$ by v because $V - V_D$ is smaller than the volume, smaller than the total volume of the reactor, which is, and V by v is nothing but the space time. So, in this case, the tracer will actually leave, they will actually leave the reactor early, because some of the, part of, some part of the reactor is actually inaccessible.

And so, the space time is actually, space, the actual space time, the space time based on the volume which is available in the reactor is actually smaller than the actual space time of the reactor. And so, the E-curve would actually look like; there will be δ function. And that will actually be centred at τ_{SD} . And the space time will be much later. That will be the E-curve.

And similarly, the F-curve will be. So, that is the E-curve and the F-curve for a plug flow reactor with a dead volume. So, what we have seen in this lecture is looking at the different RTD functions for different operations of a CSTR and the, and different operations of a plug flow reactor. And we will continue from here in the next lecture. Thank you.