Chemical Reactions Engineering II
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Lecture - 37
Non-ideal Reactors: Dispersion model

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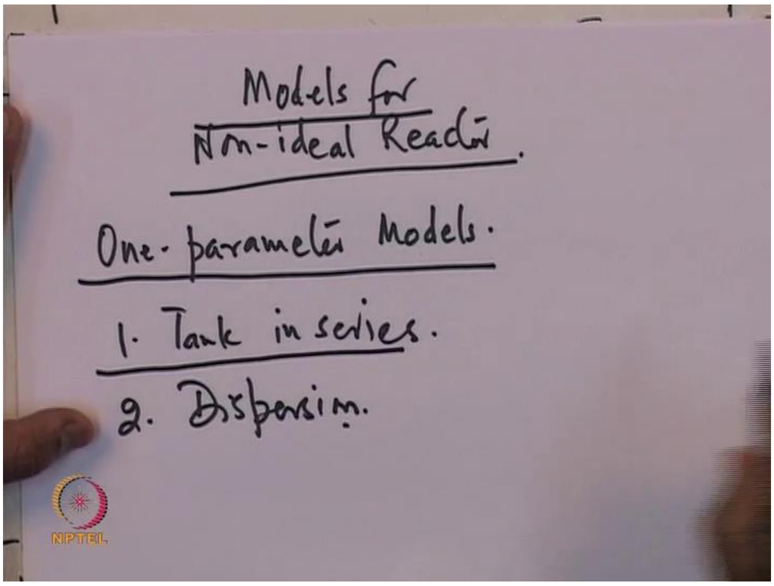

Models for Non-ideal Reactor.

One-parameter Models.

1. Tank in series.
2. Dispersion.

Good morning. So, we will quickly revise what we learned in the last lecture, we are looking at models for Non-ideal reactors. You know, non ideality comes because of the non ideal flow patterns and we have to somehow characterize this non ideality. So, we looking at 1 parameter models, before this; in the earlier chapter, we looked at a 0 parameter models with 2 extreme situations maximum mixedness and complete segregation. Now, in this particular chapter we are looking at models with some parameters in involved in it. And these parameters have something do with the flow patterns inside a reactor, the extend of mixing and so on.

So; we will just moving away from 0 parameter models, the problem with 0 parameter models I told you that gives you bounds on conversion does not tell you that exact conversion; whereas now, we are looking at a model with a parameter. So, it is going to give us some idea about the conversion, exact conversion. If the model that we using is. So, we going for simple model now is a 1 parameter model you can have model with many parameters, but right now we just looking at 1 parameter model.

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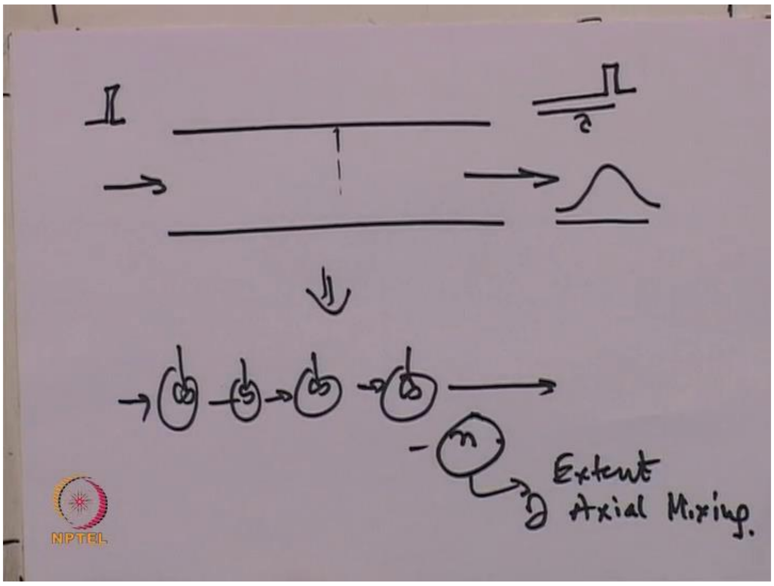

That the 2 types of models is it we have look that the first is tank in series and the 2nd 1 is dispersion of course, we have just looked at this 1 in detail and today we are going to talk about dispersion model, but just to quickly revise what is tank in series model. We have tubular reactors, say tubular reactors and is a flow that is taking place in this direction. Now, a plug flow reactor is a reactor where the mixing in the radial direction is maximum, but there is no mixing in axial direction, but at the velocity profile is flat and if I have a pulse injected here or tracer injected here, then I will see the same tracer after a time tau here.

That is e cover and something that is known to you now; now If this pulse gets disturbed when it comes out, then it may be because of some extend of back mixing. So, if it comes out like this there is a possibility that some back mixing is occurring here. It is not just a plug flow behaviour, but it is hampered by some kind of back mixing. This may occur because of the concentration waves moving or this they might be some disturbance in the flow, internals for examples say part column whatever, but I want to characterize this extend of back mixing.

So, what I am going to look at is this as a series of small c s t r's and this n number of c s t r write and this n characterizes extent of axial mixing. So, this n is parameter a given tubular reactor, if I say that, I have n number of c s t r's in series which are equivalent to this tubular reactor then n become a parameter this n can be 1 2 3 4 5 6 and infinity. So, infinity means it is a plug flow reactor and n is 1 means is a c s t r because complete mixing and in between these 2, you have partial back mixing and if and yes n will n is large means less mixing n is small means there is good amount of back mixing that is occurring.

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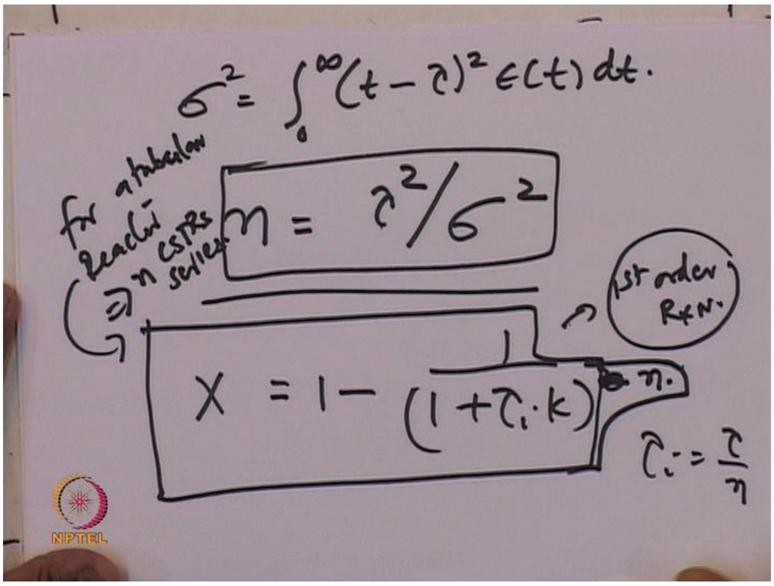

$$\sigma^2 = \int_0^\infty (t-\tau)^2 E(t)\,dt.$$

for a tubular reactor ⇒ n CSTRs series

$$\boxed{n = \tau^2/\sigma^2}$$

$$\boxed{X = 1 - \frac{1}{(1+\tau_i \cdot k)^{n}}}$$

1st order RxN.

$$\tau_i = \frac{\tau}{n}$$

Then we derived equation for n in terms of… now, how do I get a value of n; n is a; obviously, obtained by the tracer experiments. So, tracer experiments is a tool for any given reactor under the condition whatever flow rates and all we are operating it that tool gives you the parameter that is nothing but, n. So, if I get e curve the variance in the e curve tracer experiment the E curve and the various in the E curve, you know what is variance sigma is equal to 0 to infinity sigma square t minus tau square Et dt.

