Chemical Reaction Engineering
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Lecture No. #38
Non-ideal flow and reactor performance
Introduction

Friends let us start discussion on the last topic of this course and in this, we are going to look at some non-ideal flow patterns or non-ideal flow of fluid in the reactors and its influence on the conversion yield selectivity and so on.

Now, why is this non ideal flow important or what is it that we have not considered, so far that this becomes an important discussion? If you recall for majority of the discussion, so far, we assumed our reactors to have ideal flow patterns namely, complete mixing such as stirred tank reactor or no mixing such as plug flow reactor, but as you can well imagine that reality will be somewhere in between. And here are few examples which may occur inside the reactor; so that we need to worry about how this reaction will reaction will proceed.

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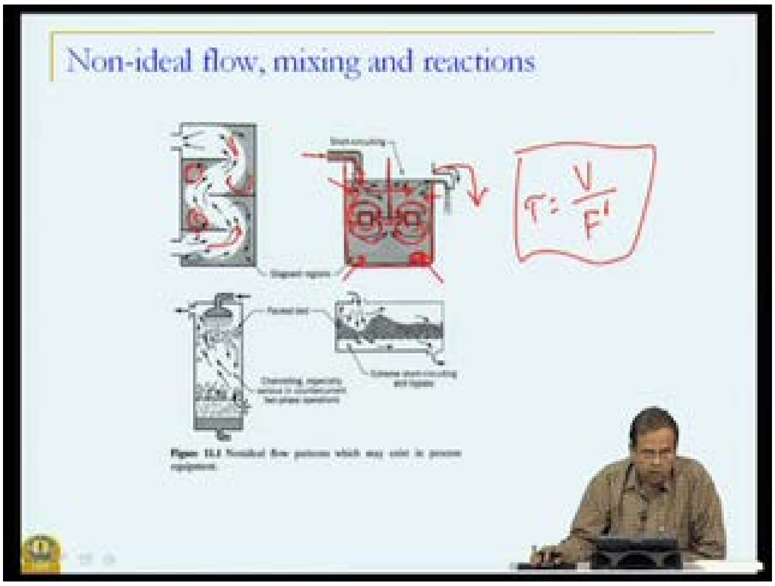

To begin with let us, let us look at some of the typical flow patterns inside the inside the reactor. For example, let us say that we have a stirred tank reactor and that is something that we use quite frequently. So, we have a stirred tank reactor here we have a stirred tank reactor over here and the liquid is coming in from one side and is leaving from other side.

Now, our idea that reactant is well mixed is essentially, because of this impeller that we have in the in the reactor. So, this impeller is set at certain agitation speed and that causes mixing by setting up the flow patterns such as such as shown over here. Now ideal flow pattern or ideal mixing or ideal reactor is the one where, we say that the, there is a complete homogeneity inside the reactor, so if you look at the reactor contents in this zone, in this zone, in this zone or anywhere inside these reactor the concentrations are uniform; and it is the same as what is coming out of the out of the reactant.

So, now let us look at what happens actually when you carry out these exponents. So, for example, it is likely that when some fluid comes inside the reactor. Some of this fluid instead of entering into the main reactor, actually just simply goes out of the reactor by bypassing almost entirely the reactor; that is one possibility, other possibility is that some of the liquid comes to this region, which is corner of a reactor and stays there for a long time or sometimes what seems like forever and therefore, does not participate in what else is whatever else is happening in the reactor; or in other words our assumption that all fluid elements on an average has spent residence time tau equal to volume divided by the volumetric flow rate is not necessarily a good assumption.

Some of the fluids spend times much less than this residence time, such as the fluid which is bypassing. Some of the fluid stay stays much longer than this residence time, such as the fluid element which has got caught into this dead zone; and remaining fluid depending upon when it gets time to escape the reactor comes out at differing amount, after spending differing amount of amount of time.

The same thing can be observed in a column reactor for example, if you have a plate kind of reactor for gas-liquid contactor, we have gas coming in from the bottom, we have liquid coming in from the from the top and these two have to contact each other for for reaction to take place. Now, depending upon the kind of flow for example, there may be some fluid which just keeps re-circulating in these zones over here. Some fluids which, just takes the shortest route and leaves. So, in other words fluids spend times which are different than these average residence time in the in the in the reactor.

The same thing can be said for trickle bed reactors or packed bed reactors and so on. So, the idea is that, now if you look at look at these reactor, we say that these reactor is a confined a piece of equipment, or if piece of equipment where our reaction is confined, we do not consider reactions in the inlet or after they have exited the reactor. But now if the if the fluid elements are not residing in these reactor for same amount of time, some are coming out quickly, some are coming out very late; or in other words there is a distribution of the residence time as far as, a distribution of times as far as, how long the fluid has spent in the reactor. The conversion in the reactor definitely is going to be going to be significantly affected, based on how these reactions reactions take place.

So, while talking about the real reactors and real real performance of the reactor, we have to consider how is the distribution of this times that these fluid elements have spent in the reactor is it is it favorable, unfavorable and so on, we will see in some of the examples and and then look at its look at its influence. But there is another aspect also which we have to we have to consider.

