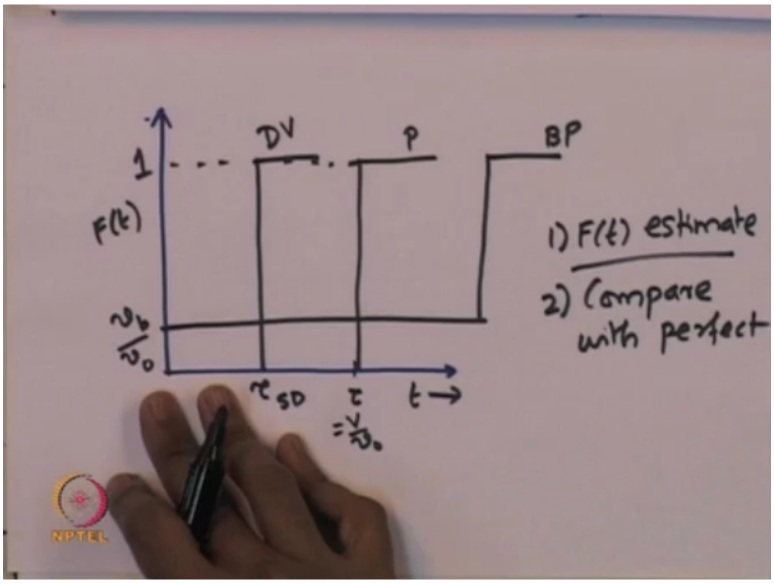
Chemical Reaction Engineering - II
Prof. Ganesh A Viswanathan
Department of Chemical Engineering
Indian Institute of Technology - Bombay

Module - 12
Lecture - 57
Modelling Non-Ideal Reactors I

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 modelled as a plug flow reactor. Specifically, we looked at what is the residence time distribution if the plug flow reactor was operated under normal conditions. 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 dead volume in the reactor. So, now if we compare the, let us now compare the distributions of these 3 modes of operation for a tubular reactor.

(Refer Slide Time: 01:20)



So, suppose if this is the, if this is 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 tau which is essentially given by the volume of the reactor divided by the volumetric flow rate with which the fluid is actually flowing through the reactor. And then, it actually is a, it looks like a step function and this is 1. So, that is for the perfect operation.

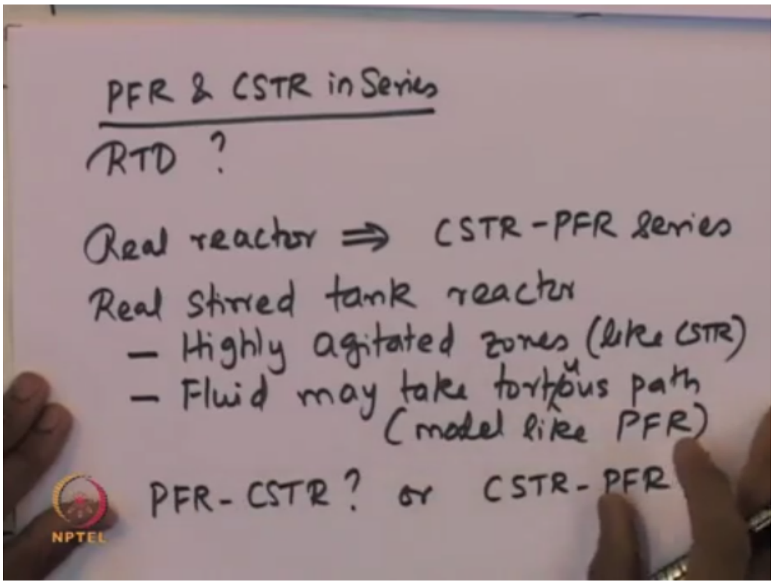
Now, suppose if there is a bypass in the reactor, then what happens is that, there will be a jump in the F-curve. So, the jump will be, start at v b by v nought. So, that tells you the extent of bypass which is actually present in the reactor. And then, the, because the space time is now larger than the space time of the reactor if it was conducted 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 operation. 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 a 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 actual volume of the reactor.

