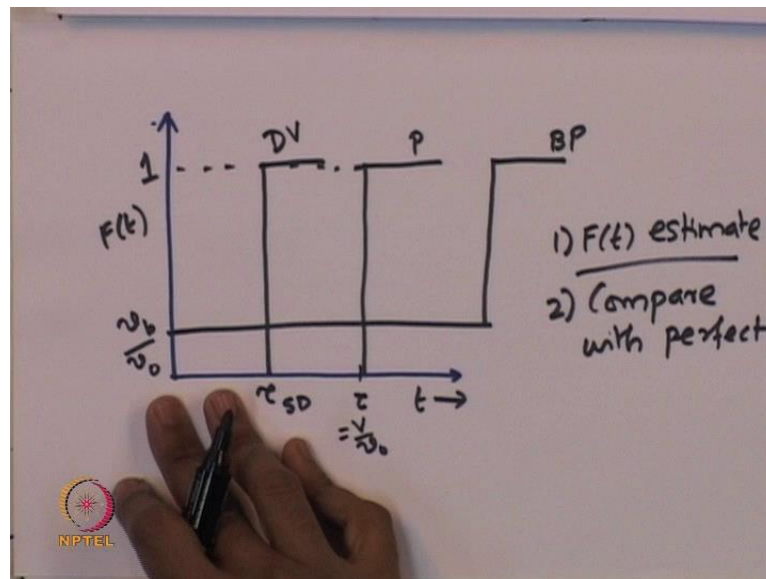


Chemical Reaction Engineering II
Prof. A K Suresh
Prof. Sanjay Mahajani
Prof. Ganesh Viswanathan
Department of Chemical Engineering
Indian Institute of Technology, Bombay

Lecture - 34
Modeling non-ideal reactors

Friends, in the last lecture we looked at different operations of CSTR and we stopped at what is the residence time distribution curve for different operations of a tubular reactor modeled as a plug flow reactor. Specifically, we looked at what is the residence time distribution if the plug flow reactor was operated under normal condition; that is if the residence time distribution is actually a delta function. And then we looked at what happens if there is a bypass in the reactor and then we looked at what happens when there is a dead volume in the reactor. So, now if we compare let us now compare the distributions of these three modes of operation for a tubular reactor.

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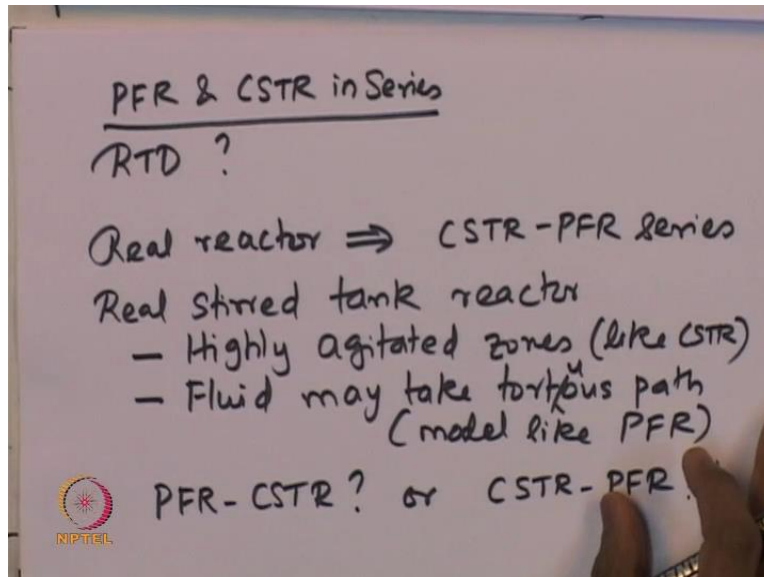
So, suppose if this is the time axis and this is f of t which is the f curve, and if it is a normal operation, then the f curve will start at the space time of the reactor τ which is essentially given by the volume of the reactor divided by the volumetric flow rate with which fluid is actually

flowing through the reactor and then it actually is a it looks like a step function and this is one. So, that is for the perfect operation. Now suppose if there is a bypass in the reactor, then what happens is that there will be a jump in the f curve. So, the jump will start at v_b by v_{naught} . So, that tells you the extent of bypass which is actually present in the reactor and then because the space time is now larger than the space time of the reactor if it was conductor under perfect operation or if there was no bypass.

Therefore, the fluid stream that enters the entry of the reactor is now going to take longer time to leave the reactor as compared with the perfect operations; therefore, the f curve will essentially look like this if it is a bypass operation if there is a bypass inside the reactor. And then if suppose there is dead volume which is present here, then the net volume which is available for net active volume which is available is for the fluid stream to access is actually smaller than the actually volume of the reactor. So, therefore the residence time the apparent space time of the reactor is actually going to be smaller than that of the space time of the plug flow reactor which is actually operated at a perfect condition.

So, therefore, the fluid stream leaves faster than the normal or perfect operation of the reactor. So, this is $\tau_s d$. So, the method is first one should actually estimate the f curve experimentally and compare with the perfect operation case. And this actually will provide a clue whether there is a bypass in the reactor or whether there is dead volume which is actually present inside the reactor. So, this is a story for the single CSTR and the single plug flow reactor. So, now let us look at the combination of reactors. So, we observed earlier that RTD function is actually used to model the real reactors as combination of ideal reactors. So, let us take a very simple example of combination of two ideal reactors.

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So, let us consider the plug flow reactor and CSTR in series. So, what will be the RTD function for this case? So, remember that the real reactors can actually be model as a combination of a plug flow and a CSTR, and let us assume that there is a real reactor which is actually modeled as a CSTR plug flows as a CSTR and plug flow operated in a series mode. Now when is it possible to approximate it as a CSTR plug flow series model? So, consider the situation of a real stirred tank reaction. So, one could intuit that there will be highly agitated zones which will be present in the real stirred tank reactor.

So, these zones will typically behave like a CSTR. So, they behave like a CSTR and then there will be situations where the fluid may take tortuous path before it actually leaves the reactor, so which means that it sort of behaves so that particular fluid stream which actually takes such tortuous path can actually be modeled like a plug flow reactor modeled like a PFR. So, this kind of a situation one can actually use a combination of CSTR and plug flow reactor in order to model the real reactor.

