Chemical Reaction Engineering - II

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Lecture - 49
Residence Time Distribution (RTD): Introduction

Friends, starting from this lecture for the rest of the course we will be looking at the non-ideal reactors, how to characterize non-ideality in reactors, so for this will be particularly looking at the distribution of residence time for chemical reactors.

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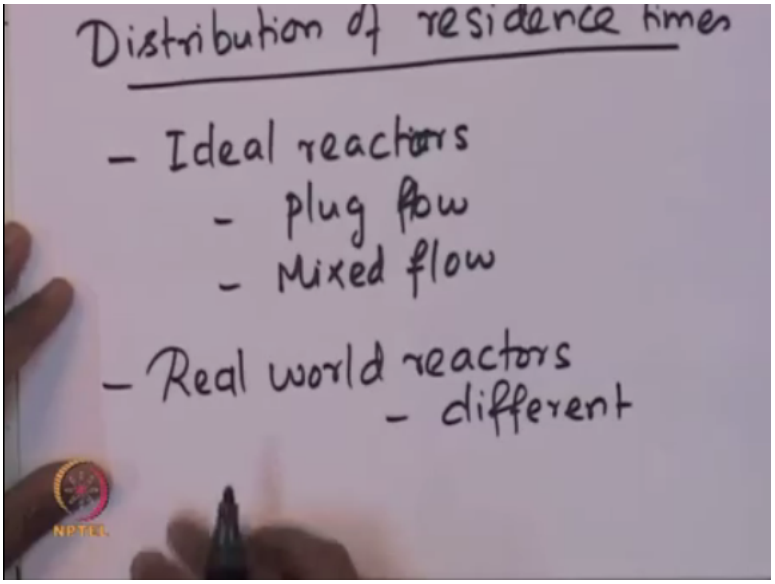

Distribution of residence times

- Ideal reactors
  - plug flow
  - Mixed flow
- Real world reactors
  - different

Particularly, we are looking at the distribution of residence time. Now it turns out that the ideal reactors that is the all the reactors that we have looked at so far they are all ideal reactor that is the Plug flow and the Mixed flow reactors these are all ideal reactors. And it turns out that the real-world reactors they really do not behave like the plug flow or the mixed flow reactors. So the real-world reactors are slightly different.

Real-world reactors they behave differently. And it is actually important to diagnose and understand when they deviate from ideal behavior. So we have seen how to write performance equations for ideal reactors like plug flow reactors or under mixed conditions and we have also know how to write performance equation for CSTR which is not necessarily an ideal situation, we will see what is meant by ideal situation and where does CSTR fall into that category.

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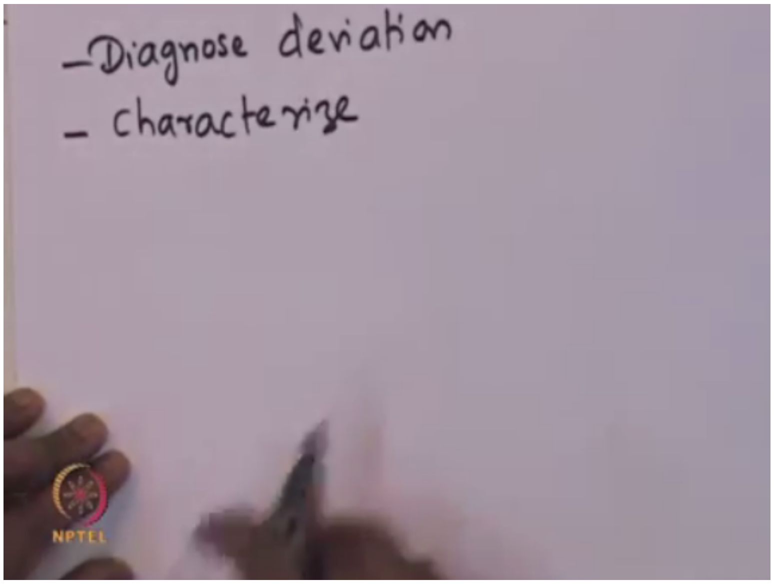

- Diagnose deviation
- Characterize

So it is important to diagnose the deviation from the ideal behavior. So suppose if there is a reactor if I assume that it is a plug flow reactor and I write a performance equation I find out what is the concentration profile of the reactant let us say in the effluent that is after when the stream leaves the reactor. Now the real world reactor perhaps may not attain that kind of conversion and so the and that sort of indicates that the reactor does not behave like a plug flow reactor. So the question is how do I diagnose such kind of a deviation.

