Mathematical Modelling and Stimulation of Chemical Engineering Process
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Lecture 21
Modelling transport phenomena problems - part 1

Hello everyone, in this week we are going to study about different transport phenomena based problems that occur in different physical systems and we often encounter them in trying to relate or trying to estimate different process parameters or system design or performance prediction.

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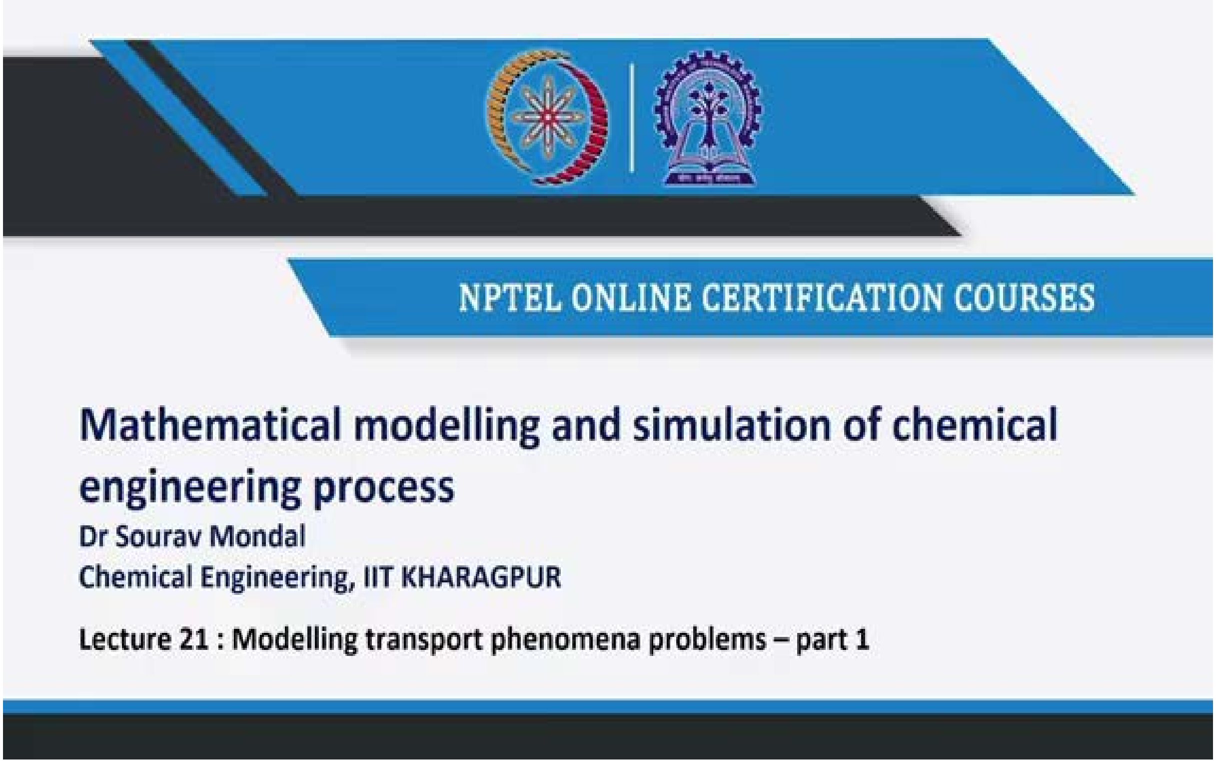

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Mathematical modelling and simulation of chemical engineering process

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Lecture 21 : Modelling transport phenomena problems – part 1

Now, in this class we are going to talk about a problem which is often encountered during combustion.

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CONCEPTS COVERED

- Transient gas liquid absorption
- Gas liquid absorption with chemical reaction

So, and this absorption of gas in liquid or liquid in gas is a very common thing in Chemical Engineering Process and the biggest application is this in the case of fuel droplet burning or if you have a gas liquid mass transfer taking place, droplet based chemical reaction. In all of these cases, the mass transfer plays a big and a very important role.