Now the question is what should be the order in which they should be combined? So, should it be CSTR that follows the plug flow reactor or it should be the plug flow reactor which follows the CSTR? So, when it is in series combination, question is which one comes first and which one comes later? So, let us analyze this by considering one by one.

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Consider CSTR-PFR

C_{A0}

CSTR τ_s C_{Ai} PFR τ_p C_A

- Pulse tracer
- CSTR output conc.
 $C_{Ai}(t) = C_{A0} \exp(-\frac{t}{\tau_s})$
- Output will be delayed τ_p

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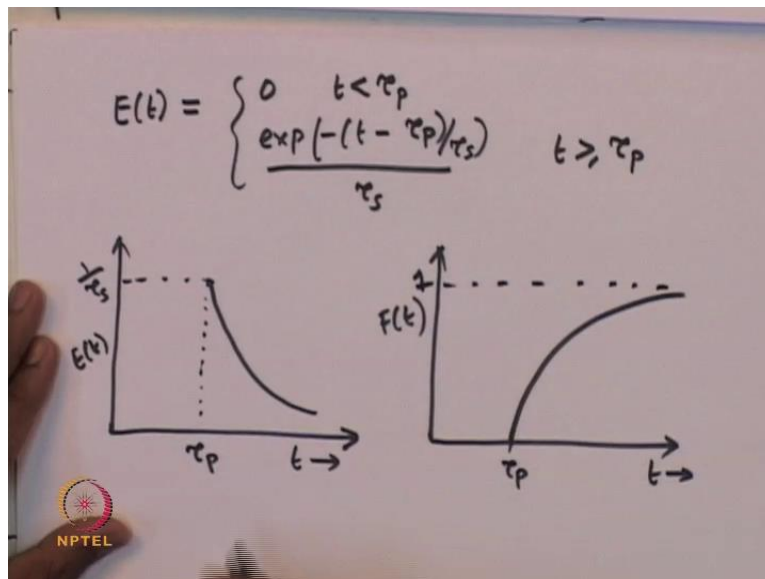
So, let us consider the first case of CSTR being the first reactor and the plug flow reactor follows the CSTR, CSTR followed by a plug flow reactor. So, suppose if there is a CSTR and let us assume that the concentration with which a certain tracer is actually flowing into the reactor is actually c_{A0} . Let us assume that there is some species and then if c_{Ai} is the concentration with which the species leaves the CSTR and remember that it is a CSTR, it is well mixed. Therefore, the concentration of the species inside the CSTR which is uniform because it is well mixed will be equal to the concentration of the species in the effluent stream.

And then now this is followed by a plug flow reactor and as it goes through the plug flow reactor, let c_A be the concentration of the species that actually leaves the plug flow reactor. Now if τ_s is the residence time of the CSTR and if τ_p is the residence time of the plug flow reactor, then let us say at the tracer that is introduced is actually a pulse tracer. Let us assume that it is a pulse tracer. The objective is to find the RTD function for this combination; eventually, the objective will be to find the conversion if these two reactor are actually operating in series mode. So, let us start with a pulse tracer to find out what is the RTD function.

Now we know that the CSTR output concentration we know what is the mole balance for the tracer; we have seen many number of times. So, the CSTR output concentration based on the mole balance is basically c_{Ai} by solving the mole balance was given by c_{Ai} as a function of

time that should be equal to c_0 into exponential of minus t by τ_s where τ_s is the space time of the CSTR. Now the output of the CSTR is actually fed into a plug flow reactor, and, therefore, it simply brings a delay in actually taking the species from the entry of the reactor to the exit of the reactor. So, therefore, the output from will be just delayed by the space time of the plug flow reactor τ_p . So, therefore, the output will simply be delayed by the space time of the plug flow reactor at the output of the plug flow reactor itself. So, therefore, based on these observations, we can actually intuit what is going to be the residence time distribution function E of t .

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So, the residence time distribution function will simply be because the output is now going to be delayed, there will be no output that will actually come out of the plug flow reactor till the residence time of the plug flow reactor which means that E of t is going to be zero for t less than τ_p , which is the space time not the residence time. It is space time of the plug flow reactor, and for other times, it will simply be whatever RTD function for the tracer that actually goes through the CSTR; that is simply delayed by the space time of the plug flow reactor. So, therefore, we know what is the RTD function for the CSTR; we simply have to introduce the delay of in the plug flow reactor that of the space time of the plug flow reactor.

So, therefore that will be equal to minus t minus τ_p which is the space time of the plug flow

reactor divided by τ_s which is the space time of the CSTR divided by τ_s and this is for τ greater than or equal to the space time of the plug flow reactor. So, that is the RTD function and so now we can simply plot this function. It will start at τ_p because the plug flow reactor is now going to introduce certain delay and this will be 1 by τ_s and there will be an exponential decay exponential fall. And then similarly we can draw the f curve.

And it will start at τ_p because the plug flow reactor is going to introduce certain delay and the delay is actually the delay time is equal to the space time of the plug flow reactor. And then there will be exponential increase in the f curve and goes all the way up to 1. So, that is the residence time distribution for CSTR followed by a plug flow reactor. Now let us look at the other option where the plug flow reactor comes first and the CSTR comes later.

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PFR - CSTR Series

→ PFR → CSTR →

- Pulse enters PFR
- Delay by τ_p
- Appears at CSTR entry.

