Chemical Reaction Engineering - II
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Module - 12
Lecture - 58
Modelling Non-Ideal Reactors II

So, we know that the R T, residence time distribution function is actually used for diagnosing various aspects of the non-ideal reactor.

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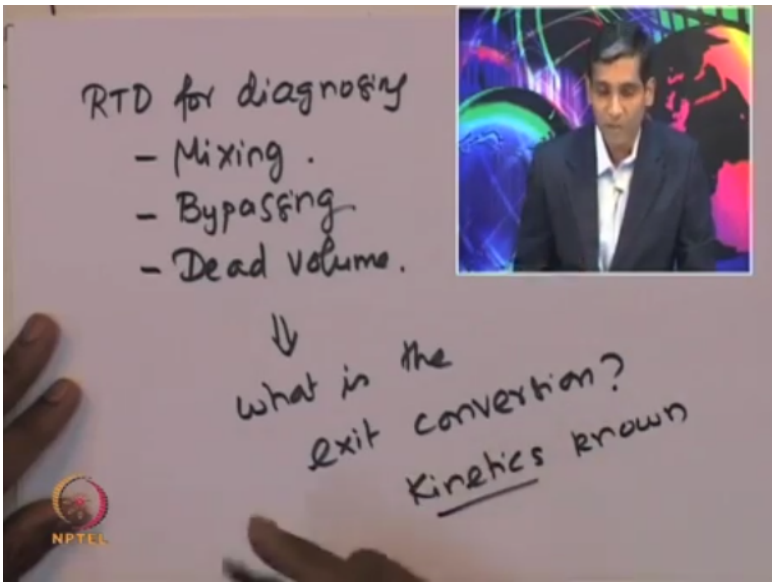

For instance, RTD for diagnosing the mixing, extent of mixing. And we will look at it in a little bit more detail in this lecture and in the next lecture. And then, it is also used for detecting bypassing in the reactor if it is present. And it is also used for detecting dead volume once again if it 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 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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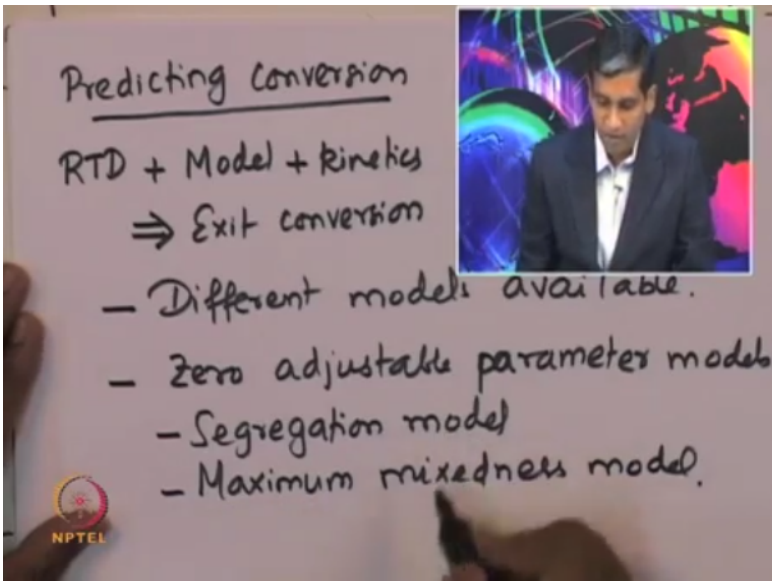

So, predicting conversion actually has a strong impact. So, knowledge of conversion of a particular reaction actually has a strong economic impact because the design of things around it can actually be planned accordingly. And therefore, if one is able to predict the conversion, it actually goes a long way in terms of designing the reactor and designing other processes which is associated with this particular with the reaction of interest.

And this has a strong economic implications for the industry which is actually involved in conducting that reaction and generating, synthesising 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 2 systems, 2 reactor systems which have same RTD functions.

But will it be possible to estimate the conversion in these 2 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 needs to know what is RTD function. And one needs to know what is the model that represents the non-ideal reactor, that captures the process which is 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 device methods to find out what is the exit conversion of the species. So, there are different models which are available. So, 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 of, some other future lectures.

So, first we are going to look at the zero adjustable parameter models. And these are essentially 2 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 2 types of models to predict the conversion of a real-world reactor. So, the residence time distribution, what does residence time distribution function give. What does it give?

