Chemical Reaction and Engineering
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Lecture no. # 39
Non ideal flow and reactor Performance

Friends, let us continue our discussion on non-ideal flow in the reactor. And in the last session, we stopped at a point where we were trying to figure out how to determine residence time distributions from experimental experimental measurements. So, let us recap little bit of what we saw in the last class, and we were looking at for an arbitrary input that we put in the reactor. What output can be expected and how do we extract knowing this output the residence time distribution?

So, the input is what we call a tracer which has to be a material which does not undergo any transformation in the reactor; either physical by way of getting adsorbed on to the surface of the reactor or it is internals or the chemical transformation, because of prevailing condition in the reactor. So, a tracer is expected to enter the reactor and depending upon the flow conditions in the reactor is expected to leave the reactor. And it is this exit point at which we are examining this tracer concentration, and thereby determining the residence time distribution.

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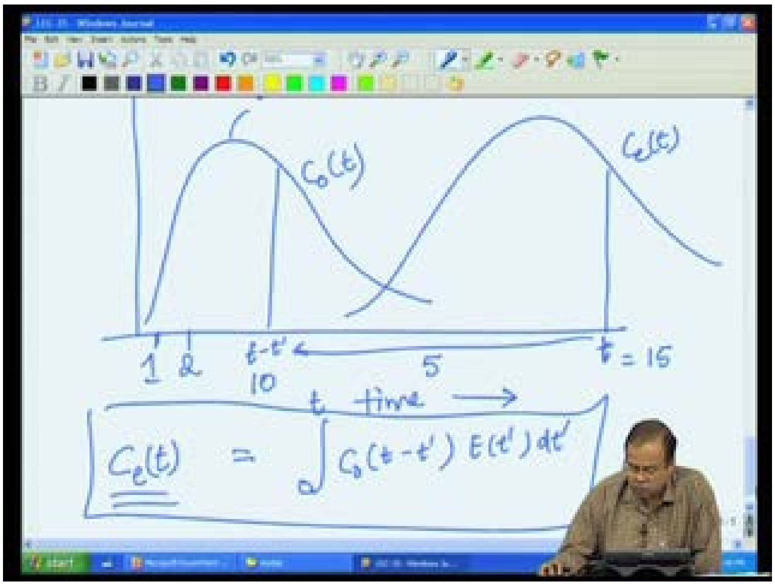

$$\underline{\underline{C_e(t)}} = \int_0^t C_0(t-t')\, E(t')\, dt'$$

So, let us go back and say that C naught of t is my is my input which I can be any arbitrary arbitrary form as shown over here. C naught of t and I measure the output which is some C e or the exit concentration of this tracer at time t. And we also talked about a specific example saying that suppose we say that time is my 15 minutes or seconds whatever is the unit. At this time, what do I expect to see in my react to begin with, let us say I expect to see what I had put in at time t equal at 10 minutes, and that fluid element which has a residence time of about 5 minutes. So, what I have put in at 10 minutes and then after spending 5 minutes, it comes out is what I expect at t equal to 15.

But that is not the only thing I can expect. I can expect what I have put in at 1 minute and which has a residence time of 14 minutes before it comes out or what I have put in 2 minutes and at the residence time of 15 minutes or 13 minutes. Or in other words, I can expect what comes out is a result of what I have put in at time t minus t prime and which has spent time t prime in the reactor. And since I am looking at all such possibilities, I will write this as an integral; that is what comes out of my reactor. C e of t is adding up all those contributions from material which is put in at t minus t prime and having spent time t prime in the reactor and this is what, we call convolution convolution integral. Why is it called convolution integral?

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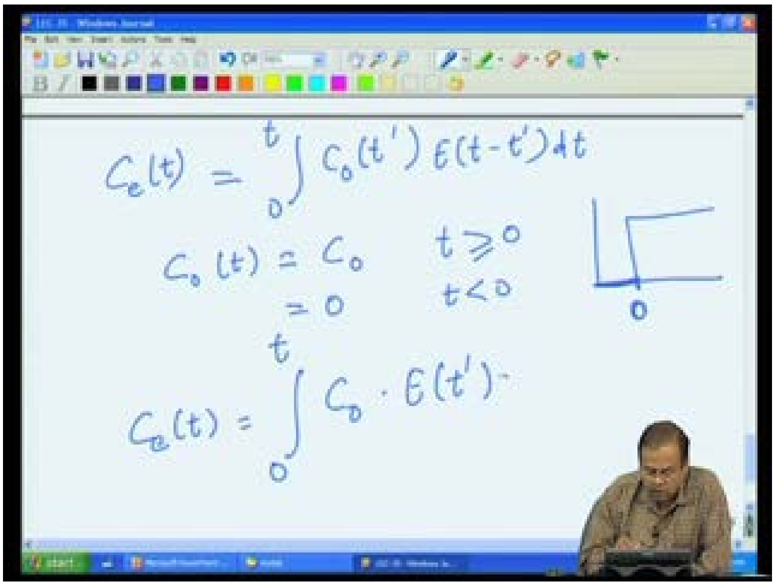

$$C_e(t) = \int_0^t C_0(t') E(t-t') dt$$

$$C_0(t) = C_0 \quad t \geq 0$$

$$= 0 \quad t < 0$$

$$C_e(t) = \int_0^t C_0 \cdot E(t')\cdot$$

Because I can as well write this in a other way manner; that is all contributions of what I have put in at t prime and which has a residence time of t minus t prime is what comes out of the reactor. So, this t minus t prime and t prime can be interchanged. Simply, put when I say that what I expect at 15 minutes is what I have put in for 10 minutes and which has a residence time of 5 minute. Or what I have put in at 5 minutes and which has a residence time of 10 minutes. So, t minus t prime can be can be 10 t prime of 5 or t prime of 5 and t minus t prime of 10.

So, it is it is interchangeable and hence, we call such integral as a convolution convolution integral. So, having known what I expect at C e of t? Now, let us take a specific experiment for let us say that we put in a step input. What is a step input? A step input is C naught of t is some constant value; C naught for t greater than or equal to 0 and it has a value 0 for t less than 0. Or in other words, if this is my 0 time C naught of t is 0 for t less than 0 and a constant value at t equal to t equal to 0. So, now if I if I put that value in my convolution integral, what will I get? I will get C e of t is integral 0 to t C naught in to E of t prime dt prime right. I am using the first part of this.

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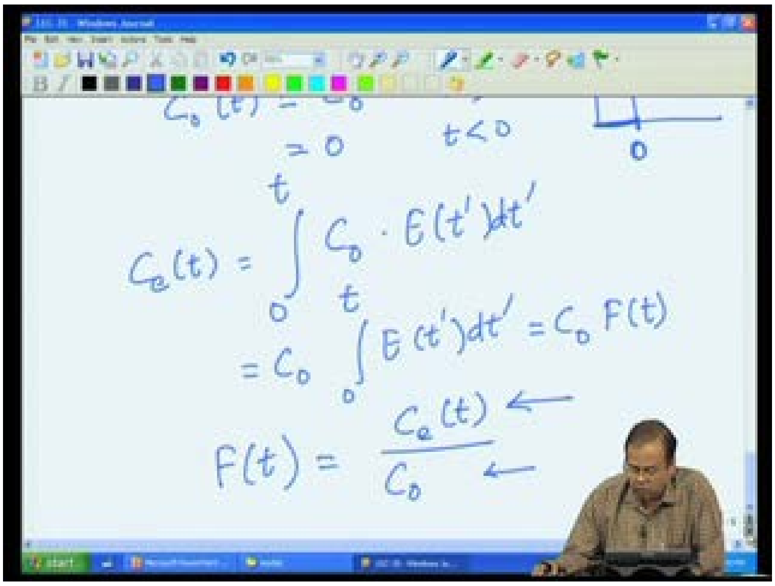

$$= 0 \qquad t < 0$$

$$C_e(t) = \int_0^t C_0 \cdot E(t')dt'$$

$$= C_0 \int_0^t E(t')dt' = C_0 F(t)$$

$$F(t) = \frac{C_e(t)}{C_0}$$

C naught of t minus t prime is a constant; C naught for t greater than 0, which is nothing but C naught integral 0 to t E of t prime dt prime. So, what does it integral 0 to t E of t prime dt prime? This is nothing but F of t or in other words I will get my cumulative age distribution F of t as C e of t divided by C naught. So, I do a simple experiment. I put in the step; I make a step change in the tracer concentration and keep it at that level and measure the exit concentrations. So, I know C naught and can measure C e of t. So, I am measuring my external exit concentration at all times and the ratio of the two is nothing but my cumulative age distribution.

