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**Lecture - 6 Non – ideal Reactors: Tank – in – serious model**

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Reactor Models<br>Jor non-idea writer ideal Rxtrs.

We are going to start a new chapter today which deals with design of non-ideal reactors. So, we going to look at reactor models for non-ideal reactors let us take, a review of what we have learnt so far as per as non-ideality in reactors is concerned as you know, there are ideal reactors like: CSTR, PFR in which the flow pattern is well define. In these reactor flow pattern is well defined whereas, non-ideal reactors the flow pattern can take any particular shape in term like if you look at e curve.

Now, this flow pattern tells you, how the flow is flowing inside a reactor or somehow like it does not follow a very particular or specific pattern. Now, in order to get a converse final aim is to have a reactor design. And this reactor design somehow you have to incorporate this non-ideality. So, I cannot assume any reactor to be plug flow reactor or a CSTR. So, they can be non-ideal flow patterns which will affect the rate reactor design.

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So, in the last chapter will look at 0 dimensional model for non-ideal reactors. So, in this you have typical e curve right and this e curve of course, is as you know e is the exit age distribution; that means, I have a reactor this inlet going outlet. And what you seeing in outlet gives you, this particular pattern. Now, they can be many different possibilities, which of the flow patterns which would give raise to this e curve. And what happens inside a reactor is, not exactly reflected in the exit age distribution is something like that we already learned.

So, so there are different possibilities in terms of what happens inside a reactor, the mixing pattern inside a reactor. So, mixing is not well incorporated in the e curve. So, then we looked at 2 different extremes: so 1 extreme is a completes aggregation model and another extreme is the maximum mixedness model. Now what let me quickly revise, so it founds a nice platform of a further discussion as for is this chapter is concerned.

So, let me quickly revise what these 2 models are, so maximum mixedness model means, that mixing is maximum. So, mixing between what? So, if you look at this e curve there are different segments every segment right. So, these segments whether will have will be flowing through the every segment will have a residence time. And that is why like will have a fluid element, we will have a specific residence time and it is have a distribution of residence time.

So, will have different segments spending different residence times in the reactor right and the extent of in terms of a mass or volume of this particular element spending this much residence time the reactor that may vary right that is nothing but e curve. So, you have this different segments or different elements spending different residence time. Now we talking about, a mixing between these 2 elements or several elements.

Now, there is an extreme where these elements then mix there well mix right. And there is another extreme where, these elements they do not mix at all. So, they going parallel, they do not talk to each other, they do not interact with each other. So, that is segregation; completes segregation and there is another extreme where these are completely mixed. Now, how it happens and all you will not going to look at a in detail, but that is a meaning of it. Why we look at these extremes, because these 2 extremes would give us a bound on conversion.

So, it gives a range given an e curve like this I make an assumption that is completes aggregation of these elements. And, then calculate a conversion and, then another extreme where there mix thoroughly mix before the come out inside a reactor. And calculate a convergents and these 2 convergents are likely to be different and they are going to different for most of the reactions, but they are going to same for just 1 case remember what is it, when the reaction is first order.

And I think it has been discussed to well before why first order reaction, internal mixing does not matter whereas, any other order internal mixing matters a lot that. So, if you go for the complete segregation model and maximum mixedness model. These 2 models are going to give you different convergents, different extend of reactions. Intrinsic current is same, rest all volume the reactor everything is same, e curve is same, but internal mixing will matter.

So, what happen in this case I am not going to get a exact conversion why? Because, the 0 dimensional model I am just going to look at a extremes. So, I get bounds, I get a range, I may say that, fine for given volume this is the possible range of conversion that I am likely to get if the e curve is like this for a non-ideal reactor. So, it may vary from 0.45 to 0.55, so that is a idea I get right I do not get a exact conversion that is a limitation of this model.

So, this is 0 dimensional model it talks about, the extremes as for as a mixing inside a reactor is concerned e curve only gives you partial information of the flow pattern it does not tell you about a internal mixing. And for the first order reaction of course, it does not matter. So, it inside getting a bound and I just getting a single value I do not have to worry about, whether it is complete segregation or whether it is maximum mixedness.

