Chemical Reaction Engineering – II

Prof. Ganesh A Viswanathan
Department of Chemical Engineering, IIT Bombay
Indian Institute of Technology – Bombay

Lecture - 50
RTD: Non-Ideal Reactors

So let us take another example of CSTR a well-mixed CSTR.

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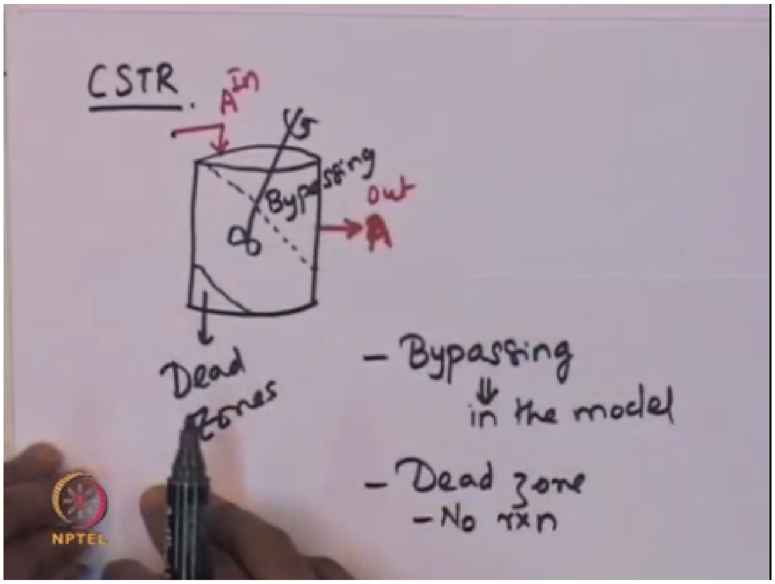

Suppose we take a well-mixed CSTR, so CSTR is a tank that is a tank and it has a mixer so let us assume that it is rotating in this direction. And if this species is actually entering through entering into the reactor suppose this is the feed stream, species A is entering into the reactor at the feet where are the feed stream and let us say that the outlet of this reactor is at this location so this is the out and this is the in stream.

And what happens is that often the inlet and the outlet streams of the reactor may actually be placed close to each other for various reasons and because of that what happens is that some of the fluids would actually quickly some of the fluid that is entering the CSTR would actually quickly leave the reactor and in fact that process is called as bypassing so the some of the fluid stream particles which are actually entering into the reactor would actually bypass and leave the reactor.

And as a result what is created is some of the some locations of the reactor are actually underutilized or unutilized and those zones are called as the dead zones. So what is been observed is that the there is bypassing of fluid stream and because the inlet and outlet may be placed close to each other and so some of the fluid particles will quickly bypass. And of course if one needs to model such kind of a reactor this has to be incorporated in the model.

And the second problem is the presence of a dead zone where the reactants are actually where the where there is no reaction occurring in the dead zone so there is no reaction. And not just that there is no reaction there is actually no exchange of materials from the dead zone to the well-mixed zone.

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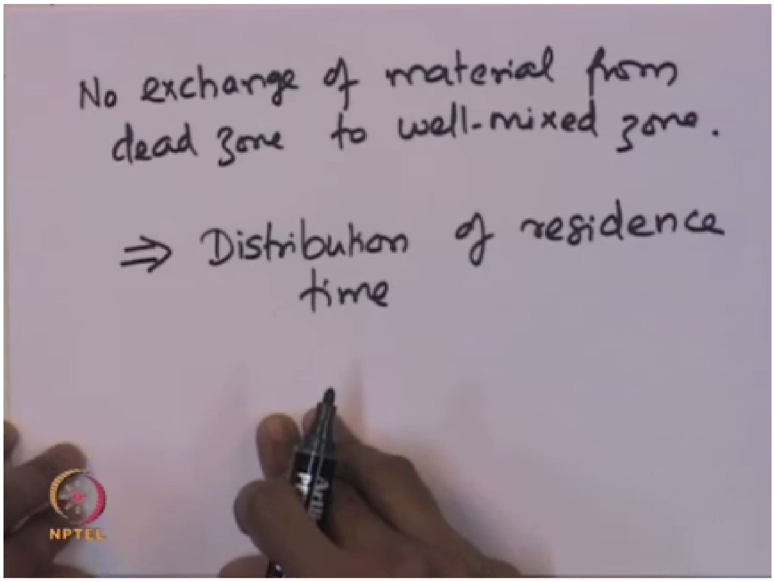

No exchange of material from dead zone to well-mixed zone.