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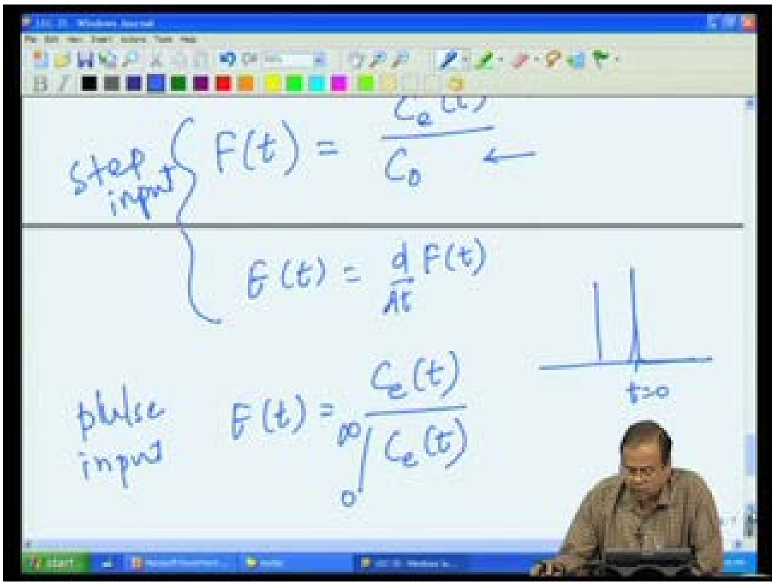

step input

$$F(t) = \frac{C_e(t)}{C_0}$$

$$E(t) = \frac{d}{dt}F(t)$$

pulse input

$$E(t) = \frac{C_e(t)}{\int_0^\infty C_e(t)}$$

Now, how do we get how do we get E of t? That is exit age distribution from this. I know my F of t is nothing but integral 0 to t E of t prime dt prime. Or in other words, e of t is nothing but d dt of F of F of t. I can do a similar exercise with at t equal to 0. Suppose I put pulse input, pulse input is in one shot. I give this give this input and so tracer is put only once at time equal to 0 at some appropriate concentration and then I measure measure the concentration in the in the exit. If I do that, I get if I put the same thing in my convolution integral, I will get my exit age distribution is nothing but e C e of t; that is exit concentration divided by 0 to infinity integral C e of t.

And this is my response for pulse input; all this all this is for my step input. So, I can do any one of these two experiments and find out, what my exit age distribution is; what my cumulative age distribution is. And knowing these two, I can also find out what is my internal age age distribution. So, this is how experimentally we can determine determine our our exit exit age distributions. Now, we can also determine the exit age distribution or develop a model for this. Now, what is the need for doing this? The need for doing this is that once we determine our exit age distribution.

For example, such as such as E of t from my pulse experiments or from my step inputs, I would like to propose a model for how this reactor reactor behaves. And if I want to do that, I must be in a position to determine from a model what is my exit age distribution or cumulative age distribution that I expect. Now, if that is the case, then tries to map it with the experimental experimental results. So, that I will have an equivalent model for my reactor; we will take one or two example to see how it how it works. So, now we are going to therefore see how we determine exit age distributions from model based analysis.

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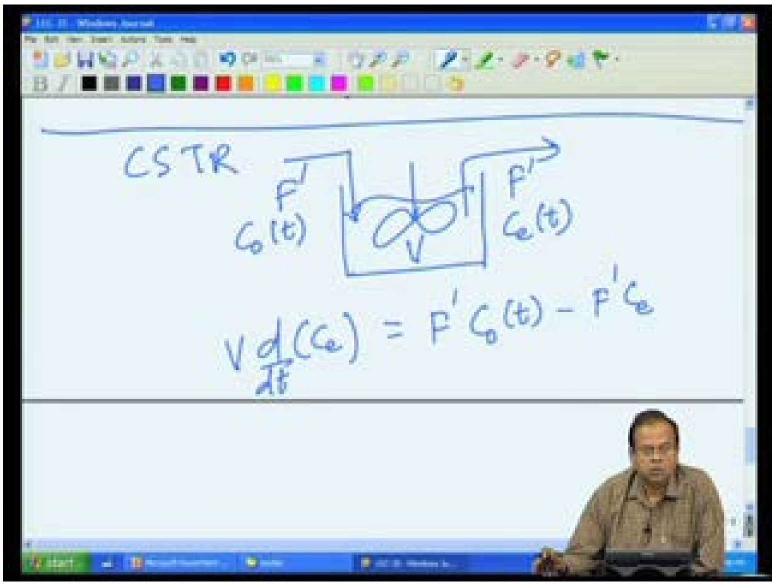

$$V\frac{d(C_e)}{dt} = F'C_0(t) - F'C_e$$

And let us start with a CSTR; because that is the simplest kind of reactor model that we can think of and then, we will look at plug flow also and some combination there off. So, what happens in a CSTR? I am putting in my fluid at volumetric flow rate of F prime; the volume here is V. Let us say that C naught of t is my inlet concentration; F prime is the volumetric flow rate that comes out. C e of t is my it my is my exit exit concentration. So, now how how is the dynamics of this system system defined? I can go back and do a mass balance equation, which in this case will be the accumulation is what is coming in minus what is going out as simple simple as that. Now, in this let us say that my inlet experiment or my experiment is such that my I have done a step input.

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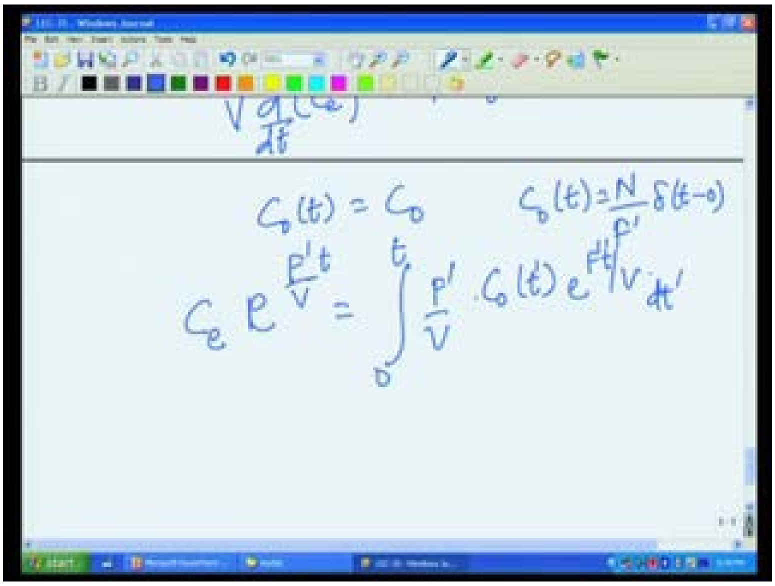

$$V\frac{d(C_e)}{dt}$$

$$C_0(t) = C_0 \qquad C_0(t) = \frac{N}{F'}\delta(t-0)$$

$$C_e\, e^{\frac{F't}{V}} = \int_0^t \frac{F'}{V}\, C_0(t)\, e^{F't/V}\, dt'$$

So, C naught of t is some value some value C naught or let us say that we have we have done a pulse experiment. It can be either either one of them, where C naught of t will be N by F prime in to delta of t minus 0. This is how, we represent represent a step a step input. So, if we now go back to this go back to this mass balance equation, we can solve this actually and say C naught e raise to F prime by V in to t is equal to integral 0 to t F prime by V in to C naught of t in to e raise to F prime t by V dt prime. That is, this is just a linear equation linear equation. So, I can get integrating factors and express this solution in this particular term. So, let me to make it clearer let me. So, all I have all I have done is integrate this integrate these differential equation using integrate integral integrating factor.

