Lecture - 38
Non – ideal Reactors: Dispersion model Introduction to multiparameter models

Good morning. So, will quickly revise what we learn in the last lecture, in the last lecture we look at dispersion model; overall we just looking at models for Non-ideals reactors. First model was tank in series; the second one is dispersion model.

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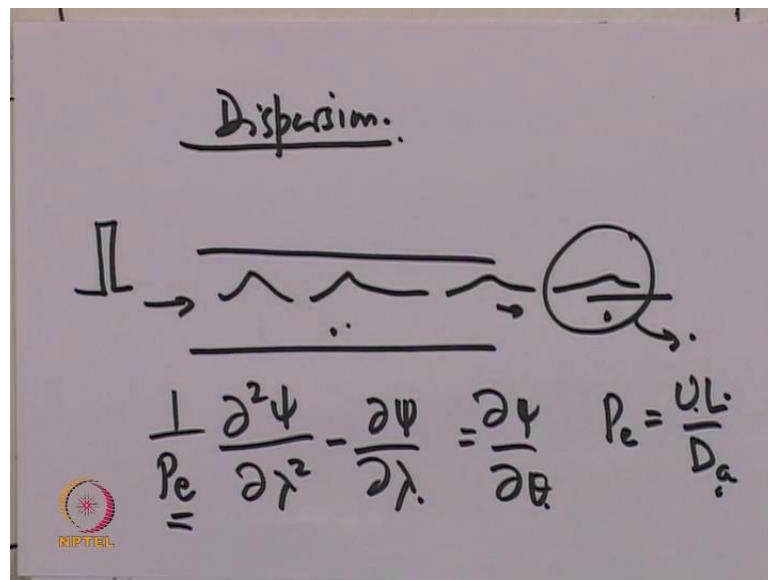
So, in Dispersion model we assume tubular reactor geometry and then of course, we say, we characterize this flow pattern by through a parameter called peclet number. So, we say that, we have a tracer that is injected and the inlet which gets into the form like this. So, it becomes flat, when it comes out flat in the sense of course, it gets distributed I would say. Now, we want to see the behaviour and that this particular behaviour is that depends on the extend of back mixing, which in turned depend on the peclet number for the given system.

So, we derive equation for this or other we formulated differential equation for this; which was 1 by Pe dell psi dell to psi by dell lambda square minus dell psi by dell lambda is equal to dell psi by dell theta, where theta is dimensionless number lambda is dimensionless length at P. Peclet number, which something that characterizes the extend

of mixing, which is nothing but UL by Da, where Da is a dispersion coefficient. And this is length and U is a velocity and this dispersion coefficient is nothing but something similar to a diffusion coefficient, but that there diffusion is by fix law where talking about migration due to concentration driving force. Here if the, it has a slightly broader meaning in the sense is not just diffusion, but it takes care of other effects also and somehow characterize this extend of mixing that is occurring or the flow that is occurring outside the convective flow.

So, the 2 type of flow now, convective and dispersive now. So, this is something that takes care of dispersion and conviction is of course, taken care of by the velocity term. So, this is particular term, where you have velocity coming in picture. So; now, this peclet number have I told you that, if it goes to infinity means you have typical ideal plug flow reactor. If it goes to 0 means, you have a CSTR. So, that 2 extremes of plug flow, peclet number and in between these 2, 0 to infinity you will have number of peclet. So, peclet number giving an idea about the extend of back mixing occurring in the real reactor.

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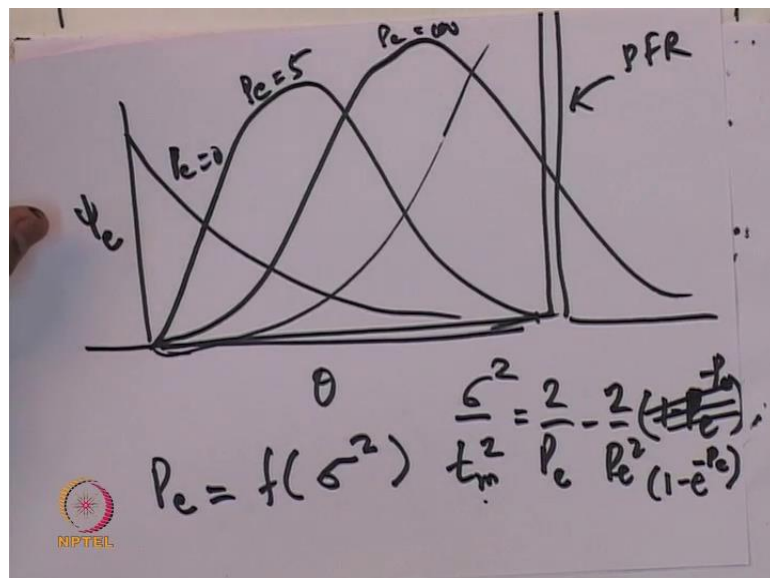
Now, if you have this equation and of course, the corresponding boundary conditions you solve them and you get a behaviour like this, for different values of peclet number. This is the exit concentration, of course and for peclet number equal to 0; you have CSTR then for the peclet number higher than that you have a behaviour like this, peclet