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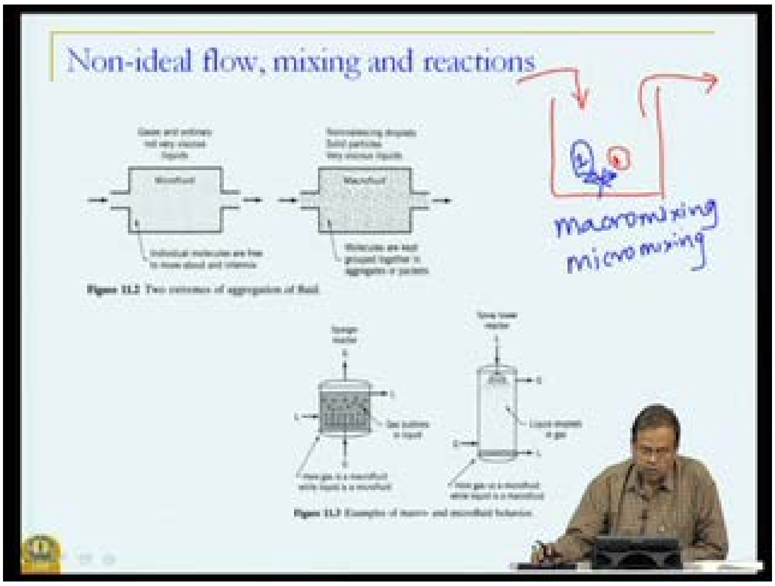

So, let us say that we have our reactor we have our reactor and there is some fluid element coming in, so now, if you if you look at our our reactor, we will find that there is there are fluid elements, which have spent different amount of time.

Now, what is a fluid element? Fluid element is just nothing but a concept to say that, the small volume of the of the reacting fluid is the small, but is also large in some sense, that is large enough. So, that we can define the continuum properties of the of the fluid medium for example, concentration and so on.

So, our our fluid element is not small, such as it is at a molecular level, but there are lots of these molecules. So that, we can describe the properties of these fluid elements, such as density, concentration by the continuum property. Concentration such as k g moles per meter cube and so on.

So, let us say that some fluid element has spent this has has comes inside the reactor and after some time another fluid element comes in the reactor, it spends some time and so on. So, one aspect we just now saw is to see, how long these fluid elements are there in this in this reactor, that is that is one of the important important consideration for us, but apart from the fact that we we have to consider how long they have spent, we also have to worry about, how does these fluid elements interact with each other? That is these fluid elements, which have come at differing amount of time in the reactor; and spending some time inside the reactor do they do they mix with each other, do they interact with each other or do they just remain as an isolated entities spend some amount of time and simply simply leave these reactor.

Now, a gut feeling tells us, that not only the time that they spend, but the quality of their interaction with each other will also make a difference as far as, the reaction reactor performance is concerned. And in other words the mixing at a micro level, that is mixing at the at the fluid element level is also of equal equal importance.

What are again one can look at this phenomena as two extremes, it is always helpful to look at the limiting cases, so that the actual cases fall somewhere in between. One limiting case is complete segregation, where this fluid element 1 and 2 never interact with each other. So, fluid element 1 enters the reactor let us say spends 5 minutes in the reactor goes out, fluid element two comes after 5 minutes after the first one has has entered spends 7, 8 minutes, whatever it takes, then leaves the reactor. So, there is no interaction between these fluid elements and this is a situation of what we call complete segregation.

The other extreme is maximum mixedness, that is these fluid elements interact with each other as soon as, they come into contact with each other. So, the fluid element which, which has which has come inside will mix with the other fluid elements and then leave the leave the reactor. So, we have to worry about not only the residence time distribution, but the quality of mixing in the in the reactor; and this gives rise to idea of what we call micro mixing? A term often is used to describe the residence time behavior and we call such term is used macro mixing. So, we have macro mixing and micro mixing and then there are several other other ideas, which which become important, when we want to discuss when we want to discuss the the reactor performance for non-ideal flow behavior.

So, let us, let us try to, try to now, define few terms and try to understand, how we can determine the behavior of fluid flow inside the reactor, how do we characterize it; and then later on we will come to the part, where we try to use this characterization methods to describe the behavior of the reactor.

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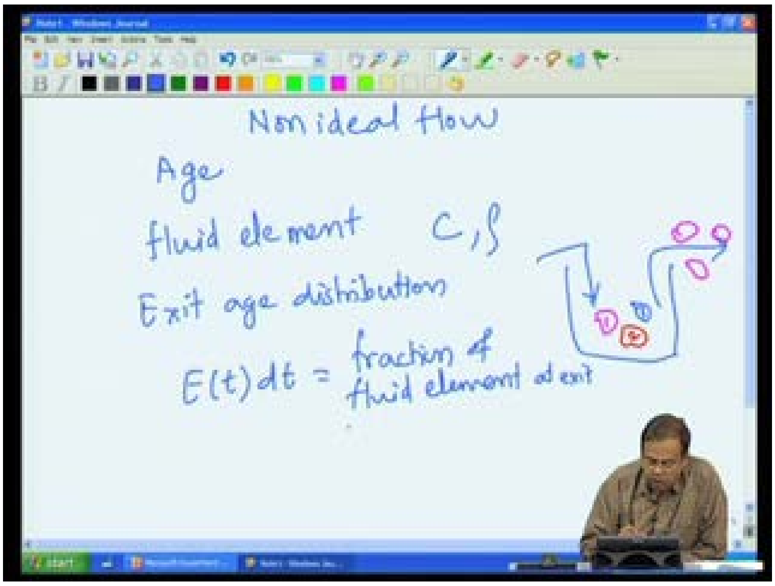