So, therefore the residence time, the space time of, 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 conditions. So, therefore the fluid stream will actually be, leave faster than the normal or perfect operation of the reactor. So, this is tau S D. So, the method is, first we should actually, first one should actually estimate the F-curve experimentally, 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 weather is there is dead volume which is actually present inside the reactor. So, this is the story for the single CSTR and the single plug flow reactor. So, now let us look at the, a 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 a combination of 2 ideal reactors.

(Refer Slide Time: 04:33)



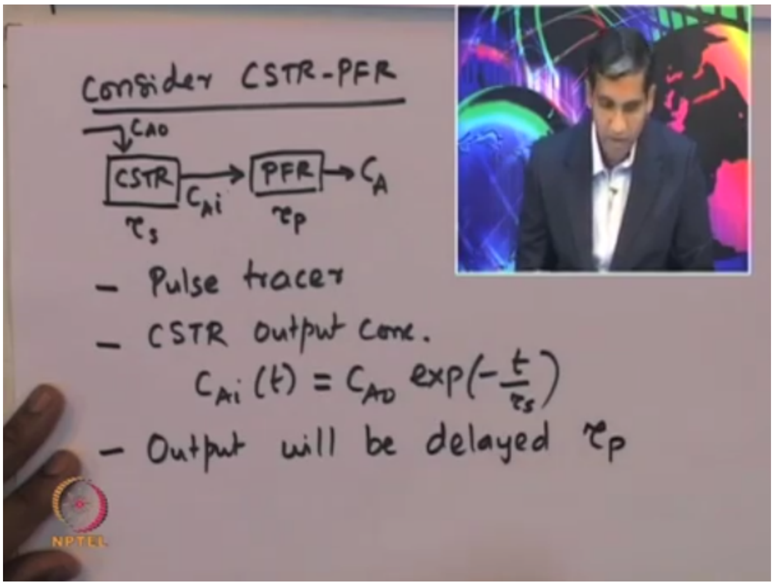
So, let us consider the plug flow reactor and CSTR in series. So, what will be the RTD function for this case? Now, remember that the real reactors can actually be modelled as a combination of a plug flow and a CSTR. And let us assume that there is a real reactor which is actually modelled as a CSTR plug flow, as a CSTR and plug flow operated in a series mode. Now, where is it possible, when is it possible to approximated as a CSTR plug flow series model?

So, consider the situation of a real stirred tank reactor. So, one could include that the, 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 modelled like a plug flow reactor, modelled like a PRF. 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 analyse this by considering one by one. So, let us consider the first case of CSTR being the first reactor and the plug flow reactor follows the CSTR.

(Refer Slide Time: 07:10)



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 A nought. Let us assume that there is some species. And then, if C A i 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 = the concentration of the species in the effluent stream.

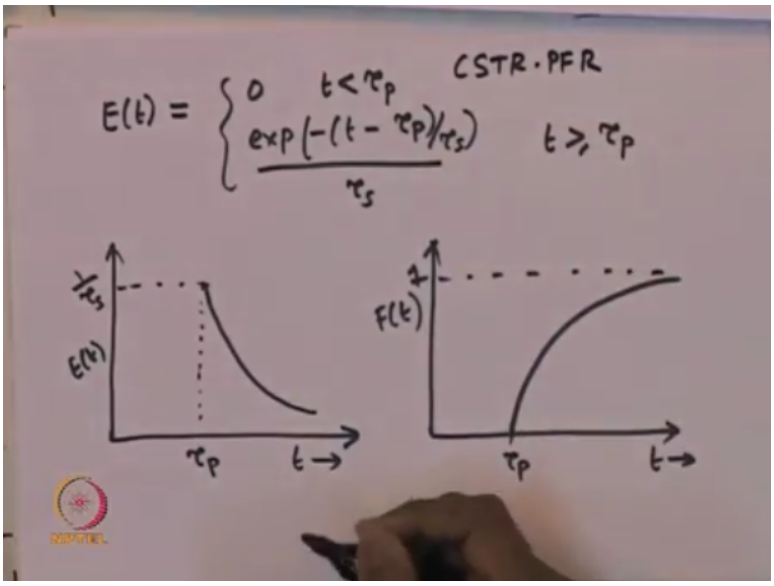
And then now, this is followed by a plug flow reactor. And as it goes through the plug flow reactor let C A be the concentration of the species that actually leaves the plug flow reactor. Now, if tau S is the residence time of the CSTR and if tau P is the residence time of the plug flow reactor, then let us say that the tracer that is introduced is actually a pulse tracer. Let us assume that it is a pulse tracer.