number say 5 then you start seeing some lag than peclet number say 100 or so. And then you have something like this, going up and then at value of peclet number closed to infinity very large, you see a plug flow behaviour. So, this is a quick revision of what we learned in the last lecture.

So, I told you that once peclet number known again, I can draw this profile other way around if the profile is known I can draw, I can get a value of peclet number; now how was the profile known you do experiment in the boundary. So, you have a reactor you do tracer injection and you whether the exit concentration and get this profile. Once you have this profile from this profile, you go back and calculate peclet number. So, you know what is reactor is all about or what kind of mixing is occurring here and then you can predict the conversion you applied for the reactive flow that is what we are going to see now.
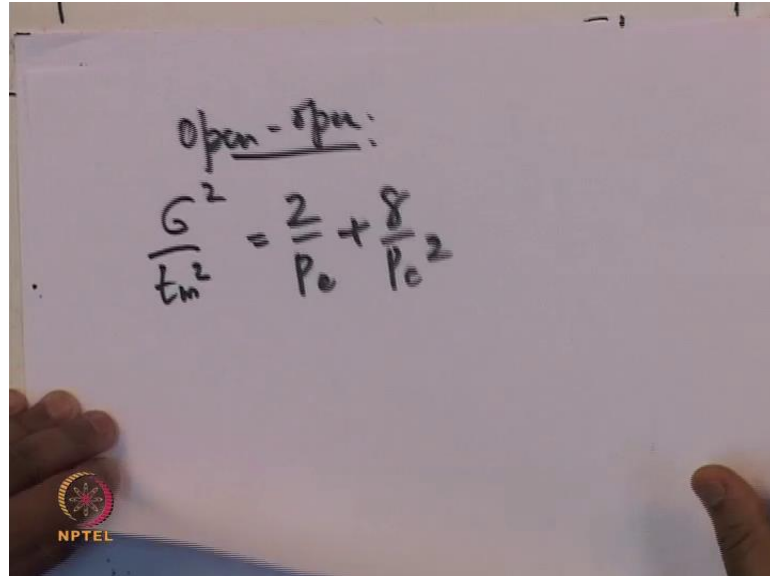
So, before that now peclet number is related to derivation or variation variance. Now what is that relation I told you last time, sigma square divided by tau m square tau m is nothing but tau t a is nothing but tau is a mean residence time 2 by Pe minus 2 by Pe square 1 minus e raise to minus Pe. So, this is 1 minus e raise to minus Pe. So, this is relationship. So, you know this is a residence time this is Pe and sigma. So, in the case of tangent series I had a relationship between Pe and sigma and n now instead of n, I have Pe.

So, in tangent series I have a parameter called n here its peclet number. So, once you now peclet number how to get a conversion. So, let us go back to the reactor now, I have a tubular reactor, I write differential balance for it and get a conversion. So, let me right differential balance for the reaction case now, earlier it was only non reactive tracer injection. Now, I have a reaction case before that, this is something that I have obtained for obtained for close-close vessels. You know what I mean by close-close; that means, before the inlet and after the outlet Da is equal to 0 there is no dispersion happening.