So, variance now this variance is related to n. What is the relationship n is equal to you have already looked at a tau divided by sigma square, now what is tau? tau is a residence time, total residence time, volume of the tube divided by the volumetric flow rate. Volumes of the tube do not talk about or rather do not confuse it with the volume of c s t r's. So, given a tube somebody asked me, whether this will behave like a plug flow reactor or not tell me. This is flow rate that I am operating; what will i do, i will do trace experiment, I will see whether I get a nice pulse just getting repeated or very close to something that, I have injected after time tau, if it is not happening it is not a plug flow reactor.

If it is get dispersed, as I showed before it is a slightly disperse or the pulse get distributed rather over a time. In that case, there is definitely some back mixing occurring and there is a way to characterize this back mixing. And I will do a tracer experiment, I will get the E curve from E curve, I will get a variance because in this, just E curve is to be known otherwise everything else is not. If I get I curve variance once the variance is known, tau is nothing but, volume divided by volume it will florid.

I get a value of n; n is number of c s t r, now once you have a value of n, you have x that is conversion for series of c s t r given by tau ik square is raise to n. Now, tau I is nothing but, tau divided by n. And k is rate constant this is for the first order reactions do not forget this. And for second order again, I can derive some equation, if not I will just go on doing calculations step after step. So, it has allowed me to get a conversion for the given value of n; it should be. So, this is the conversion for a tubular reactor that corresponds to n c s t r in series.

Now, 1 thing I forgot to tell you last time is this n, now after doing this excise and getting the value of n did not be integer, n can be 3.5 it can be 4.75. So, this value of n now, as such number of series c s t r, number means what it should be integer, but just ignore rather forget it. Whatever value of n comes just put it here and once you do that whatever value x come that is a reactor value of x, which is close to what you get in the real reactor, which is a tubular reactor neither p of r nor c s t r; must be noted that, this is possible that is using non integer value of n only for the first order reaction, for other orders analytical expression is not available for the conversion after n reactors.

In such cases, n will have to be rounded of to the next highest integer. Will solve some example or I will tell you the method logic to solve the example, as we go ahead, but before that lets look at the dispersion model. So, this is where I stop, as for as the tank in series model concerned. You know, n is a parameter, n is to be obtained once you get n you get a value of conversion for a given reaction for a tubular reactor. Now let us go ahead and discuss the other model that is dispersion model. Now, once you have 1 model why to have another model convenient some time some model work well some time they do not work.

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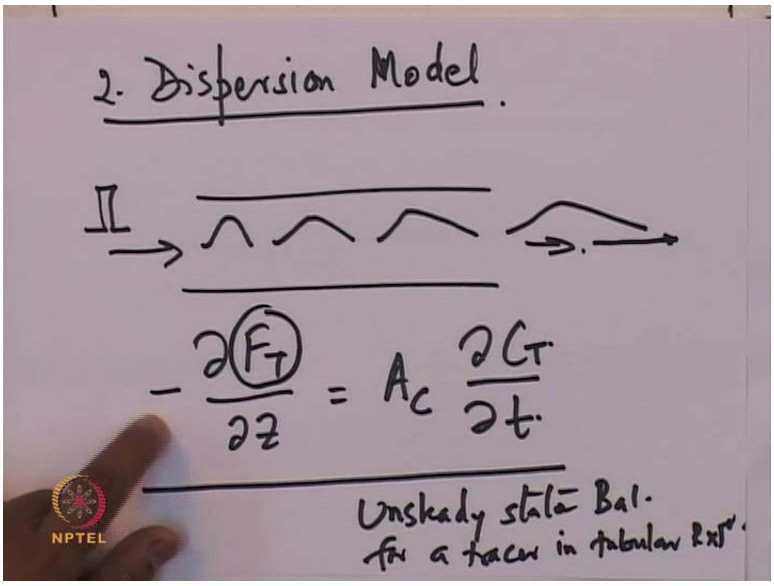

2. Dispersion Model.

$$-\frac{\partial (F_T)}{\partial z} = A_c \frac{\partial C_T}{\partial t}$$

Unsteady state Bal. for a tracer in tubular Rxr.

So, I probably after discussing dispersion will have will spend some time relating this 2 model as well. So, there are 2 model available, just we should know both of them. So, that because there both of them are popular in industry; now, dispersion model, in this case, dispersion is what; dispersion is again a synonym for a axial mixing that is occurring of course, it can be radial direction also. So, just dispersion it can be any direction, but as for as tubular reactant is concern we talking about axial mixing.

But it can be radial also, can be club this 2 to together and get overall dispersion. Now again, you have a tubular reactor; if you inject a tracer because of back mixing is going to get something like this. If it spreads, it becomes flat in that case extend of back mixing is is very large. This a behaviour and that I am going to see, now can we give a mathematical treatment to this. The first model that we look at, this assumption that you have series of c s t r tank in series, but here I am not going to do that, I am just going to look at the way I do it for a plug flow reactor to the differential balance, take a differential balance.

Now, for unsteady state for suppose I inject a tracer how it behave with a respective time, I have to write unsteady state balance p of r is a da by dv is equal to r is a steady state balance. Now, I have a tracer injected r terms that reaction term is 0 no reaction taking place and non reactive conditions. So, you have flow taking place, but at the same time tracer concentration at any given point is going to change with respective time. So, accordingly I will have an equation. So, what is the equation unsteady state equation for a p of r. So, it is going to be d FT, FT is a flow rate of the tracer, now will say Fa for a that is a rector.

Now, instead of a now I have T here. So, d FT by dz is equal to Ac into d CT by dt. So, this is unsteady state balance for a tracer in the tubular reactor. Tubular reactor, why I am writing this balance, I am giving you mathematical treatment to this. As time pro c how this are going to change respect to z and time as well. So, this equation describes everything. Now, what is FT; is a normal situation FT now this is very important for plug flow reactor what is FT? We say that is only conviction, that is v into c that is volumetric fluoride into concentration that is for a normal reactor, but in this case it is the flow is not taking place only because of conviction, but there is an additional term which is cause by axial mixing, which is cause by dispersion.

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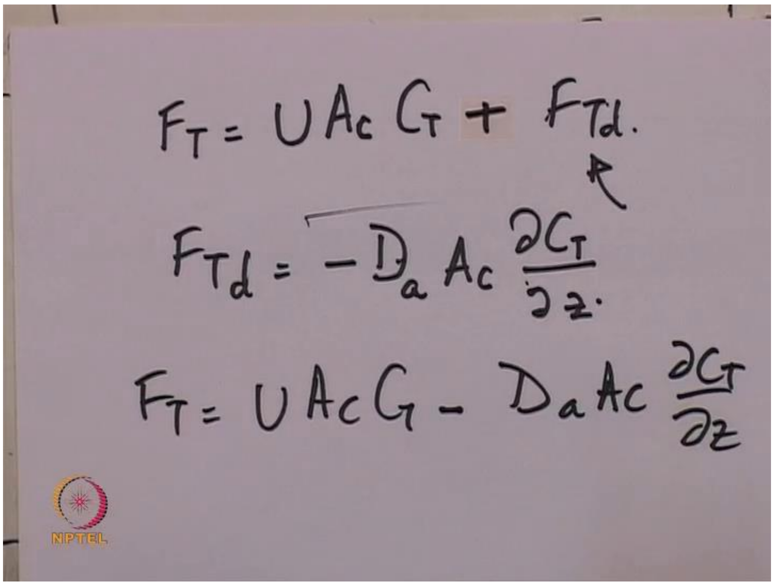

$$F_T = U A_c C_T + F_{Td}.$$

$$F_{Td} = -D_a A_c \frac{\partial C_T}{\partial z}.$$

$$F_T = U A_c C_T - D_a A_c \frac{\partial C_T}{\partial z}$$

So, this FT this lets try and write expression for this FT; this FT is of course, U into Ac into CT. What is this, this is convection, but it is not just this apart from this, is an additional term that is coming out of dispersion. So, let me call this as a FTd and what is FTd. This FTd is because of dispersion now normally it is written as some coefficient will talk about this later; Da into Ac look at how it, look at her expression is quite similar to fix law, this is quite similar to fix law Da Ac into dell CT by dell z. So, without Ac is flux. So, I am multiplying it by Ac, what is Ac, Ac is a cross sectional area.