So, this is a quick revision of what you learned before. And now let us, go ahead now this is a problem with 0 dimensional model; where it gives most of the times for in non first order reaction the range of convergent. Because, we consider 2 extremes we not looking at what is happening inside.

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One Parameter Model.<br>1. Tank- in-Sevies. Tank- in-sevies.<br>Dispersion Model  $\overline{h}$ 

Now, in this chapter we are going to look at different models: 1 of them is 1 parameter model. So, I have adsorption additional parameter that is going to give me some idea about, the convergent. It will help me get the exact value of convergent for the given e curve. Now, remember that this model that we are going to discuss or other the 2 types of 1 parameter model we going to discuss they applicable to particular geometry I will elaborate this point later, but remember that.

In 1 parameter model, we have 2 models that we going to discuss that are tank in series and dispersion model. Now let us consider a tube that is why I said it is applicable to a particular geometry. Again I tell you why am tell later tell just talk more on this a tube this is flow that is taking place. And you may have different extends of back mixing that is occurring. Now, if you are very flat profile what it means, is a you have a plug flow reactor, what is a e curve that I am going to get is a direct delta function.

So, the e curve for the plug flow reactor is direct delta function, but this tube a reactor that I am talking about, is not a plug flow reactor not necessarily behaving close to a flow reactors. You know not a single real reactor is behaves like adsorption ideal CSTR or PFS it is close to those reactors in extreme situations. But they do not exactly follow the patterns that we assume, but anyway lie for if you are very close to a plug flow reactor, if you getting a e curve is matching with direct delta function.

So, some extend like a make adsorption assumption that be behave like a plug flow reactor and I can design a reactor accordingly. Considering, some possibility of conversion being plus minus, but that is ok, because by making assumption of plug flow reactor it reduces the complexity or legal in calculation it makes my calculations simpler; it helps me to get some quick estimates of convergent for a given volume or for given convergent the estimate for the volume. So, let me get back to this you have a tubular a reactor in which there is possibility of back mixing; that means, I am not going to get adsorption e curve which is similar to direct delta function or a plug flow reactor.

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So, what is likely to happen see will have e curves e t versus t. Now, for a plug flow reactor I am going to get something like this infinite right you know the meaning of it. And this is nothing but tau which is volume divided by volumetric flow rate it is an ideal situation. Now, what I am going to see in the reality is somewhat like this possible I may see something like this; I may see something like this why does this happen?

It happens, because there is mixing in axial direction, if there is no mixing I am going to see something like this right. But because of mixing some fluid elements may spend more time, because they go back and then forth. So, it possible that day spend more time in a reactor and they come later; some fluid elements may spend a less time just componset for those for gone a head or those lagging behind.

So, it is possible that you get a distribution right. So, it's I am talking about a tubular reactor where there is possibility of back mixing, you may have packing it may provide some because tutorcity and all it's quite possible that you are you do not have the exactly plug flow type behavior. Now so these are the different e curves how do I interprets these e curves and this is happen only because the back mixing. So, I need to a corporate effect of back mixing in this particular behavior that I have observed all right.

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So, let's consider any e curve right once this e curve is obtained, I have a tubular reactor I do a pulse injection experiment and look at an exit age distribution I am going to see this. Now, this is something given to you from this you are going to come up with a model I am going to determine a parameter; now mixing is characterized, by like you have a say let us have a hypothetical mixture or agitator in the reactor.

So, in the tube itself I can say that tube is consisting of various compartments. If you have infinite such comportments in a given volume total volumes small small compartments. What is it mean? Infinite it means that, you have flow similar to a plug flow reactor. Now, you reduce a number of compartments what is it mean? That means, this some back mixing happening you go on reducing, go on reducing; mixing extend of mixing would increase right. Consider an extreme, where you have just 1 compartment there has to be compartment.