RTD:- $E(t) = \begin{cases} 0 & t < \tau_p \\ \frac{\exp(-(t-\tau_p)/\tau_s)}{\tau_s} & t \geq \tau_p \end{cases}$

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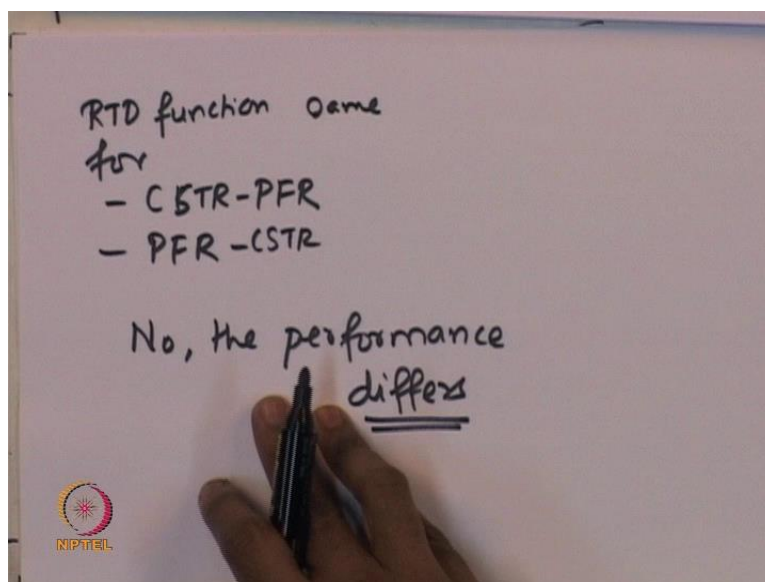
So, let us look at the PFR CSTR which actually follows the plug flow reactor. So, the depiction is you have a PFR and then there is a CSTR and there is the final outlet stream actually comes from the CSTR. So, the pulse first enters the plug flow reactor and then pulse when enters the plug flow reactor because of the nature of the plug flow reactor, there is simply a delay of the delay time or space time of the plug flow reactor is actually introduced. So, there is a delay by the space time of the plug flow reactor and then after this delay, the tracer actually appears as the entry of the CSTR and then it follows the CSTR the residence time distribution function of the

CSTR.

So, the RTD function can simply be $e^{-t/\tau}$. So, nothing is going to appear till the space time of the plug flow reactor reach because from the RTD function of the CSTR, the e -curve starts from time t equal to zero; that is the tracer will actually appear start appearing immediately after the tracer is actually pulse treasure is fed into the CSTR. But because it is presented in series, the delay that is introduced by the plug flow reactor of the time period of the space time of the PFR that will actually be the delay in the overall residence time distribution function as well. So, therefore, there will be no output in the plug flow reactor CSTR see this combination till the space time of the plug flow reactor reached.

And after that, it will simply be the residence; this will be controlled by the residence time of the CSTR. So, therefore, the residence time function will be $e^{-(t-\tau_p)/\tau_s}$ where τ_s is the space time of the CSTR, and this is for t greater than or equal to τ_p . So, what one can clearly see is that if you compare the residence time function of the plug flow reactor and CSTR which is appearing in series with the residence time function of the situation of the CSTR and the plug flow reactor that is the plug flow reactor follows the CSTR. So, this is for CSTR and plug flow reactor actually follows the CSTR. These two residence time functions are exactly one and the same.

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So, therefore, what one can actually observe is that the RTD function is same for CSTR followed by a plug flow reactor in series and plug flow reactor followed by a CSTR. So, it does not matter what quarter in which the CSTR and the plug flow reactor are placed, the residence time function of the series combination that is CSTR and plug flow reactor will continue to be the same. Now does it mean that the properties of this combination are same, so no; that is not true actually. The properties will not be same; in fact, the performance actually differs significantly and it completely depends upon what is the order in which the CSTR and the plug flow reactor combination is actually placed.

So, therefore, RTD function being same for both reactors does not necessarily mean that the performance of these two reactors will be same. So, in fact, in this case, the performance will be different. First order reaction case is actually an exception; only for first order reaction, the conversion will be same irrespective of the order in which the two reactors that is CSTR and PFR are actually placed.

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II order reaction
 $A \xrightarrow{R} P$

C_{A0}
 v_0 → [CSTR] → C_{Ai} → [PFR] → C_A
 τ_s τ_p

Mole balance for CSTR
 $v_0(C_{A0} - C_{Ai}) = kC_{Ai}^2 V$ $v_0 \Rightarrow \text{const.}$
 $\Rightarrow \tau_s k C_{Ai}^2 + C_{Ai} - C_{A0} = 0$
 $\Rightarrow C_{Ai} = \frac{\sqrt{1 + 4\tau_s k C_{A0}} - 1}{2\tau_s k}$

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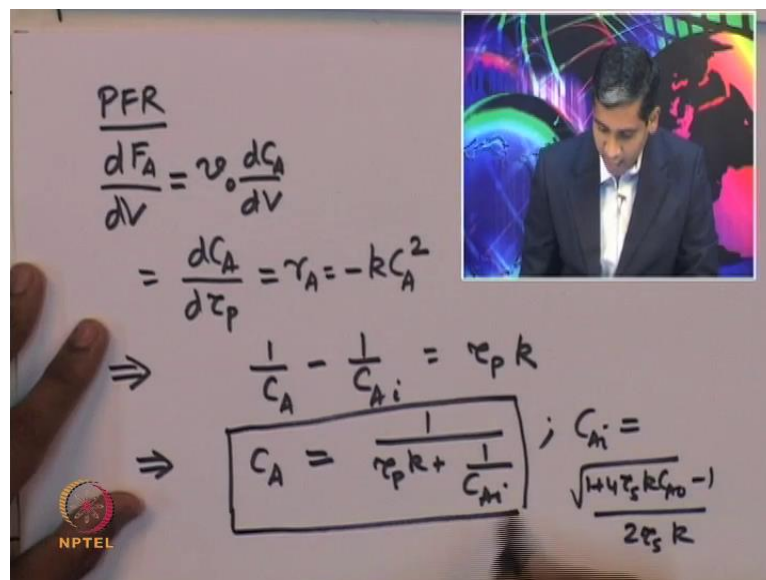
So, let us take an example of that, so let us take a second order reaction; let us take a second order reaction of a going to products and the corresponding specific reaction rate is k. And so now this can be depicted as so let us consider the combination of CSTR followed by a plug flow reactor. So, if c_{a0} is the concentration of the species fed into the CSTR and if c_{ai} is the

concentration with which the species leave the CSTR and if c_a is a concentration with which the species actually leaves the plug flow reactor and the space time of CSTR and plug flow reactor not τ_s and τ_p .