We, the objective is to find the RTD function for this combination. Eventually the objective will be to find the conversion if there are, these 2 reactors 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 A i. By solving the mole balance is given by C A i as a function of time. That should be = C A nought into exponential of – t by tau S. Where tau 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 in, to the exit of the reactor.

So, therefore the output from the, will be just delayed by the space time of the plug flow reactor tau P. So therefore, it will, 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.

(Refer Slide Time: 10:06)



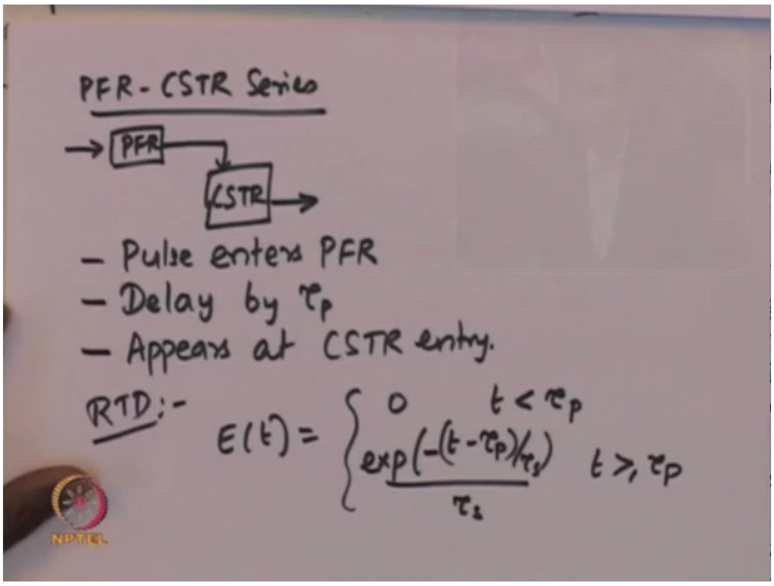
So, the residence time distribution function will simply be; because the output is now going to be delayed, there will be no output that will actually come out of the plug flow reactor till the residence time of the plug flow reactor. Which means that E of t is going to be 0 for t < tau P. Which is the space time, not residence time, the space time of the plug flow reactor. And for other times it will simply be, whatever RTD function for the tracer that actually goes to 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 = – t – tau P which is the space time of the plug flow reactor divided by tau S which is the space time of the CSTR divided by tau S. And this is for t greater than or = 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 tau P because the plug flow reactor is now going to introduce a certain delay. And this will be 1 by tau S. And there will be an exponential decay, exponential fall. And then, similarly, we can draw the F-curve. And it will start at tau P because the plug flow reactor is going to introduce a certain delay.

And the delay is actually, the delay time is = the space time of the plug flow reactor. And there will be an exponential increase in the F-curve. And it 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.

(Refer Slide Time: 12:19)



So, let us look at the PFR for 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 a, the final outlet stream actually comes from the CSTR. So, the pulse first enters the plug flow reactor. And then, there will be a, 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 spacetime of the plug flow reactor is actually introduced.