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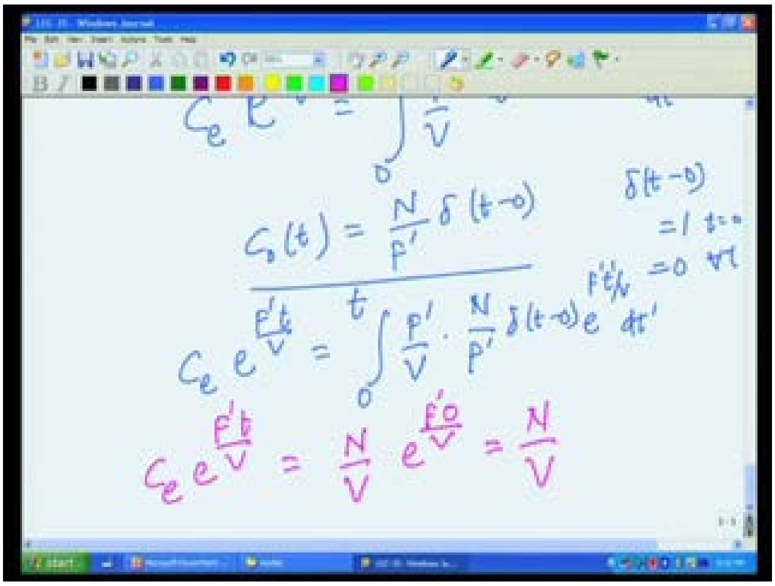

$$C_0(t) = \frac{N}{F'}\delta(t-0)$$

$$\delta(t-0) = 1 \quad t=0$$
$$= 0 \quad \forall t$$

$$C_e e^{\frac{F't}{V}} = \int_0^t \frac{F'}{V}\cdot\frac{N}{F'}\delta(t-0)e^{F't'/V}dt'$$

$$C_e e^{\frac{F't}{V}} = \frac{N}{V}e^{\frac{F'0}{V}} = \frac{N}{V}$$

So, now I say that my C naught of t; that is if I am doing a pulse experiment, then that is nothing but N by F prime delta of t minus 0. What is all this N by F prime delta t minus 0? You know what value delta t minus 0 has? It has a value unity at t equal to 0 and 0 for all other times. So, what happens here? If N is the amount of if N is the amount of tracer that I have put in amount divided by the flow rate gives me the concentration C naught of t. So, now going back taking this value and putting it over here. We have C e F prime t by V as integral 0 to t F prime by V in to N by F prime delta t minus 0 e raise to F prime t prime by V dt prime.

I am just substituting over there. So, now what do I get? If I if I simplify, this this is nothing but C e e raise to F prime t by V. What is this function? This function because delta is step function has a value 1, when t is equal to t is equal to 0 and otherwise, it has a value 0. So, what will be the value of integral 0 to t? It will be simply N by V; F prime gets gets cancelled; e raise to F prime; this has a value only when t is equal to 0 by V which is nothing but N by N by V. So, what is our C e of t?

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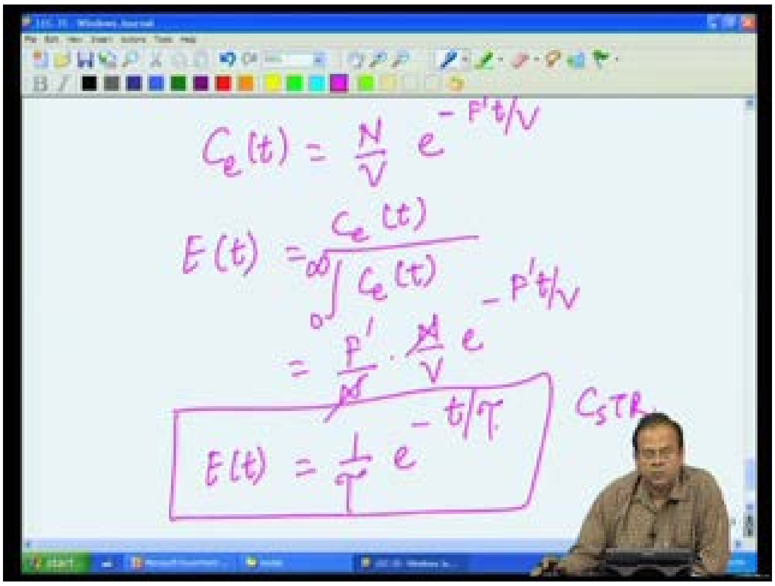

$$C_e(t) = \frac{N}{V} e^{-F't/V}$$

$$E(t) = \frac{C_e(t)}{\int_0^\infty C_e(t)}$$

$$= \frac{F'}{\cancel{N}} \cdot \frac{\cancel{N}}{V} e^{-F't/V}$$

$$\boxed{E(t) = \frac{1}{\tau} e^{-t/\tau}}$$

CSTR

Using this, our C e by t C e of t is nothing but N by V e raise to minus F prime by t by V and for a pulse experiment, what is our exit age distribution? E of t is nothing but C e of t divided by integral 0 to infinity C e of t C e of t. So, if we if we do all this integral 0 to infinity, C e of t F prime is nothing but the amount that we have put in. We get this is nothing but F prime by N or our C naught in to N by V e raise to minus F prime by t by V which after cancelling this what is F prime by V? F prime by V is nothing but our mean residence time tau; e raise to minus t by t by tau. So, this is my exit age distribution for a CSTR, for a CSTR constantly stirred tank tank reactor.

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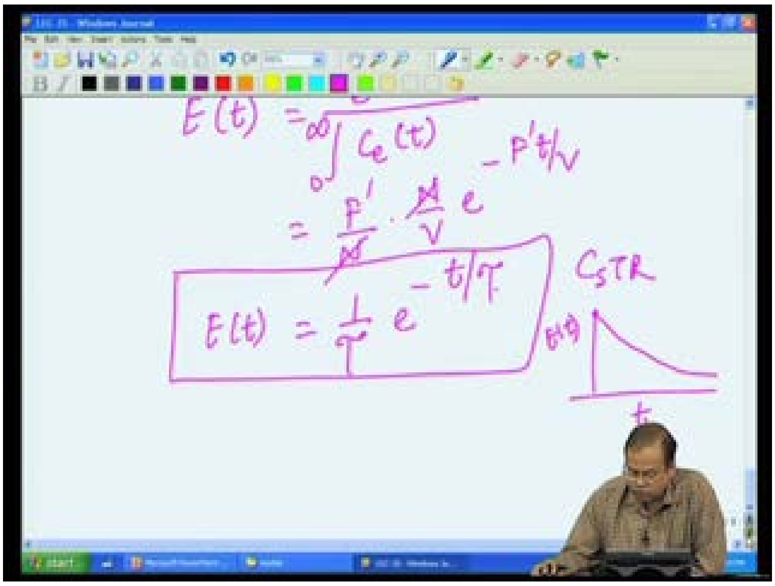

$$E(t) = \frac{}{\int_0^\infty C_e(t)}$$

$$= \frac{F'}{\cancel{N}} \cdot \frac{\cancel{N}}{V} e^{-F't/V}$$

$$\boxed{E(t) = \frac{1}{\tau} e^{-t/\tau}}$$

CSTR

So, how does it how it will look like? It will look like something like this E of t. When t is equal to t is equal to 0, this has the maximum value namely 1 by tau and then, it will exponentially decrease as time time increases. So, this is how my residence time distribution will look for CSTR. Now, for a plug flow reactor, if we if we do a similar similar analysis, what do we expect will happen for a plug flow reactor?