So, we start our discussion on non-ideal flow patterns or non-ideal flow and reactor behavior, by defining few quantities and the first quantity we define is age of the fluid element. Again, fluid element a small volume small in relative, in relation to the size of the reactor. But large enough so that, we can define the properties in a continuum domain such as concentration, density and and so on.

So, we define the age of the fluid element is as the amount of time, the fluid element spends inside the reactor, since, its entry to the exit. So, that is, that is what we call the age. So, once again the age of the fluid element is the amount of time, that has elapsed since, the entry of that fluid element inside the inside the reactor.

Now, given this fluid element and this definition of age, let us try to define certain, certain distribution, that we, that are used to characterize these fluid; and the first one we are going to define is what we call exit age distribution exit age distribution. So, as the name suggest, we are looking at what is happening in the exit of the exit of the reactor; and we said that different fluids spend, different amount of time inside the reactor and hence, we know that there is a distribution of this age exit measured, at the exit point in the reactor.

So, what it simply means is suppose this is my reactor this is my reactor and I am introducing some fluid elements and I am just, this is purely arbitrary, suppose this is this is 1, then this has come sorry, followed by this is my reactor. So, let us say, this fluid element is followed by 2 3 and so on, 1 2 3 are sequential times; and needless to say that, they are they are at some point of time, they will come out of the reactor reactor also. And therefore, if I place myself in this exit and calculate, how, what is the, what is, examine these fluid elements, and then define we give a term E of t to denote exit age distribution and E of t d t is nothing but the fraction of the fluid fluid elements, that is the fraction of the fluid elements at exit. So, we are looking at, what is happening at exit exit stream which has age between time t and t plus d t.

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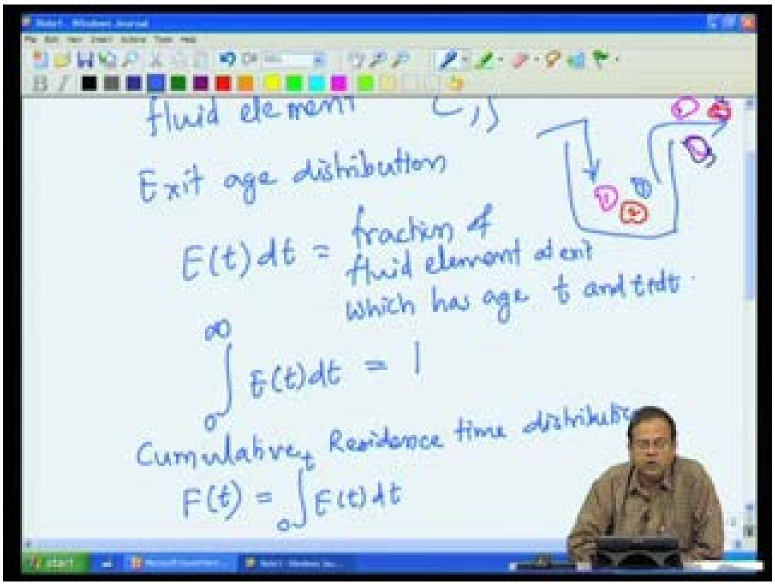

So, E of t d t is the fraction of the fluid elements in the exit stream, which has age between t and t plus t plus d t. So, this is how I define my exit age distribution? We will take an example little later on but first let us go through some of these definitions. So that, we can look at the example, all all together.

Now, given the fact those fluid elements, once they enter the reactor, they may spend differing amount of time, but eventually they all come out of the reactor. If that is the case, then if I look at this fraction, that is E of t d t, which we said is a fraction of fluid elements between age t and t plus d t; and if I add all these fractions from time t going from 0 to infinity. What does this mean? This means that, I am looking at these fluid element in the exit stream and seeing, what is it is, how much, what fraction has spend time between t plus d t; and enumerate all this between time t equal to 0 to a very large time let us say infinity; then this all must add up to 1 or in a continuum domain integral E of t d t must be 1.

And simply put what it means is that if I introduce a fluid element inside the reactor, it may spend some different amounts of time, but eventually all of this comes out of the reactor. So, it could have age anywhere between 0 to infinity or very large value, but if I add up all those, all those they all must add up to 1, because all fluid elements which have entered has to come out of the, of the react. So, this is my exit, exit age, age distribution.

Let me now define, another distribution with the help of this exit age distribution. Now, this is what is called cumulative residence time distribution, now let us go back to our, our figure. So, I have all these fluid elements now, suppose this has spent, so let me, let me just call them as 1 2 3 and so on.