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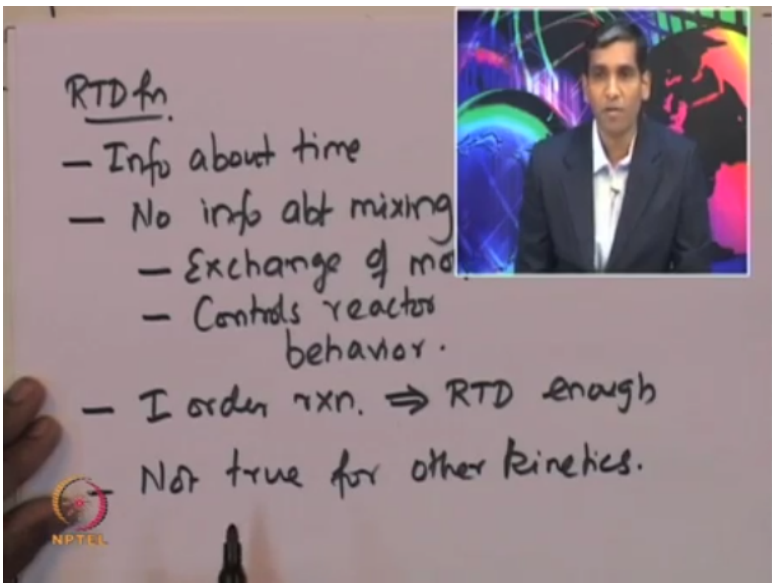

It actually gives information about time spent by various fluid elements inside the reactor. But, it does not provide any information about the mixing. There is no information about the mixing of the fluid elements inside the reactor. Now, what is mixing? Mixing is essentially, it is the exchange of 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 behaviour of the reaction and it actually strongly controls the conversion of that particular reactant in the reactor. So, it actually controls the reactor behaviour. 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, what is required is actually a complex model of the reactor.

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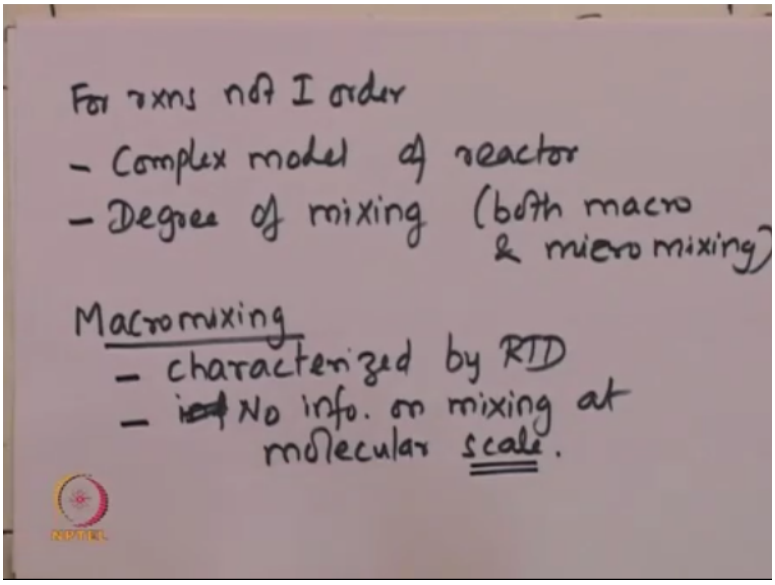

For reactions which are not first order, the complex model of reactor is required. Complex model of the reactor is actually required to find, to predict the conversion of the species which is undergoing the reaction. And also, in addition to that, the degree of mixing both macro and micromixing information is required. So, these terms macro and micromixing will actually be defined in a short while. So, let us first look at the macromixing.

So, there are 2 types of, 2 levels of mixing which, one is the macromixing and the other one is the micromixing. So, the macromixing is essentially, is the extent of mixing which is actually characterised by the RTD function itself. So that is the, it is characterised by the RTD function, the residence time distribution function. And an important aspect of micromixing is that the information about mixing at the molecular scale is actually, does not occur if the fluid is actually under a a macromixing 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 actually is flowing through the reactor essentially consists of atoms and molecules. So now, there may be exchange, the may be interactions and exchange of matter at the molecular scale. And in other extreme there may be situation where 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 1 molecule of the 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 ignored or the information is not available. So, let us next look at what is the, what is micromixing. Let us define micromixing.