Now suppose if I have diagnosed that such kind of a deviation and how do I characterize such a reactor which does not behave like the ideal reactor such as the plug flow and the mixed flow reactors.

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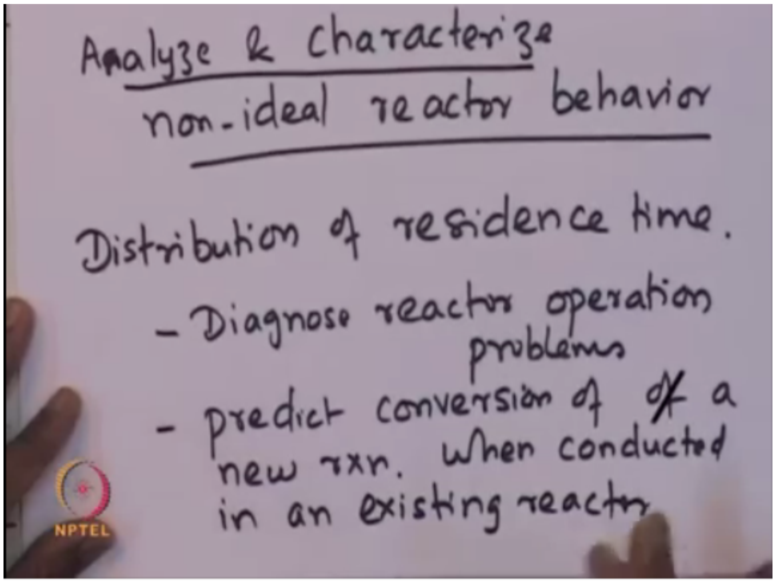

Analyze & Characterize
non-ideal reactor behavior

Distribution of residence time.

- Diagnose reactor operation problems
- predict conversion of ~~of~~ a new rxn. when conducted in an existing reactor

So the objective of the rest of the rest of the syllabus of the course is basically to look analyze and characterize non-ideal reactor behavior. So that is going to be the objective for the rest of the course. So now the key piece of information that is actually used in order to analyze and characterize non-ideal reactor behavior is the distribution of residence time. Residence time distribution of a reactor quantifies the time spent by various fluid particles in the reactor and is a characteristic of mixing that occurs in the reactor.

So in the rest of this lecture we are going to look at several examples of a non-ideal behavior that has been observed experimentally and observed in real systems and also look at some of the definitions of what is residence time and what are the different ways to capture the residence time distribution etc so that is going to be the objective of this particular lecture. So this distribution of residence time is actually used to diagnose the reactor operation problems.

It is also used to predict conversion of a new reaction when conducted in an existing reactor. So these two are important aspects suppose if there is a reactor that is already being characterized. Now if you want to conduct a new reaction in that reactor is it possible to predict the behavior of that particular reaction in that reactor, so that is an important question and in addition to that suppose if there is an experiment that has been conducted in a small scale.

And then we want to scale it up to a next level to increase the productivity of that particular product which is desired then it is important to actually characterize the non-ideal behavior where it helps in scaling of the reactors. So let us look at a specific case of gas liquid CSTR.

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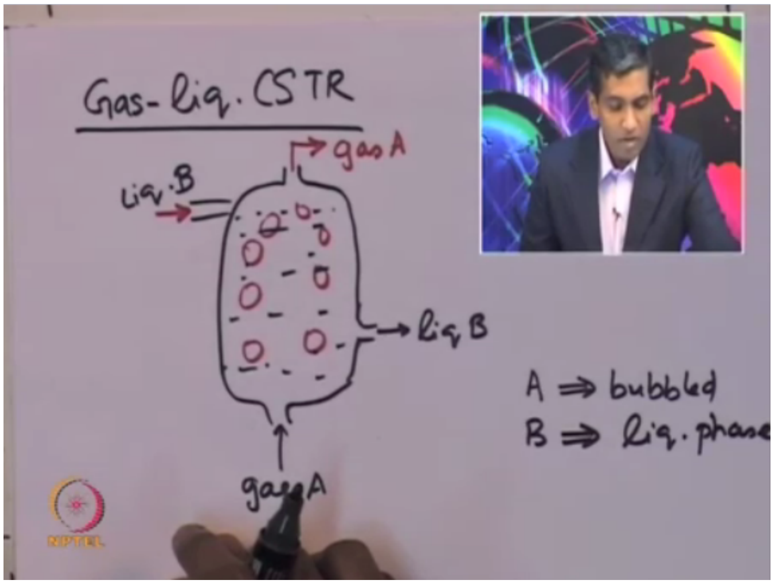