Now, when I look at these, look at these fluid elements and let us say that, I want to know, what fraction of these fluid elements, has age which is less than, let us say 3. So, I will count all the fractions which have 1, 2 and 3 or in other words; if I look at my exit age distribution E of t d t and I want to find out, what is the fraction of this fluid, fluid stream, which has age less than or equal to t time t sometime t; then I will add up or in a continual domain integrate, all those times between time t equal to 0 to t equal to time t and this will give me, what I call cumulative residence time distribution or which we denote by F of F of t.

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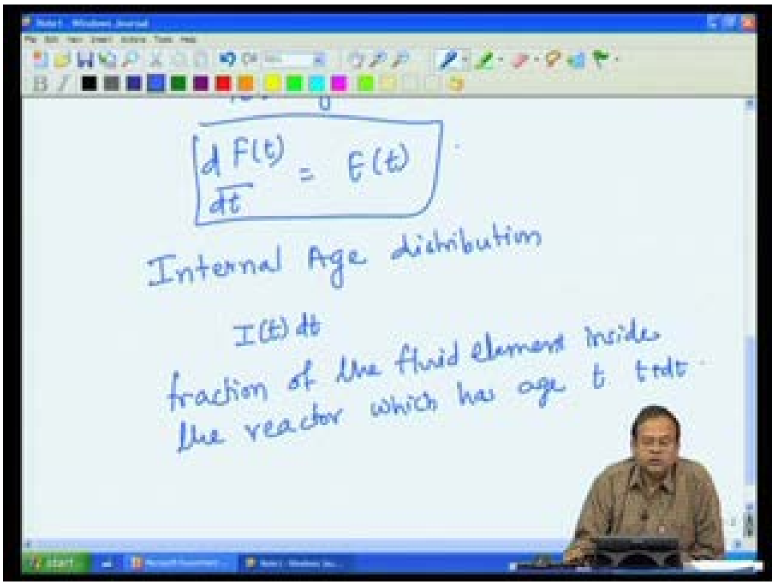

So, what is cumulative time distribution, cumulative time, residence time distribution F of t is the fraction of the fluid element, which has age less than t, time t and as the as the integral suggest, it is a cumulative distribution. So, this is the second distribution, that we have we have define.

In order to, avoid the confusion between the time t and this integral notation. So, let us call it just t prime. So, now, if I take derivative of this d F of t d t by integration formulas, we know, that this is nothing but E of t sorry E of t. So, the relationship between the cumulative distribution and exit age distribution is clear from this particular, particular notation.

Now, there is yet another another distribution which needs, we need to we need to define. Now, the very fact that we have now identified, that fluids spend different amounts of time in the, in the reactor, leads to the, to the fact that the quality of fluid inside the reactor is not same as the fluid which is coming out of the reactor; in terms of the amounts of time or ages of this fluid, fluid fractions. They must be somehow related, but it is not necessary that, this 2, this 2 are exactly, exactly same.

Or in other words the age distribution, if you look at what is happening inside the reactor, need not be same as the distribution that we observe at the exit of the exit of the reactor. And this, this introduces yet another another distribution, which is called internal age distribution. Internal age distribution I of t d t is nothing but the fraction of the fluid element, inside the reactor which has, age between t and t plus t plus d t. So, that is that is my internal age distribution.

And these are important for example, in fluidized bed reactor, where catalyst is let us said deactivating. So, the distribution of what is happening inside the reactor. We we will be of importance, because that is what will determine the reactor or how much reaction conversion has taken place and so on. So, how are these two quantities quantities related, that is internal age distribution and exit age distribution.

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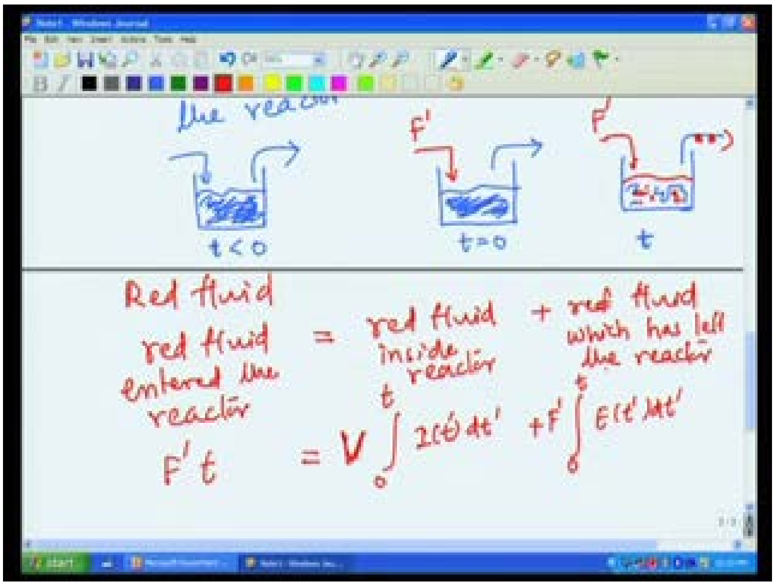

So, let us take an example, let us say that I have a reactor I have a reactor and this is filled with all fluid which is blue color, just for sake of sake of orbit. So, for time less than the starting time and therefore, we call times less than the starting time or t 0 or 0 to be simply put. So, suppose this is what is what is happening.