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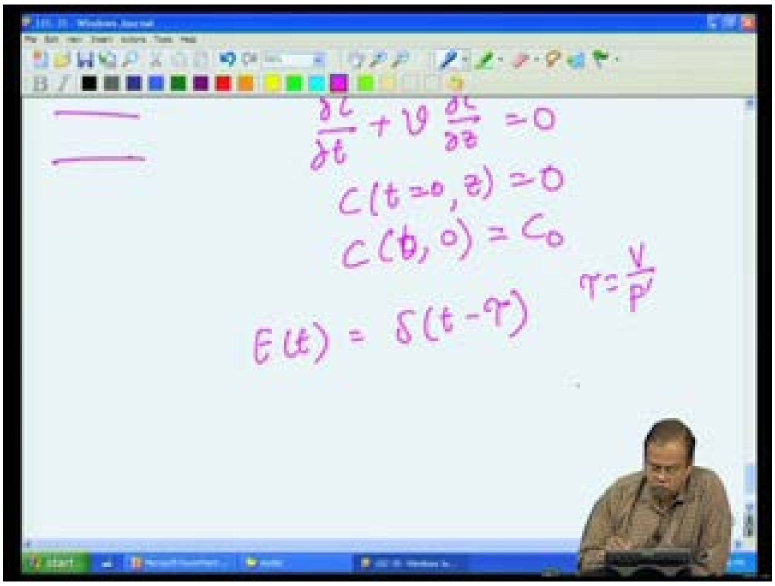

$$\frac{\partial C}{\partial t} + v\frac{\partial C}{\partial z} = 0$$

$$C(t=0, z) = 0$$

$$C(t, 0) = C_0$$

$$\tau = \frac{V}{F'}$$

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

The appropriate way to do to do this is to write the transient mass balance equation, accumulation and transport transport term with C of t equal to 0 at all z is 0. And C of time t equal to 0 and sorry at z any time any time t and z equal to 0 is some value when some value C naught. So, if we do this solve this equation by characteristic line method partial differential equation and get the get the response, you will get. Once again what is tau? Tau is my residence time, which I define as V by F prime; whether it is a plug flow reactor or a stir tank reactor; my definition of residence time is seen.

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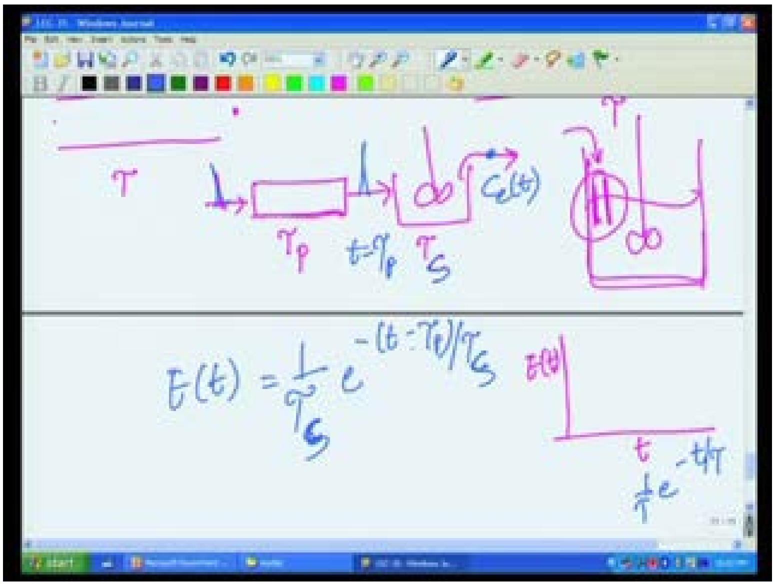

So, what will I expect as a as a exit age distribution for a plug flow reactor? If I have if I have residence time t, then all the fraction or the fluid element comes out exactly at that particular point. So, what we are saying is if this is the residence time for these reactor and if we have put tracer at t equal to 0, then as a as a as a pulse input; then we will not see any of the tracer till time t equal to tau. Why? because it is a plug flow. So, this tracer will move like a plug for amount of time equal to the residence time and then it will come out of the reactor. And once it will come out in a single shot; because once again there is no mixing action mixing in the reactor. So, our E of t will look something something like this; that is a direct delta function, delta t minus tau.

Again, delta has a value unity at t equal to tau and value 0 for all other values of values of t. So, that is what our plug flow reactor residence time will will look like. So, these are the residence time distributions for the ideal reactors; that we saw namely stir tank reactor and plug flow reactor. But let us say that my actual reactor is neither of the two. But suppose I want to model it as a mixed reactor. As a mixed reactor, that means what? As plug flow reactor, let us say followed by a stir tank reactor where will I get such situations? So, what we are saying suppose our real reactor is something like this; the fluid is coming in for some amount of time. There is very little mixing in this region, let us say. So, it behaves like a plug flow.

So, I show it as a plug flow and then for the remaining portion of the reactor; there is uniform mixing. So, it behaves like a like a stir tank reactor. So, my original single reactor is now let us say, combination of this two this two reactors is a combination of this two this two reactors. Now, what kind of residence time can I expect? One can ofcourse go back and do the mathematical analysis. But let us try to argue it on the basis of on the bases of what what do we what do we expect. So, suppose this residence time is tau p and this residence time is tau c. So, now we are trying to look at the exit age distribution for this reactor. Now, given the fact that, after I have put let us say I have put I do the same experiment.

I have put a pulse input in my in my in my reactor. So, it is a tracer. So, let us try to tracer and try to see what the concentration of this tracer is in the exit stream namely C e of C e of t. Now, what will I expect here? I will expect that this tracer will not enter the reactor until time tau p has tau p has elapsed; because it is a plug flow. So, at time T equal to tau P, we will see a pulse of tracer which will be input to the input to the reactors; the stirred tank reactor. So, after time t equal to tau P, this reactor behavior is similar to having a single reactor and the pulse input which we saw in the in the previous CSTR example. So, we should expect this response; but not from 0 time; but from time t equal to t equal to tau P; because till such time has elapsed such as tau P.

We go on we do not expect the tracer to come in to the inlet of the CSTR. So, in other words, we can we can expect E of t as 1 over tau S or tau C which is a residence time for stirred tank continuous stirred tank reactor; e raise to minus t minus tau P by tau C. For sake of being consistent with the notations which we will find in text book; let us call this residence time in a stir tank reactor as tau S. So, what is our single stirred tank reactor residence time? 1 over tau e raise to minus t by tau, single CSTR. So, we see that this behavior will be shown except the difference being only after time t equal to t equal e minus e minus tau P.

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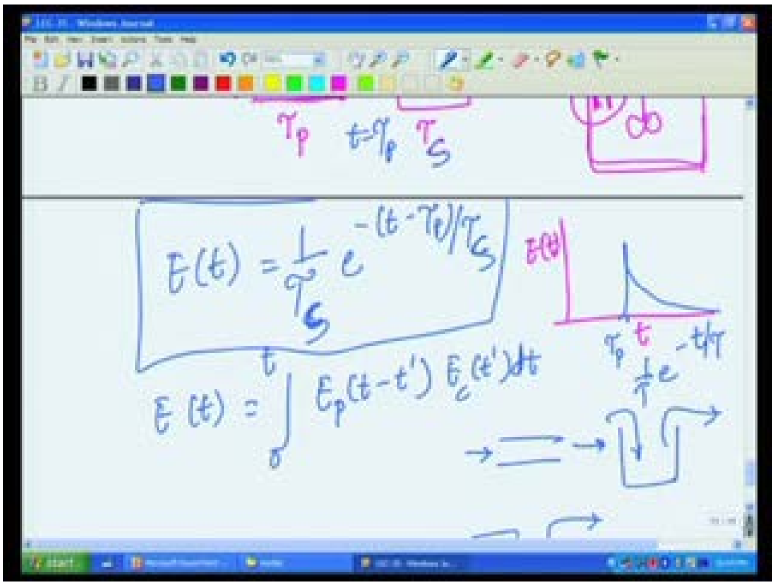

$$E(t) = \frac{1}{\tau_s} e^{-(t-\tau_p)/\tau_s}$$

$$E(t) = \int_0^t E_p(t-t')\,E_c(t')\,dt$$

Which actually, we can once again use the convolution integral; because these are processes in series. We can write this as t minus t prime E C of t prime dt; where E P is the exit age distribution for a plug flow reactor and E C is the exit age distribution for the stir tank stir tank reactor. So, if you take the appropriate values, put them put them into that is this is for single plug flow single stirred tank; put it together. We will get the exit age distribution which will look exactly exactly like this; that is for for. Now, this is the situation just to refresh ourselves. We had plug flow reactor followed by a stirred tank reactor. Now, let us try argue out, what will happen if we have a stirred tank reactor followed by a plug flow plug flow reactor? So, what what do you expect will will ah ah happen over here? Here, once again so if you if you actually put all these two together, this is what we will we will expect. At tau equal to tau P, we get our pulse followed by a CSTR behavior.