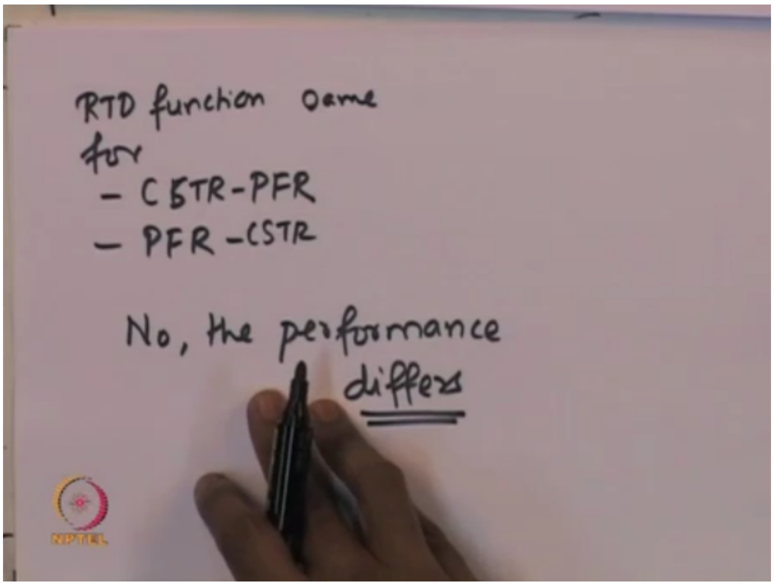
So, there is a delay by the space time of the plug flow reactor. And then, after this delay, the tracer actually appears at the entry of the CSTR. And then it follows the CSTR, the residence time distribution function of the CSTR. So, the RTD function can simply be E of t. So, nothing is going to appear till the space time of the plug flow reactor is leave, reach, because the, from the RTD function of the CSTR, the E-curve starts from term t = 0.

That is, the, there the tracer will actually appear, start appearing immediately after the tracer is actually, pulse tracer 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 series combination till the space time of the plug flow reactor is reached.

And after that, it will simply be the, this will be controlled by the residence time of the CSTR. So, therefore the residence time function will be – t – tau P divided by tau S, where tau S is the space time of the CSTR. And this is for t greater than or = tau 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 2 residence time functions are exactly one and the same.

(Refer Slide Time: 15:33)

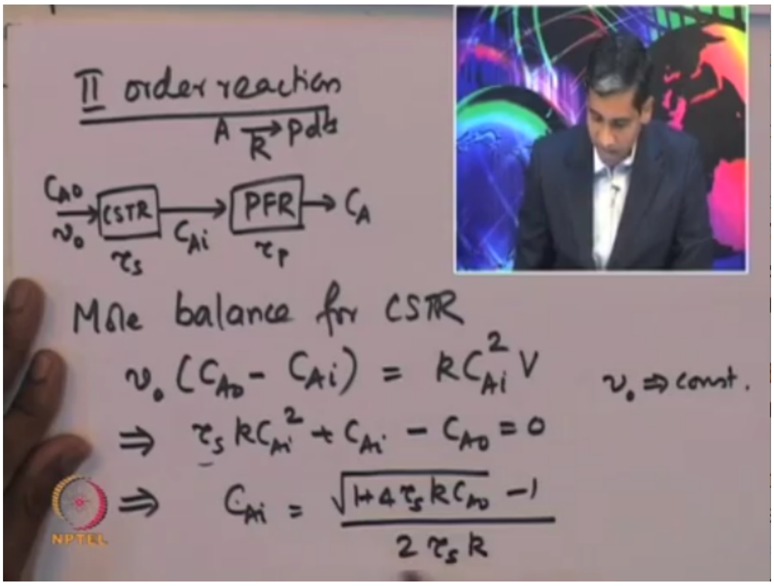


So therefore, what one can actually, one observes is that the RTD function is same for CSTR followed by a plug flow reactor in series and plug flow reactor followed by a CSTR. So, it does not matter what, in which the CSTR and the plug flow reactor are placed, the residence time function of the series combination, that is CSTR and plug flow reactor will continue to be the same.