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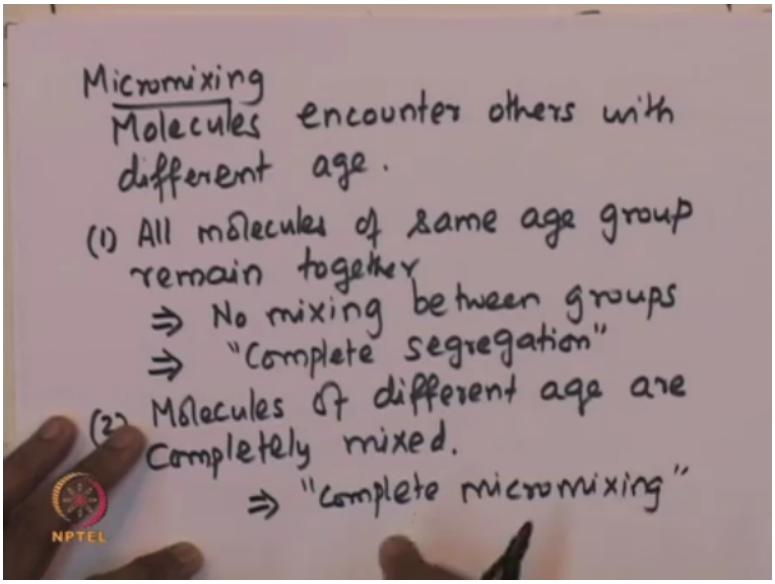

So, micromixing, that describes the, how molecules with different age. Now, suppose we consider a reactor, where there is some fluid which is already present inside the reactor. And then, there is a new set of fluid elements which are actually flowing into the reactor. Now, the age, that is the time that is spent by the fluid particles which is already 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 who, which has spent a larger time inside the reactor, how do they encounter when a fresh set of particles are actually, first set of fluid

elements are actually pumped into the reactor. So, that the aspect which actually characterises this is what is the micromixing. Where we look at how molecules encounter other molecules which are actually having a completely different age or the time that they have spent inside the reactor is different from the ones which are actually entering afresh into the reactor.

So now, there are 2 aspects associated with micromixing. The first aspect is where all molecules of same age group remain together. So, irrespective of how the molecules actually are flown inside, those molecules which actually spend certain amounts of time, they all remain together. And freshly entering molecules, that is a new set of molecules which have, which are currently entering the reactor, they also cling together and they all remain together.

So, the first state of micromixing is the situation where all molecules of same age, they are actually remaining and they are glued together in 1 group. So, this kind, this actually means that there is no mixing between groups. And this state, 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 particles 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 2 systems, they mix with each other and they get completely mixed. So, therefore one cannot virtually distinguish where the particles of which has 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 micromixing. So, these 2 states of complete segregation and complete micromixing, they have strong implications on the performance of the reactor. Now, for a given residence time distribution function; so, remember that the residence time distribution, it only characterises the macromixing 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 2 limits of micromixing. That is the, a complete segregation and the complete micromixing.

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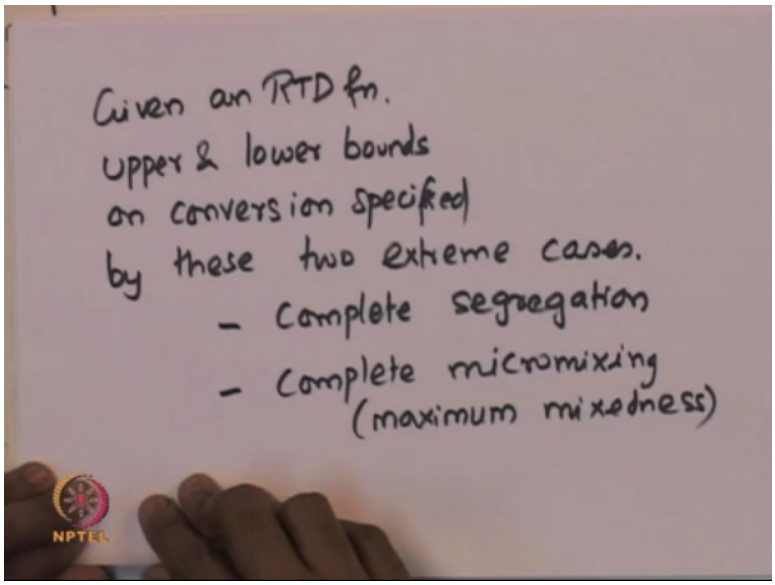

So the, for a given RTD, given RTD function for a real reactor, the upper and the lower bound conversion actually are specified, are actually specified by these 2 extreme cases. That is, complete segregation and complete micromixing. So, the complete micromixing is also called as maximum mixedness. So, the 2 0-parameter, 0 adjustable parameter model is essentially the model that corresponds to the complete segregation and the other model corresponds to the maximum mixedness model.