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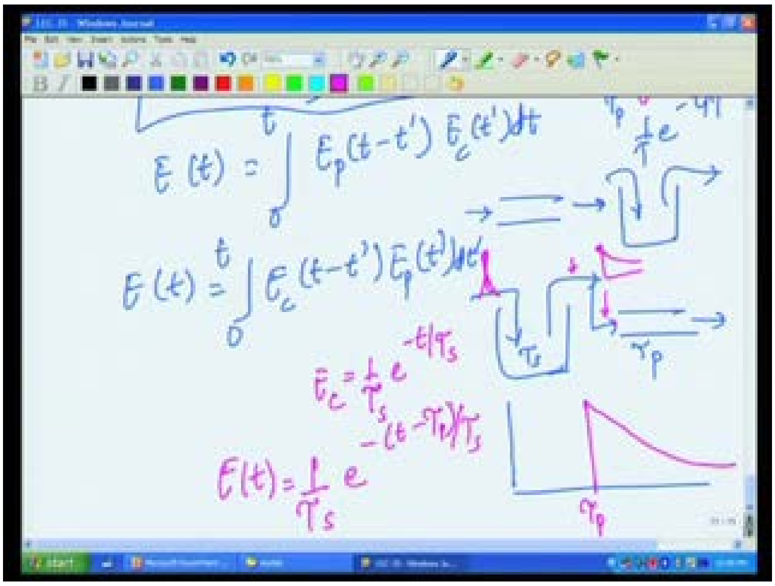

Now, we can argue using this formula that this can be also argued use of convolution integral as E C of t minus t prime E P of t prime dt prime. What does what does what does this this imply? Let us try to try to argue it. So, tau S is the residence time for this; tau P is the residence time for this. So, what we have now is a stirred tank reactor followed by a plug flow plug flow reactor. Now, what will happen here? We let us now put this pulse here. Moment we put this pulse, we will start seeing the response coming out. For example, if we were to have just this stirred tank reactor, our E C or E at the exit at this point will be 1 over 1 over tau S e raise to minus t by tau S. Tau S is our…

However, what will we see right from the beginning at the exit of the reactor, when there is a plug flow reactor in between? At time t equal to 0, remember suppose I have to draw a small sketch at time t equal to 0; this is what is the input in the in the reactor. But we will not see that, until time tau P has elapsed. Why? Because for a plug flow reactor nothing will be nothing that is coming out in the reactor will be seen in the exit of the reactor till tau P time has elapsed and there is no mixing. So, whatever that comes in at some time t will be seen at time t plus tau P at this particular location. Or whatever is put in let us whatever is coming into our plug flow reactor at time t equal to 0 will be seen at time t equal to tau P right.

So, this is what we will see at t equal to 0. What will we see at the next instant? We will see at the next instant, what has come in the reactor after the next instance of 0; that we will see after tau P. And if we if we complete this, this is what the residence time distribution will look like, which is very similar to the residence time distribution for this case. Or in other words, now our E of t will once again be 1 over tau S e raise to minus t minus tau P divided by tau S. Or to put it simply, we will have the same residence time whether it is a plug flow followed by CSTR or CSTR followed by followed by plug flow plug flow reactor.

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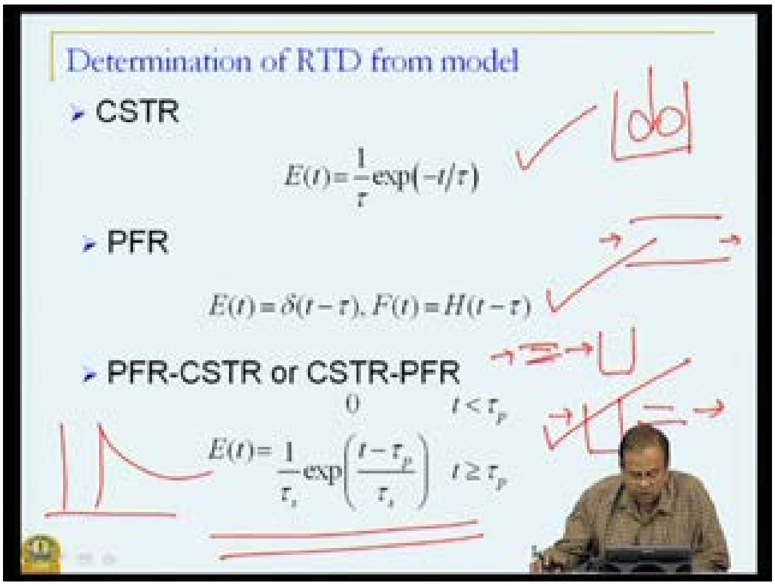

Determination of RTD from model

- CSTR

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

- PFR

$$E(t)=\delta(t-\tau),\ F(t)=H(t-\tau)$$

- PFR-CSTR or CSTR-PFR

$$E(t)=\begin{cases}0 & t<\tau_p\\ \frac{1}{\tau_s}\exp\left(\frac{t-\tau_p}{\tau_s}\right) & t\geq\tau_p\end{cases}$$

So, to summarize to summarize let us let us try to summarize it. In this particular particular slide over here, if we have a single CSTR, this is my this is my residence time distribution. If I have if I can describe my reactor by single plug flow reactor, this is my residence time residence time distribution. But if my real reactor is actually partly behaving like a stirred tank reactor and partly behaving like a plug flow reactor. So, either initially plug flow reactor followed by CSTR or CSTR initially followed by plug flow reactor. My residence time distribution will be given by E of t is 0, till such time as the residence time of the plug flow reactor tau P and beyond that time, it is 1 over tau s exponential t minus tau p divided by tau S, where tau P and tau S are the residence times of plug flow reactor and stirred tank stirred tank reactor.

So, whether a reactor behaves like a single stir tank reactor or reactor behaves like a plug flow reactor or reactor behaves like a plug flow plug flow followed by CSTR or CSTR followed by plug flow reactor, we have different residence time. Infact, PFR-CSTR or

CSTR-PFR combination gives us the same residence time; but it is different than if we have if we have these two kinds of reactors. So, this is this is what I mean, when I said if you can determine from the model. So for example, our experimental determination of residence time or experimental determinations of exit age distribution suppose it looks something like this. It means that my reactor is neither a stirred tank reactor nor a plug flow reactor; but a combination of plug flow reactor and CSTR reactor.

However, the exit age distribution alone is not able to distinguish between these two these two combinations. So, the question then arises does it matter? do I What do I expect when actual reactions takes place? We have been talking about these macro mixing and the kind of flow pattern that one can expect and based on this flow pattern, what will be the distribution of the residence time in the in the reactor? That is the age. How much time does the fluid element spent? So, now let us let us take a stirred tank stirred tank second order reaction and try to see how does it influences the how how does this flow influences now the conversion in the reactor?