Now, does it mean that the properties of this combination is 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 2 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 2 reactors, that is CSTR and PFR are actually placed. So, let us take an example of that. So, let us take a second order reaction.

(Refer Slide Time: 17:06)



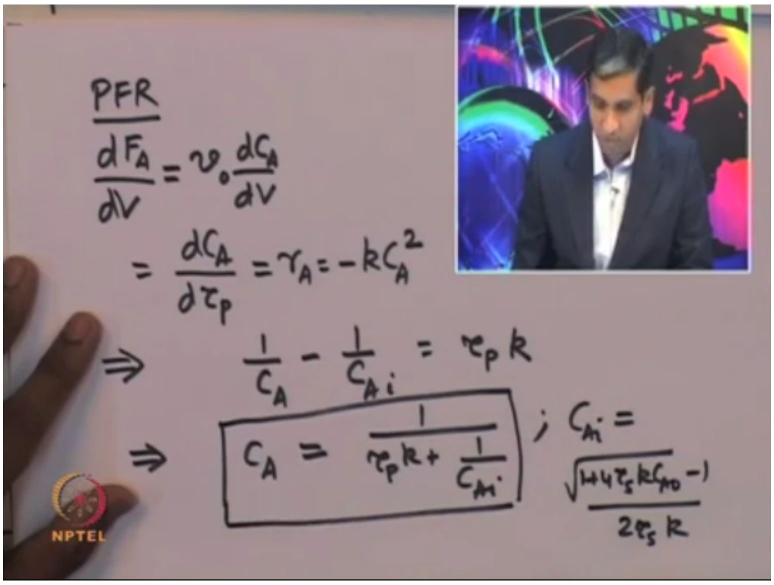
Let us take a second order reaction of A going to products. And the corresponding specific reaction rate is k. And so now, so, this can be depicted as, let us consider the combination of CSTR followed by a plug flow reactor. So, C A nought is the concentration of the species fed into the CSTR and if C A i is the concentration with which the species leaves the CSTR. And if C A is the concentration with which the species actually leaves the plug flow reactor.

And the space time of CSTR and plug flow reactor are tau S and tau P. So now, we can write a mole balance for CSTR. And the mole balance is that v nought into C A nought – C A i. So, that is the rate at which the species actually enters the reactor. And this is the rate, molar rate at which the species actually leaves the CSTR. And that should be = 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 nought 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 nought is constant, if we assume that the volumetric flow rate is constant, then we will find that this equation can be simply rewritten as tau S into k into C A i square + C A i – C A nought = 0. So, that is the quadratic equation C A i. C A nought is a measurable quantity which is known and tau which 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 + 4 tau S into the specific reaction rate multiplied by C A nought – 1 whole divided by 2 times tau S into k. So, that is the concentration of the species that actually is in the effluent stream that is leaving the CSTR. So now, let us write a similar mole balance for the plug flow reactor.

(Refer Slide Time: 19:43)



Let us write the mole balance for plug flow reactor. So, that is given by d F A. F A is the molar flow rate of the species that is flowing into the plug flow reactor, divided by d V which is the V is the volume of the reactor. That should be = v nought into d C A by d V. And that is = d C A by d tau P. Assuming that the volumetric flow rate is constant, then tau P is the space time which is the volume of the reactor divided by the corresponding volumetric flow rate.