So, this is the expression for the dispersion flux due dispersion and why it happens, it happens because of concentration is a front that is moving of the tracer. So, it is a concentration difference that causes the dispersion, this is analogues to diffusion and is expression is analogues to fix law. I am not calling this as a fix law, because I the coefficient that, I am using here that is Da, is not a regular diffusivity, is not a normal diffusivity, not bulk diffusivity that redefine the fix law. This is something that combines all the effects. Now I am ask me whether it would it has a capability to combine all the effects it may not have. In that case, your 1 parameter model does not work, that is it.

But if, for some reason of somehow if for a given geometry and flow pattern, if it is able to take care of all these dispersion effects in 1 parameter then you done; that means, you model perfect and go ahead use it and predict the conversion from the reactor for given volume. So, that is the mining of it. So, I am expressing dispersion by this particular term. Now, you may ask you what can flow by done laminar or turbulent, now it can be proved that, this expression works well even for laminar flow this works well for turbulent as well. So, this can be diffusivity in the case of turbulent flow or it can be in the because of the laminar molecule jumping from 1 layer to another layer which are otherwise not mixing.

So, 1 layer moves to 1 velocity, the other layer moves to other velocity in laminar flow and there is exchange of some molecules this is not ideality. So, is not exactly laminar, but then that case, this particular exchange can be incorporated here in this term diffusivity. If time permits will try and derive an expression separately for laminar flow and show that it can be explain in this phase, but right now there is go ahead. Let us not worry about much because laminar or turbulent flow, we say that this is applicable to any of flow that is laminar or turbulent.

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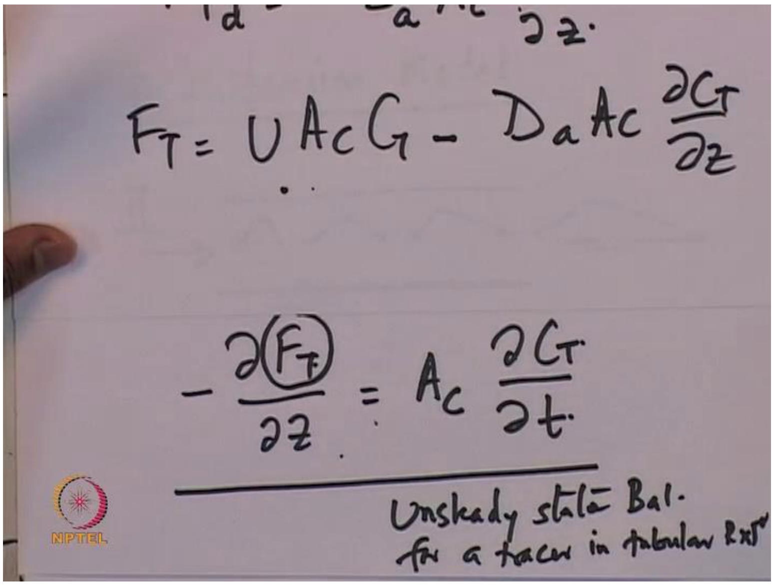

$$F_T = U A_c C_T - D_a A_c \frac{\partial C_T}{\partial z}$$

$$-\frac{\partial (F_T)}{\partial z} = A_c \frac{\partial C_T}{\partial t}$$

Unsteady state Bal. for a tracer in tubular Rxtr

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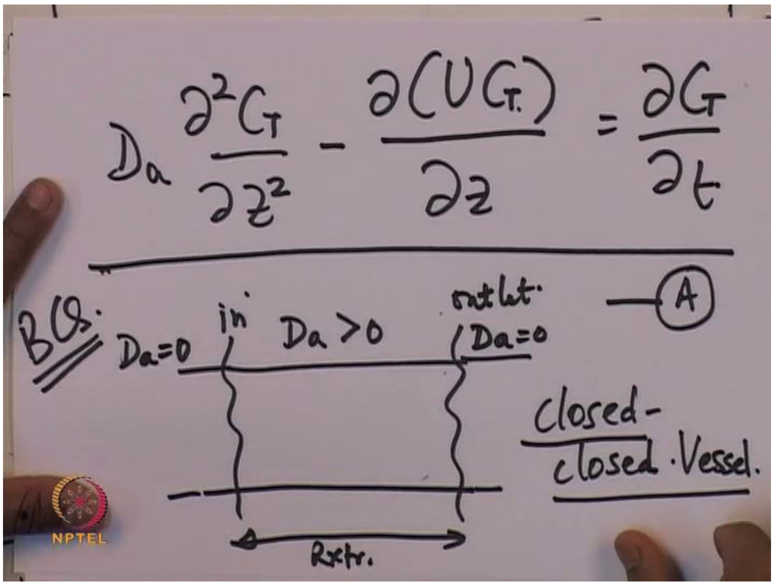

$$D_a \frac{\partial^2 C_T}{\partial z^2} - \frac{\partial (U C_T)}{\partial z} = \frac{\partial C_T}{\partial t} \quad — \text{Ⓐ}$$

B.Cs:

Closed-closed Vessel.

So, let us put this term here, FT is equal to U Ac CT minus Da Ac dCT by dz. Now, we have, you already have this equation; we have this equation and in this equation FT is given like this. So, let us substitute for FT here. So, substitute for FT here. Remember FT otherwise was this only for a plug flow reactor now that, we are considering dispersion we have a additional term you going to put this here. So, if you substitute for FT what you get is this Da dell CT by dell z square. Now, you will get a second order partial differential equation, dell U CT divided by dell z is equal to dell CT divided by dell t.

Second order, is obvious because FT comes in like you have dF by d z you know. And FT now, d CT by dz, you have d CT by d z term in FT. So, that is why, you have this expression. So, this is the expression that I am going to deal with and with this equation now, I have tracer concentration changing with respective time and z. If I solve this equation, I will get the response in says, there is a the tracer how its spreads and all that, at any given time and length in the reactor. So, let us remember this equation and in order to solve this particular equation and I need boundary conditions. Now, this boundary conditions, they have quite peculiar and we going to spend some time in knowing what is boundary conditions are.

Now, you have a tubular reactor, you have the inlet and you have the out let. Now talking about BC that is boundary conditions, differential equation needs boundary condition otherwise you cannot solve this equation. Now how I look at it, you we will say is not that difficult what big deal is in let concentration is a out let concentration. So, see this is your second order partial differential equation, how many boundary condition you need here you need 1 initial condition and 2 boundary condition. So, there are some assumption to be made here and some of the assumption they works so well.

You have a flow taking place, dispersion is happening now where is a dispersion happening, dispersion is happening here; that means, Da value of Da is greater than 0 in the reactors. So, this is a reactor. So, value of Da in this domain is greater than 0; now, this is before this is in let this is after the out let. So, before the inlet I have a choice whether dispersion is happening here as well or not. So, let me consider a situation where Da is equal to 0 here and DA is equal to 0 here.

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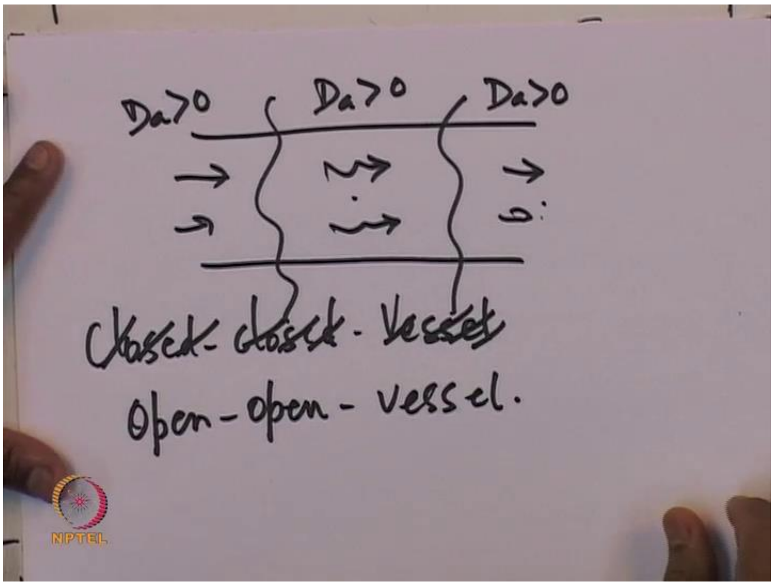

So, no dispersion is happening in the outgoing channel and in incoming channel. It all depends what can system you have, what kind of nosal you have here and here, but if I assume this then this is called is closed-closed Vessel and we have corresponding boundary condition will come to that, but this is the situation where I have a closed closed Vessel; that means, this is no dispersion here and there is no dispersion here. The there is another extreme where I have open-open case or open-open vessels.