Accordingly we wrote the equations at those boundaries and got a boundary condition, but then it can be open-open vessel as well, it can be open-close it can be close-open. So, depending on what I assume, I will get a different boundary condition and if your boundary condition is different than your value of peclet number is also going to change. So, the expression that I have got always remember is for a closed-closed Vessel. Very

important; for open-open vessel, you can derived it, but then of course, I am not going to spend some time on this, all given in its standard text books.
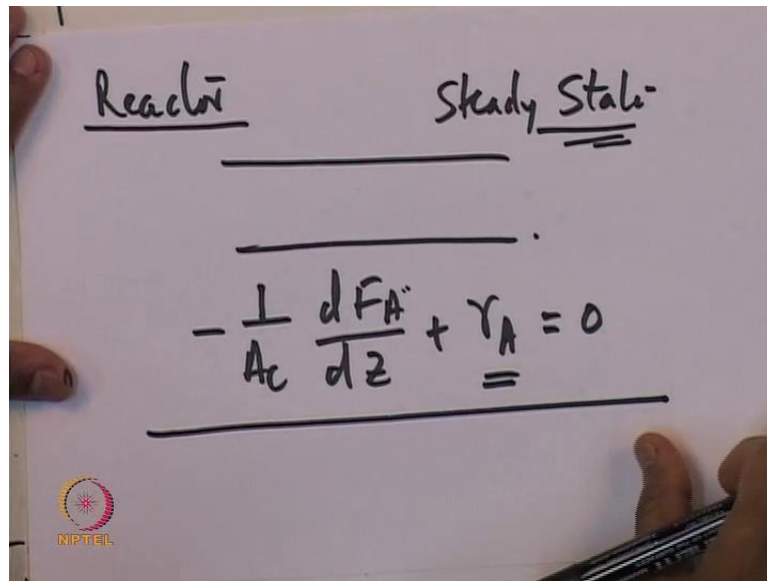
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So, what I get there is sigma square divided by tau and square or tm square is equal to 2 by peclet number plus 8 by peclet number there is raise to 2. So, I will get a relationship for open-open Vessel like this. What you need to remember is there is a relationship between sigma and p it changes as per the boundary condition that I am using for a open-open system it must be noted that tm is not equal to tau. So, once you get sigma from E curve, you can calculate a value of p, if you not sure about what happen there is inlet what kind of vessel it is open-open try and get a get all value of possible Pe depending on which boundary condition, your depending on the boundary conditions. And for every peclet number can be help me to conversion. So, you will get some idea atleast.

So, let us go ahead for the reactive case reaction happening in a tubular rector. In fact, our main aim to design a reactor, but for time that will spend so far is to be this characterise flow pattern. Let us go ahead, if I take a differential balance at steady state now. So, very important earlier all was unsteady state now, it is a continues reactor it is steady state operation. So, this plug is similar to what we see in plug flow only thing is now the FA is different any way. So, let us write it DFA by d a z; now it is not dell FA it is DFA because it is steady state, no time no change with respective time. Why rA, rA is a rate of reaction it in comes in the rate equation rA is equal to minus k c a or whatever depending on what kind of reaction it is first order, second order I can be anything.

So, I have this differential equation now, in this differential equation this FA is not U into CA, it is not just U into CA, but it has diffusion or dispersion term also present there. So, if I substitute for FA based on those 2 terms convective and dispersive or dispersion rather, then what I see is this DA into U. So, divided by u dCA by d z square minus dCA by dz plus r A by U is equal to 0, this U will come here. So, that is. So, these 2 terms is nothing but what is this, d FA by dz. So, this is 1 by U is equal to this. So, dFA by dz that is equal to dA into this into U into dCA by dz. So, I just substitute for this and then I have divided by U also for this terms I am dividing it by U, dividing entire LHS by U. I hope this is clear, you just substituted for FA you know what is FA is equal to you have been already seen this. FA is equal to U into CA minus dA dCA by dz into Ac. You see, in this.

So, this is the equation now for the reactor, is have the reaction term. I am not expanded this it can be rate equation minus kCA or whatever, depending on first order or second order. Now, let me write rA is equal to minus kCA in the first order reaction and go ahead. So, what was see Da by U is into d2 CA by d z square minus dCA by dz minus k CA divided by U is equal to 0; I have just substituted for rA, non dimensionalize this further what do I get, if I just non dimensionalize it, I would get divided by l.

So, 1 by Pe d2 CA, d2 psi by d lambda square minus d psi, see look at this I am going 1st, but I think it because you already done similar exercise before. Now, difference is that you have the reaction term that will here. So, for CA it will be psi into k psi into k into L divided by U, Why see, what I am doing here is I am multiplying or rather since I am writing Pe here; that means, I have to multiplied by L here. So, I am multiplying by L here. So, L L got cancelled. So, have L appearing here is equal to 0. So, this is my dimensionless equation, is my dimensionless equation and I go ahead and solve this of course, it need boundary condition, but before that will define 1 more parameter 1 more dimensionless number, which is called as the of course, it has many other definitions as well, but here, psi into Da is equal to 0, what is this Da? Do not confuse this Da with dispersion coefficient.