So, now we can write a mole balance; write a mole balance for CSTR and the mole balance is that v naught into c_a naught minus c_a i. So, that is the rate at which the species actually enters the reactor and this is the molar rate at which the species actually leaves the CSTR, and that should be equal to k into c_a i square into v , where this is the rate at which the species a is actually consumed multiplied by v which is the volume of the CSTR. So, simply by dividing this by v naught which is the volumetric flow rate? So, volumetric flow rate with which the fluid is actually entering the combination of reactors; so if we assume that v naught is constant if we assume that the volumetric flow rate is constant, then we will find that this equation can be simply written as τ_s into k into c_a i square plus c_a i minus c_a naught equal to zero.

So, that is a quadratic equation c_a i c_a naught is the measurable quantity which is known and τ_s is again a measurable quantity. So, from this, we can solve this quadratic equation and we will find that c_a i is given by square root of 1 plus 4 τ_s into the specific reaction rate multiplied by c_a naught minus 1 whole divided by two times τ_s into k . So, that is the concentration of the species that actually is in the effluent stream that is leaving the CSTR.

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The image shows a handwritten derivation on a whiteboard for a Plug Flow Reactor (PFR). The equations are as follows:

$$\begin{aligned} \text{PFR} \\ \frac{dF_A}{dV} &= v_0 \frac{dc_A}{dV} \\ &= \frac{dc_A}{d\tau_p} = r_A = -kC_A^2 \\ \Rightarrow \frac{1}{C_A} - \frac{1}{C_{A_i}} &= \tau_p k \\ \Rightarrow C_A &= \frac{1}{\tau_p k + \frac{1}{C_{A_i}}} \end{aligned}$$

Next to the boxed equation, the initial concentration C_{A_i} is given by:

$$C_{A_i} = \frac{\sqrt{1 + 4\tau_p k C_{A_0}} - 1}{2\tau_p k}$$

The NPTEL logo is visible in the bottom left corner of the whiteboard image.

So, now let us write similar mole balance for the plug flow reactor. Let us write the mole balance for plug flow reactors; so, that is given by dF_A , F_A is the molar flow rate of the species that is flowing into the plug flow reactor divided by dV which is the V is the volume of the reactor that should be equal to $v_0 \frac{dc_A}{dV}$. And that is equal to dC_A by $d\tau_p$ assuming that the volumetric flow rate is constant and τ_p is the space time which is the volume of the reactor divided by the corresponding volumetric flow rate. And that should be equal to r_A , which is $-k c_A^2$. So, that is the mole balance, and by solving this, we can actually obtain that the solution of this equation is $1 - k \tau_p c_A$.

That should be equal to the space time of the plug flow reactor multiplied by the specific reaction rate. So, from here, we can see that c_A can actually be expressed as $1 - k \tau_p c_A$ where c_A is essentially given by c_A is given by the quadratic function that we actually derived a short while ago. This is the concentration with which the species actually leaves the CSTR. So, that is actually given by square root of $1 + 4 \tau_p k c_{A0}$ minus 1 divided by $2 \tau_p k$. So, that is the specific reaction rate. So, this is the concentration of the species that actually leaves the plug flow reactor.

Now we want to compare the performance of the combination of CSTR and plug flow reactor where the plug flow reactor follows the CSTR and the other combination where the CSTR actually follows the plug flow reactor. Now we found that the residence time for these two are same, and we are attempting to find what is the conversion of the species for a second order reaction for both these combinations.

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PFR - CSTR

$C_{A0} \xrightarrow{\text{PFR}} C_{Ai} \xrightarrow{\text{CSTR}} C_A$

PFR $\therefore \frac{1}{C_{Ai}} - \frac{1}{C_{A0}} = \tau_p R$

$\Rightarrow C_{Ai} = \frac{1}{\tau_p R + \frac{1}{C_{A0}}}$

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So, let us now take the second combination where the CSTR follows the plug flow reactor and the depiction is c_a the concentration which we see species actually enters the plug flow reactor and if v is the corresponding volumetric flow rate, so that is the plug flow reactor and c_{ai} is the concentration with which the species actually leaves the plug flow reactor and then it enters the CSTR. And c_a is the concentration with which the species actually leaves the concentration of the species in the effluent stream of the CSTR. So, now from the plug flow reactor mole balance, we can find that $\frac{1}{c_{ai}} - \frac{1}{c_a}$ that should be equal to the space time of the plug flow reactor multiplied by the corresponding specific reaction rate. So, from here, we can estimate that c_{ai} is equal to $\frac{1}{\tau_p k + \frac{1}{c_a}}$. Now from the CSTR mole balance, we can actually find that from the mole balance of the CSTR.

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CSTR

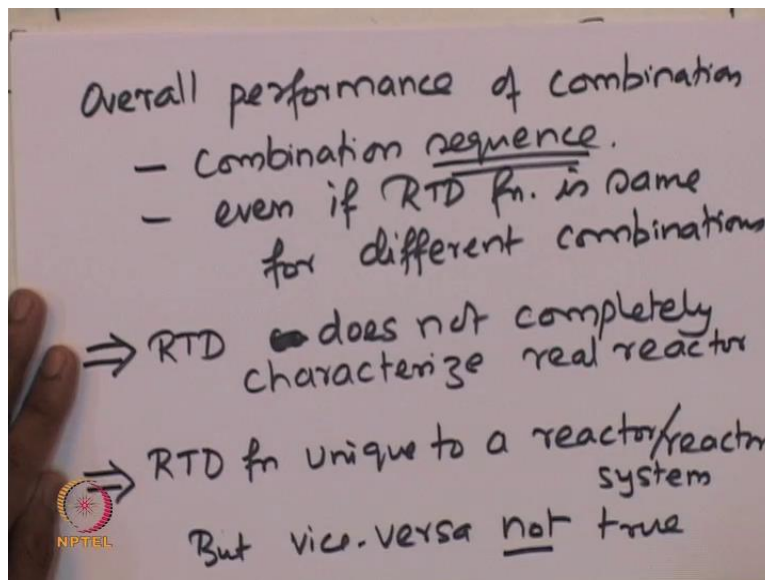
$$C_A = \frac{\sqrt{1 + 4\tau_s k C_{Ai}} - 1}{2\tau_s k}$$
$$C_{Ai} = \frac{1}{\tau_p k + \frac{1}{C_{A0}}}$$

Performance depends on how the CSTR & PFR are combined

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We can actually find that c_a is equal to square root of $1 + 4\tau_s k$ into c_{ai} minus 1 divided by two times τ_s into k , so where c_{ai} is actually given by 1 by τ_p into k plus 1 by c_{a0} . So, clearly, the expression that you get for the concentration of the species that is actually leaving the CSTR if there is a plug flow reactor which is preceding the CSTR is completely different from the expression that you get for the situation where the plug flow reactor actually follows the CSTR. So, what it suggests is that the performance of the reactor depends on how the CSTR and plug flow reactor are combined. So, it is important how they are combined, which means that whether CSTR appears first or CSTR appears later actually matters when we actually estimate the performance of the combination of reactors.