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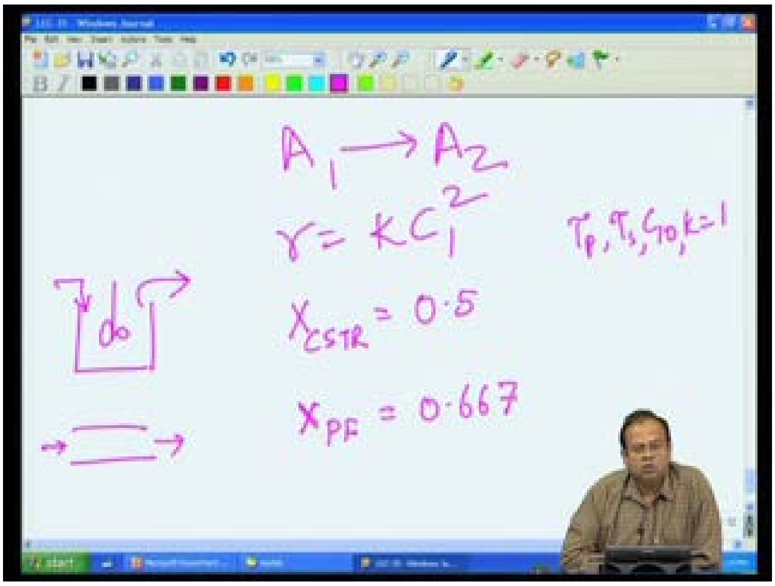

So, what we are what we are saying is that let us say I have a reaction A 1 going to A 2 and the rate of this reaction is given by a second order reaction. Why not first order? first order will why not First order will become clear in few minutes. So, let us say that we have a second order second order reaction. So, we can we can say that, we can we can look at what will be the reaction conversions or concentrations in the exit, if we have a

CSTR. So, if we have a CSTR a single CSTR and all our usual inlet, outlet, inlet concentrations, outlet concentrations and so on.

And we are going to put tau P, tau S, all concentrations rate constant everything to unity value; just to make a make a point. So, if we use CSTR CSTR balance, we can get the exit concentration and the conversion and it turns out the conversation for CSTR in this particular case is 0.5 is 0.5. What I have done? I have just taken the simple example of putting all numerical values of all constants to one and you can you can actually get this get this value. Suppose it was a plug flow reactor as you can expect, the conversion in the plug flow reactor for the same residence time will be higher; because it is a second order reaction. So, that gives you a value of 0.667.

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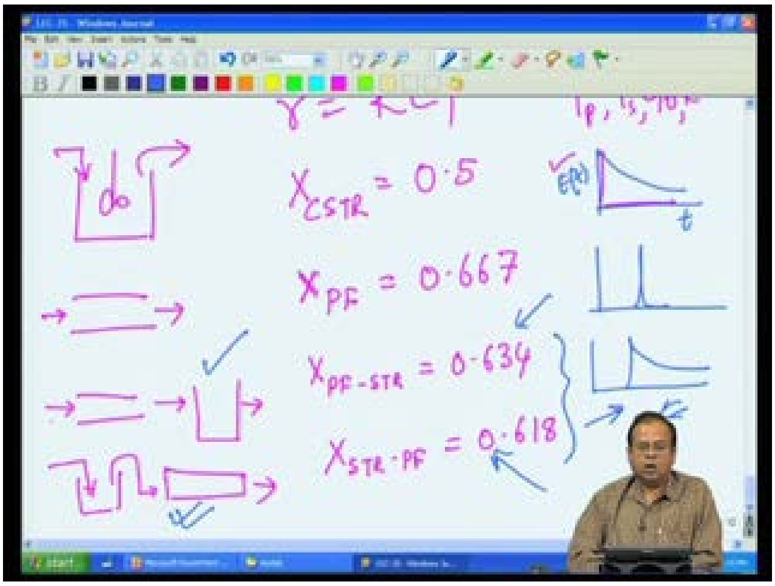

Now, let us say that I consider this as a case of CSTR a plug flow reactor followed by a CSTR. And then, if I do this same calculation, first use plug flow reactor. Then, find the inlet and then calculate the exit concentration of a stirred tank reactor. So, idea is to go in a sequential manner. So, inlet calculates the concentration at the exit of the plug flow reactor. Take the concentration of the exit of the plug flow reactor as the inlet concentration for CSTR. And using CSTR mass balance, calculate the exit concentration from CSTR. We will get X. So, I will now call it as PF followed by stirred tank reactor.

We get 0.634. I can ofcourse do the same thing same thing for stirred tank rector followed by a plug flow reactor. Repeat the same process; inlet to first stirred tank reactor; exit of stirred tank reactor which is inlet of plug flow reactor. And from that, you calculate the exit of plug flow reactor. We get the conversion which I called as STR dash PF as 0.618. Now, what does this what does this imply? It implies the following. If you have different residence time distributions, you get different conversions; that is, this residence time is different. So, what is a residence time distribution here?

I will I will put it in a different color. This is my E of t versus t. In this case, in this case and for both these cases, it is the same residence time distribution. We just now saw it few minutes back. So, what does it what does it mean? It means different residence time gives you different conversion. So, definitely non-ideal flow pattern influences the conversion; but it tells you more than that. It says that even though the residence time distribution is same, you may get two different levels of conversion which implies that residence time alone is not sufficient to describe the conversion in a in a reactor. Just to give you a clue as to what is what is happening over here?

Both this combination give us give us the same residence time. But what was happening in the first reactor? In the first reactor, the fluid elements do not mix as they travelled in a axial direction in the reactor. And then, later on they mixed completely in a stirred tank reactor; that is this particular case. In this case, the fluid elements initially mix well together. But then, later on they do not mix as they travel to plug flow reactor. Or in other words, whether there is a mixing early in the reactor or late in the reactor also amounts also accounts for differing conversions; because residence time distribution is same; but conversions are different.

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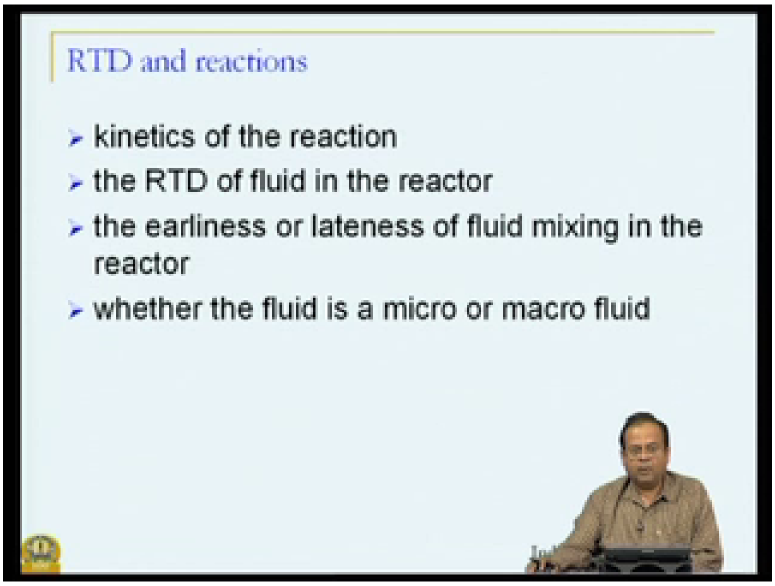

RTD and reactions

- kinetics of the reaction
- the RTD of fluid in the reactor
- the earliness or lateness of fluid mixing in the reactor
- whether the fluid is a micro or macro fluid

So, it is the quality of mixing which is causing this particular particular difference. To summarize kinetics of the reaction, it will influence the conversion. If it is a first order, you will get one conversion whatever is the reactor that you are using. The RTD in the reactor that is how the liquid is flowing through the reactor determines the conversion. So, it is different for stirred tank reactor and different for plug flow plug flow reactor. But earliness and lateness of fluid missing in the reactor also influences influences the behavior of the of the fluid in the in the reactor. And whether the fluid is macro fluid or micro micro or macro a little tongue twister there; so, micro or macro, it will determine the performance.