Suppose I take a tank and let us say that the gas A is being bubbled through the liquid so let us say that the liquid is filled let us say the tank is filled with liquid and bubble A is actually bubbled through this liquid inside and then it leaves the reactor from the top, so that is gas a which is actually entering from the bottom and it is being bubbled inside and then it leaves from the top of the reactor.

Now suppose there is another liquid B which is now flowing through this reactor start flowing through this reactor and the gas is simultaneously bubbled through this liquid so the liquid leaves from the exit stream for the liquid. So now, so A, species A is actually being bubbled and species B is actually the liquid phase which is going through the reactor. So now one can actually realize that there are three processes which are actually occurring here.

So remember this is a gas liquid reactor so the reaction is actually occurring between the species A which is in the gas phase.

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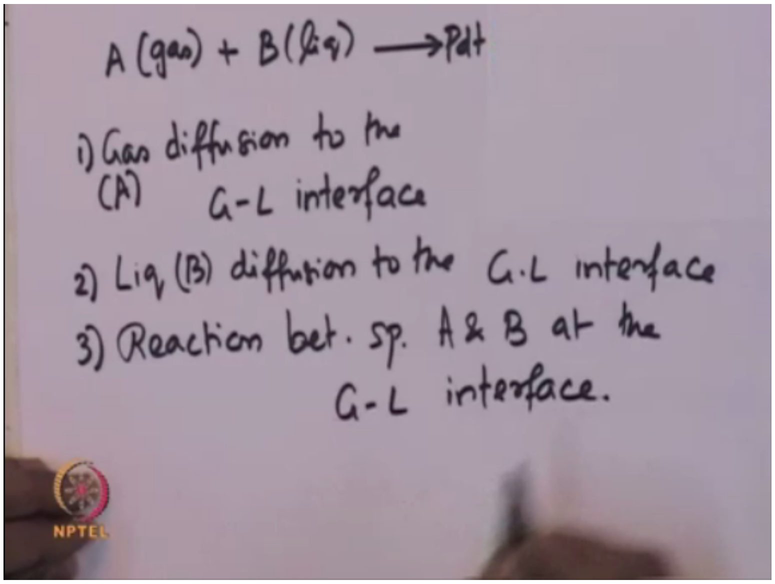

$A\,(\text{gas}) + B\,(\text{liq}) \longrightarrow \text{Pdt}$

i) Gas diffusion to the
(A) G-L interface

2) Liq (B) diffusion to the G.L interface

3) Reaction bet. sp. A & B at the
G-L interface.

The reaction is between species A in the gas phase and species B in the liquid phase and that leads to formation of certain products. So now if this reaction has to happen, the species A which is present in the gas phase has to diffuse and come to the interface between the liquid and the gas stream. So the first process is the gas diffusion to the gas liquid interface. Now suppose I assume that the gas was immiscible in the liquid then the reaction has to occur at the gas liquid interface.

So there is an interface between the gas stream which is present inside the bubbles and the fluid stream which is actually present around the bubbles. And so therefore the gas species has to diffuse from the bulk inside the bubble to the gas liquid interface in order for it to get in contact with the liquid with which it has to react. And similarly, so this is basically diffusion of species A, and similarly the species B has to actually undergo diffusion that should has to be a diffusion of species B to the gas liquid interface.

So only after this these two processes have occurred the reaction between these two species can occur so therefore, the third step is the reaction between species A and species B at the gas liquid interface. It has been assumed that the reaction occurs at the interface. However, the reaction need not be confined to the interface as were the cases that were covered in lecture 26. So these are the three processes which are actually occurring now in order for the reaction to actually occur.