So, 1 compartment what is it mean? A compartment with agitator good mixing complete back mixing in that compartment what is it mean its CSTR, this is an another extreme. So, what is it mean? So, you have on 1 side you have a CSTR, on the other side you have PFR; CSTR means are 1 compartment, PFR means finite compartments in between you have a reactor which has partial back mixing right.

So now, you would have guess what is a parameter that I am talking about, it is a number of compartments, every compartment is CSTR perfect back mixing right. So, its number of CSTR or number of tanks which are in series that are going to that number is going to be a parameter for this model.

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Fine, so why I am saying it is a tubular reactor. So, let us a consider reactor which is a very regular geometry say I have a reactor like this, this is an inlet, outlet. Now, there are flow patterns, then there are possibilities of some isolated zones right. And you have the

output here and what you going to see, is a behavior like this any general e curve. Now, this particular e curve does not look like the e curve of it tubular reactor why.

Because, for tubular reactor like let us, look at all the possibilities now, you have a plug flow reactor, CSTR e curve right CSTR. Once CSTR is this what will happen to 2 CSTR like a in the case of 2 CSTR you are going to get something like this. Then 3 CSTRs, 4 CSTRs see what is happening now? As you go on increasing number of CSTRs you are approaching the plug flow reactor this is a of course, going to infinity this is becoming narrow, it starts its seeing a delay here.

So, what is happening as we go on increasing the value of n that is number of compartments, number of CSTRs in series. The behavior it goes it follows this particular the train goes from CSTR to PFR, but look at these curves the nature of these curves. These curves and to compare it compare these curves with this particular curve I am getting a very irregular shape here or other very an unusual like there are many punctuations are up down and all that. Why does that happen? It happens because of the regular geometry here and that define the geometry flow pattern is a quite complex.

So, this flow pattern and this flow pattern they are not matching. So, can I apply a tank in size model for this reactor? I cannot do that Why because there is no curve that fits well in this particular shape. So, again 1 parameter model has its own problems, it is applicable to most of the times to tubular reactor, where the e curve is like this or 1 of these rather. Its continuous thing, it is continuous things, the no ups and downs, no recirculations or recycle with have behavior. So I will go back to my statements that, 1 parameter models are good for tubular reactors where you get e curve with a nature like this clear?

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So, let us go ahead and do some mathematical derivations how do a find out number of tanks that I have in series for a given tubular reactors say I have an e curve. How do a find it? So, let us derive an expression for the e curve for a tank in series suppose I have n number of tanks in series let us try with 3 tanks in series first. And, then explain this concept to n times, so let us have 3 tanks in series fine.

So, let me write it write a let expression for a e curve I mean I am going to give pulse here, I am going to see what happens here. So, this is my e curve and this is what I am going to get likely to get fine. Now, can I get explanation for this? But I know CSTR behaves. So, let us write e t into delta t this is a fraction you know meaning of this I am not going to repeat.

So, e delta t is a fraction that comes in between t and t plus delta t that is equal to the volumetric flow rate I am going to assume an volumetric flow rate remains constant throughout into c3 t. So that means, c3 is a concentration that at the outlet of tank number 3, so 1 2 and 3 right tank number 3 c3t into delta t divided by N0. What is N0? N0 is a total amount of pulse that have injected.

How do a calculate N0? N0 is nothing but based on c3 t, because now I am get read of N0 I am just looking at concentration outlet see and visualize a realize realistic experiment that I am doing, I am looking at a concentration at outlet. So, tank expires everything in terms of concentration at outlet. Now, N0 is a total amount of pulse or

other the tracer rather that have injected. N0 is equal to 0 to infinity c3 is t dt total amount that is come out into of course, the volumetric flow rate see, concentration right concentration into volumetric flow rate into time. So, I just integrate right I just integrate from 0 to infinity. So, that much amount have injected as tracer, so let becomes N0, so let us go ahead fine.

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Let me substitute for N0, so what I get is e t is equal to v C3 t right it says this is delta t. So, e t is equal to c3 t divided by so I have got a patience for e t based on the concentration at the outlet. Now, the c3 I need to get that in terms of the residence time, initial concentration or inlet concentration. And I know these are all CSTR, let me write an steady state balance for CSTR.