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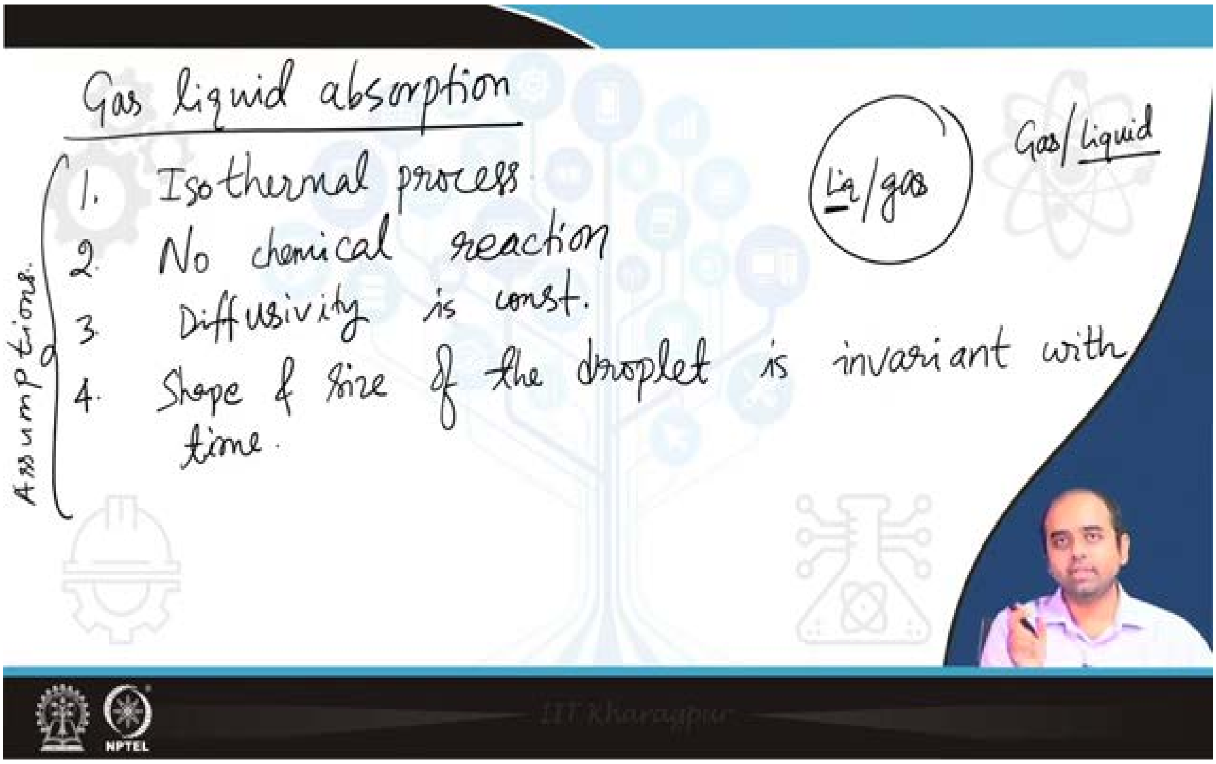

Gas liquid absorption

Assumptions

1. Isothermal process
2. No chemical reaction
3. Diffusivity is const.
4. Shape & size of the droplet is invariant with time.

Now, let us try to consider or try to visualize the picture let us say you have a, a droplet, a droplet could be of, the droplet could be of a liquid or gas, so if it is a liquid droplet, then the outside environment should be gas, so it could be like liquid droplet dispersed in a gaseous medium or liquid droplet spray, so this is an ideal example of the scenario of a fuel droplet burning.

And if you are considering gaseous droplet, then you can consider that gas bubbling through a liquid pool or something you are having two phase boiling systems or you can think of bubbling of argon gas during in molten steel furnaces to improve the homogenization or its composition. So, there could be several such applications where do you encounter this gas liquid absorption.

So, before starting to try to model this mass transfer phenomena from liquid to gas phase or from gas to liquid phase, it is very important to first list down or try to write the different assumptions that we are considering in this problem. So, the first assumption that we are considering let us say it is an isothermal process, we are not going to consider any temperature effects in the problem.

So, of course, a fuel droplet burning or the case of gas bubbling through a chemical reactor are not isothermal process, they are not in practical scenarios they are not. But this would be the first assumptions that we would want in our problem to simplify it and so that the base case scenarios can be obtained reasonably with not much of complexity to the problem. That is the reason why we try to add as much assumptions as possible to the problem and then later on to have a more practical, to have a more detailed understanding of the process you can ignore some of the assumptions and get to more realistic scenarios.

The second assumptions we can think of let us say for the time being no chemical reaction, we will talk about today what happens when you have chemical reaction. But let us say for the first case we do not consider any chemical reaction. So, we ignore any chemical reaction effects. We also consider that the diffusivity whether its liquid to gas or gas to liquid whatever diffusivity is constant and it does not depend on the concentration of the mixtures or the components. We also consider that the shape of the droplet, both shape and size of the droplet is constant with time.

Now, of course this is not always the case as we have talked about the burning of a fuel droplet, so as it burns the oil droplet shrinks, so it becomes like a shrinking core scenario. So, it may not be true always but this is, but if you consider them to be the shape as well as the size to be constant this will significantly simplify the problem and but still it will preserve the essence of the mass transport phenomena or the physics of the mass transport process.