Where Da is greater than 0 here as well, Da is greater than 0 here as well Da is greater than 0 here as well. Why not, is sometime like we showed arrow like this and not straight why this is 1 indication where flow is not ideal indicate not like plug flow reactor. So, it is all depend how we want to show it. In the indication is like arrow is distorted means some back mixing happening. So, this is called as closed-closed Vessels, now you may have situation where you have open-closed or closed-open depending on what is happening in the... So, you have a choice and depending on that decide what kind of boundary condition is applicable my particular case, because every time we have different expression.

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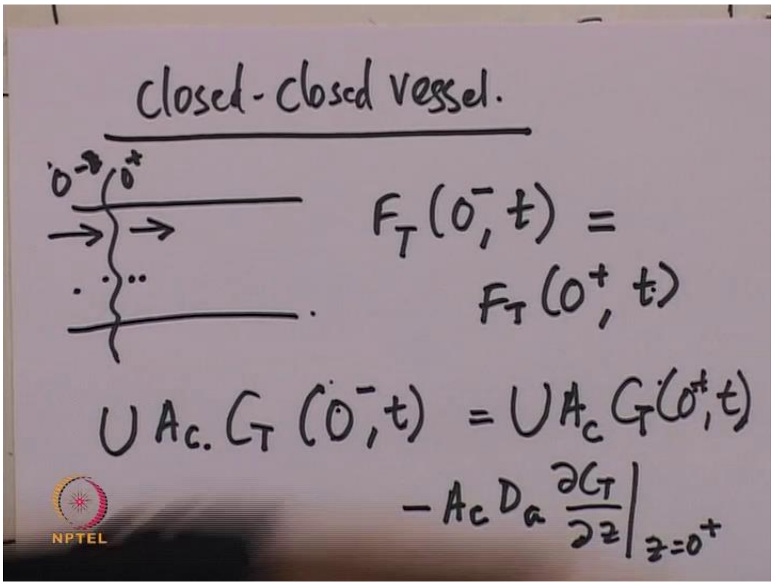

Closed - Closed Vessel.

$$F_T(0^-, t) = F_T(0^+, t)$$

$$U A_c . C_T(0^-, t) = U A_c C_T(0^+, t) - A_c D_a \frac{\partial C_T}{\partial z}\bigg|_{z=0^+}$$

So, let us look at get I say, this is open-open, earlier was closed-closed. This is open-open. So, you may have several possibilities and you decide what you want, we can be closed-closed, it can be open-open, it can be close-open or it can be open-close all possibilities. So, depending on that you get a expression for the boundary condition. So, let us write expression for a closed-closed Vessel. So, let me draw it again, at in let you have flow taking place. So, whatever coming in is going out at this particular boundary.

So, I have expression FT tracer 0 minus, see here it is 0 minus that is 0 plus FT 0 minus at any given time is equal to FT 0 plus at any given time. At that particular time of course, this 2 times are same. So, that is obvious know that is obvious there is no accumulation at the inlet. So, whatever comes in goes out. So, Molar Fluoride FT tracer coming in is equal to coming in at inlet is equal to coming inside a reactor. So, let said expression for FT, now FT in there is no dispersion here closed-closed, there is not dispersion here.

So, it is velocity a into cross section area into concentration 0 minus t concentration at in let that is 0 minus at particular time. And multiplying it by U and AC; what should I write here now, for this; can I just write this U that is velocity, Ac CT 0 plus t, is that sufficient? The answer is no, this is not sufficient because inside it is not just the conviction or the velocity driven flow, but it is dispersion as well. So, will have an additional term, which is given by Ac into Da right dCT by dz at z is equal to 0 plus.

So, FT coming in from here is this and FT here is this plus this. So, this 2 concentration are different, why because this is an additional term, which will make sure that is concentration changes. If this term was not there than U Ac will get cancel in this 2 concentration would be equal, but this term is responsible for making this 2 concentration different.

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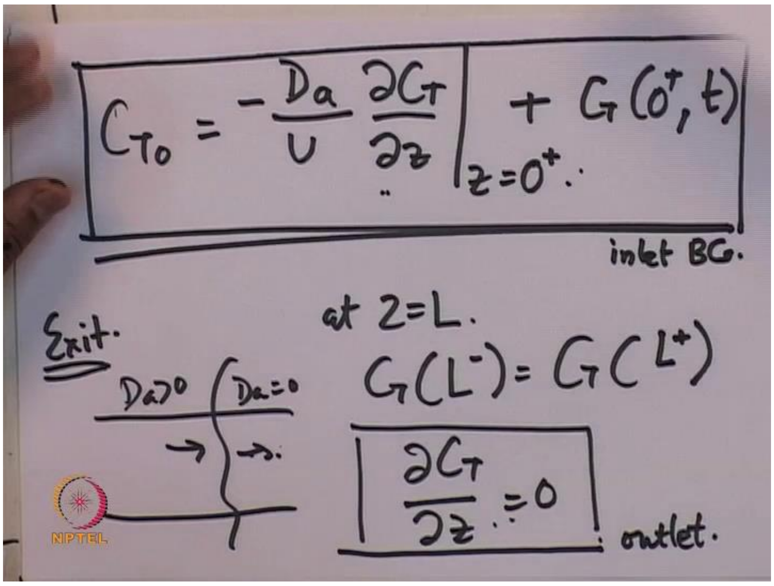

$$\boxed{C_{T_0} = -\frac{D_a}{U}\frac{\partial C_T}{\partial z}\Big|_{z=0^+} + C_T(0^+,t)}$$

inlet BC.

Exit.

at $z=L$.

$$C_T(L^-) = C_T(L^+)$$

$$\boxed{\frac{\partial C_T}{\partial z} = 0}$$

outlet.

So, let us simply this further; CT 0 is equal to minus Da divide by U dCT by dz at z is equal to 0 plus plus CT 0 plus t. So, this is 1 boundary condition that is, at inlet. So, in let boundary condition I am saying, in let BC; this I have to exit or outlet what happens that out let. So, let me get back to this figure or let me draw it here again. So, Da is greater than 0, Da is equal to 0 here, this are continues flow. So, at z is equal to L CT at l minus is equal to CT at L plus. The concentration here is same as concentration here concentration this to point are going to be same. So, what it means, this d CT by dz is equal to 0. So, this is the boundary condition at the outlet. So, these are the 2 boundary conditions that I have.