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CSTR 1 V1 that is a volume of CSTR d c1 by dt you learned this unsteady state balance for CSTR is equal to minus v C1 right. Shall I write here? This is what this is going out this is going out, this is accumulation coming in Shall I write this? No, because what I am looking at see traces experiment, pulse experiments, I am injecting a tracer. And, then after that at 0 time an injecting tracer and after then I am observing the response.

So, after that is there anything that is coming in as per as a tracer is concerned no right. So, I have injected and stopped it now it is only the inlet that is flowing, the solvent that is flowing. The tracer is not coming in, after 0 plus and this is equation I have written is for time 0 plus onwards let me 0 onwards. So, this term is not there, this term is not there.

So, I have only this equation for the concentration in the first time I am writing it for a first time. Now, later on I will do it first, second, third and then finally, I will get expressions for c3 that is my objective. So, here from this I get a concentration and outlet of tank 1, where I have the boundary condition at time is equal to 0 time is equal to 0 C1 is equal to C0, but solve this equation its very simple right.

So that is nothing but C1 is equal to c0 e raise to minus t by tau 1 what is tau 1? tau 1 is equal to v1 divided by v. This is a volumetric flow rate, this is a volume of first tank this is a expression for C1 that is the concentration and outlet of first tank. So, let us continue now, so this acts as a inlet for a second tank. So, let us a write an expression for the second tank.

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Tank number 2 what is it? v2 d c2 by dt is equal to v C1 coming in minus v c2 I cannot neglect this. This is changing with respect to time and 0 plus C1 will have some value. So, there will be 2 terms as per as tank 2 is concerned, but tank 1 inlet was 0, because tracer was 0 at tank 0 plus right. Before we go ahead let me, make an assumption that v1 is equal to v2 is equal to v3 all v's are equal same V just was simplicity right.

Let me say vi, because I am not use v for something and hence later I am not use v for the total volume let me call this is vi. So, let becomes vi here fine, so let me simplify or other solve this further for C1 I have the expression. What is that? This 1. So, this expression I will substitute for C1 what I get is this dc2 by dt is plus c2 by now I will say, tau i. Why tau i.? So, what is tau i? tau i is equal to Vi divided by v which is constant that is volumetric flow rate given to you.

So, C2 divided by tau i is equal to C0 divided by tau i into e raise to minus t by tau i I am just substituting for C1 and expressing everything in terms of tau i now. So, you know what is tau i? So, I get an expression for differential equation for C2 right now again, for this I need a boundary condition at t is equal to 0, C2 is equal to 0 right. So, this equation I solve this using this boundary condition, so this is famous or this is a couple of method of integrations factor e raise to t by tau i. So, this expression can be solving using integration factor or integrating factor e base to tau by.



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So, t by tau i and I get the solution for it; which is given by C2 is equal to C0 t divided by t tau i into e raise to minus t by tau i. See concentration and outlet of the second tank is a express in terms of initial concentration time anyway, I want to know how it changes with time and of course, tau i right. I will eliminated C1 what is my aim? I am my aim is to get C3 in terms of C0 t and tau i.

So, let us do it now I follow same methodology for tank 3 substitute for C2, because now in tank 3 in inlet is C2 right and I will solve this equation fine. So, what I get is, C3 is equal to, so you can try it out again a same methodology I get what I get is this e raise to minus t by tau i. So, you have 2 appearing here right see the difference, not much difference but of course, you have the you have the exponential term there. And, but instead of t now it becomes t square i have 2 appearing here tau instead of tau i I have tau i square. So, let us go ahead now I have the expression for the e curve or other the e for the entire reactor that tanks in series.

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$$
\epsilon(t) = \frac{0 \cdot C_3(t) \Delta t}{\Delta t \cdot 0 \cdot \int_0^{\omega} C_3(t) dt}
$$
  

$$
\epsilon(t) = \frac{C_3(t)}{\int_{0}^{\omega} C_3(t) dt}
$$

What is that? This 1 now I have the expression for e, I have the expression for C3; substitute this C3 in e curve or other the e expression for e.