Now, let us say, that at time t equal to 0 time t equal to 0, we start putting in red fluid in this in this reactor, start putting in red fluid in this reactor, what was there in these reactor, the inside fluid was fluid was all blue. I will let us say start putting in this red color fluid. So, what will happen at some time greater than greater than 0, that is at some time down the, after the start up of these red fluid, what will happen? We are putting in we are putting in red fluid, but now inside the reactor inside the reactor, there will be some red fluid some red fluid along with my original blue fluid, which will be also coming out. So, what will be coming out will have both red and blue fluids.

So, let us try to see, how this situation can be can be described. So, what I am going to do is, I am going to take a balance on the red fluid balance on the red fluid, at time some time t and I am going to say that the flow rate of this fluid is F prime. So, at time t at time t, the red material which has entered the reactor, so between 0 to t up to time t, some red material has entered the reactor and what has happened to this red fluid? This must be the red fluid, which is inside the reactor plus the red fluid which has left the reactor, right, because these red fluid can go nowhere else. The fluid that has been introduced in the reactor either is found inside the reactor or it has already left the reactor through the exit exit exit stream.

So, if I say my F prime F prime is my flow rates so which is constant, then in time t how much of the red fluid have I have I send in, if F prime is the is the red, then F prime t is the volume of the fluid which I have introduced in my in my reactor

Now, what has what has happened to this fluid? If I say that of the fluid of the reactor reactor volume V. If I of t d t is the vocalized-noise fraction of the fluid having age residence or age between t and t plus d t, then up to time t, the total fraction of the red fluid which is inside the reactor will be given by, adding up all these fractions between time 0 to 0 to t, right.

Now, how much how much of this, how much of this fluid has left the reactor between between the time time d t, that will be given by if F prime is the is the flow rate and we have our cumulative age distribution, so the fluid element which has which has left the reactor up to time t is the cumulative cumulative age age distribution, right.

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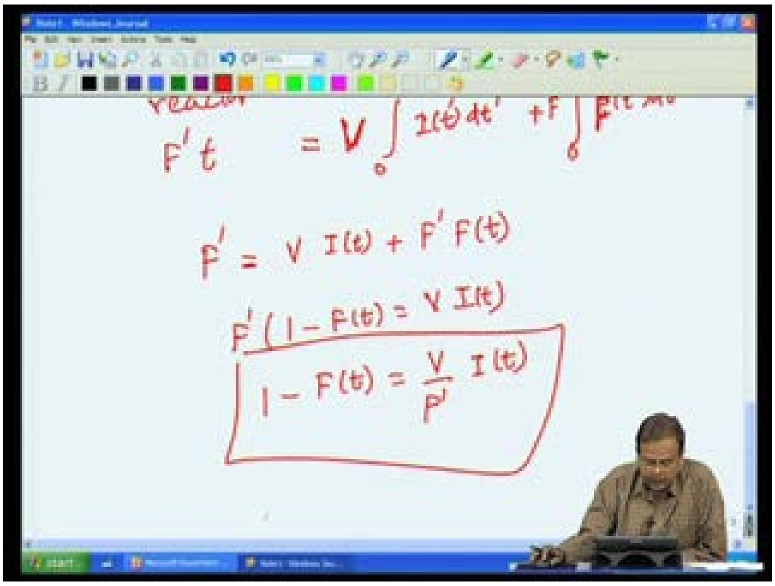

So, if I differentiate this, I get F prime equal to V of I of t, d t sorry not d t. So, if I differentiate these equation, what I get is, V into I of t plus F prime into F of F of t, they should be F of t. So, in other words we get F prime into 1 minus or or 1 minus F of t equal to V by F prime of I of I of t. So, that is the relationship between my different residence time and what is F of t, F of t I know is integral 0 to t E of t prime d t d t prime.

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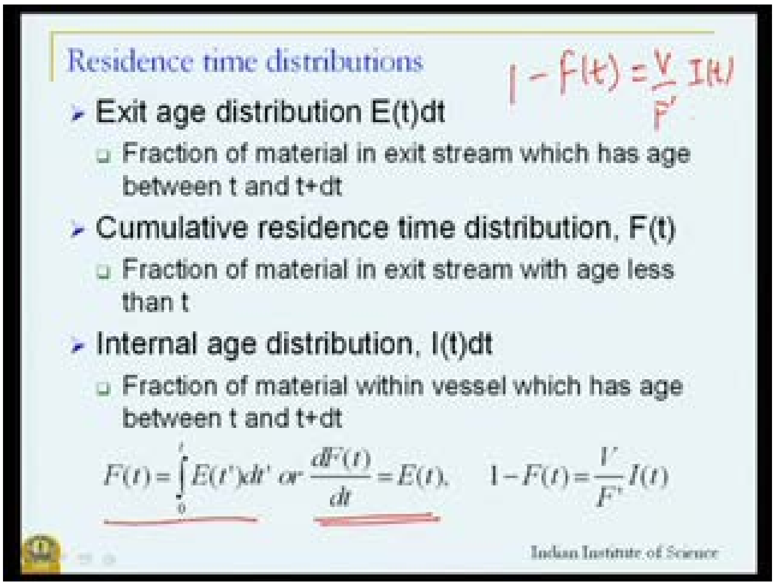