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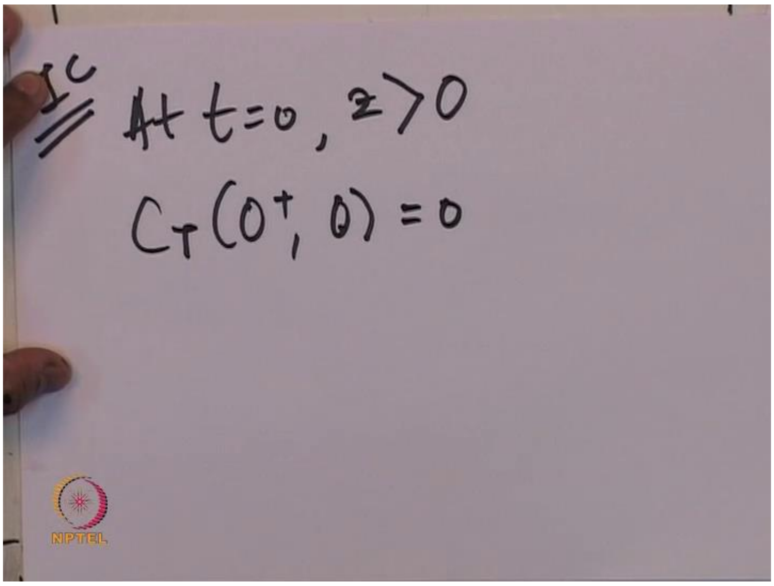

IC

At $t=0$, $z>0$

$$C_T(0^+, 0) = 0$$

So, this 2 boundary conditions and where our equation, is equation here. So, this equation and this 2 boundary conditions what else to I need, I need initial condition what is that initial condition, at time is equal to 0 what is the value of concentration at all lengths. So, at time is equal to 0 initial condition IC initial condition at time is equal to 0 and z is greater than 0; that means, at any length CT 0 plus 0; that means, time 0 is equal to 0 of course, it can be at any length 0 plus means onward 0 or initially the concentration 0 because I have injecting the tracer at time 0 I saw at time 0 inside a reactor concentration is 0.

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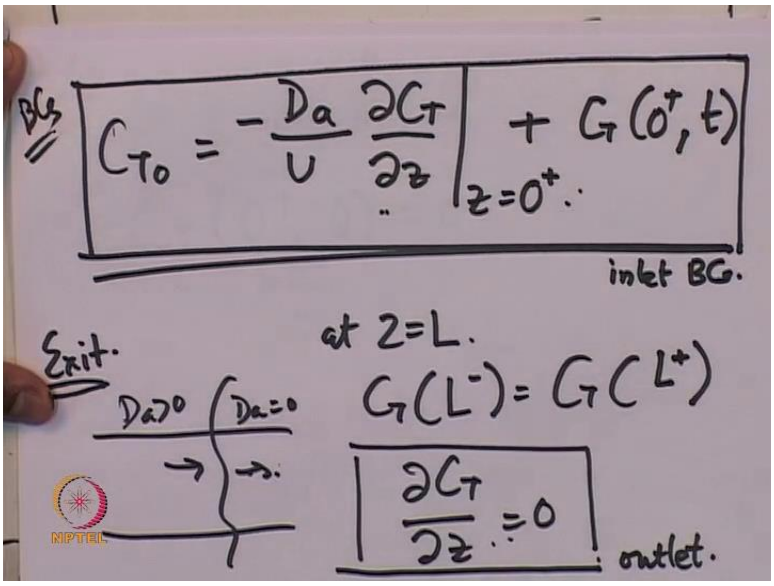

BCs

$$\boxed{C_{T0} = -\frac{D_a}{u}\frac{\partial C_T}{\partial z}\Big|_{z=0^+} + C_T(0^+, t)}$$

inlet BC.

Exit.

at $z=L$.

$$C_T(L^-) = C_T(L^+)$$

$$\boxed{\frac{\partial C_T}{\partial z} = 0}$$

outlet.

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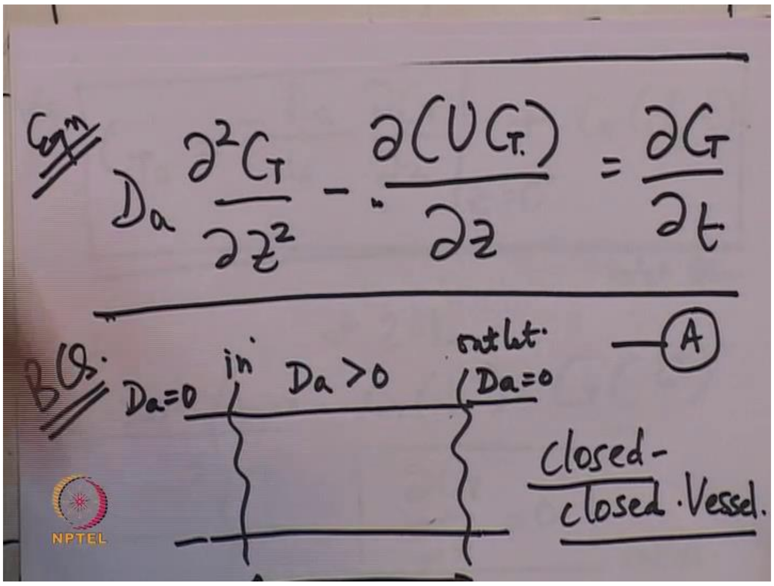

Eqn

$$D_a \frac{\partial^2 C_T}{\partial z^2} - \frac{\partial (U C_T)}{\partial z} = \frac{\partial C_T}{\partial t} \quad \text{—} \ (A)$$

So, this is initial conditions. So, initial condition than you have boundary conditions. So, this are the boundary conditions and this is your equation main differential equation, I can solve this equations together to get the tracer concentration how it changes inside a reactor, why we are doing all this; because we want to see, how the tracer get tracer spreads, why we want to know how the tracer is spread because that is going to tell me the flow pattern inside a reactor. So, I am I wont able to characterize a flow pattern like what I did in the case of tank in series, at I characterize flow pattern in terms of a number called number of times.

Similarly, I am going to get a parameter here will see what parameter that will characterize a flow pattern. So, let us solve this equation will see; now see, the main difference what we see before and after, before it means; in the tank in series model there we just discretized it, the entire domain The volume in different times. Now, I am looking at differential equation. So, there is discrete dynamic stair, here it is a continues dynamics. I am writing it differential equation here, there I was a writing difference equation see this different you come across this particular way of formulating a problem in many cases, the distillation column absorption, column see number of stages pet column try column similar.

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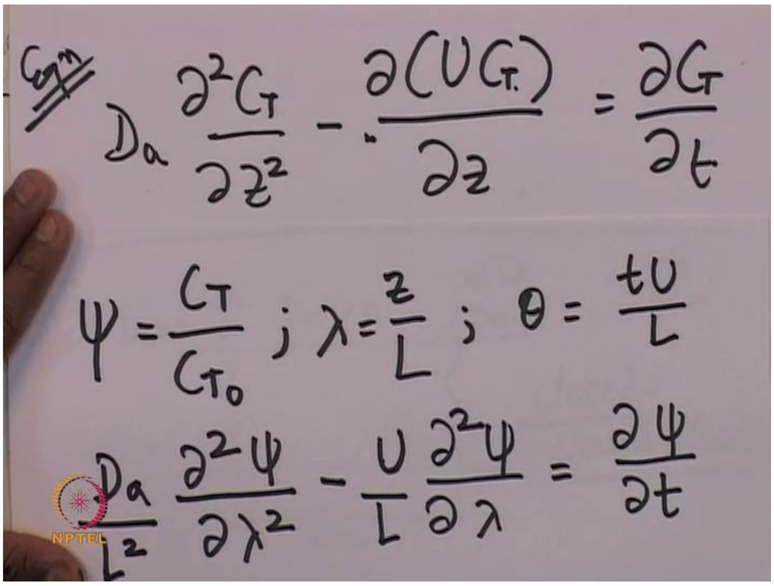

Eq^n

$$D_a \frac{\partial^2 C_T}{\partial z^2} - \frac{\partial (U C_T)}{\partial z} = \frac{\partial C_T}{\partial t}$$

$$\psi = \frac{C_T}{C_{T_0}}\ ;\ \lambda = \frac{z}{L}\ ;\ \theta = \frac{tU}{L}$$

$$\frac{D_a}{L^2}\frac{\partial^2 \psi}{\partial \lambda^2} - \frac{U}{L}\frac{\partial^2 \psi}{\partial \lambda} = \frac{\partial \psi}{\partial t}$$

So, now let us go ahead before that we need to Non-dimensionalize this equation, because where we non-dimensionalize we will come with the parameter that is going to decide everything. Now what is this, the non-dimensional form the equation is going to be like this. So, let us start this equation. So, let me this is a differential equation, I want to non-dimensionalize this. So, let me define non-dimensional concentration psi CT is by CT is 0 lambda z by L theta. In fact, theta we will come back to this, it will come on zone. You know typically what happens when we do now, non-dimensionalize equation.