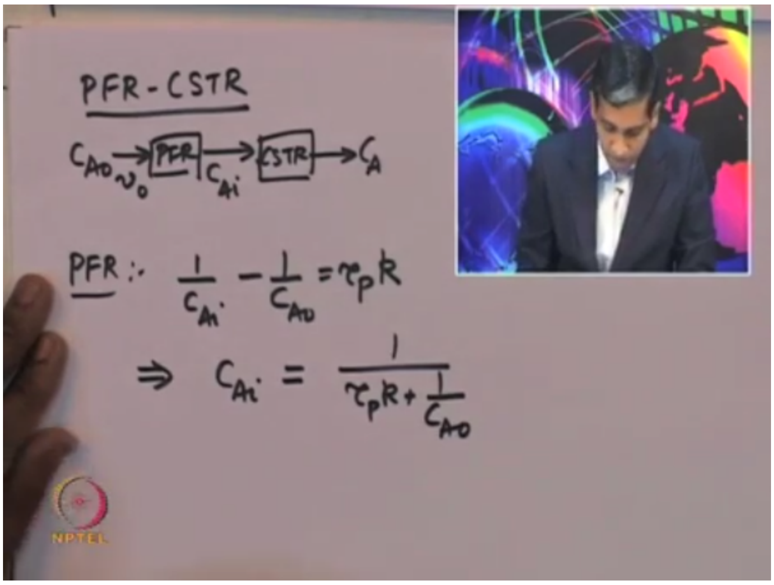
And that should be = r A which is – k into C A square. So, that is the mole balance. And by solving this, we can actually obtain that the solution of this equation is 1 by C A in – 1 by C A i. That should be = the space time of the plug flow reactor multiplied by the specific reaction rate. So, from here, we can see that C A can actually be expressed as 1 by tau P into k + 1 by

C A i. Where C A i is essentially given by C A i 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 S k C A nought – 1 divided by 2 tau S into 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 2 are same. And we are attempting to find what is the conversion of the species for a second order reaction for both these combinations.

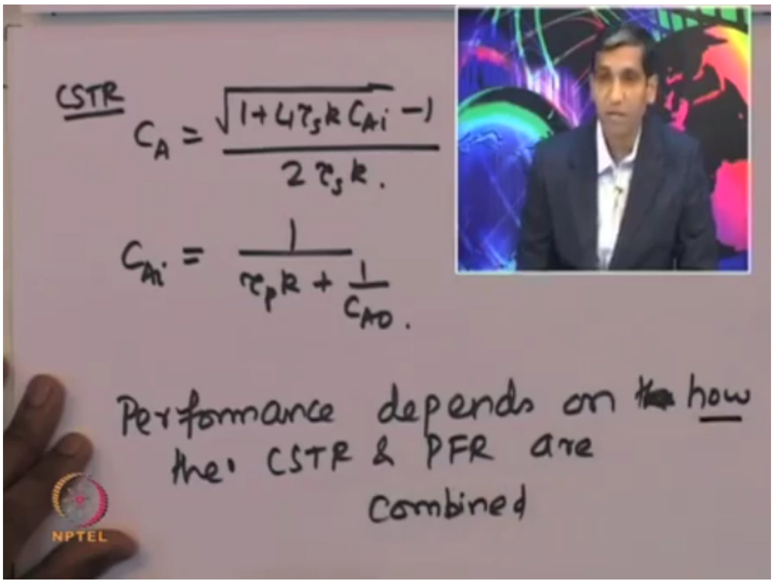
(Refer Slide Time: 21:53)



So, let us now take the second combination where the CSTR follows the plug flow reactor and the depiction is C A nought. This concentration with which the species actually enters the plug flow reactor. And if v nought is the corresponding volumetric flow rate. So, that is the plug flow reactor. And C A i is the concentration with which the species actually leaves the plug flow reactor.

And then it enters the CSTR and CA is the concentration with which the species actually leaves the concentration of the species in the effluent stream of the CSTR. So now, the from the plug flow reactor mole balance we can find that the 1 by C A i – 1 by C A nought, that should be = the space time of the plug flow reactor multiplied by the corresponding specific reaction rate. So, from here, we can estimate that C A i is = 1 by tau P k + 1 by C A nought. Now, from the CSTR mole balance, we can actually find that, from the mole balance of the CSTR, we can actually find that;