⇒ Distribution of residence time

So in addition to that no exchange of materials from dead zone to well-mixed, so clearly this suggests that there will be a distribution of residence time, so there will be distribution of residence time even in the case of where there is a CSTR with bypassing occurring inside the reactor.

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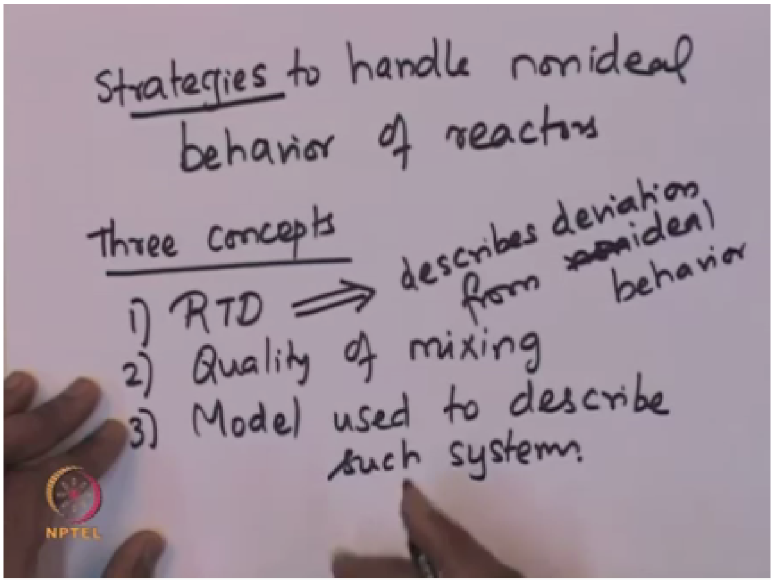

Strategies to handle nonideal behavior of reactors

Three concepts

1) RTD ⟹ describes deviation from ideal behavior
2) Quality of mixing
3) Model used to describe such system.

So all these three examples are actually a good motivation to think that there is a requirement for strategies to handle non-ideal behavior, so it is important to come up with strategies to handle the non-ideal behavior of reactors and this is very common because the ideal reactor such as the plug flow and the mixed flow reactors are commonly the not they are not a good representation of the real-world reactors they do not behave exactly like they plug flow and the mixed flow.

And in fact we will see in one of the in the future lectures that the one can actually clearly show using the residence time distribution that the real reactors do not necessarily behave like a plug flow or the mixed flow. So there are three concepts which are involved here there are three concepts that one need to understand in order to come up with strategies to handle the non-ideal behavior of reactors. So the first one and that is the Residence Time Distribution.

So that is the amount of time that is actually spent by a given fluid particle inside the reactor. And the distribution says how much time different fragments of the fluid particles are actually spending time inside the reactor. Then the second important aspect is the Quality of mixing. So what is the extent of mixing that is actually undergoing inside the reactor due to various reasons. So one needs to understand and characterize the nature of extent of mixing in order to be able to understand the non-ideal behavior of reactors.

And then the third aspect is basically to Model used to describe such systems. So one needs to come up with ways by which you one can actually model such kind of non-ideal behavior and so we are going to see that what are the various ways by which we can actually characterize the non-ideal behavior using these three concepts. And several examples will actually be shown to explain each of these concepts. And in fact the RTD the residence time distribution it actually is used to describe it describes the deviation from non-ideal, oops from ideal behavior.

So the residence time distribution actually describes the deviation or it sort of captures the deviation from the ideal flow behavior and we are going to look at how it captures in a short while.