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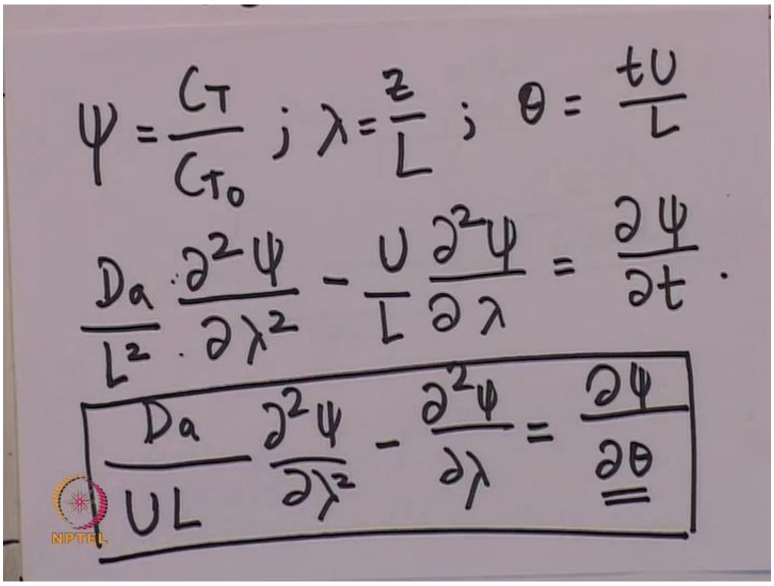

$$\psi = \frac{C_T}{C_{T_0}}\ ;\ \lambda = \frac{z}{L}\ ;\ \theta = \frac{tU}{L}$$

$$\frac{D_a}{L^2}\frac{\partial^2 \psi}{\partial \lambda^2} - \frac{U}{L}\frac{\partial^2 \psi}{\partial \lambda} = \frac{\partial \psi}{\partial t}.$$

$$\boxed{\frac{D_a}{UL}\frac{\partial^2 \psi}{\partial \lambda^2} - \frac{\partial^2 \psi}{\partial \lambda} = \frac{\partial \psi}{\underline{\underline{\partial \theta}}}}$$

If it do this. So, let us see, you have Da d2 psi by d lambda square now here; what will see you have L square minus, you can take it out assuming that velocity is not changing with respective z and t. So, this is the of course, is not a not down not dimensional, I am not d dimensionalize is a time yet. Now if, I define theta equal to t U by L or in other words, suppose I multiply this equation by L by U. So, let us multiply both the sides by L by U, there what do I get, Da divided by UL, I am multiplying it by L by U. So, UL this will go away L by U means, what, when it comes in denominator you have this is happening. See L by U multiplied by L by U comes in denominator 1 upon U by L and I take this the t into U by L.

So, I get d theta dell theta. So, this is a dimensionless equation theta have got. If it is not clear you can do it on your own and check. So, dimensionless concentration dimensionless length, dimensionless times; what is the unit of this second meters per second and meter. So, now, you let U by L has a unit per second. So, that is why, I am using U by L as parameter here or other ,I have club this 2 to get dimensionless time and Da by UL what is the unit of Da, meter square per second. This is meter per second and this is meter. So, this is again dimensionless number, raise to all and dimensionless this is the dimensionless numbers.

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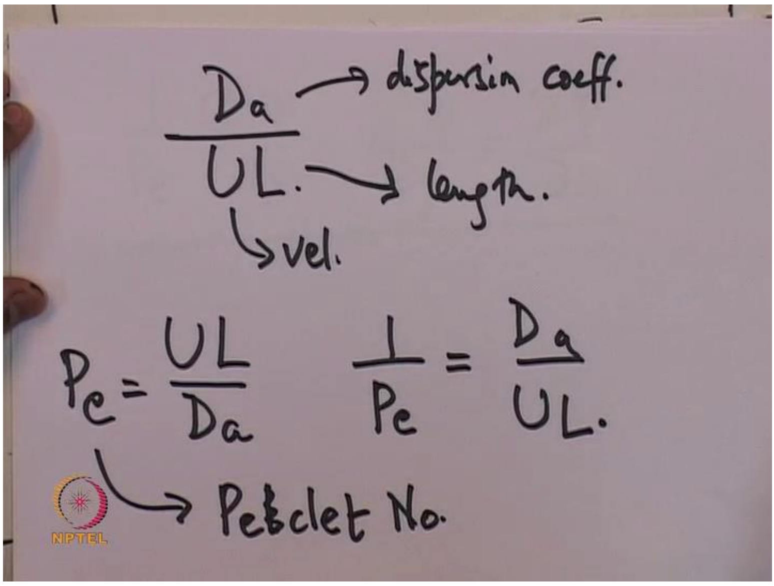

$$\frac{D_a \xrightarrow{} \text{dispersion coeff.}}{\underset{\searrow \text{vel.}}{U}L. \xrightarrow{} \text{length.}}$$

$$P_e = \frac{UL}{D_a} \qquad \frac{1}{P_e} = \frac{D_a}{UL.}$$

$P_e \xrightarrow{}$ Peclet No.

.

So, let us spend time on this particular number Da by UL; this is a dispersion coefficient velocity and length. This is very famous number, which can this is number that characterizes the mixing; is named after an engineer called peclet, but of course, the peclet number is inverse of this; that means, UL by Da. So, peclet number is UL by Da or in other, words 1 upon Pe is equal to Da by UL. Peclet number that t is silent. So, so it say peclet number, the very famous number.

So, let me put that number in the equation again, you remember that equation. So, here so Da by UL is 1 divided by Pe by p. So, this is my equation. So, this peclet number before we go ahead and try and understand meaning of it. If peclet number is very large, peclet number is very large; that means, the dispersion is small velocity is very large what is it mean, it means I am going towards what kind of flow, plug flow because dispersion is less velocity is very large no dispersion or a very small dispersion peclet number is very large. If it is infinity then it is plug flow reactor, in other words if dispersion coefficient is very large, then peclet number will become very small.

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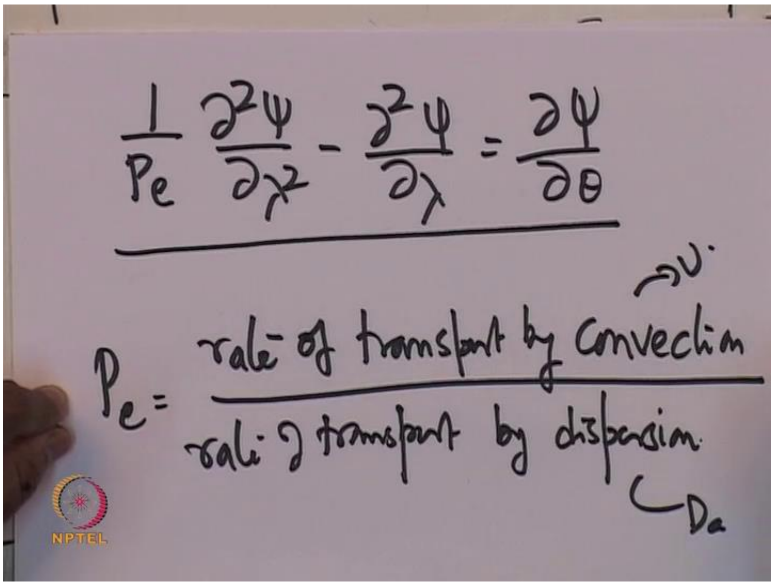

$$\frac{1}{Pe}\frac{\partial^2\psi}{\partial\lambda^2} - \frac{\partial^2\psi}{\partial\lambda} = \frac{\partial\psi}{\partial\theta}$$

$$P_e = \frac{\text{rate of transport by } \overset{\to U}{\text{convection}}}{\text{rate of transport by } \underset{\hookrightarrow Da}{\text{dispersion}}}$$

What is meaning of large dispersion; that means, back mixing happening and what is that situation it is nothing but, a back mixed reactor CASTR when peclet number is 0. So, 2 bounce, see it is quiet similar to number of CASTR in series number of tank in series. So, this is a differential equation or continues dynamics, there it was discrete dynamics. Theoretically it both are falling in line let me similar. So, peclet number can be define in words, as peclet number is equal to rate of transport by convection see those 2 term UL and or in the U numerator U; U is convection is a velocity divided by rate of transport by dispersion, because in the denominator you have Da here. You have U and of course, L that is characteristic length comes because of like you have to somehow Da means, not is meter per second.