So, this is a Damkohler number and you have already seeing this number before probably in reaction Damkohler in part 1. So, this becomes non-dimensional or dimensionless equation, Damkohler number let us define it, like what we did for peclet number. What is Damkohler number?

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Damkohler number is a rate of consumption of a by reaction, see in the in the numerator you had k you remember, let me write it KL by U. So, in the numerator you have k. So, this divided by rate of transport of a by convection. So, this is Damkohler number. So, CA is what is happening to A in the rector, A is moving ahead because of conviction and A is reacting. So, Da tells you the relative importance or relative potential of these 2 terms or magnitude of this term. What is important conviction is important it comes in denominator reaction less. So, Da is less, higher the value of, larger the value of Da it is says that reaction is more compare to conviction.

So, Damkohler number, I am not going to spend more time on this because you already discuss this or learn in this chemical engineering, chemical reaction, engineering part 1 and in the. So, this is a definition for Da for first order reaction, for second order or n'th order reaction, Da is nothing but a Damkohler number is nothing but k into CA 0 n minus 1 into n divided by U . So, this term as a P Damkohler because that concentration will also come in picture that is and the initial concentration or inlet concentration rather, but raise to n minus 1 n is the order.

So, we have this equation, I will get back to the main equation because that we should not forget. So, this is the main equation that I have got, in that I have 2 dimensionless numbers peclet number that characterize this the extend of back mixing or dispersion. And Damkohler number that characterize this is the important reaction, as against

conviction and for in order to solve this equation I need boundary equation is again, 2 boundary conditions 1 Pe you remember this, closed-closed vessel, we have use this for at lambda is equal to 0; that means, inlet and the outlet we have d psi by d lambda is equal to 0, that is what lambda is equal to 1 how to write closed-closed vessel.

So, these 2 boundary conditions I do not need a boundary condition I do not need initial condition now. This is the equation because this is steady state equation, 2 boundary conditions. I solve this equation for psi that is dimensionless concentration of say A what I get is this, psi at why see psi is changing with respective length, but where, what position do I want to value of psi. I want to value of psi the insist exit because that going to decide convergent, psi is a convergent concentration.

So, best if I know the concentration and calculate the convergent. Now this, psi at outlet; that means that lambda is equal to 1 or z is equal to L. So, psi at lambda equal to 1 is equal to, after I solve this equation what I get of course, this is nothing but CAL that is outlet concentration divided by inlet concentration and in terms of convergent it is going to be 1 minus x and you get a very big expression, analytical expression if I solve this equation and I am just writing, I am not spending time for C is mathematical derivation here. What is a more important is, I get a value of convergent based on what? They will be 2 numbers here, which are the 2 numbers, peclet number and Damkohler number.

So, this is nothing but look at this expression no need to bahite this expression, but then you should know, that is an equation like this possible. What are we doing? We are looking at a tubular reactor, non-ideal reactor with axial mixing and this mixing is characterize by number called peclet number, this is closed-closed boundary condition is very big expression. So, what do you see here, on the right hand side peclet number what else you expect here, Damkohler number. This not Damkohler number, but something called q why because, it quite complicated now, this is q is nothing but a function of Damkohler number.

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So, where q is equal to root of 1 plus Da divided by Pe into 4. So, 4 da by Pe. So, I get expression for psi which is nothing but 1 minus x. So, x is nothing but 1 minus psi. So, 1 minus this quantity will give me the time convergent; just write it again, x is equal to 1 minus 4q exponential Pe by 2 divided by 1 plus q square exponential Pe q by 2 minus 1 minus q square exponential minus Pe q by 2, this conversion. So, now compare this with what q got in the case of tank in series model, what was it x is equal to 1 minus 1 divided by 1 plus tau i k raise to n.