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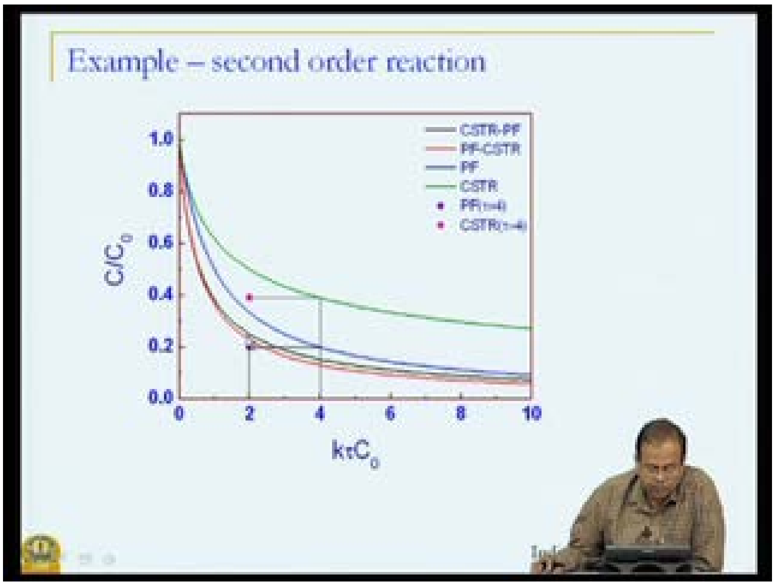

Example – second order reaction

This is again again the same same illustration; that same reaction second order reaction. Let us see, what happens as asthe dimensionless parameter K C naught into tau; because now the dimensionless parameter has K; not only K tau, but C naught concentration also. So, this is what this is what will will happen. Let us lets us look at an example, where we carry out a reaction; second order reaction and results that you are seeing is what is the exit concentration as a function of different residence residence times. Different colored lines are showing different combinations. For example, the black one is CSTR followed by plug flow reactor.

The red 1. So, that is that is CSTR followed by plug flow reactor. The red one is plug flow reactor followed by CSTR. The blue one is a plug flow reactor reactor alone and the green one is a is a CSTR. So, at first glance, we ofcourse conclude that Cs; we are looking at exit concentration. So, higher the value of exit concentration, lower is the lower is the conversion. So, at any value of this dimensionless parameter, we see that CSTR single CSTR gives you low performance; because exit concentration is high. So, conversion is the lowest. The plug flow reactor performs much better.

But combination of stirred tank reactor followed by plug flow reactor performs better than either single reactor or stirred tank reactor. And the last one that is plug flow reactor followed by a stirred tank reactor performs performs even even better. The results shown for blue line and red line or red dot; these are actually the lines are results when all residence times were for the same value of K K tau and C naught. But for example, if you look at it in this manner that a plug flow reactor with tau equal to 4, CSTR is this; my my plug flow is this. And CSTR followed by plug flow or plug flow followed by CSTR is this particular combination.

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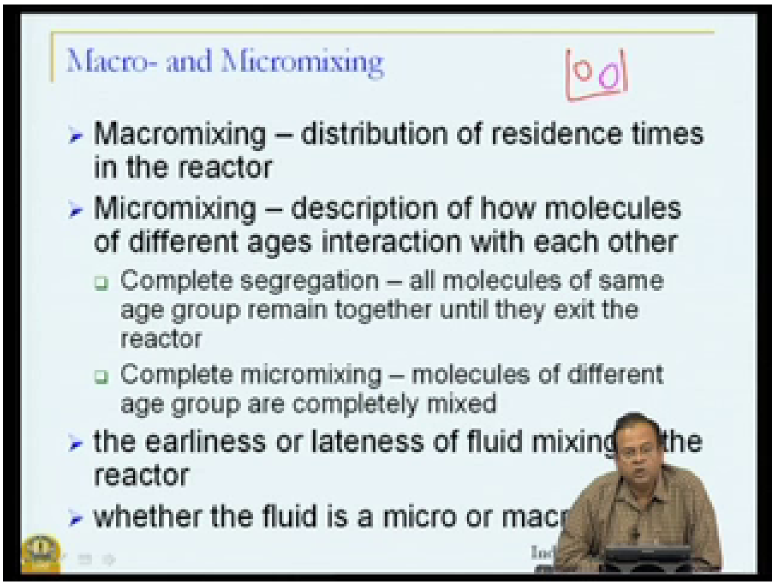

Macro- and Micromixing

- Macromixing – distribution of residence times in the reactor
- Micromixing – description of how molecules of different ages interaction with each other
  - Complete segregation – all molecules of same age group remain together until they exit the reactor
  - Complete micromixing – molecules of different age group are completely mixed
- the earliness or lateness of fluid mixing the reactor
- whether the fluid is a micro or macr

So, what is it what is it that we are talking about? Summarize this macro mixing is a distribution of residence times in the reactor. So, how depending on the flow conditions, the age of the fluid element in the reactor reactor matters. Micro mixing, on the other hand is a description of how molecules of different ages of in the reactor. So, fluid elements of different ages; how do they interact with each other? And it is here that once again we can draw two distinctions limits; first, we that there is complete segregation.

That means I have a reactor I have a reactor which has fluid elements of different ages. So, some are shorter age; some are longer age and so on. If these fluid elements do not interact with each other; that is all molecules of the same age group remain together, until they exit the reactor. So, there is no cross talk. This is the situation of complete segregation. On the other hand, if molecules of different age groups are completely mixed, we have what we call complete micro mixing. So, two different extremes complete segregation and complete micro mixing.

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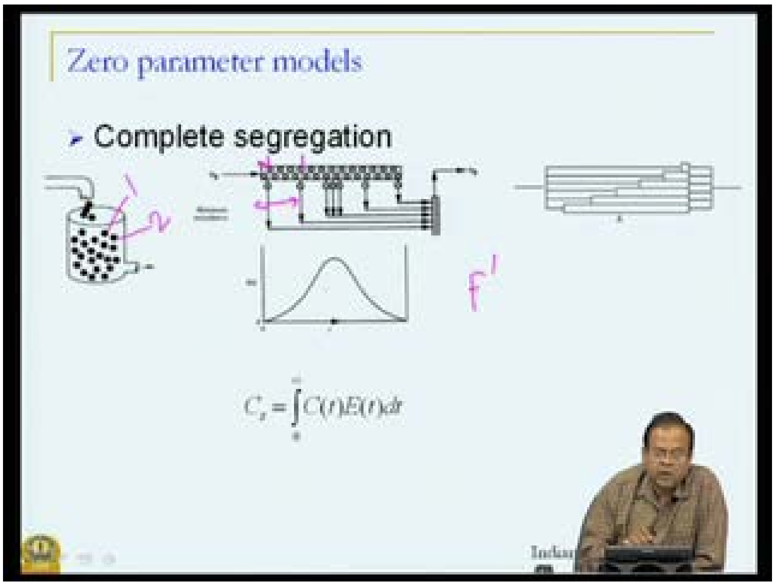

Zero parameter models

- Complete segregation

$$C_s = \int_0^\infty C(t)E(t)dt$$

So, how do we how do we deal with this situation. Let us say that we have we can look at the situation of complete segregation which we call 0 parameter models. Let us let us look at it in a way that equivalent in the time domain is what happens in a plug flow reactor in a in a residence time domain. So, let us say that either we can look at the reactor complete segregation reactor in the way we look at the stirred tank reactor. So, these fluid elements for example have different ages. So, this has 1; this has 2; it does not matter numbers and they do not interact with each other. But come out at time equal to 1, after it spends time equal to 2 and so on. Other way of looking that is if you have a plug flow plug flow reactor, then the fluid elements do not interact with each other is equivalent to saying that having put in some material.

It comes out; some fluid elements come out at this particular point. So, it will have age corresponding to this particular particular residence time, whatever that is. For this, it will have a residence time fraction of this. So, it comes out little later in the reactor and so on. Or in other words to visualize a situation of complete segregation, I can look at it as a plug flow reactor with exit at different locations along with the reactor. And how are these exit or what are these flow rates? Suppose if I say that F prime is my flow rate in the inlet, then I will I will reconstruct the flow rates at these different exit points in such a way that my residence time distribution matches with what I experimentally experimentally observe. So, that is that is one way of looking.