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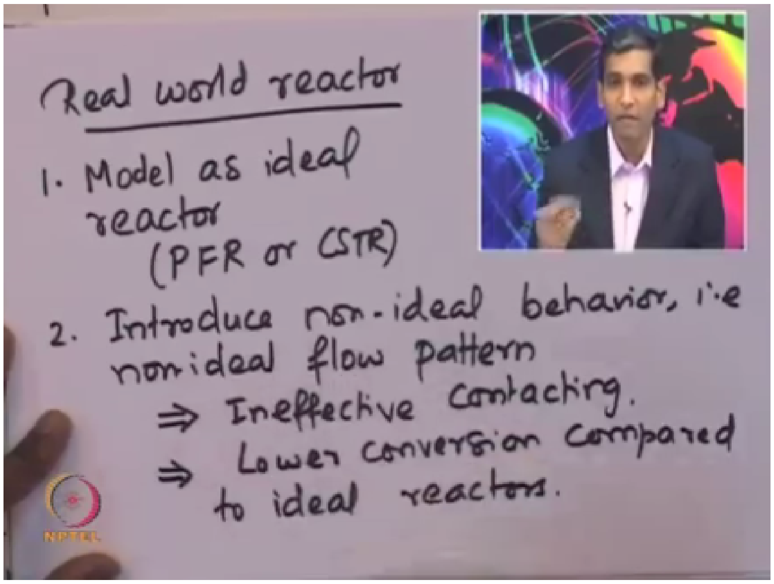

Real world reactor

1. Model as ideal reactor (PFR or CSTR)
2. Introduce non-ideal behavior, i.e non-ideal flow pattern
   - ⇒ Ineffective contacting.
   - ⇒ Lower conversion compared to ideal reactors.

So the first step towards handling this handling a real-world reactor that is the actual reactor which may be present in industry. So the first step is basically to water them as an ideal reactor. So the first step is to assume that the reactor is an ideal reactor. What it means is that it needs to be modeled either as a PFR or a CSTR so one can actually model it as a plug flow reactor or a CSTR reactor.

Remember that even in a CSTR the residence time is not same for all the particles that actually goes through the reactor however it is a thoroughly perfectly well-mixed system so it has certain ideal properties and we will see the short while how to characterize them. And then suppose if this model does not predict the actual behavior of the reactor then one needs to actually introduce the non-ideal behavior that is the non-ideal flow pattern needs, one introduce the non-ideal flow pattern.

And in fact in order to introduce a non-ideal flow pattern one has to actually account for the ineffective contacting while some of these; for example let us take the packed bed reactor case the some of the fluid actually enters and leaves the reactor immediately because of the channeling effect and so the contact that actually these fluid stream has with the catalyst particles present inside the reactor is not very effective and therefore one needs to account for such kind of ineffective contacting.

And also one needs to affect account for low conversion compared to ideal reactors. So one needs to account for these two factors if one has to introduce the non-ideal behavior into the ideal reactor model, so once we know once we know that the reactor behaves like a non-ideal reactor then we need to account these two aspects into the modeled to capture the dynamics or the behavior of the reactor. Now the question is how do we account these two factors.

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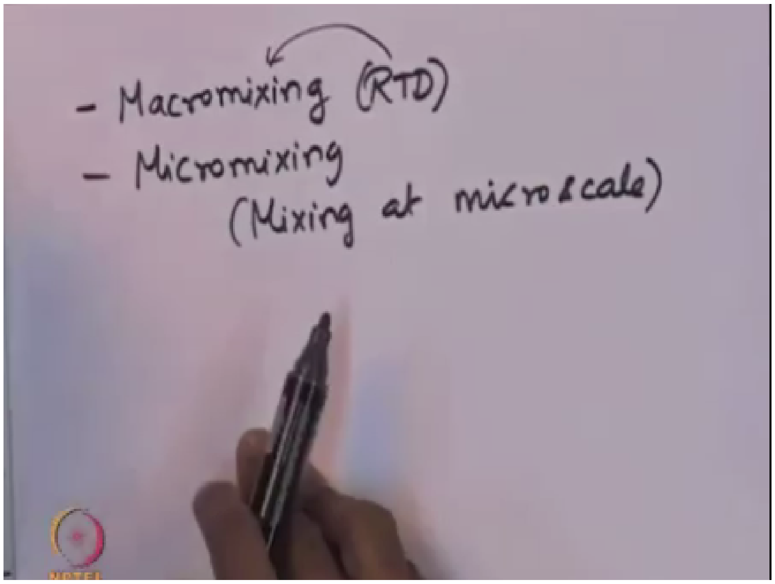

- Macromixing (RTD)
- Micromixing
  (Mixing at microscale)

So the first so one needs to actually look at the Macromixing, macromixing which is basically the residence time distribution which captures the macromixing one needs to account for macromixing in the system and the other aspect is the Micromixing that is the, so this is the mixing at micro scale. So one needs to account for these two factors and in fact these two factors will actually help in characterizing the non-ideal behavior of the reactor. So let us first look at the residence time distribution which actually account for the macromixing.