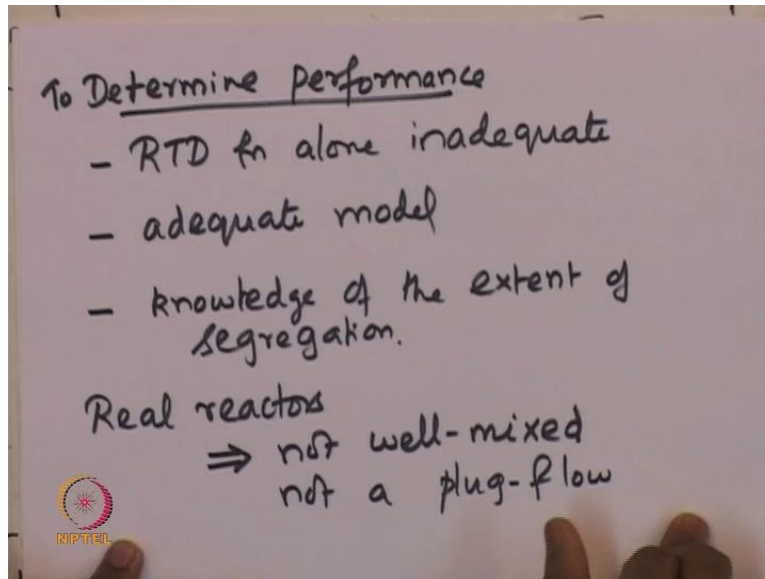
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So, therefore, this clearly suggest that the overall performance of the combination of reactors depends on overall performance of combination reactors actually depends on the combination sequence and not just the combination even if it depends on the combination sequence even if the RTD is the same. So, even if the RTD function is same for different combinations, the overall performance of the combination actually depends on the actual sequence in which the reactors are actually placed. So, this clearly shows that RTD function actually do not completely characterize the RTD; RTD does not completely characterize the real reactor situation.

In fact, it only says what is the nature of the residence time distribution, and it cannot directly tell what is the actual overall performance of the reactor? In fact, additional piece of information is actually required, and this also suggests that RTD the residence time distribution function is unique to a reactor slash reactor system combination reactor system, but vice versa is not true. That means that the reactor per reactor system is not unique to a given RTD whereas a RTD can actually be unique to a given reactors slash reactor system. And what we demonstrated just now is that depending upon the combination in which it is placed, the overall performance could be different, but both combinations have exactly the same RTD function. So, now what all this points to is that in order to determine the performance of the non-ideal reactor which is the original objective of the whole topic of residence time distribution is.

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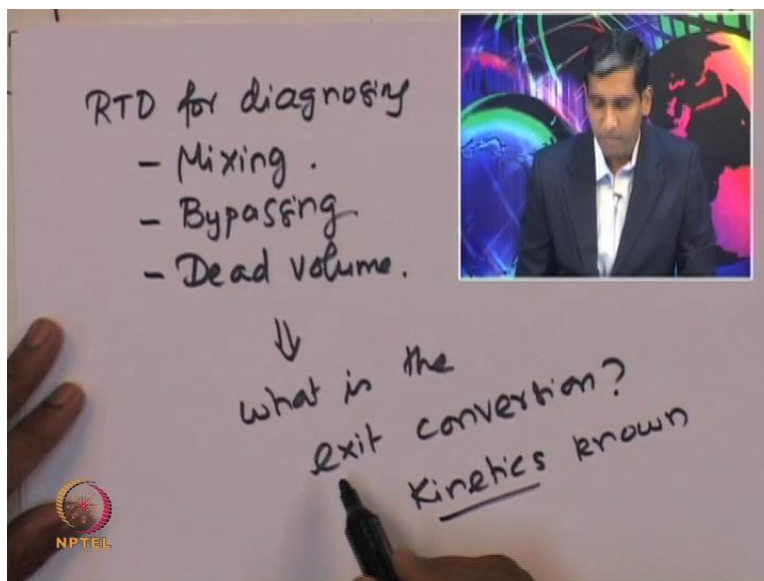
To determine the overall performance, one needs to know what is the RTD? But RTD function alone is insufficient; RTD alone is inadequate. In fact, one needs to know additional piece of information if one need to characterize or one needs to find out what is the performance of a real world reactor. So, in addition to RTD, adequate model of the non-ideal reactor is required; one each to know what is the appropriate or the correct model of the non-ideal reactor without which the performance can actually not be estimated. So, just the RTD function is alone not adequate; one needs to know what is the adequate model.

And in addition to that more importantly even if the model is known, the knowledge of the extent of segregation needs to be known, which means that what is the degree of mixing of the fluid elements inside the reactor; that information or that knowledge has to be available in order to estimate the overall performance. So, what all this points do is that, simply knowing the RTD function is insufficient; there is clear need for adequate model in addition to the RTD function and more importantly what is the degree of mixing or what is the extent of mixing of fluid elements inside the reactor that needs to be known, and that is what we will see for the next few lectures.

So, now in real reactors, the real reactors are actually not very well mixed; they are not very well mixed. And, in fact, they do not even behave like a plug flow. So, so far we have seen in the first

course of reaction engineering and also in this second course of reaction engineering, there are actually CSTR models and what happens is there is different order reaction in CSTR. What happens if it is in a plug flow, but unfortunately it turns out that the real reactors are not well mixed and they do not behave like a plug flow, so which means that one needs to come up with the various different kinds of approach; a different approach in order to model the non-ideal reactor in order to estimate the performance of such real world reactors.