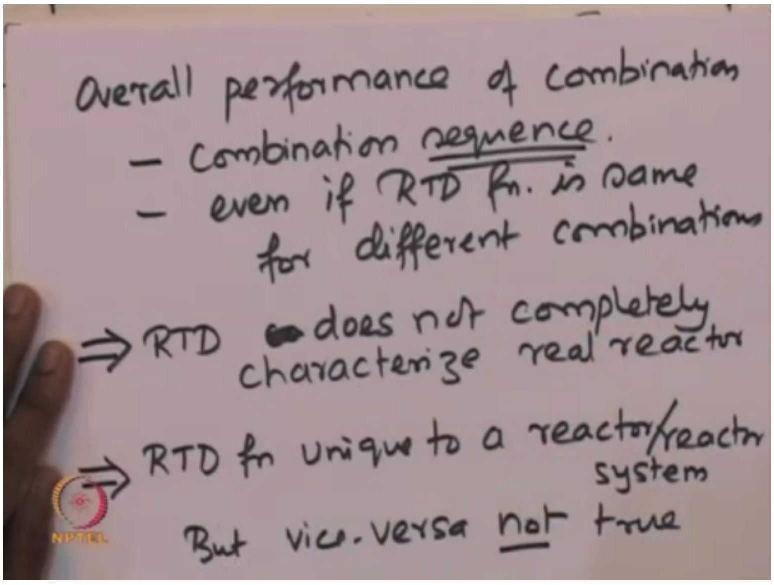
(Refer Slide Time: 23:10)



C A is = square root of 1 + 4 tau S k into C A i – 1 divided by 2 times tau S into k. So, where C A i is actually given by 1 by tau P into k + 1 by C A nought. 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 actually, when we actually estimate the performance of the combination of reactors. So, therefore this clearly suggests that the overall performance of the combination of reactors depends on;

(Refer Slide Time: 24:46)

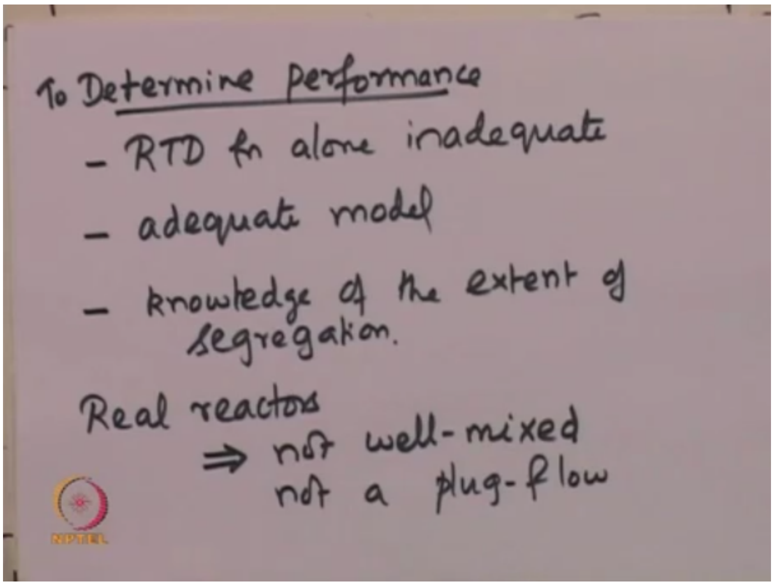


Overall performance of combination reactors actually depends on the combination sequence and not just the combination, even if, it depends on the combination sequence, even if the RTD is the same. So, even if the RTD function is same for different combinations, the overall performance of the combination actually depends on the sequence, actual sequence in which the reactors are actually placed. So, this clearly shows that RTD function actually does not completely characterise, RTD does not completely characterise 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 / reactor system combination. Reactor system, but vice versa is not true. That means that the reactor / reactor system is not unique to the given RTD.

Whereas an RTD can actually be unique to a given reactor / 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 the, 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 to determine overall performance.

(Refer Slide Time: 27:44)



So, determine the 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 needs to characterise 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 needs 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, is 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 to is that simply knowing the RTD function is insufficient. If there is a, 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, that are actually, CSTR models and what happens if 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 are, they do not behave like a plug flow.

So, which means that one needs to come up with the various different kinds of approach or a different approach in order to model the non-ideal reactor in order to estimate the performance of such real-world reactors.