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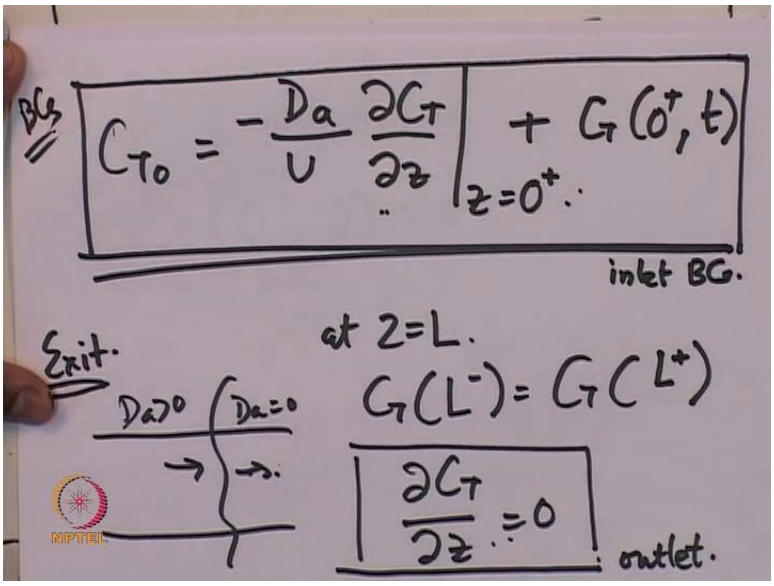

BCs

$$\boxed{C_{T_0} = -\frac{D_a}{U}\frac{\partial C_T}{\partial z}\bigg|_{z=0^+} + C(0^+,t)}$$

inlet BC.

Exit.

at $z=L$.

$$C(L^-) = C(L^+)$$

$$\boxed{\frac{\partial C_T}{\partial z} = 0}$$

outlet.

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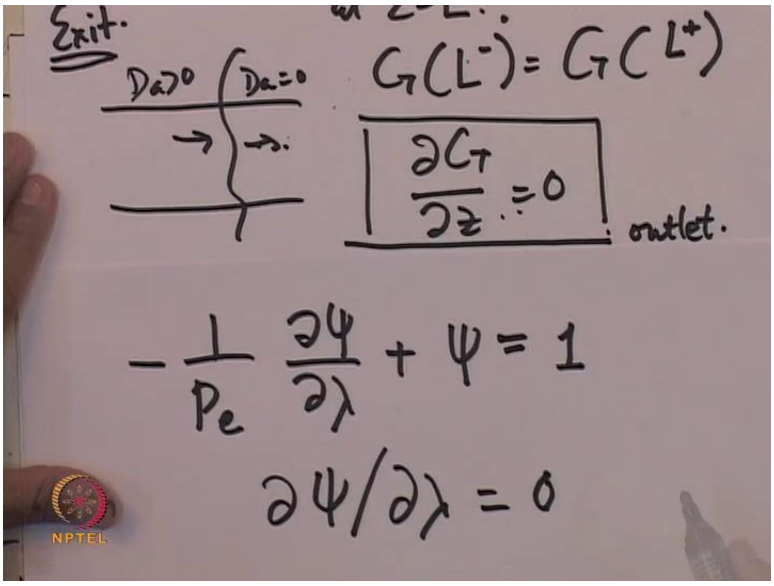

Exit.

$$C(L^-) = C(L^+)$$

$$\boxed{\frac{\partial C_T}{\partial z} = 0}$$

outlet.

$$-\frac{1}{P_e}\frac{\partial\psi}{\partial\lambda} + \psi = 1$$

$$\partial\psi/\partial\lambda = 0$$

So, that Da by delta has to come. So, you have that L coming in expression profile otherwise, remember this you will come in the numerator and Da in the denominator and peclet number will characterise is the back mixing, larger the peclet number, smaller is the back mixing and smaller the peclet number larger back mixing. Peclet number infinity will plug flow peclet number 0 means CASTR. So, so this where the boundary conditions I had, if I am non-dimensionalize them. So, the first 1 looks like this, the first 1, if I am non-dimensionalize this, it becomes 1 by Pe into dell psi by dell lambda plus psi is equal to 1, you can derive it. If I am non-dimensionalized this, this, this; the expression that I get, because this is I am just dividing both the side by this number, this number CT0 and divide CT0 CT0 1 and then I get this.

So, this is the non-dimensional form the boundary condition 1, then the boundary condition 2, this is the boundary condition 2, this was boundary condition 1, this is a boundary condition 2. Now, I get let us go as simple d CT by dell CT by dell z is equal to 0 means, dell psi by dell lambda is equal to 0. So, this 2 boundary conditions and of course, I will have the initial condition, which say that concentration is 0 everywhere at time is equal to 0. So, psi is equal to 0; let me write it, psi is equal to 0 at all lambdas when theta, what is theta; time is equal to 0. I am working in terms of dimensionless numbers.

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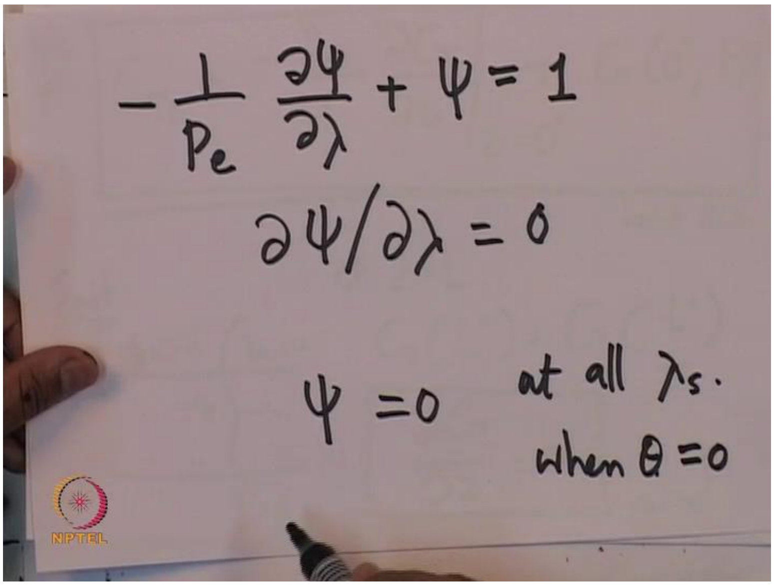

$$-\frac{1}{Pe}\frac{\partial\psi}{\partial\lambda}+\psi=1$$

$$\partial\psi/\partial\lambda=0$$

$\psi=0$ at all λs.