So now let us, let us look at some of the definitions, some of the properties and and and so on. So, going back to our our material or distributions, that we have already already seen, we say that exit age distribution E of t d t is nothing but the fraction of the material in the exit stream, which has age between t plus t plus d t and t plus d t. Cumulative age distribution F of t is the fraction of the material in the exit stream, which with age less than t and internal age distribution I of t d t is the fraction of the material within the vessel, which has age between t and t plus d t.

So, exit age and internal age two different quantities - one looking at the exit stream, another one looking inside the reactor, but these two are not independent of each other. Because fraction cumulative residence time distribution F of t is nothing but adding up all those fractions from time 0 to t. So, that is our relationship that is our relationship between the F of t and E of t or alternatively expressed in this particular form. And we also just now saw that 1 minus F of t is V by F prime into I of t. So, thereby internal age distribution and exit age distribution and cumulative residence time distributions are all related to related to each other.

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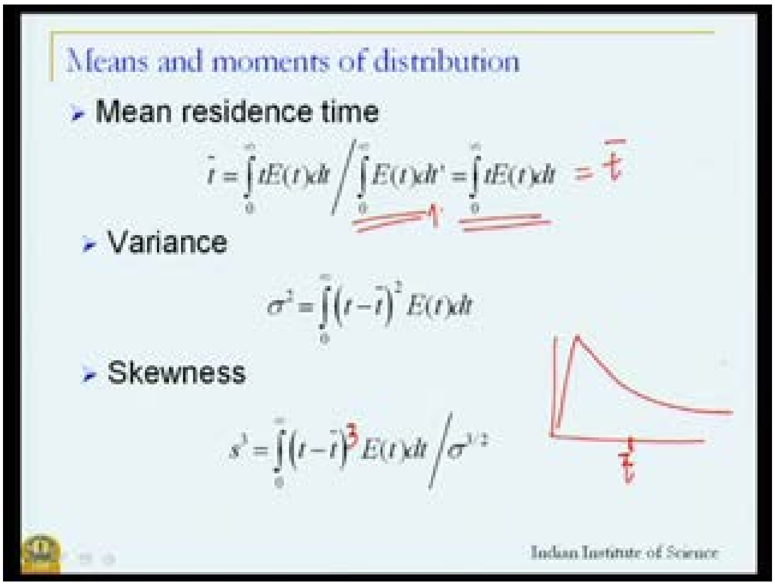

We will come to how we get these distributions in just few minutes, but let just continue this characterization of these residence residence time; and we have various the moment you have, we have distributions, we can characterize these distributions by looking at various moments of these distribution. The first moment the second moment and so on.

So, mean residence time for example, it is nothing but t into E of t d t, 0 to infinity divided by E of t prime, d t prime, again limit between 0 to infinity, but this quantity we earlier saw is nothing but 1. So, this is my mean residence mean residence time, the first moment of the distribution. Variance that is t minus t bar, that is mean residence time the whole square E of t d t, gives me the distribution around this around this mean and the skewness the skewness, this should read q, t minus t bar cube, E of t d t that is the third moment, divided by sigma raise to 3 by 2, that is s cube it tells us, whether the fluid is coming out much before, that is skewness as the as the term term indicate; for example, this is my mean residence time we will see the example, but if my distribution is something like this, that is lot of fluid is coming much before or whether it is coming, much after the mean residence time, it tells me the skewness.

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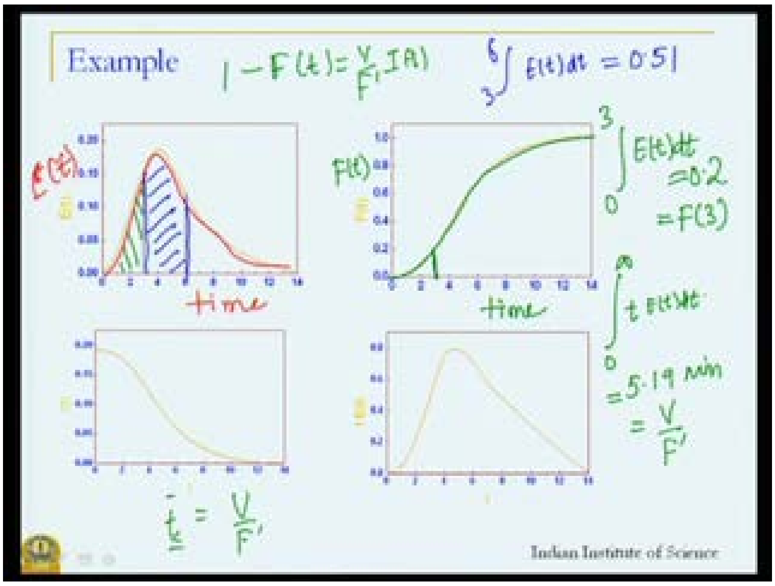

So, let us take an take an example and and look at look at, how we characterize this or what is meant by, so let us say that on x axis, we have time and on y axis, we have E of t. Our distribution that we were we were looking at and let us say that distribution is something like this.