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So, we know that the residence time distribution function is actually used for diagnosing various aspects of the non-ideal reactor. For instance, RTD for diagnosing the extent of mixing and we will look at it in a little bit more detail in this lecture and in the next lecture, and then it is also used for deducing bypassing in the reactor if it is present. And it is also used for deducing dead volume once again if it is present, but it does not give any clue about what is the conversion of the species which may be undergoing a certain type of a reaction; maybe it is a first order, maybe it is a second order or some other type of kinetics.

So, it does not tell us what is the so the question is what is the exit conversion; what is the exit conversion of the species? So, can we use RTD to actually find out what is the exit conversion? And suppose let us assume that the kinetics of a particular reaction is known, then are there methods or are there ways by which we can use RTD function which is used for diagnosing

various aspects of the functioning of the reactor, but can we extend that and do something, develop a method in order to estimate what is the exit conversion of a particular species. So, the next topic that we are going to look at starting from this lecture is actually going to be predicting the conversion of a real reactor.

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Predicting Conversion
RTD + Model + kinetics
⇒ Exit conversion

- Different models available.
- Zero adjustable parameters models
- Segregation model
- Maximum mixedness model.

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So, predicting conversion actually has a strong impact. So, knowledge of conversion of a particular reaction actually has a strong economic impact because the design of things surrounded can actually be planned accordingly, and therefore if one is able to predict the conversion, it actually goes a long way in terms of designing the reactor and designing other process which is associated with this particular with the reaction of interest. And this has strong economic implications for the industry which is actually involved in conducting that reaction and generating synthesizing a certain required product certain desired product.

So, let us look at how to predict conversion if we know what is the residence time distribution function. So, there may be two reactor systems which have same RTD functions, but will it be possible to estimate the conversion in these two reactors even if the RTD functions are same. And the answer is yes, it is possible, and there are methods to do this. So, the information that one needs to know is of course one need to know what is the RTD function and one needs to know what is the model that represents the non-ideal reactor that captures the process which are

occurring inside the non-ideal reactor or real world reactor. And one needs to know what is the kinetics of the reaction that is actually being conducted inside the reactor.

So, if we know this, then one can actually devise methods to find out what is the exit conversion of the species. So, there are different models which are available. So, in the next couple of lectures, we are going to look at a couple of these models and other models will actually be dealt with in some other future lectures. So, first we are going to look at the zero adjustable parameter models, and these are essentially two types of models. The first one is called the segregation model and the second one is the maximum mixedness model. So, we are going to look into details of these two types of models to predict the conversion of a real world reactor. So, the residence time distribution, what does residence time distribution function give?

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The slide contains the following text:

RTD fn.

- Info about time
- No info abt mixing
 - Exchange of ma
 - Controls reactor behavior.
- I order rxn. \Rightarrow RTD enough

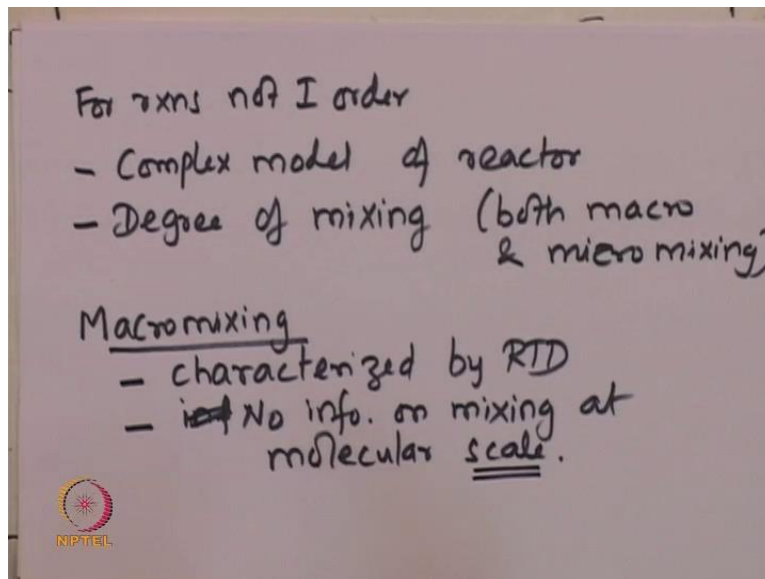
Not true for other kinetics.

The slide also features an NPTEL logo in the bottom left corner and a small video inset in the top right corner showing a man in a dark suit and white shirt speaking.

What does it give? It actually gives information about time spent by various fluid elements inside the reactor, but it does not provide any information about the mixing. There is no information about the mixing of the fluid elements inside the reactor. Now what is mixing? Mixing is essentially it is the exchange of molecules or matter which is actually in the fluid stream. So, the exchange of matter between different sections of the fluid stream is what is called as mixing and what does it do, why is mixing so important? Because it actually controls the behavior of the reaction, and it actually strongly controls the conversion of that particular reactant in the reactor.

So, it actually controls the reactor behavior. It has strong implications on the performance of the reactor, and now an exception to this is that the first order reaction is actually a special type where only RTD information RTD function is actually enough to predict the conversion. And in fact, we will see in one of the future lectures that how is it that the first order reaction for a first order reaction just the knowledge of RTD function is sufficient to predict the conversion, and what is the reason why this is the case? And this is not true for other kinetics. So, the degree of mixing is actually the information about the degree of mixing is actually required for all other kinetics other than the first order reaction. So, for reactions which are not first order.