So, we write that the shape and size of the droplet is invariant with time. So, these are generally the assumptions and with these assumptions we can try to frame the mass transport model. So, these are the assumptions. So, let us look into how we can write a species balance in a small elemental section in this droplet.

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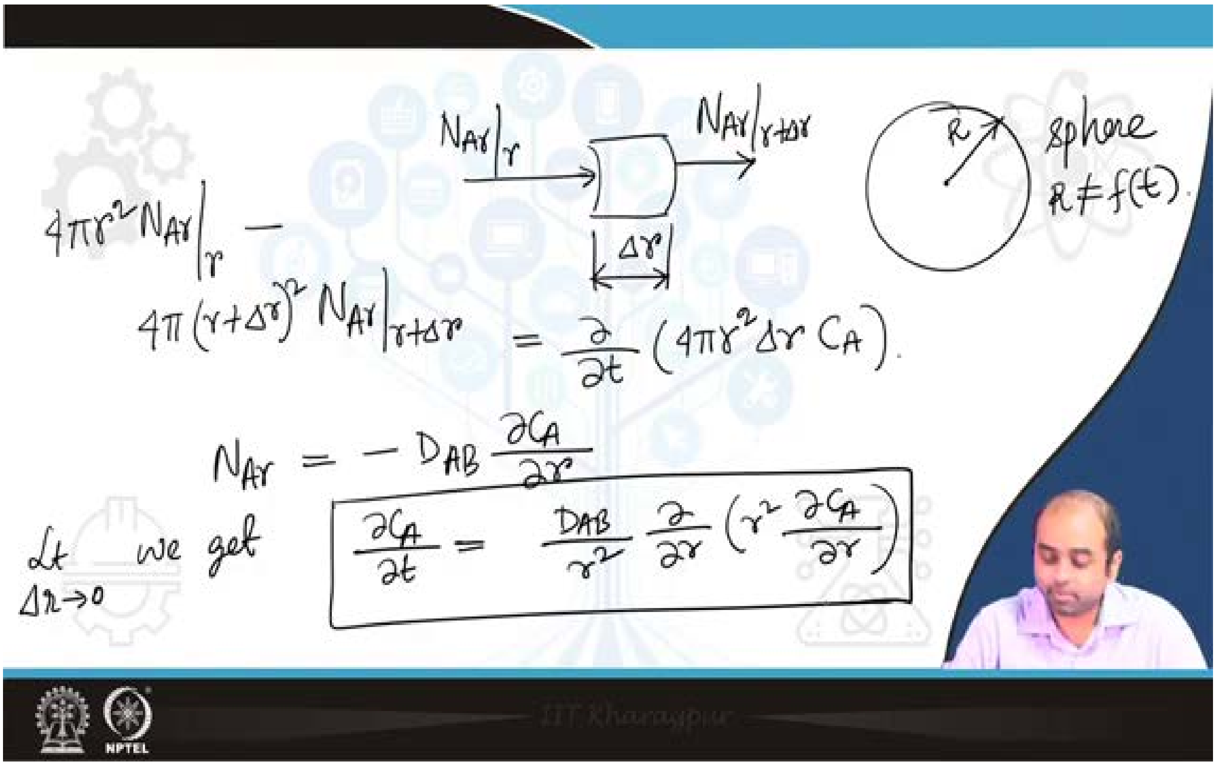
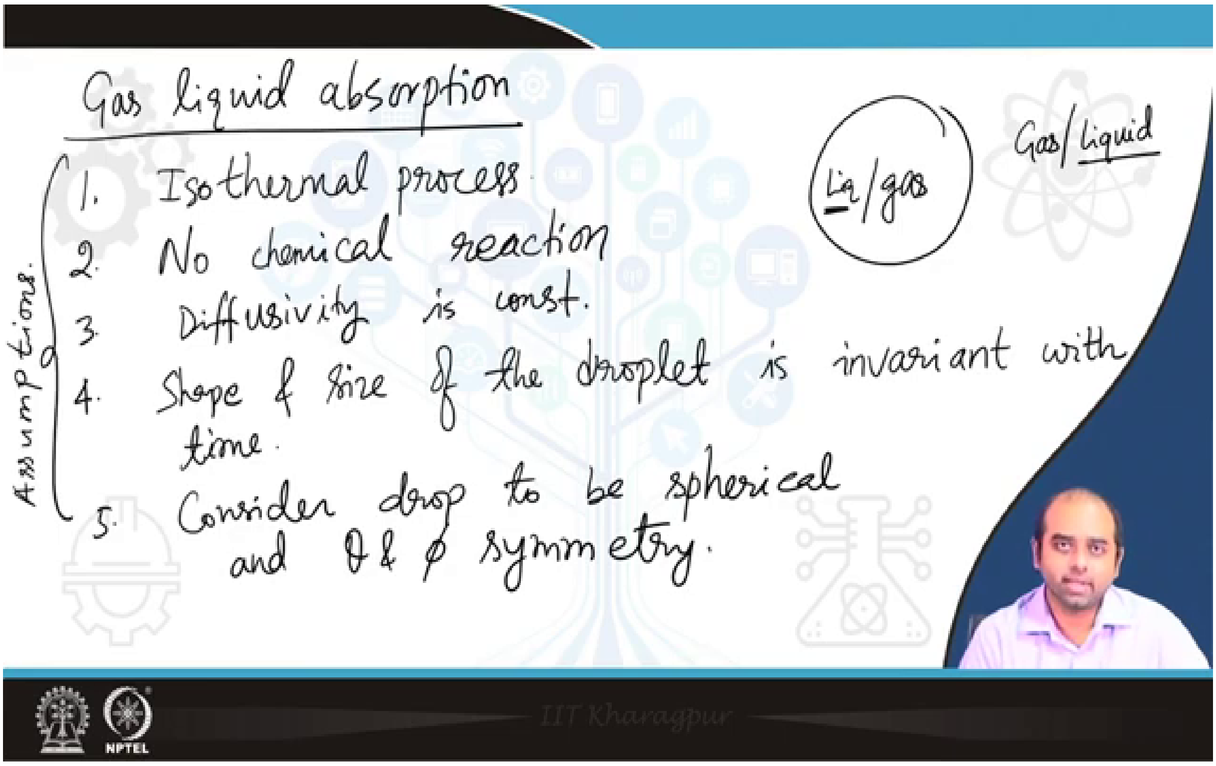