So now, if we want to, for example, look at the area under this curve between time t equal to 3 to t equal to 6. So, this area under the curve or in other words, integral E of t d t between 3 to 6 which numerically for this distribution has a value 0.51, so what does it what does it mean? It means that 51 percent of the fluid elements come out of the reactor between times t equal to 3 to 6, whether it is minutes or seconds or hours is immaterial at this at this moment that will depend on what this time scale time scale is.

So, E of t, again E of t d t is the fraction having age between t and t plus d t. So, if I said the if I sum up all those fractions between time 3 minutes to 6 minutes which is, what is done when we integrate, it tells us what fraction of the fluid element has residence times between 3 minutes and and 6 minutes.

Now, in the same example, this area under the curve between 0 to 3 minute, shown in the green color, so 0 to 3 E of t d t, which here is roughly 0.2. So, what does it what does it tell us, it tells us that roughly 20 percent of the fluid element has residence time less than 3 minutes. Because I have added all those fractions between the times limit 0 and 0 and 3. This is nothing but my F of 3 that is F of t. So, if I if I integrate between 0 to 3, I get a value of F of 3, so on this plot I have time and F of t. So, at time t equal to 3 minutes the value is 0.2.

And then I can change these limit of 3 to 1 2 3 4 and generate, what we call the cumulative residence time residence time distribution residence time distribution. We had just now seen the relationship between I of t and F of t, namely 1 minus F of t is V by F prime I of t, now what is V by F prime? So, if we take this distribution and do this integral 0 to infinity; that is the first moment of these distribution and you know how to integrate numerically given these distribution, this works out to be 5.19, let us put some minutes, units, minute in this particular.

So, what does this what does this tell us? This tells us that the reactor for which we have got this distribution time like this, the mean residence time or the average residence time is 5 point 5.19 and it turns out that is nothing but V by F prime. So, if we know or t bar is nothing but V by F prime, so if we can experimentally calculate these distribution, then we can we can we can then, calculate what is, if we if we can calculate, the distribution we know, what is the mean residence time and then any of this quantity V or F prime if it is known, we can we can estimate that using this using this relationship

So, now let us let us try to find out, how do we experimentally determine these residence time distributions and for this, we have to do experiments naturally; and that is the whole idea, right. So, what kind of experiments experiments can we do? We can for example, introduce some tracer elements, so let us say that, this is my reactor and need not be stirred tank reactor, can be a tubular tubular reactor reactor as well.

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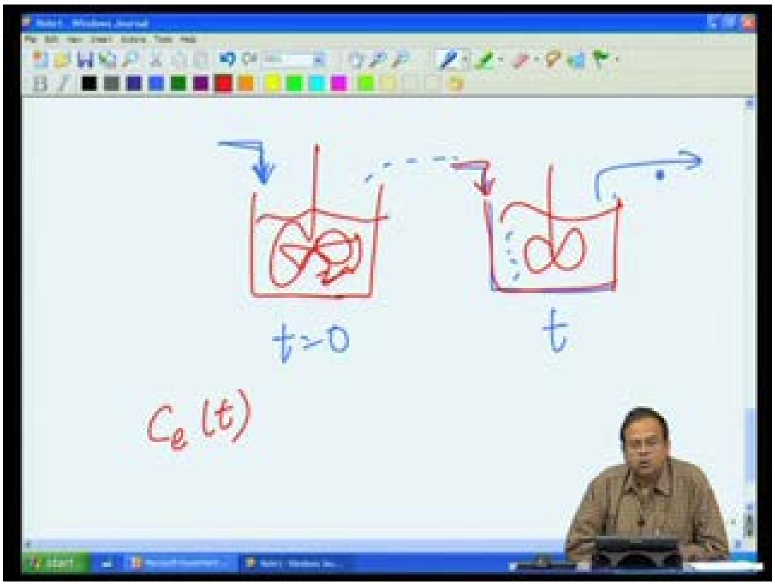

So, as we saw in the previous case, where we introduce red fluid or whatever, we can introduce a tracer at time t equal to 0; and then monitor the progress of this tracer at large longer times or times since, its entry and then calculate what fraction has come in and what is the concentration and so on. So, that is how we can determine the residence time, we need one more piece of information, we will come to that in just a minute.

What kind of tracer can we introduce there are so many, we can introduce a die, we can introduce a salt solution. Something which does not undergo any chemical transformation inside the reactor or something which does not undergo a physical adsorption onto the material of the of the reactor. So, the idea here is that you introduce a perturbation or tracer, which can be a die or which can be a salt solution or something which changes the p h and so on and so forth; or introduction of acid that is, such that this tracer does not undergo any chemical degradation or transformation in the reactor; or does not get adsorbed onto the material of the reactor.