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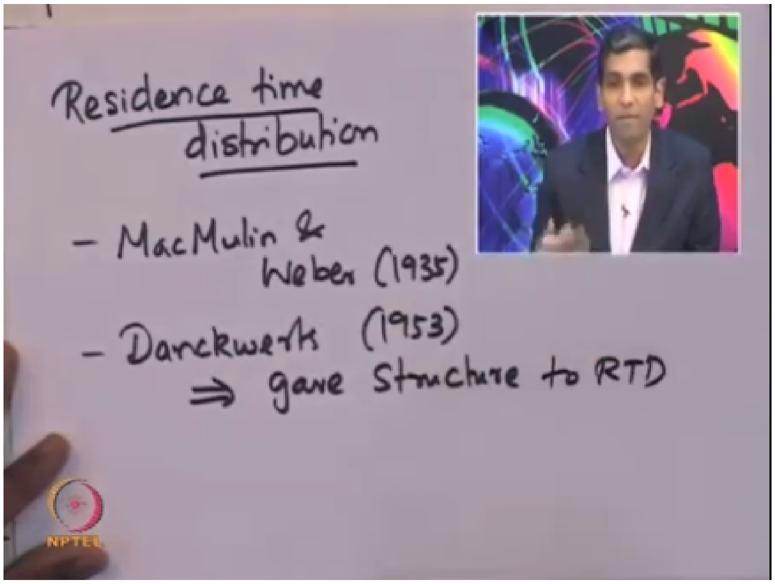

Residence time distribution

- MacMulin & Weber (1935)
- Danckwerk (1953)
  ⇒ gave structure to RTD

So the residence time distribution was actually originally proposed by MacMulin & Weber in 1935. However, it is actually ignored for nearly two decades later Danckwerts came and actually gave a special structure to the residence time distribution and defined various types of possible distributions. So it was Danckwerts in 1953 gave structure to RTD, in fact he came and took the idea of MacMuline & Weber and developed it further and gave some special structure to RTD.

Therefore, most of the RTD work is actually attributed to the seminal work done by Danckwerts in 1953. So now we said that the plug flow reactor is an ideal reactor. So why is it an ideal reactor?

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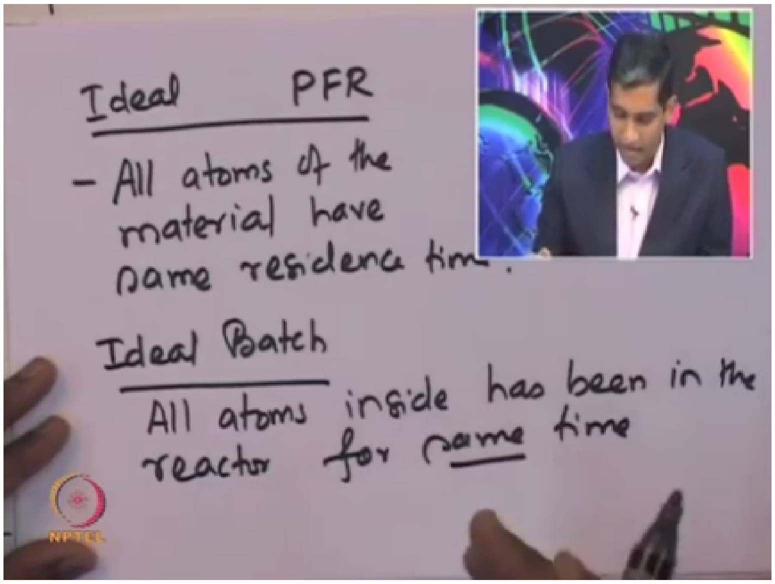

Ideal PFR

- All atoms of the material have same residence time.

Ideal Batch

All atoms inside has been in the reactor for same time

So let us look at the ideal plug flow reactor. So plug flow reactor can actually be is be an ideal reactor under certain situations. So what are the properties of an ideal plug flow reactor? So in an ideal plug flow reactor all atoms and materials all atoms of the materials have same residence time. So suppose there is a fluid which is actually flowing through a plug flow reactor then all fluid particles are actually entering the ideal plug flow reactor they spend exactly the same amount of time inside the reactor before they leave the plug flow reactor.