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So, what I get is see final, so see objective is to get e expression for e. So, I substitute for C3 and let me write this first, so that C3 right. Now, what is this? This is the total amount of the tracer that I have injected, can I get it in terms of initial concentration C0? Possible what is it?

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 $=\frac{U_{o}(\text{d}U)\int_{o}^{\infty} \zeta_{s}(t) dt}{V_{i}}$  $\zeta$ cvdt =  $\gamma$ . Co

If you look at it what happens at time 0 you have C0 is equal to N0; that is a total number of moles or whatever unit can be grams or moles whatever. You have that much amount of tracer divided by V1. So, this is something present at time is equal to 0 sharp in the reactor V1 is a volume and it can be Vi also in our case.

So, let me call this is Vi; which is nothing but the total amount right is V0 which is nothing but v rather into C3 t dt right divided by Vi. So, from this what is this v by Vi tau 1 by tau. So, this till is tell me that this integration is nothing but tau i into C0 right. And I am just expressing it in terms of initial concentration, because this is appearing the final equation right.

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 $c, c \Theta$ H  $C_{3}$  to dt =  $r_{i}$  G

So, let me get back to this equation this is for the e curve I am substituting for C3 that I have just derived C3 that have derived here.

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I will substitute it here and then I will have a very simple equation e t is equal to C0 C0 will get cancel. And I will have t square divided by 2 tau i now it cubed, because it is 1 tau I have just come from that denominator integration term e raise to minus t by tau i. Now, this is for 3 tanks if you applies same logic do it 4 tanks, 5 tanks, 6 tanks, n tanks then what I am going to get is this is for n tanks is t raise to see 3 tanks 2 here n minus 1

divided by see n minus 1 factorial into tau i raise to n see the logic, then e raise to minus t by tau i this is for n tanks in series.

So, I have got an expression for e curve for n tanks in series; a general expression for e curve for the n tanks in series and that is what I want right. So, when I get e curve I have e curve, so in this is 1 parameter that is n that I can calculate from this. So, this will this will obtain from experiment in the laboratory for a reactor; it tabular reactor under a flow conditions that are desired for the reaction. But of course, I do the experiment nonreactive condition you know that just look at a residence time distribution right.

So, from this experiment I get e curve from e curve I get n, because I had I have an expression for tanks in series e curve and once again get n then I can calculate a conversion. What is n? n tells you the extent of back mixing n infinity means, if PFR, n1 means its CSTR. And in between 1 and infinity you have the extent of back mixing characterized by the number n fine. Let's go ahead and simplified further equation looks bit a complicated.

So, from this you have going to defining a term called a variance of course, you know what is variance when we had distribution the variance that means, how much at particular time in the values of away from the average.

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So, the something called as variance before that will define a term non-dimensional term theta equal to t by tau, where tau is that total residence time what is it mean? That means, tau is n into tau i is individual residence time for every tank n into tau i is a total residence time. So, if tau i is equal to Vi by v then tau is equal to V which is nothing but V1 plus V2 and so on divided by V that why I said now I have been using V for something else the total volume.

Why? Because see I do not have tanks, I am just assuming a tubular reactor to be set of tanks. So, all I know is the total volume right, so I need to expression in terms of total volume finally, right this total volume is V1 plus V2 plus V3 plus V4 and so on. So, the residence time based on total volume is tau right for individual reactor is what tau i now it is tau. And, then I have a dimension less number theta express in terms of tau that is t by tau.

So, I have the expression for e t I will write it again to raise to n minus 1 divided by n minus 1 factorial tau i n right e raise to minus t by tau i. Now, this will get reduce to e theta now t will be express in terms of dimension less time theta while do that, then all these will get converted to n into n theta raise to n minus 1 see t will become n theta. Because, see t right then e raise to minus n theta divided by n minus 1 factorial. So, this is the expression for e in terms of dimensional less time instead of actual time you going to use this further that why you expressed like that.