So; this is dispersion model, this is tank in series models so; obviously, this is simpler compare to this, but does not matter, this is no like you have everything in computer where we can calculate the conversion not an initial. What is more important closer you to the reality and so look at the entire exercise what we have done so far.
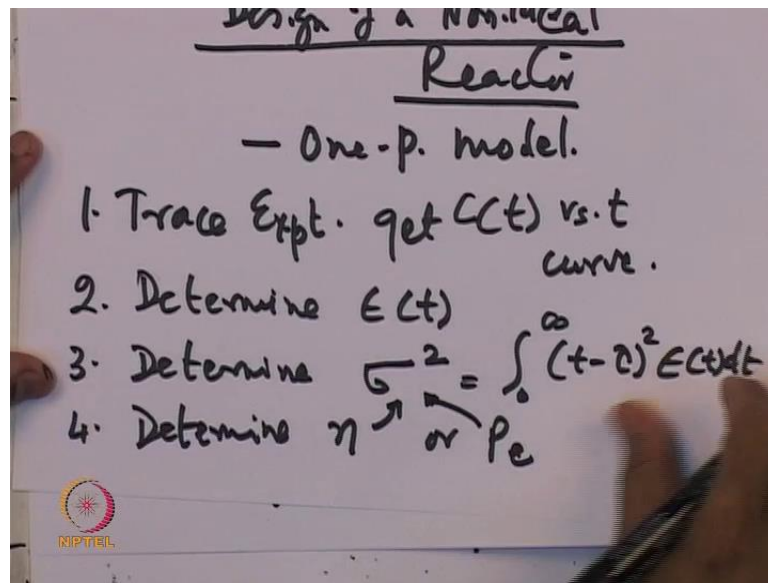
If I want to design a reactor how do I do it a based on parameter. So, let me right down in step design of a non-ideal reactor using 1 parameter model what I do first; I do tracer experiment in the lab get C t verses t curve, then determine E T, third determine variance sigma or sigma square and you know the definition on this. Once you get sigma determine, if it is tank in series n, you know this is related to this or Pe this is again related to this, upto this point I am looking, I am no pattern. Now, using this parameter what I need to do is, just get a conversion; now for first order reaction conversion x; first order reaction, I have the analytical expression, but depending on the order I will have a probably do it numerically especially in case of form dispersion model.

So, get conversion by a solving reaction enabled balance for a real case. So, in this particular, some for a first order of course, I will repeat 1 minus 1 by 1 plus tau i k raise to n this is tank in series model. And here it is a big expression for a dispersion model this will be function of Pe and Da. So, this is the overall procedure, this is for design, I say that, this is a design problem and I have written logarithm to calculate conversion. So, this is not really design problem, is like you are given the length of or the volume that is the reactor to calculating a conversion, but then it can be other way round somebody says 50 present conversion, design reactor for me.

So, what will I do? I will just do, the entire exercise assumes some flow rate calculates a conversion not matching where the flow rate is, but I would do a entire exercise again. This become trial and error method, it is it is a bit complicated, but is no way because the flow pattern or a flow rate that going to decide residence time is likely to changed your E curve also, it is likely to change your mixing also. So, every time whatever flow rate that you want to operate it as, is always better to do experiment and see whether you have the right kind of E curve or you have taken into consideration non-ideality and accordingly to the value of Pe and Pe or n.

So, this procedure tells you for a given volume, what is the conversion possible. Problem can be solve iteratively to get volume for a desired conversion. So, this is how it works, because you want to incorporate flow patterns. If we had assume reactor to be ideal

closed to p of r or CSTR things would have been much easier, like what we did before, but now, I want to take into the consideration the flow patterns. And this is remember this is only for reactor, which is giving me behaviour closed to tubular reactor.

If you have a very irregular geometry, then this is not going to fit your Pe or n values or not going to, there not enough 1 parameter model are not enough or then not adequate to rather express or characterize your flow pattern. You have to go for multi parameter model, will see that later. So, this works for particular E curve, always remember that I have told you in the beginning of this particular first lecture. This chapter that, if you have very viearod like E curve, you do not think of you using a parameter model for it. It should be look like CSTR then going from CSTR to p f r. So, let us solve problem of course, I am not going to do numerical calculation, but again like whatever have writen words here, let me try and explain more detail if 1 has to solve problem. So, the first… So, who. So, what is given to you C t verses t.

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So, this is what you would expect in a problem, the tracer concentration time and concentration, unit can be grams per letter or moles per letter here it can be say taken many in order. So, 1, 2, 3, 4, 3, 4, 5 whatever and here again you has some numbers. So, at 0 time 0, then probably 1 then 7 20 and then it may come down again say 8 3 what. So, this is the, this is typical behaviour like this. So, this is given to you, what else we need to design and reactor value k at the rate constant and what order.

So, that independently some would have determine it for you, in a differential reactor in laboratory and then they would have values of k rate constant activation it is running the reaction and all frequency of reactor or order. So, these are all parameter for this reaction kinetics. So, this is what is given to you and from this we need to determine the conversion, using different models now, as a problem may be calculate conversion for a CSTR PFR 1 parameter models it can be tank in series and can be dispersion.