when $\theta=0$

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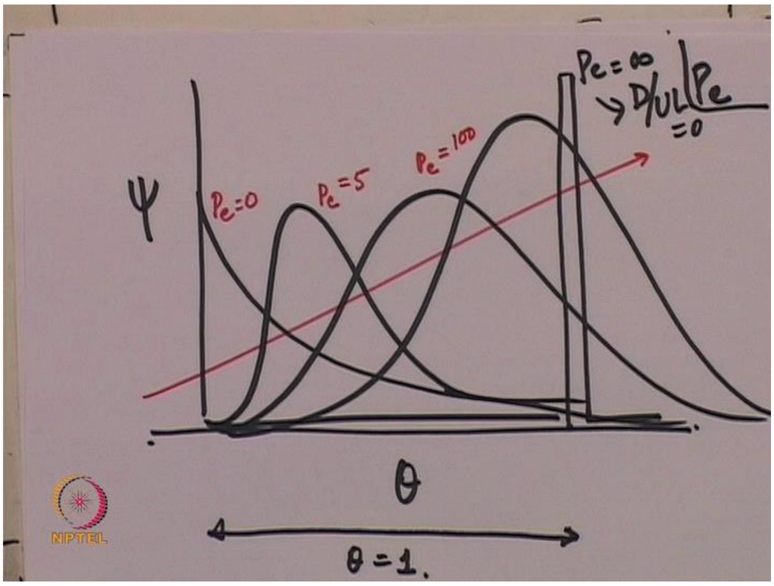

So, with this now I have equation to be solved, 1 equation ordinary partial differential equation and second order with 3 boundary conditions of course, 2 boundary condition and 1 initial condition in dimensionless form. I what, I will get is the plot of tracer concentration says psi verses theta, how will I. So, what is the tracer concentration the out let tracer concentration out let exit concentration, because I am not looking at, what I am inside of course, it is going to be in between what you get at out let and what you get in the what you injected inlet.

But, normally see what do I realise, I realise out get concentration because I do pulls experiment or I do tracer injection experiment. So, this is out let concentration, when I solve this equation, when I solve this equation at z is equal to L or at lambda is equal to 1 what is the concentration. So, this is what I am going to see. So, what kind of profile will see here? So, it all depends on the peclet number, if peclet number is very large means, dispersion is 0 or say in peclet number is infinite dispersion is 0. What is the tracer concentration that I am going to see it is exactly similar to what I have injected, I am going to see plug flow behaviour.

So, what is that; this is what I am going to see, this is, what is this? This is theta equal to is a dimensionless time theta equal to 1, why? Dimensionless time it is t into U by L or L by U is tau that is residence time. So, this time is tau actual time, actual time divided by tau that is theta is equal to 1. So, this is when peclet number is infinite or some time it will have let talk in terms of D by UL.

So, D by UL be 0 or this corresponds to D by UL equal to 0. Another extreme peclet number 0 famous E curve for I am not plotting E curve plotting concentration, but it is the qualitative behaviour is say similar to the E curve. And then in between these 2 see now, this plot has to become this means, the transition is like this; this will move this peak will normally increase like the height of a… So, because it is going to go up.

So, this is the typical behaviour that I will see, as the value of peclet number increases. So, here peclet number is 0, here the peclet number is probably say some value 5, peclet number what 100 and so on. So, this is the typical behaviour and this is quite similar to what we have seen before means, what for a tank in series model, in tank in series model will look at how this profile, how this E curve or the tracer concentration changes with respective time with respective time or E curve, how does it look like with respective n rather number of tank in series.

So, it goes from CSTR into p of r similar thing is happening here; that means, n in tank in series model is equivalent to peclet number if the case of dispersion model both are similar. So, once you have the E curve now is other way around, once you have the E curve you can calculate a peclet number. I have drawn this for several values of peclet number, but if you do the boundary experiment for tracer equation get some E curve, I can calculate a corresponding peclet number from this. And peclet number will characterize the extend of mixing, like the number of tangent series in the previous model. So, as simple as that.

So, do tracer experiment get E curve or concentration verses times for the tracer determine the value of peclet number. what next then if you have the value of peclet number then you have to calculate a conversion when actual reaction is taking place. So, far we just look at a tracer experiment without any reaction you have characterized the flow patterns in terms of extent of back mixing and that is through the value of peclet number 1, once you get a peclet number we have go for the reaction model. Now, how to get a value peclet number. So, the 1 can derive, of course 1 can solve this equation we have to solve this equation numerically by the way it is a differential equation.

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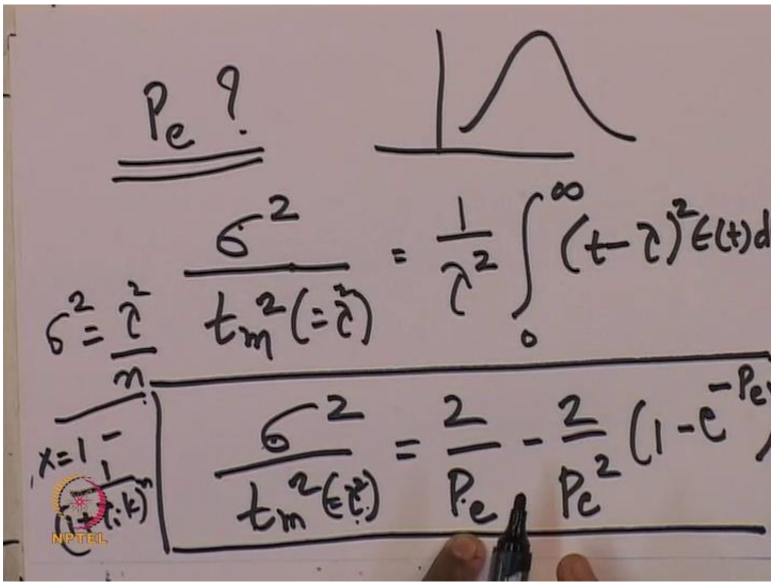

P_e ?

$$\frac{\sigma^2}{t_m^2(=\tau^2)} = \frac{1}{\tau^2}\int_0^\infty (t-\tau)^2 E(t)\,d$$

$$\sigma^2 = \frac{\tau^2}{n}$$

$$x = 1 - \frac{1}{(1+\tau k)^n}$$

$$\boxed{\frac{\sigma^2}{t_m^2(=\tau)} = \frac{2}{P_e} - \frac{2}{P_e^2}\left(1 - e^{-P_e}\right)}$$

So, I have not given you analytical expression for this, but you have to solve this equation numerically or analytical expression is also possible it comes in the form of a series mathematical series, but then that is not important. You the expression is not important, how it looks like what is it qualitative behaviour is important and once I have the expression or I have the profile or E curve rather. How to get a value of peclet number. So, 1 can get a appropriate number approximate value of peclet number from this.

Now, once I have the E curve, from this E curve or concentration tracer concentration verses time curve. I know that sigma square that is variance divided by mean residence time which is nothing but tau that is a our residence time, in this particular volume divided by volumetric flow rate. Tau square infinite 0 infinite t minus tau square Et dt should be noted, that tm is equal to tau is valid only for closed-closed system. This is the something that, I know is definition of sigma variance.

Now, from this differential equation I can derive the expression for sigma in term of Pe like, What I did before in terms of number of tank in series, sigma square was equal to tau by n or tau square by n square. So, here again I am going to get a expression for sigma in terms of peclet number. So, that expression happens to be sigma square tau m this is nothing but, tau is equal to 2 by Pe minus 2 by Pe square 1 minus e raised to minus Pe; slightly complicated no need to remember this equation.

But then you know there is a relationship between sigma Pe and t m or rather tau. And we had a similar relationship before as well, between sigma tau and m there was n here that was relatively simpler. Now this is slightly complicated, but of course, no need to worry about it, early relationship was sigma square is equal to tau square divided by n. Now, instead of this relationship I have this relationship here, I had n is a parameter now I have Pe as a parameter that is the only difference.

So, once I get sigma square from my curve that is mean variance, I get sigma square from mean variance. I can get a value of Pe that is peclet number and once you have peclet number, you have characterized the flow pattern then the next job is to get a conversion for the reaction of interest. So, far no reaction similar to what we did once you get a value of n, then for the first order reaction I say that x is equal to 1 minus 1 by 1 plus tau i k raised to n remember. So, this is what I did after getting a value of n; now my next job here is after getting a value of Pe I need to get a conversion in terms of Pe. So, that is what we will we are going to see in the next lecture. How to get conversion from Pe.

Thank you very much.