Now suppose we can assume that the liquid which is actually flowing from the top of the off the tank. So as, if you look at the tank again, so the liquid which is actually flowing from the top of the tank through the tank and leaves the bottom of the liquid so this is this can be assumed as a continuous liquid phase, so we can assume that the liquid is actually a continuous phase.

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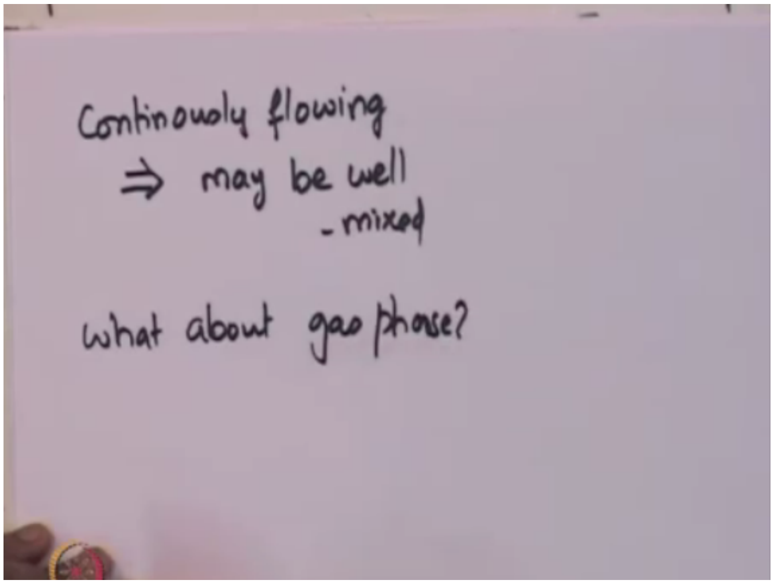

Continously flowing
⇒ may be well
-mixed

what about gas phase?

So the liquid is actually continuously flowing. And in fact it perhaps it can also be assumed that it may be well-mixed. It can be assumed that it may be well made that is the concentration of the species in the liquid phase is almost uniform inside the reactor. Now that is not really true but maybe we can assume for the time being that it is well-mixed in order to actually appreciate what is happening inside the gas liquid CSTR and particularly in order in order to appreciate the nature of the non-ideal behavior.

Although in reality even the liquid phase will not necessarily be well-mixed but if it is a continuous phase and it may be assumed to be well-mixed for the time being. So the is what about gas-phase? In fact, comparing gas phase the liquid phase can actually easily be assumed as a, a well-mixed phase. Now what about gas phase, before we understand what happens in the gas phase let us try to actually understand how the, what are the different properties are actually controlled in the reaction rate. In fact, it is that which gives an insight as to what is the nature of the fluid flow in the gas phase.

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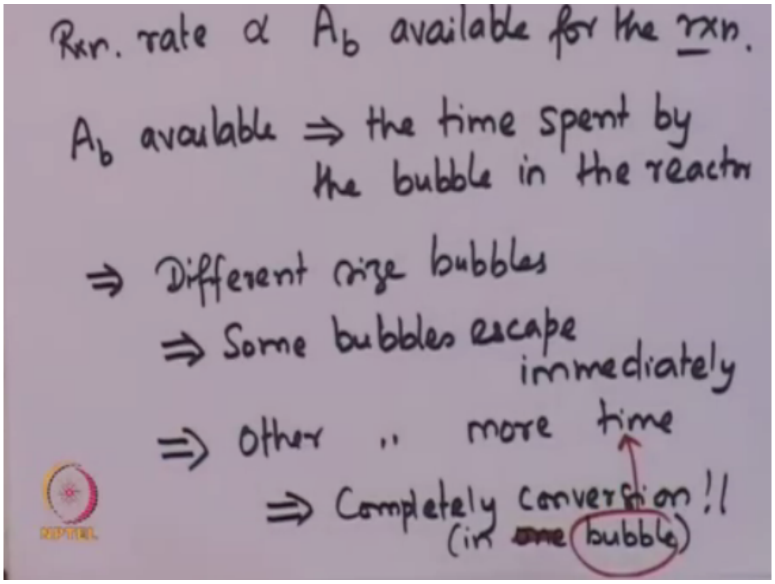

Rxn. rate α A_b available for the rxn.