Now, just 1 question before we go ahead see is not solve a equation whatever we know and get a value, but then if it is a first order reaction or it is a positive reaction CSTR give me 1 bound, conversion will be minimum or maximum conversion would be CSTR positive order reaction, conversion will be minimum. PFR will give me another bound, conversion will be maximum and in between you have this mixing happen because of which conversion will be in between PFR and CSTR the tubular reactor.

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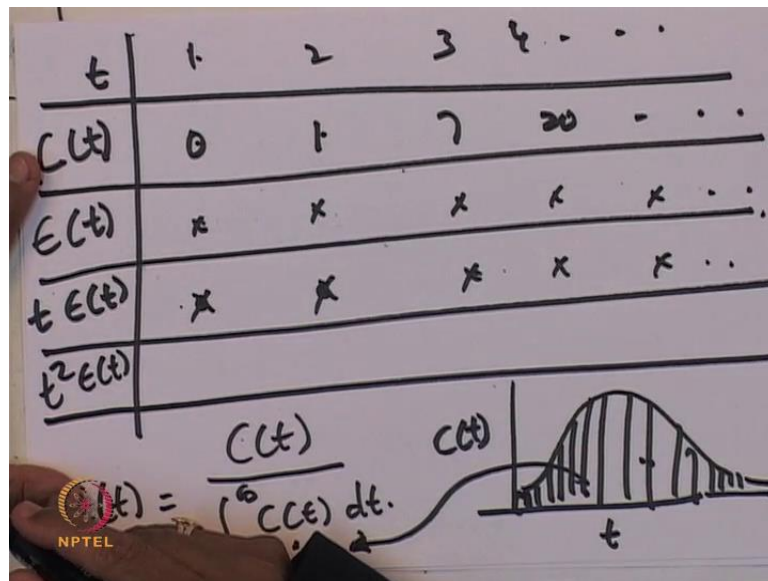
So, only thing is it because partial the back mixing conversion get effected and since this is the positive order reaction, back mixing is not desired for a convergen higher. Like convergen will get affected adversely with back mixing. Of course, we need initial inlet concentration and all for all this exercise. So, how to I proceed, I have t 1 2 3 4 and so on. Ct concentration, measured concentration 1 0 1 7 20 and so on. I need to get Et; how do i get Et, is equal to Ct divided by integration 0 to infinity Ct d t now how. So, Ct is known for particular time, I need to know this, how may the tracer that I have injected.

So, the entire concentration I have a plot of Ct verses time, if I want to get this value, what I have do; I just take the area under the curve from the 0 to infinity may meet x axis do not need to go further. So, this area is nothing but this denominator and this explaining in the procedures. So, this gives me Et; so I will have some value is here, I am not going to write this value I have some values here. So, I got Et from Et what do I find out.

First thing is I need to get a average residence time, I want the value of tau remember every where tau came in picture, the tau is require. How do I get average residence time or mean residence time, mean residence time is this expression for mean residence tau put tm is equal to 0 to infinity t et dt again, tau is equal to tm is valid only for closed-closed systems.

So, what I need here is from this plot I will calculate t into Et and I have value. So, t into Et I will have some values it looks like 0. So, let me right cross; I am just simply multiplying these 2 numbers t Et, I am explaining those only the procedure there are because being calculations in the lecture it bit difficult. So, t Et and then from this once I know t Et, I can plot t Et verses t. So, whatever plot I get area under the curve, I do not know the nature of this, it can be anything, all I need to do is get area under the curve and that is nothing but tau.

So, in this stay I have determined the value of tau that is mean residence time. So, this is a, this particular row would be give me that t Et by multiplying this 2 and then area under the curve. When I plot this are against this that is time this against this and I have get mean residence time. What do I need next, then what I have do is I take t square now you know why I am doing this, instead t i have t square, why will I need t square because I need to calculate variance you know the expression for variance.

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What is the expression for various, expression is this sigma square is equal to 0 to infinity t minus tau Et dt, if I expand this it is t square Et dt minus 2 tau t Et dt plus tau square 0 infinity Et dt. You know, what this is this is nothing but 1. So, this becomes tau square and what is this, this is tau. So, this going minus 2 tau square plus tau square; that means, it minus tau square. So, these 2 terms I know, what I need is only this. So, this is 2 be found out, by plotting t square into Et dt t square Et verses time. What a plot I am going to see, I do not know nature of this, I take the area under the curve.