So that is an important characteristic of an ideal plug flow reactor. And what about an ideal batch reactor? What about ideal batch reactor? So ideal batch reactor is one where all atoms inside has been in the reactor for same time, so all atoms that are actually present inside the batch reactor ideal batch reactor they actually have they have been there all atoms have been there for exactly the same amount of time as each of them. And so therefore the time that is actually spent by these atoms inside the reactor called the residence time.

And both these ideal plug flow reactor and the ideal batch reactor they actually have all the molecules inside they have exactly the same residence time. So there are actually only two classes of ideal reactors. In fact, there are only two classes of reactors in which the residence time can actually be same.

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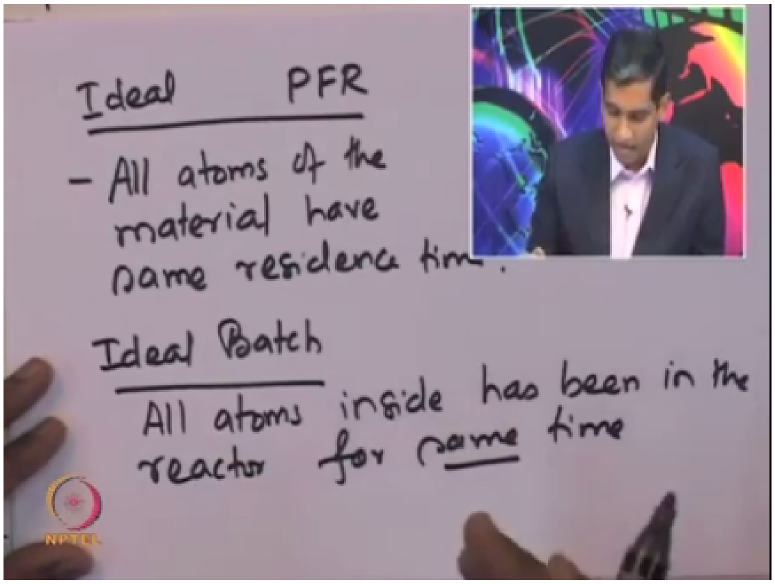

Ideal PFR

- All atoms of the material have same residence time.

Ideal Batch

All atoms inside has been in the reactor for same time

So it is the Ideal Plug Flow and the Ideal Batch Reactors, two classes with same residence time. So all other reactors that is going to be a distribution of residence time including CSTR. So suppose what happens in the CSTR, CSTR is something that has been commonly studied in this course in many different in the first course of the reaction engineering and so.

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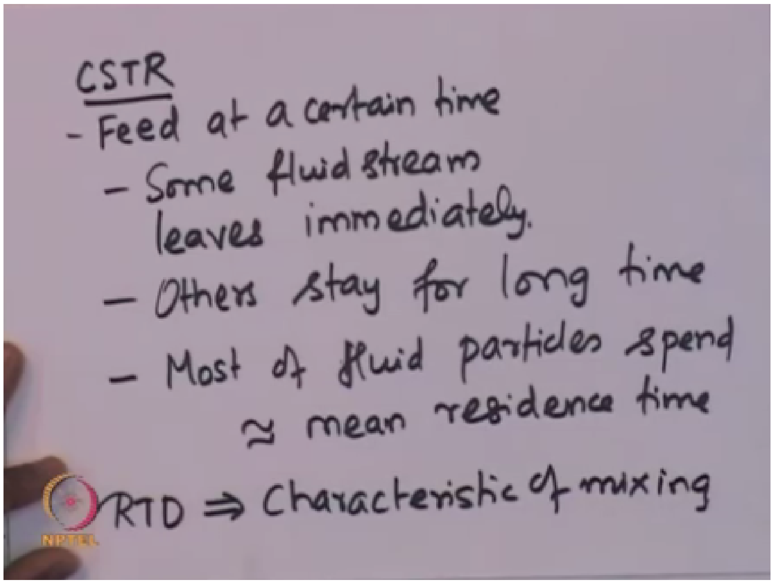

CSTR

- Feed at a certain time
  - Some fluid stream leaves immediately.
  - Others stay for long time
  - Most of fluid particles spend $\simeq$ mean residence time

RTD $\Rightarrow$ Characteristic of mixing

So what happens in a CSTR? How can we describe, what have what is the nature of the residence time distribution in the CSTR? So suppose if you take a tank and then we feed a certain speed certain species into the tank which is undergoing a reaction. So if we consider the feed at a particular time suppose we look take at the feed at a particular time; suppose we consider feed at a certain time then as the feed stream actually enters into the reactor the feed stream.