A_b available ⇒ the time spent by the bubble in the reactor

⇒ Different size bubbles

⇒ Some bubbles escape immediately

⇒ Other " more time

⇒ Completely conversion !!
(in ~~one~~ bubble)

So the reaction rate is actually proportional to the surface area, suppose Ab is the surface area of a particular bubble, so remember that the gas which is actually flowing from the bottom to and leaves the top of the reactor is actually bubbled inside, so it forms bubbles and then the bubbles raise inside the liquid stream and then while it raises the reaction occurs in the gas liquid interface and then the bubble leaves the reactor.

So the reaction rate is actually proportional to the surface area of the bubble which is available for reaction. It is the surface area of the bubble which is actually available for the reaction to occur. Now the surface area of the bubble which is available for the reaction what does it depend upon, it actually depends upon the amount of time that the bubble actually spends inside the reactor. So therefore, the surface area of the bubble available, so remember it is not the surface area just the surface area of the bubble.

It is the surface area of the bubble which is available for the reaction to occur when the bubble is actually rising from the bottom to the top of the reactor. And that depends upon the time spent, so that is depends upon the amount of time that the bubble actually spends inside the reactor. So the there are; the gas bubbles when it is actually generated when it is purged into the liquid they are generally not of same size so different gas bubbles are going to be of different sizes.

So therefore, so different sized bubbles one can expect different size bubbles to be created and these different sizes are actually simultaneously they are rising up and because this the bubbles are of different sizes different bubbles are going to rise at different velocities. So therefore, clearly some bubbles may actually escape immediately, so some bubbles actually they will escape immediately which means as soon as they are created they will quickly go to the top of the liquid stream and then they will leave the reactor.

And so the amount of time that these bubbles would have spent which have left immediately will be extremely small. Now others might spend more time other bubbles may spend more time inside the reactor and as a result of this the amount of species which is present in the gas phase can actually get completely consumed because the bubble is now spending sufficient time inside the reactor for all of the reactant to actually diffuse from the gas phase and reach the gas liquid interface and actually contact the liquid phase, species in the liquid phase and the reaction to occur. So therefore some of these bubbles gets completely converted.

So the gas species present in some of these bubbles gets completely converted. So there can be complete conversion or complete consumption of all the species in each of these bubbles. So when I say complete conversion it means that in one bubble which actually spends more time inside the reactor or in the bubble, in bubble which actually spends more time inside the sufficiently more time inside the reactor, so that is what is meant by complete conversion in that particular bubble.

So now as a result of this observation that difference bubbles spend different amount of time inside the reactor and that some bubbles actually leave immediately and some bubbles actually spend more time in order for all the reactants present inside that bubble to have undergone reaction or to get consumed the gas phase cannot be assumed as well-mixed.

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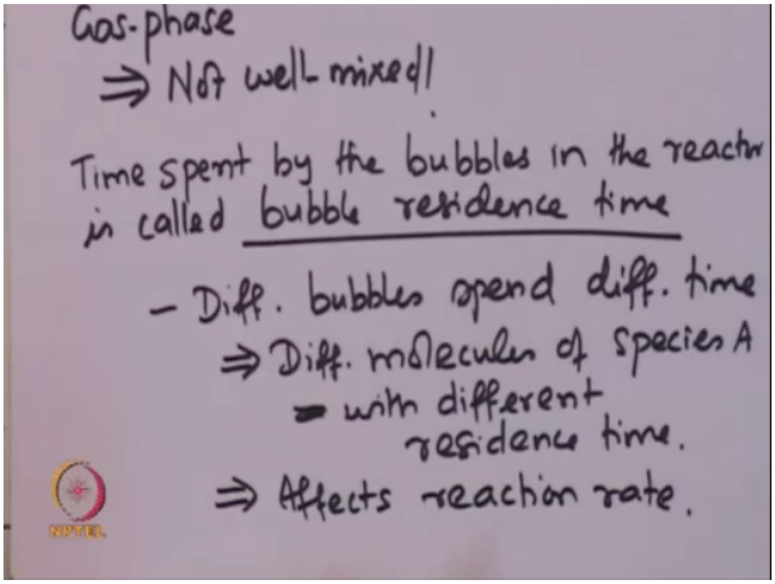

Gas-phase

⇒ Not well-mixed!