And this is nothing but this term this term minus tau square this is nothing but tau square minus tau square. So, this term this area minus tau square is nothing but variance. So, I did I get the variance, I hope it is clears. So, I have this values I plot this values against this values. This verses time get the curve and area under the curve will give me this particular term, this term minus this all is tau square I already determine tau that is mean residence time in my earlier exercise right here tau.

So, from that I get c must square that is variance, why I want variance because variance tells me the extend of distribution or dispersion. So, from variance I calculate Pe or n from sigma square, this is require these 2 are require because I want to get conversion on this. So, from this there are expressions, conversion and you know the expression. So, here it is nothing but 1 minus 1 by 1 plus tau i k raise to n for first order reaction and similarly you have expression here. You will get this 2 value now, you may ask me this value different or they are same; see they should be quite close to each other, this 2 values.

If you exercise this correct this 2 value should be very close to each other. So, you may get say I am. So, I will just right a values CSTR you may get the conversion 0.5 PFR, you may get conversion 0.7 for a first order reaction or positive order reaction and it is quite possible that for a tank in series model, you get 0.63 and dispersion, for a dispersion model you may get something close to say 0.61 or 62.

So, they have call it closed to each other, just to give an idea and they these 2 are going to be in these 2 positive order reaction effects of mixing on the reaction convergent. So, this is how it going to be as for as effect of mixing, on reactor is concern on conversion is concerned. When have a tubular reactor and we talking about first order reaction of course, it can be any other reaction the algorithm procedure will be quite similar be quite

similar. So, the many example, in assignment there many example text book like Levenspiel flogger and all like.

You can solve this examples and the clear border overall procedure then there should be much of a problem. Now, there is some co-relation between n and peclet number. So, approximately this n is nothing but peclet number by 2 plus 1 approximately. This is approximately relationship. So, there relates if you if you want to compare these 2 approaches, where the question is like whether I should go for dispersion model or tank in series model. So, that will depend on your choices, whether people like differential equation or you like algebraic equation.

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Because in a case of tank in series model you need to solve algebraic equation, in case of dispersion model, you need to deal with differential equations. Typically, the calculation voice of if you want to remember formula and all that, probably tangential series model this relatively is compare to dispersion model. Now, let us go ahead, so what we have seen here is that, we can use 1 parameter model if you have a typical E curve. So, it is a always is very important like once you do experiment tracer experiment you get in E curve you should know whether you should apply 1 parameter model or some other model.

Because some time even 1 parameter model may not fit I have been repeating this again and again because very important. It is sometime students are in impression that 1

parameter model can be use for any reaction. So, after you do a entire exercise realise that you got a value, which is or you come up with result which are of no use. Because the E curve does not represent a tubular reactor of which, can fit in either dispersion model or tangential series model.

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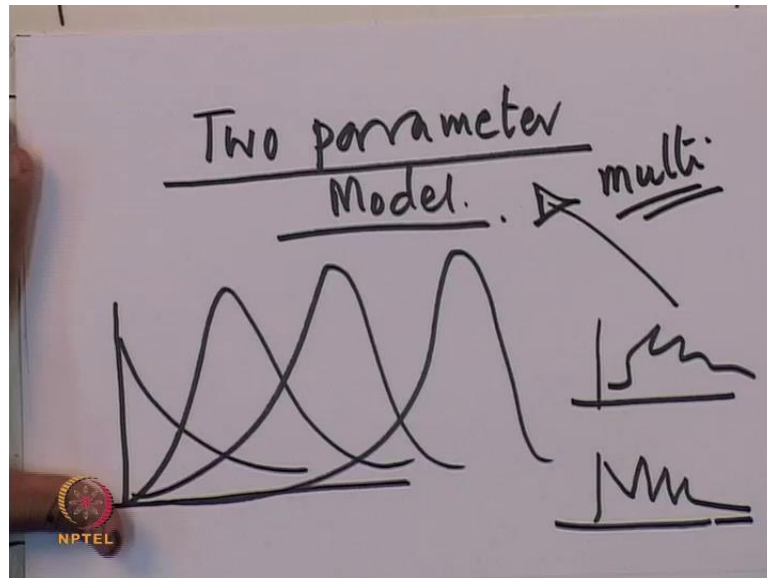
Now, we going to go 1 step ahead and look at 2 parameter model; now, why would why we need extra parameter because 1 parameter is not able to explain the flow behaviour properly as simple as that. As I say, like if I go in changing the value of peclet number or n, I get typical behaviour like this of course, this peak is going to increase, but it is not necessary that E curve falls in this categorise only will have E curve this nature only. As I said before, I may have e curve like this. It all depends on a geometry that you have; it all depends on what is happening inside.