Because it is a CSTR the feed stream immediately gets completely mixed with the materials which are already present inside the reactor. Now, not just that the feed; there may be a small fraction of the feed stream which is actually carried along with the fluid stream and it leaves the reactor. So therefore it is possible that some fluid stream some fluid stream leaves immediately some fluid stream actually leaves immediately.

And so therefore the residence time of this fluid stream which actually leave the reactor immediately is going to be very small. And in fact it is going to be different as compared with the residence time of others particles which are actually staying inside the reactor. So other particles they are going to stay for a much longer time and in fact most of the particles, it is been observed that most of spend approximately the mean residence time.

So most of the fluid particles the amount of time they spend inside the reactor is approximately equal to the mean residence time. So therefore the residence time distribution actually characterizes the extent of mixing. So in a CSTR the some fluid stream leaves immediately and the other they stay for a longer time which means that there is going to be a distribution and in fact the residence time distribution it characterizes the extent of mixing inside the reactor. So that is an important aspect. It is a characteristic of mixing.

So residence time distribution henceforth to be referred to as RTD and it is actually a characteristic of the mixing which is happening inside the reactor.

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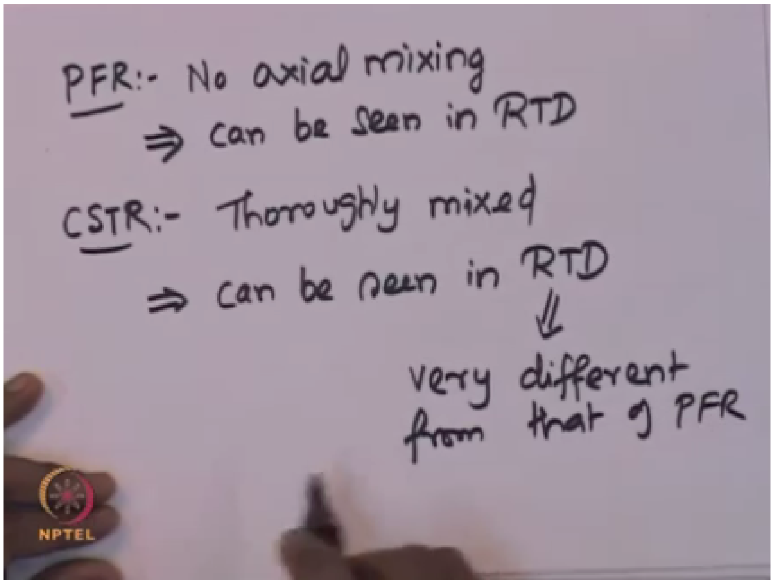

PFR:- No axial mixing
⇒ can be Seen in RTD

CSTR:- Thoroughly mixed
⇒ can be seen in RTD
⇓
very different
from that of PFR

So now if I take a plug flow reactor there is no axial miss mixing in a plug flow reactor; there is no axial mixing in a plug flow reactor which means that the if there is a tube and if it behaves like a plug flow reactor then the fluid stream which is actually entering inside they actually move like a plug which means that the fluid particles which is actually entering the reactor at a certain time they do not mix with the fluid particles which are actually entering just after it or just before it.

So therefore there is no axial mixing of fluid particles inside the reactor if it behaves like a plug flow reactor. And this can actually be seen this behavior or this aspect of no axial mixing can actually be seen in the residence time distribution and it will be shown in one of the lectures in the one of the future lectures that for a plug flow reactor there is actually no axial mixing and that can be deciphered from the residence time distribution curve itself.

And let us look at CSTR. So a CSTR is actually thoroughly mixed which means that the concentration of the species inside the reactor is going to be uniform at all times and so it is a thoroughly mixed system and that can also be seen in the residence time distribution of the reactor. So now, and in fact one will observe which will see in one of the future lectures is that the RTD of CSTR is actually very different from.