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 $=$  (t- $(\theta - 1)^2$   $E(\theta)$  de 

Now, there is a variance that we define now how do we define variance if you have a distribution the expression for the variance is, in terms of dimensional less time variance square is equal to actual variance in time divided by tau square. Now, so this is nothing but 0 to infinity theta minus 1 square e theta d theta right. I hope it is clear if you write just variance in time you will have t minus tau you have to just divided by tau square and then you get this.

So, it is a very as I said like how much you go away from tau mean residence time. So, if you expand this further what you get is 0 to infinity theta square e theta d theta minus 2. I am just expanding this, so theta minus 2 theta plus 1 so you get this. So, what is the value of this? This is equal to 1 this particular term. What about this? This particular term this is dimensionless average residence time dimensionless.

So, it is going to be 1 because it is the reference is tau for the residence time it was t e t dt, then I was tau now it is theta e theta d theta; that means, it is tau divided by tau that means, 1. So, this is this is going to be again is integration is going to be 1, this is 1, this is 1. So, minus 2 plus 1 is minus 1 0 theta minus 1, so this is an expression I am going to simplify this further.

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So, let us solve this integration what I get is or before that let me just write it again right substitute for e theta see we have derived equation for e theta. So, this is e theta I just substitute for it n n theta n minus 1 divided by n minus 1 factorial e raise to minus n theta d theta minus 1. Now, if you do all this what you get is, because take n, so will have n raise to n divided by n minus 1 factorial it come out right. And you have 0 infinity theta raise to n plus 1 e raise to minus n theta right dt that is solve this further what you get, you can do it on your own.

So, it get simplified to very simple term 1 by n and this is what I want variance is 1 by n; variance is obtained from the e curve. So, once you get variance right you get value of and number of tanks in series. So, n is equal to 1 by sigma theta square which is nothing but tau square divided by sigma square right. So, I get a value of n this is what I want right.

So, given e curve now will see how to calculate sigma from e curve, I have already told you that expression for rate. But will solve or I will tell you the procedure to get sigma from that or this sigma they from that I get n. So, e curve will give you sigma and sigma will give you the value of n right.

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How to calculate conversion for the given n, now we talking about reactor tank in series there is very simple know. I have n number of tanks how do I calculate conversion for a CSTR? I have n number of CSTR are in series the conversion say for first order reaction the conversion is 1 minus 1 by 1 plus tau i k raise to n tau i is the again see do not get confusion this 2 tau.

So, this 2 tau is the residence time for single tank what is k? k is the rate constant. And this is something like that you done before. So, let me summarize I have a tubular reactor I want to get a convergent problem can be other around for given convergent, find out a length a volume the tubular reactor, when I have a tubular reactor let us talk about given reactor in calculating convergent.

So, I have a tubular reactor what I will have to? I will not assume it has a PFR. Now we have talking about, non-ideality that can be possibility of back mixing. So, what I will do is I just pass of fluid I will do residence time distribution experiment. I will inject a tracer look at its falls it outlet I will get a e curve form it right. Once I have the e curve, then I can get a variance from the e curve; from the variance I will get a number of tanks in series for that particular tubular reactors reactor other if it is close to PFR the value of n will be very large.

If there is so much back mixing happening for some reasons value of n will be close to 1 1 2 3 whatever. So, I get a value of n once I know the value of n, I have the expression for convergent and that tells me how much is the convergent based on n. Because, rest all you know what is this rate constant; tau i is the residence time for the individual reactor how do i calculate tau i? So, I know the total volume for the tube.

So, know the total residence time from a total residence time I calculate individual residence time; residence time individual reactor. But dividing it by n; n is known right. So, I get an expression for a convergent that is for the first order, but I am of course, for second order, third order, but I have different expression it is just solving a problem for CSTR.

So, I have converted a non-ideal reactor to a an ideal reactor problem tanks in series; ideal reactor in series. So, that n varies n is the parameter thank you will continue discussion will solves a small problem of course, not numerically, but I will tell you the procedure, so let things will be clear to you fine.

Thank you