So, how do we incorporate this aspect of complete segregation and complete micromixing 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. Now, suppose if n is larger than 1, that is the order of reaction, n here stands for the order of reaction.

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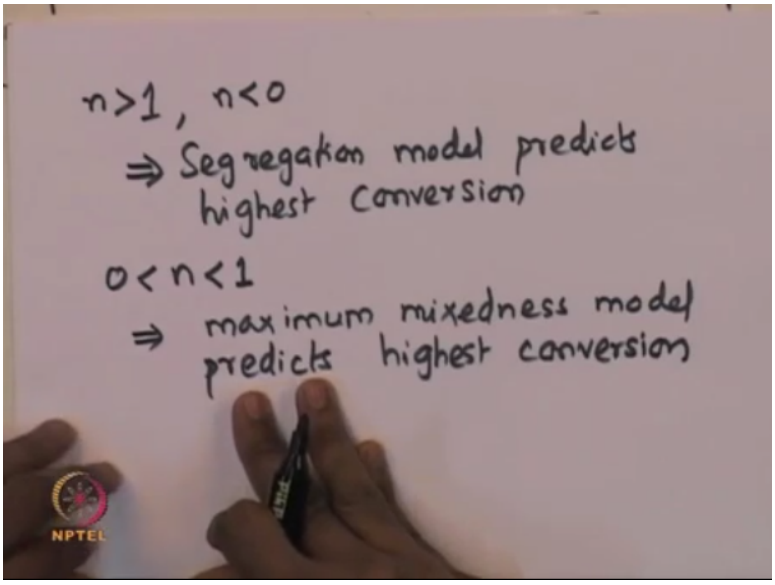

So, if the order of reaction is > 1 or if the order of reaction is < 0, that is, if it is a negative reaction, negative order reaction. Then, it turns out that the segregation model, the complete segregation model predicts highest conversion. On the other hand, for reaction orders between 0 and 1, that is even for partial fraction order reactions, it turns out that the maximum mixedness model predicts highest conversion. So now, there are a few definitions that we need to define before we attempt to consider the segregation model and the maximum mixedness model.

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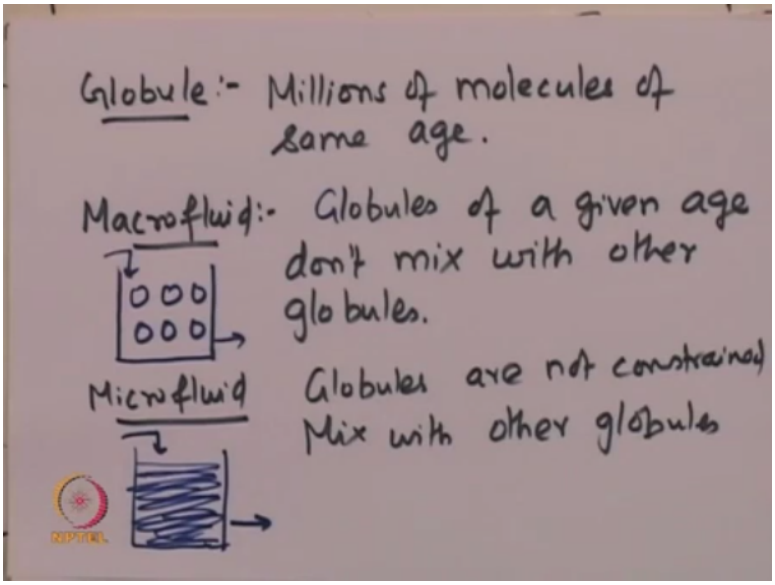

So, the first one in the definition is, what is a globule. So, a globule is basically a group of molecules, millions of molecules which are actually essentially of same age. So, basically it is millions of molecules of same age. So, that is what is a globule. And then, a macro fluid is

essentially the one where the globules of a given age, they actually do not mix with the other globules.

So, in a reactor suppose there is a fluid which is already present and it consists of many different globules and each of these globules will actually have contain 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 present 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 globules, it is globules of a given age. They do not mix with other globules. Which means that these are essentially non-coalescing globules. And so, one can actually visualise this as; suppose if there is a 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, another definition is, another type of fluid is the micro fluid where the globules are not constrained. They are not constrained 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 another 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, if this is the inlet stream and the effluent stream. 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 summarise what we have learnt in this lecture. We have looked at what is the, we have, we compared the residence time distribution for a plug flow reactor that is operated under 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 those, these 2 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 a second order reaction. And then, we observed that the, 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 macromixing and the micromixing and introduced a certain definitions and will continue from there in the next lecture. Thank you.