Time spent by the bubbles in the reactor is called <u>bubble residence time</u>

- Diff. bubbles spend diff. time

⇒ Diff. molecules of species A

= with different residence time.

⇒ Affects reaction rate.

Cannot be considered as well-mixed, so therefore it is important to consider the amount of time spent by the bubble inside the reactor while designing these kinds of gas liquid CSTR. So just to define the time spent by the bubbles in the reactor is called bubble residence time that is called the bubble residence time that is the amount of time spent by bubble inside the reactor. Now as observed earlier different bubbles spend different time inside the reactor.

And therefore different molecules of species A will have with different residence time. So different molecules of species A although all of them could have actually come into the reactor at the same time because of this feature that different bubble spend different amount of time inside the reactor different molecules species A would also have different residence time. So clearly this is going to affect the reaction rate.

It is important to note that RTD affects the conversion but does not affect the intrinsic reaction kinetics. Why is that? Because the reaction rate is a function of the available surface area and the available surface area depends upon the amount of time that is actually spent by the bubbles inside the reactor, so therefore if different molecules of species A they have different residence time that is going to clearly affect the extent of the reaction it is going to affect the reaction rate.

And therefore it is important to consider this aspect of different bubbles having different residence time into the model analysis.

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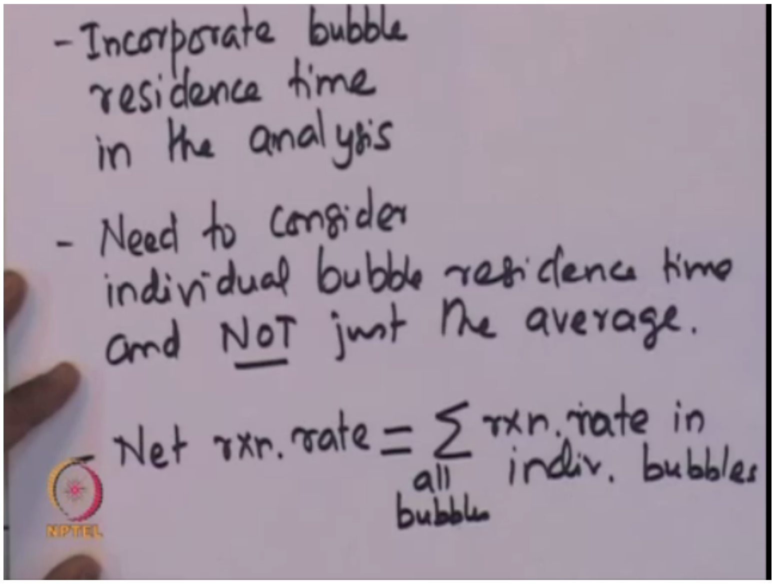

- Incorporate bubble residence time in the analysis
- Need to consider individual bubble residence time and <u>NOT</u> just the average.
- Net rxn. rate = $\sum_{\text{all bubbles}}$ rxn. rate in indiv. bubbles

So therefore it is important to incorporate the bubble residence time in the analysis of such reactor. And moreover it is actually important it need to consider it is important that one considers the individual bubble residence time and not just the average. So it is not sufficient to consider only the average residence time of the bubbles it is important to consider the residence time of each and every bubble which is actually created because the bubble is being purged into the liquid.

So, and as a result the net reaction rate is simply going to be sum of the reaction rate in individual bubbles and summed over all bubbles. So if there are 100 bubbles inside the reactor then one needs to actually find out what is the reaction rate in each of these 100 bubbles and sum them all and that gives you the net reaction rate inside the reactor, net reaction rate here refers to the observe total reaction rate and not the intrinsic reaction rate.