So the residence time distribution observed for a CSTR is going to be very, very different from the residence time distribution of a pure plug flow reactor. So at this point one needs to also know that not all residence time distributions are actually unique to the reactor type, so it does not mean that every reactor type has a unique residence time distribution and there is no one to and correlation; there is no one residence time distribution for a particular reactor type.

So what it means is that different reactors can actually show identical residence time distribution. In fact, different reactors of completely different configurations they can all show very, very similar residence time distribution. So residence time distribution can actually be used to decipher the nature of the functioning of that particular reactor or nature of the non-ideality that is present inside the reactor. So now the question is how do we detect these non-ideal behavior; how do we detect the residence time distribution experimentally?

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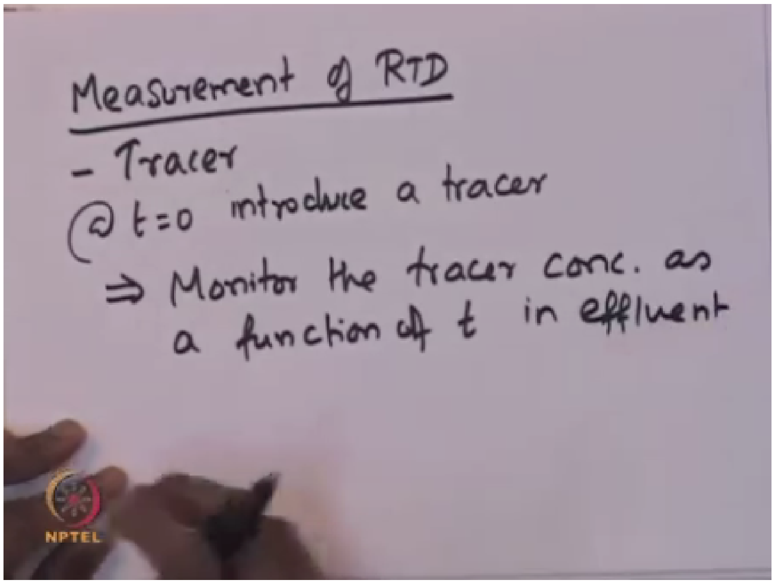

Measurement of RTD

- Tracer

@ t=0 introduce a tracer

⇒ Monitor the tracer conc. as a function of t in effluent

So it is actually possible to measure it is possible to measure the residence time distribution and in fact it is experimentally determined using what is called a tracer. So suppose if there is a reactor, a fluid stream is flowing through this reactor which is actually participating in a certain reaction which is getting consumed to form products. Now in order to find out what is the residence time distribution in order to detect whether the reactor is ideal or non-ideal we need to know what is the residence time distribution.

And the way to do that is basically to use a tracer. So what is done is @ time t=0, so a tracer is introduced so and a tracer chemical is actually introduced and then monitor the tracer concentration as a function of time in effluent. So one can actually measure the tracer concentration that actually is going to flow along with the fluid so the tracer is introduced at the inlet of the reactor and the tracer is now going to be taken forward taken by the fluid along the reactor and then it is going to leave the reactor.

So one can actually measure the concentration of the tracer material as it leaves the reactor and that way one can actually construct the residence time distribution. Now it is not possible to conduct such an experiment with any kind of tracer; the tracer has to have certain properties. So for example the tracer must actually satisfy certain important must have certain important properties in order for it to be used to measure the residence time distribution.

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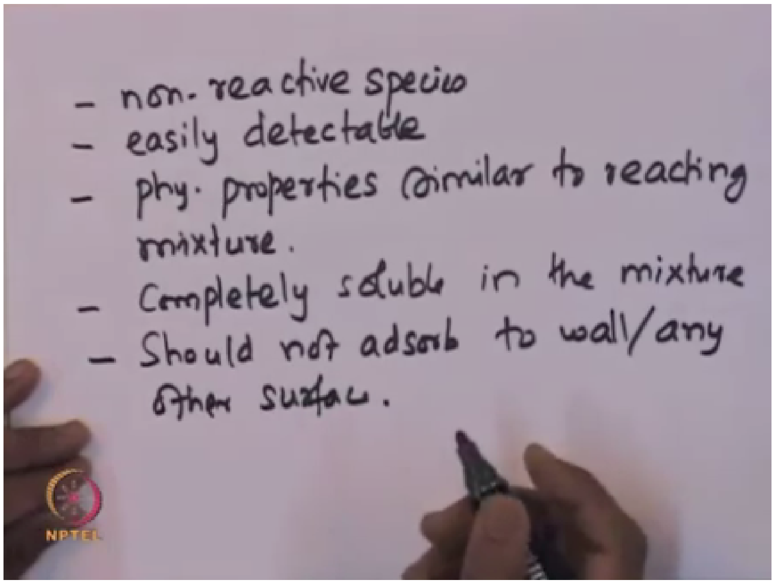