Because we want to trace this tracer and if this tracer has disappeared for some reason, such which I mentioned just few minutes back, then we have lost our purpose of tracing this, because there is one more factors than, just the fluid moment inside the reactor, which will give us different kind of kind of. So, what kind of tracers in what manner can we can we introduce, we can introduce as a as a pulse or as a step input, now what is pulse and what is step input.

So, first of all let me, let us say that we have these reactor we have these reactor, which is which is colored fluid red or colorless or whatever and then as a 1 shot 1 shot experiment, we introduce a blue tracer at time t equal to 0; and then at longer times and then I stop it. So, I have this reactor in which, I have as a 1 shot introduce this blue material, so there will be some blue material here but later on I am not introducing anymore and I simply monitor for this blue material at longer times.

So, this was only 1 shot and I go back to whatever red or whatever was there, so 1 shot pulse experiment and step experiment is something which we saw earlier, that is I introduce introduce change the color from blue to blue to red or something like this and keep it red for all times beyond my starting point.

Now, when we do that, what do we what do we do, suppose, we are we are looking at concentration of this tracer in the exit, so we monitor the concentration of this tracer in the in the exit at longer longer times. Now, what do we expect will happen to this tracer? So, let us let us just let just look at, pulse and step are the general general tracers, that we put in a pulse manner or in a step as a step input.

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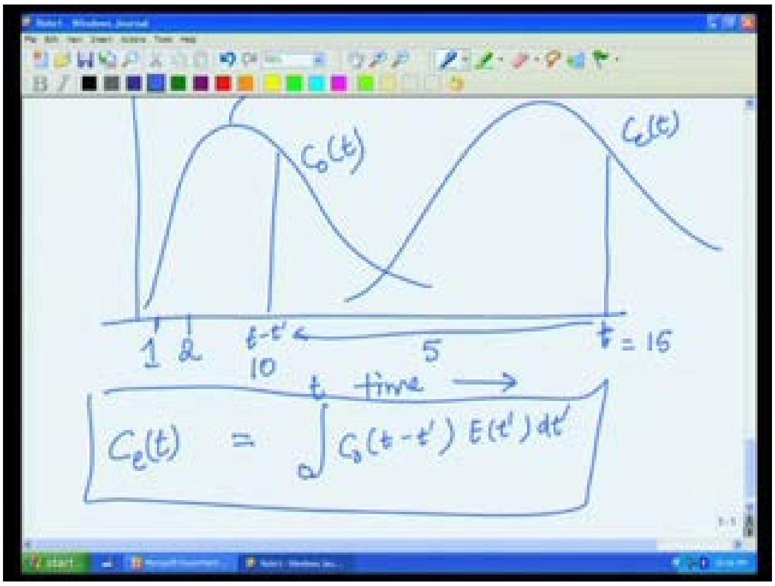

But let us consider a more general scenario; let us say that, this is our some kind of a input, so this is my input, which could be a function of function of function of time. So, I have time on on this axis. And after sometime, I mean the fluid starts coming out so let us say, that exit concentration profile is something like this. I am looking at what is the concentration at time t. So, this is my C e of t this is my C 0 or input, so I want to see, what is c E at time t and let me let me take a specific specific example, let us say that this time is some 15 minutes, time is some 15 15 minutes.

Now, what comes out at 15 minutes for example, would be what was putting at time t minus t prime, t prime is some sorts of some time or in other words what comes out at this 15 minutes is let us say what was putting at time t equal to 10; that means, I am putting my t prime 5. So, what was put in at time t equal to 10 and which has the residence time those fluid elements, all those fluid elements which had residence time of 5 minutes.

Or in other words, all the fluid element I mean, that is just one part, the fluid elements that, I will see or the concentration that I will measure at time t equal to 15, will consist of; what was put in, in the reactor 10 minutes, at time t equal to 10 minutes and which has stayed in the reactor for 5 minutes; or what was put in the reactor at 1 minute and stayed in the reactor for 14 minutes; or what was put at 2 minutes and stayed in the reactor for 10; or in general what was put in the reactor at time t minus t prime and has stayed in the reactor for t prime and what is that that fraction is E of t prime d t prime; and if I add up all these fractions from 0 to t, this is what I will see comes out of my reactor at any given time.

Once again, what I see, what comes out of the reactor at time t is what I have put in, in the reactor at time t minus some time t prime; and which has stayed in the reactor for time t prime or which comes out of the reactor after t prime.

So, for for example, for 15 minutes case the example which we saw, what comes out at 15 minutes is what material you put in at 1 minute and which comes out of the reactor after 14 minutes plus, what we have put in at 2 minutes and which comes out at 13 and so on. And so, forth up to fifteenth minute or in other words, these integral 0 to t c not of t minus t prime E of t prime d t is what gives us, what comes out of the reactor, so this is what gives us what comes out.

Now, we will we will stop here but in the next class or next session, we will see how we use these information to find out these residence time distribution; and how do we use these residence time distribution to decide on, what conversions we will get in our in our reactor. Thank you.