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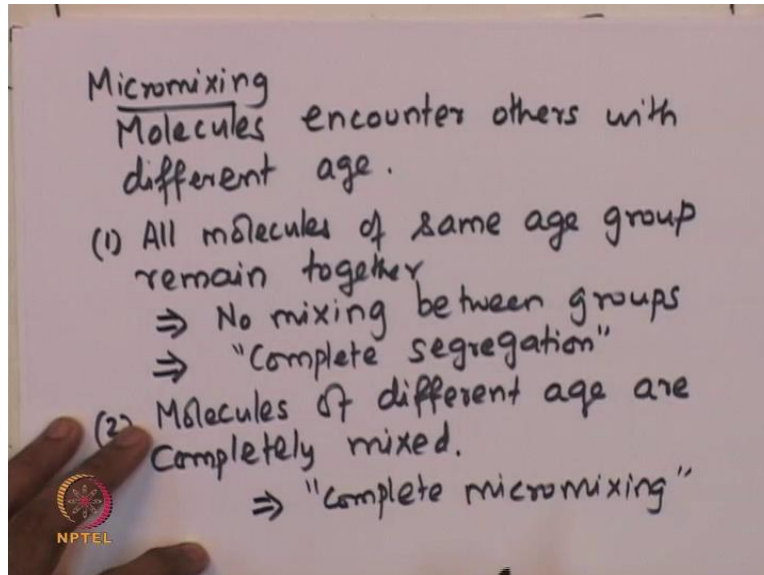
For reactions which are not first order, what is required is actually a complex model of the reactor. So, reactions which are not first order, the complex model of reactor is required. The complex model of reactor is actually required to predict the conversion of the species which is undergoing the reaction. And also in addition to that, the degree of mixing both macro and micro mixing information is required. So, these terms macro and micro mixing will actually be defined in a short while. So, let us first look at the macro mixing. So, there are two types of two levels of mixing; one is the macro mixing and the other one is the micro mixing.

See macro mixing is essentially is the extent of mixing which is actually characterized by the RTD function itself. So, that is it is characterized by the RTD function the residence time

distribution function and an important aspect of macro mixing is that the information about mixing at the molecular scale is actually does not occur if the fluid is actually under a macro mixing state. So, the no information on mixing at molecular scale; now it is important to pay attention to what the scale means here. So, remember that the fluid particles fluid elements which are actually flowing through the reactor essentially consist of atoms and molecules.

So, now there may be interactions and exchange of matter at the molecular scale, and in other extreme, there may be a situation there may be lumps of molecules which actually do not interact with each other. So, there are different scales which are actually present inside; the microscopic scale is where the molecule we look at what is the interaction or how one molecule of this species, it encounters another molecule which is actually present next to it. So, that is the microscopic scale and the macroscopic scale is actually a situation where the microscopic scale is actually completely ignores or the information is not available. So, let us next look at what is micro mixing; let us define micro mixing.

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So, micro mixing that describes how molecules encounter others with different age. Now suppose we consider a reactor where there is some fluid which is already present inside the reactor and then there is a new set of fluid elements which are actually flowing into the reactor. Now the age that is the time that is spent by the fluid particles which is only present inside the

reactor is now going to be larger than the time that is actually spent by the fluid which is freshly entering into the reactor; so, now the question is how these molecules which has spent a larger time inside the reactor, how do they encounter when a fresh set of particles are actually fresh set of fluid elements are actually pumped into the reactor?

So that the aspect which actually characterizes this is what is the micro mixing where we look at how molecules encounter other molecules which are actually having a completely different age or the time they have spent inside the reactor is different from the ones which are actually entering afresh into the reactor. So, now there are two aspects associated with micro mixing. The first aspect is when all molecules of same age group remain together. So, irrespective of how the molecules actually are flown inside, those molecules which actually spent certain amount of time; they all remain together and freshly entering molecules that is new set of molecules which are currently entering the reactor. They also cling together, and they all remain together.

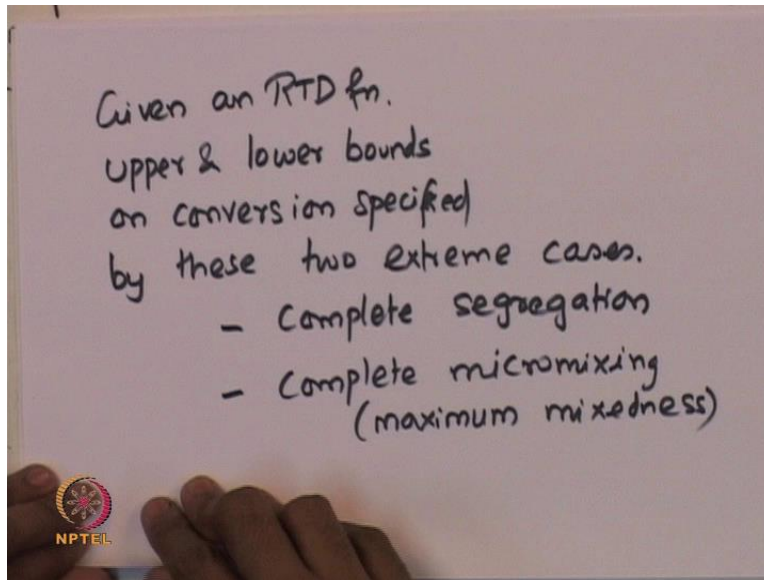
So, the first state of micro mixing is the situation where all molecules of same age, they are actually remaining and they are glued together in one group. So, this kind this actually means that there is no mixing between groups and this situation or the state of the fluid where there is no mixing between groups is what is called as a complete segregation system, where fluid particles of different age are actually completely segregated and they are actually not interacting between each other. The second situation is where molecules of different age are completely mixed.

So, consider a situation where there is a reactor in which the fluid is already present and then there is new set of fluid particles are actually added into the reactor. So, therefore, now the reactor is now having fluid particle which are of different age and so these fluid particles which are actually pumped in afresh, they actually interact with the they are actually encountered by the fluid particles which are actually already present in the reactor. And so, therefore, these two systems they mix with each other, and they get completely mixed. So, therefore, one cannot virtually distinguish where the particles of which has a higher age is actually located as compared with the particles which are actually freshly pumped into the reactor.