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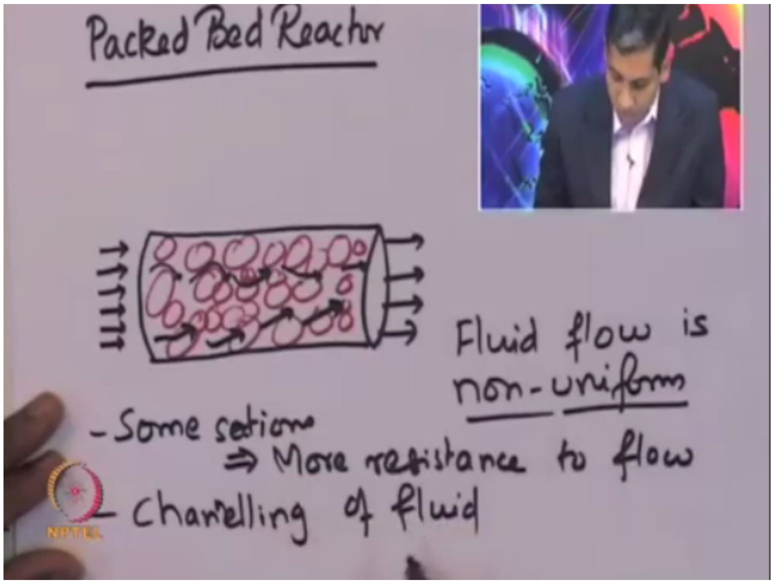

Packed Bed Reactor

Fluid flow is non-uniform

- Some setions
  ⇒ More resistance to flow
- Channelling of fluid

So now let us look at another example of a Packed Bed Reactor. So a packed bed reactor is nothing but a tube and the tube is packed with catalyst particles so let us say that these are the catalyst particles which are actually present inside the reactor. So these are the catalyst particles which are actually packed inside. And suppose if the if a fluid stream is actually flowing into the reactor.

Let us say that it has a flat profile that means the velocity with which the fluid is actually flowing and the concentration with which the fluid is actually entering the stream is actually uniform across a given cross-section. So suppose if it flows uniformly inside then because of the packing the resistance to flow is not going to be uniform at every location in a given cross-section. So therefore one can observe that the fluid stream is now going to bend and then it is going to move through the crevices of the reactor and then they are going to leave from the other side.

So clearly one can observe that the fluid behavior is not going to be uniform, so clearly the fluid flow is going to be it is to be a non-uniform fluid flow, and why would that be the case? So some sections can actually offer more resistance, so some sections will offer more resistance more resistance to flow and as a result the channeling of fluids will occur. So as can be as depicted here some; in some sections of the reactor the fluid will actually quickly go from the inlet to the exit of the reactor and leave the reactor while in the other sections they spend a lot more time.

So clearly the amount of time that is spent by every by a molecule by different molecules of the species that is entering the reactor is going to be different which means that there is going to be a;

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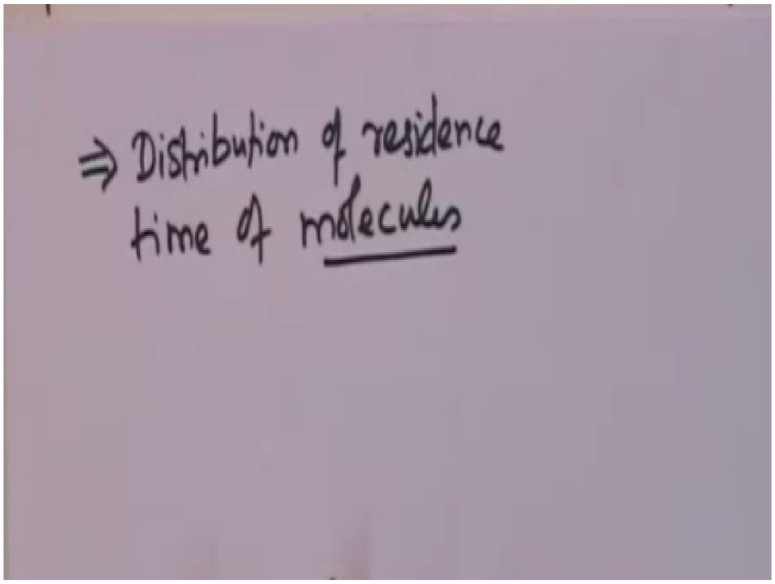

⇒ Distribution of residence time of molecules

A distribution of residence time that is clearly going to be a distribution of residence time of the molecules which are actually entering the reactor and is participating in the reaction.