- non-reactive species
- easily detectable
- phy. properties similar to reacting mixture.
- Completely soluble in the mixture
- Should not adsorb to wall/any other surface.

And these properties are basically they have to be non-reactive species; they have to be non-reactive otherwise is going to get consumed inside the otherwise it is going to get consumed because of some reaction. And if it gets consumed then one cannot observe the non-ideal behavior or non-ideal flow pattern using this particular tracer and then it must be easily deductible.

So the tracer chemical must be easily detectable that means that there must be methodologies well-established methodologies in order to measure the concentration of the tracers in a very, very in a very short time which means that the equipments must be sensitive enough to distinguish the small concentrations of the tracers. The physical properties should be such that similar to that of the reacting mixture.

So if the physical properties are not similar then it does not reflect the exact flow behavior of the reacting mixture which is of interest to actually study. So now in addition to that it must also be completely soluble, it must be completely soluble in the reacting mixture and it actually should not adsorb to wall or any other surface of the reactor, so it should not adsorb to wall or any other surface because if it gets absorbed then the some of these species are being consumed and that is not going to help in actually measuring the residence time distribution of the reactor.

So typically colored and radioactive materials along with the inert gas commonly used as tracers.

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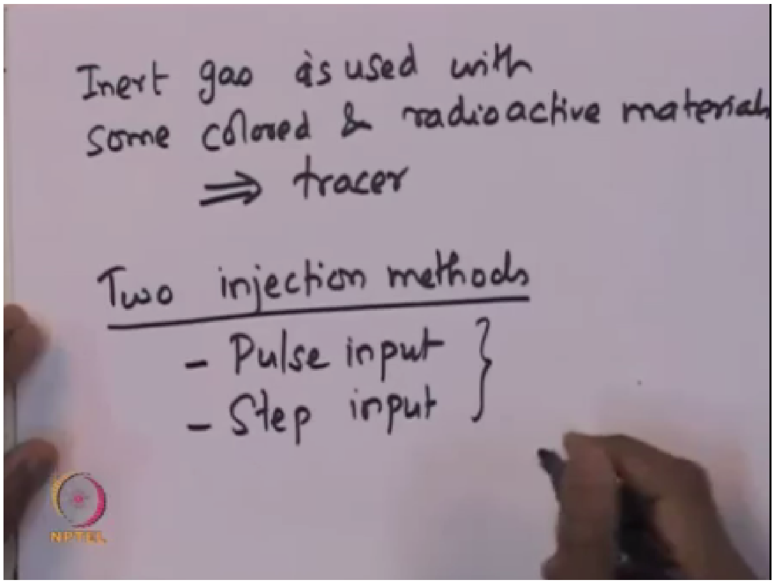

Inert gas is used with
some colored & radioactive material
$\Rightarrow$ tracer

Two injection methods

- Pulse input
- Step input

So, Inert gas with some colored and radioactive material, so these are all commonly used tracers for actually finding the residence time distribution, so there are actually two common strategies for injecting the tracer, so two strategies or methods, so there are two methods for injecting the tracer in order to study the residence time distribution. The first one is the Pulse input and the second one is the Step input, so these are the two classical methods of tracer injection in order to detect the residence time distribution, so which is what we will see in the next lecture.

And what we have seen today is basically to introduce what is the non-ideal behavior, and that to appreciate that real-world reactors do not behave like the ideal reactors such as the plug flow and the mixed flow reactors that we have studied in the in the past. And what are the definitions that is the residence time distribution definitions that are actually involved to characterize such kind of non-ideal behavior.

So what we will see in the next lecture is to look at what is this pulse input and the step input method in order to track the residence time distribution of a given system. Thank you.