So, in that case, you should be quick enough to know that; now, 1 parameter model not going to help. I have to go for a 2 parameter model or a multi parameter model. So, here we need to know what happens inside the reactor. You have a should, some information about what is happening inside a reactor. So, that I have proper guess as to how to go ahead. Now, I will give an example here. So, you have a normal CSTR like loop reactor or I would not called a CSTR is a mixing tank or mixer or reactor.

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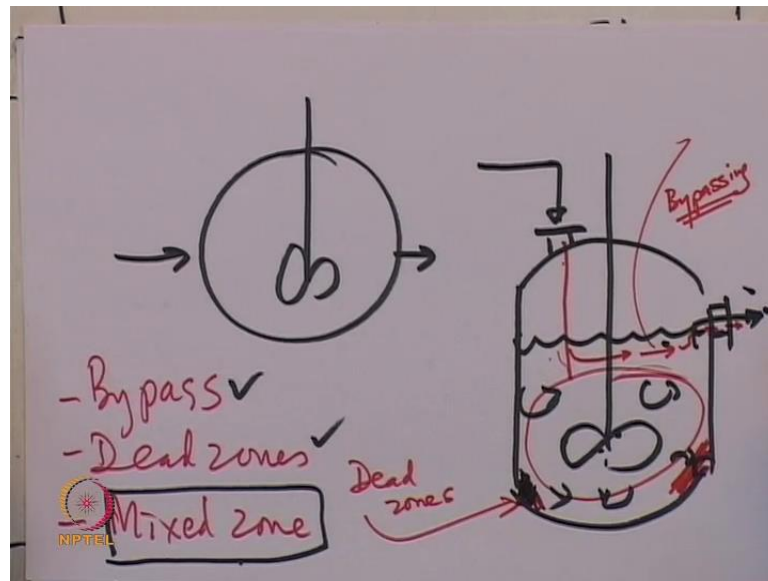
Now, this is the way I represent CSTR, but in reality I will have a vessel a vessel, in that that may have reactor agitator. I will have an agitator now, I am looking at this geometry also, it is not a schematic, but it is somewhat real picture there is have an nozzle here, I will have a nozzle here and I have feed coming in. And product stream going out from here; look at this nozzle is now, close to in that now this is the way. So, it may be overflow. So, whatever extra comes in goes out from here and there is intense agitation inside you have nice mixing happening.

So, called nice see because what is a time like a you do not have proper mixing in each recall of CSTR or in mixing tank for that matter. There always some pockets in the reactor which do not see the kind of tubular intensity, which is their near impellers. You can very well appreciate this fact see, if you want exactly same amount of turbulence intensity or mixing level everywhere the tank, then you need to put agitators, as many agitators as possible at every position in the reactor, isn't it? That should be the case, but that is not practical. So, normally you have 1 agitator or for some time you may have 1 short which you have multiple agitators or impellers amounted.

So, it is quite possible like if you away from the pro impeller, especially in the corners then there are stagnant pockets. So, what is like to be happen this particular case, see you field is coming in, right and you have certain the $z1$ possible. So, at this point is away from is this, this point is away from the agitator. So, somewhere in this part you will

have dead z1s. This is not a only the effect, another effect can be that some of the stream there stream like imagine now, this stream get divided inside several subs streams.

So, it quite lightly that some part of the inlet stream will directly go here will not see the agitators at all. What is this? This is by passing these are dead zones and in between you have perfect back mixing or in between rather in this point what you region sorry right. So, now, i have 3 things happening by pass, dead zones and mixed zones. I know how to model this. This is like a normal CSTR how do I incorporate this, in my model. So, I need to have a combined effect of all this happening here.

So, what I am going to see at exit is the effect of what is happens here, what happens here and what happens here. So, all this 3 effects or going to tell me, the convergen or not going to decide a convergen. So, if I just assume a normal CSTR a mix zone I may go wrong, I need to consider this 2 effects also, which are probably not desired, but definitely I have to consider them to design the reactor by pass and dead zones. And there is no provision to consider these effects in my 1 parameter model, that is tangent series or dispersion model there is no provision for this.

So, I need to have additional parameters, I need to complicate my model further. So, that I get these effects in calculate in my model and my predictable convergen will be more or it will be closer to the reality.

Thank you, will discuss this further in next lecture.