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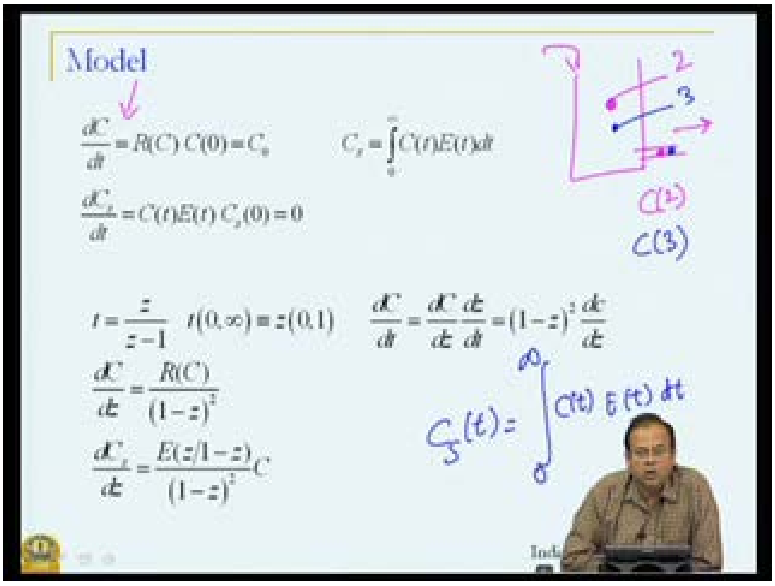

Model

$$\frac{dC}{dt} = R(C) \quad C(0) = C_0 \qquad C_s = \int_0^\infty C(t)E(t)dt$$

$$\frac{dC_s}{dt} = C(t)E(t) \quad C_s(0) = 0$$

$$t = \frac{z}{z-1} \quad t(0,\infty) \equiv z(0,1) \qquad \frac{dC}{dt} = \frac{dC}{dz}\frac{dz}{dt} = (1-z)^2\frac{dC}{dz}$$

$$\frac{dC}{dz} = \frac{R(C)}{(1-z)^2}$$

$$\frac{dC_s}{dz} = \frac{E(z/1-z)}{(1-z)^2}C$$

$$C_s(t) = \int_0^\infty C(t)\, E(t)\, dt$$

So, if you take a model for example. Let us say that we have a reaction and its dynamics is given by dC dt is equal to R of C. Now, what we are saying. For example, a fluid element of certain age spends that much amount of time and comes out. So, what would be the what would be the concentration of… Suppose there is some inlet concentration and then, there is a exit. So, this fluid element which has age as indicated by this purple line; purple color is coming out at time t equal to 2. So, let us say this age corresponds to 2 units. Then, we will have C of 2 that is concentration of the reactant species at time t equal to 2 which is the age of this fluid element is what will be one component here.

Now, what is C of 2 will be determined by the dynamic of this particular system. So, let us say we have another fluid element which has age 3. So, this one will have concentration equivalent to time which has spent which it has spent in the reactor equivalent to 3. So, what will be the total fluid concentration at any given point of time? That will be this is my residence time distribution and this is my concentration at that time. So, adding up all these fractions will give me the concentration in the exit of the exit of the reactor; this is when complete segregation occurs.

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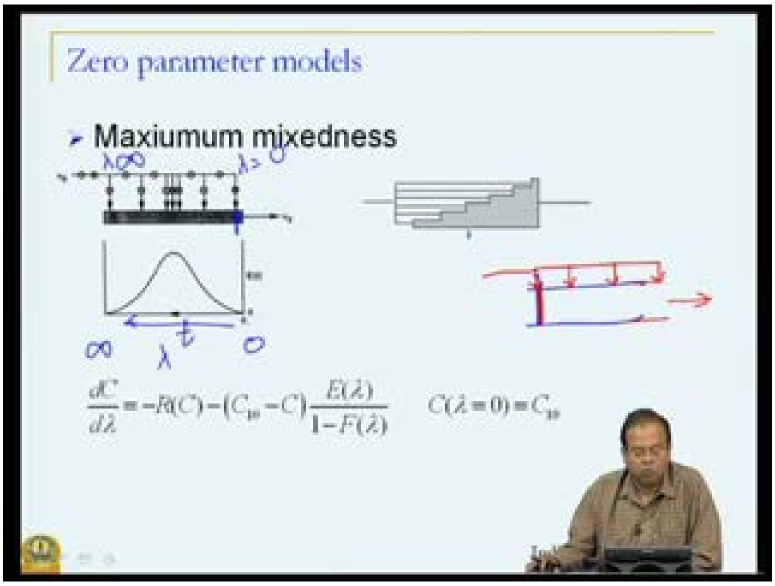

Zero parameter models

- Maxiumum mixedness

$$\frac{dC}{d\lambda} = -R(C) - (C_{in} - C)\frac{E(\lambda)}{1 - F(\lambda)} \qquad C(\lambda = 0) = C_{in}$$

What happens, when there is maximum mixedness? Now, I can turn back on to plug flow reactor and say that my maximum mixedness model is equivalent to having a plug flow reactor with inlet streams distributed along the along the length of the length of the reactor. Now, what does this what does this distribution distribution imply? If I call for example lambda as the life expectancy of a fluid element in the reactor, the fluid element which enters at the inlet has the maximum life expectancy. So, I call it lambda alpha; whereas, the fluid element which enters at the exit point in the reactor has a has a life expectancy of 0. So, if I look at lambda, this is 0; this is infinity.

So, this is equivalent to what now. The fluid element enters the reactor pretty late mixes with whatever is there along the inin in the in the radial direction; not in the axial direction. So, complete mixing and then leaves the reactor. So, my exit age distribution E of t now has to match in this particular particular direction. Once again, I will repeat. We are looking at a plug flow reactor with side entries. The reactor which enters the earliest leaves the last; the fluid element which which enters the last at the exit point leaves earliest. So, my exit age distribution is now from t equal to 0 over here to t equal to very large large values. And what happens in a plug flow reactor?

In a plug flow reactor for example, whenever a fluid enters, it mixes; because in a plug flow reactor, we say that the concentration variation along radial direction is negligible. What does it mean? That means whatever for example, I will look at the simple simple plug flow reactor; whatever is there over here and whatever is coming at the next instance like this get completely mixed along the radial direction and then it moves. So, something else comes in, it gets completely mixed. So, what does what what does this now imply? These imply that the situation of the maximum mixedness is equivalent to a situation of a plug flow reactor with side entries as shown over here.

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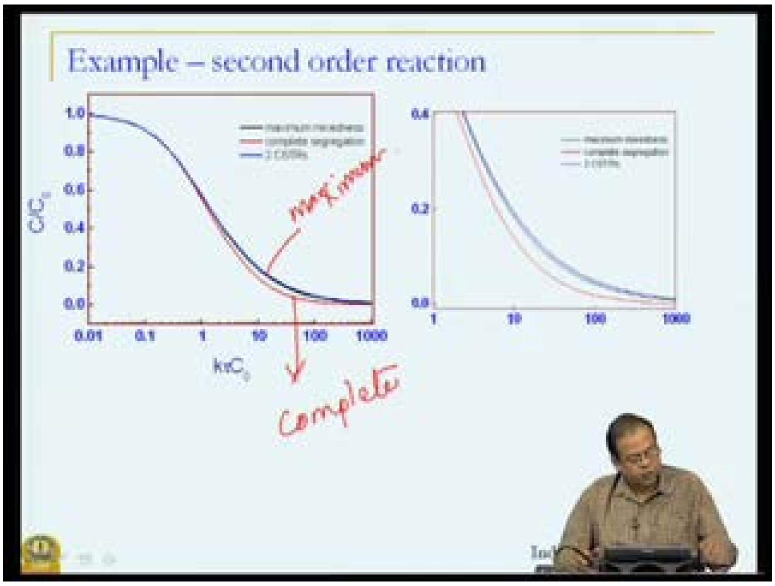

Example – second order reaction

So, if we if we do this, then we get once again for a second order reaction. We can we can see that this is again residence time versus concentration. This is the case of complete segregation; this is a case for maximum mixedness. So, complete segregation gives you better conversions compared to compared to maximum mixedness. So, with this, we will come to the end of our discussion on residential non-ideal flow and the reactor performance. We had only brief discussion for want of time, but what essentially we saw was that how residence time is determines the performance of a reactor. What is residence time? It is nothing but the distribution of the age that fluid spends in the in the reactor. So, different residence time - different conversions, but it turns out that same residence time distribution can also give you different conversions depending upon whether there is a mixing early in the reactor or late. So, we will conclude our discussion and stop here for the today’s session. Thank you.