So, that kind of a situation is what is called as a complete micro mixing. So, these two states of complete segregation and complete micro mixing, they have strong implications on the

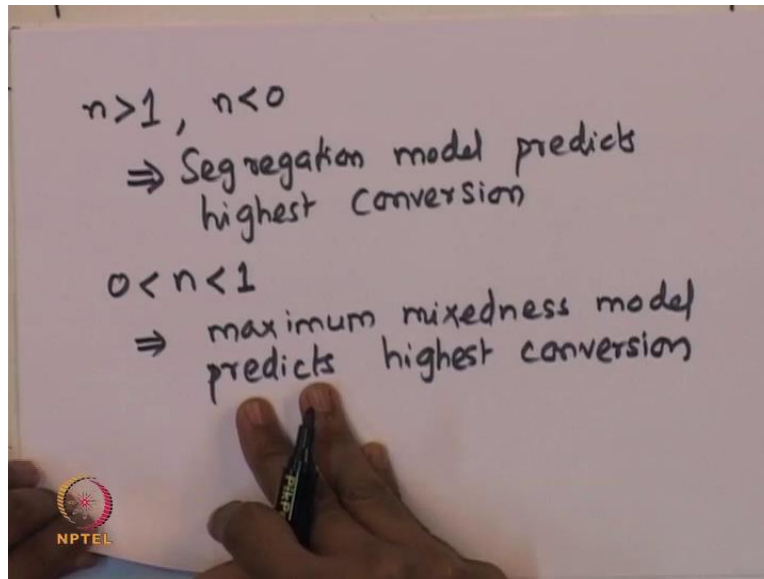
performance of the reactant. Now for a given residence time distribution function, so remember that the residence time distribution it only characterizes the macro mixing inside the reactor. For a given residence time distribution, the upper and the lower bound of the conversion that is actually achieved in the reactor is controlled by these two limits of micro mixing that is the complete segregation and the complete micro mixing.

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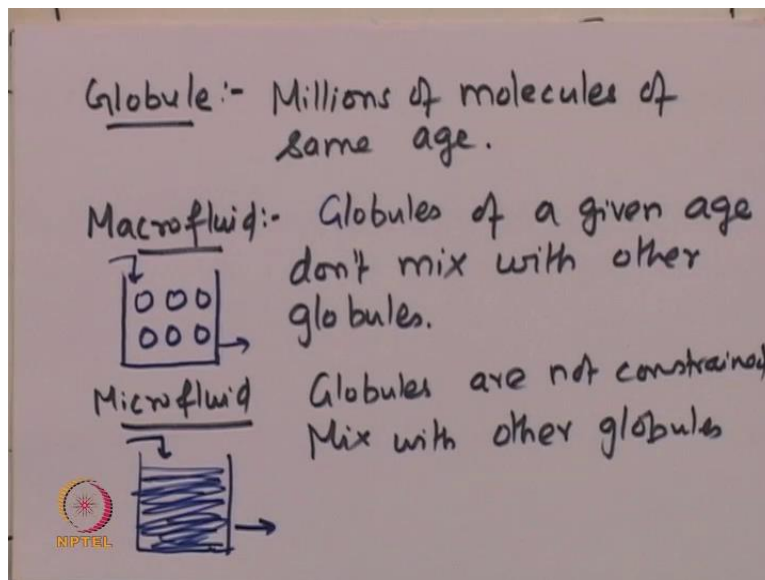
So, for a given RTD function for a real reactor, the upper and the lower bound conversion actually are specified by these two extreme cases that is complete segregation and complete micro mixing. So, the complete micro mixing is also called as maximum mixedness. So, the two zero adjustable parameter model is essentially the model that corresponds to the complete segregation and the other model corresponds to the maximum mixedness sample. So, how do we incorporate this aspect of complete segregation and complete micro mixing in the reactor model and combine that with the RTD function is what is going to be the next step which is the next step towards predicting the performance of a real reactor.

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Now suppose if n is larger than one that is the order of reaction; n here stands for the order of reaction. So, if the order of reaction is greater than 1 or if the order of reaction is less than 0 that is if a negative order reaction, then it turns out that the complete segregation model predicts highest conversion. On the other hand, for reaction orders between 0 and 1 that is even for partial fraction ordered reactions, it turns out that the maximum mixedness modeled predicts highest conversion. So, now there are a few definitions that we need to define before we attempt to consider the segregation model in the maximum mixedness model.

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So, the first one of the definition is what is a globule. So, a globule is basically a group of molecules millions of molecules which are actually essentially of same age. So, basically it is millions of molecules of same age. So, that is what is a globule and then a macro fluid. A macro fluid is essentially the one where the globules of a given age, the actually do not mix with the other globules. So, in a reactor, suppose there is fluid which is already present and it consists of many different globules and each of these globules will actually have contained millions of these molecules all of which are actually of same age.

Now macro fluid is one where the fluid in which these globules which are actually distinctly and independently represent and they do not interact with each other, and that is what is called as a macro fluid. So, let us look at what macro fluid; it is a globule of a given age. They do not mix with other globules which means that these are essentially non-equalizing globules and so one can actually visualize this as suppose if there is a reactor and there may be globules which are actually present here. And these globules will continue to maintain their identity, and they will not interact with each other.

Now on the other definition is another type a fluid is the micro fluid where the globules are not constraint. They are not constraint, and in fact, they can freely mix with any other globules which are actually present inside the reactor. So, they mix with other globules which means the

molecules present in one globule actually moves to other globule and there is exchange of molecules between different globules. So, this can actually be depicted as suppose if there is a reactor, then if the fluid that is present inside the reactor is a micro fluid, then one can actually virtually not distinguish between the particles which are actually of different ages. So, they will all be present together. They will all be completely mixed inside the reactor. So, this is the inlet steam and the effluent steam. So, the fluid which is present inside is now going to be mixed and so one will not be able to identify the globules independently.

So, let us summarize what we have learnt in this lecture. We have looked at what is that we compared the residence time distribution for a plug flow reactor that is operated in different conditions and then we looked at the combination of plug flow and CSTR in series mode. And we observed that the residence time distribution function is the same whether the plug flow reactor appears first or the CSTR appears first; however, the performance of these two reactors combination, performance of the combination of plug flow and CSTR depends upon which one comes first; whether the plug flow or the CSTR comes first and the other reactor follows the first one.

So, this we demonstrated for second order reaction and then we observed that this example sort of suggest that the residence time distribution function is not sufficient to actually predict the conversion or the performance of the non-ideal real world reactor. And additional piece of information such as a model and also the knowledge of the extent of mixing is actually required in order to predict the performance of the reactor, and so we looked at different types of mixing that is the macro mixing and the micro mixing and introduced certain definitions, and we will continue from there in the next lecture.

Thank you.