$$4\pi r^2 N_{Ar}\Big|_r - 4\pi (r+\Delta r)^2 N_{Ar}\Big|_{r+\Delta r} = \frac{\partial}{\partial t}\left(4\pi r^2 \Delta r\, C_A\right).$$

$$N_{Ar} = -D_{AB}\frac{\partial C_A}{\partial r}$$

$\lim_{\Delta r \to 0}$ we get

$$\boxed{\frac{\partial C_A}{\partial t} = \frac{D_{AB}}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial C_A}{\partial r}\right)}$$



Gas liquid absorption

Assumptions.
1. Isothermal process.
2. No chemical reaction
3. Diffusivity is const.
4. Shape & size of the droplet is invariant with time.
5. Consider drop to be spherical and θ & ϕ symmetry.

I will draw the droplet once again and we consider the radius of the droplet to be R and we have already said that R is fixed so this is, let us consider this the droplet to be a sphere or a spherical particle or spherical droplet, and the shape and the size does not change with time so R is not a function of time.

So, let us consider a small section of this, this is, consider this to be a sphere, so consider a small spherical element of delta r, let us say the flux in the radial direction is at r is N Ar and at r plus delta r is written like this. So, how do we write? So, the flux across this small elemental section, so we multiply 4 pi r square, it is the surface area of a sphere of having, or a spherical region of radius r that is N Ar, so this is the inlet flux and minus we have 4 pi r plus delta r whole square N Ar r plus delta r, so this is the inlet flux at the radius r.

And next we have the outlet or the flux that is coming out and the difference of these two is written down by the accumulation term which is the rate of change of the flux, in, rate of change of the concentration in this domain or in this volume segment, so the volume segment since this delta to be infinitesimally small we can write surface area multiplied with the thickness that is 4 pi r square delta and we write the concentration as CA.

So, now one more assumptions to this problem that we missed out is that we consider the particle to be spherical, consider drop to be spherical and assume, and have theta as well as phi symmetry, this is generally very common for spherical coordinate problems that we say that change in the concentration or the flux along the theta or the phi direction does not happen, so it is symmetric in the theta and the phi angular planes. That is the reason why we consider the change in the flux or the radial profiles only in the r direction.

So, as there is no convection to the problem, the flux if you are considering only a binary system and then it is very easily you can write the flux to be the based on the ficks law of diffusion. So, instead of grad C, I can write del C del r because theta and phi symmetry exist. So, if I take the limit of the next step delta r tending to 0 from the above equation we get del CA del t is equal to D AB by r square del del r r square del CA del r.

So, this is the differential equation for this problem where you consider only radial diffusion, unsteady radial diffusion of the species in the droplet or in the spherical particle. Now, what about the boundary conditions?

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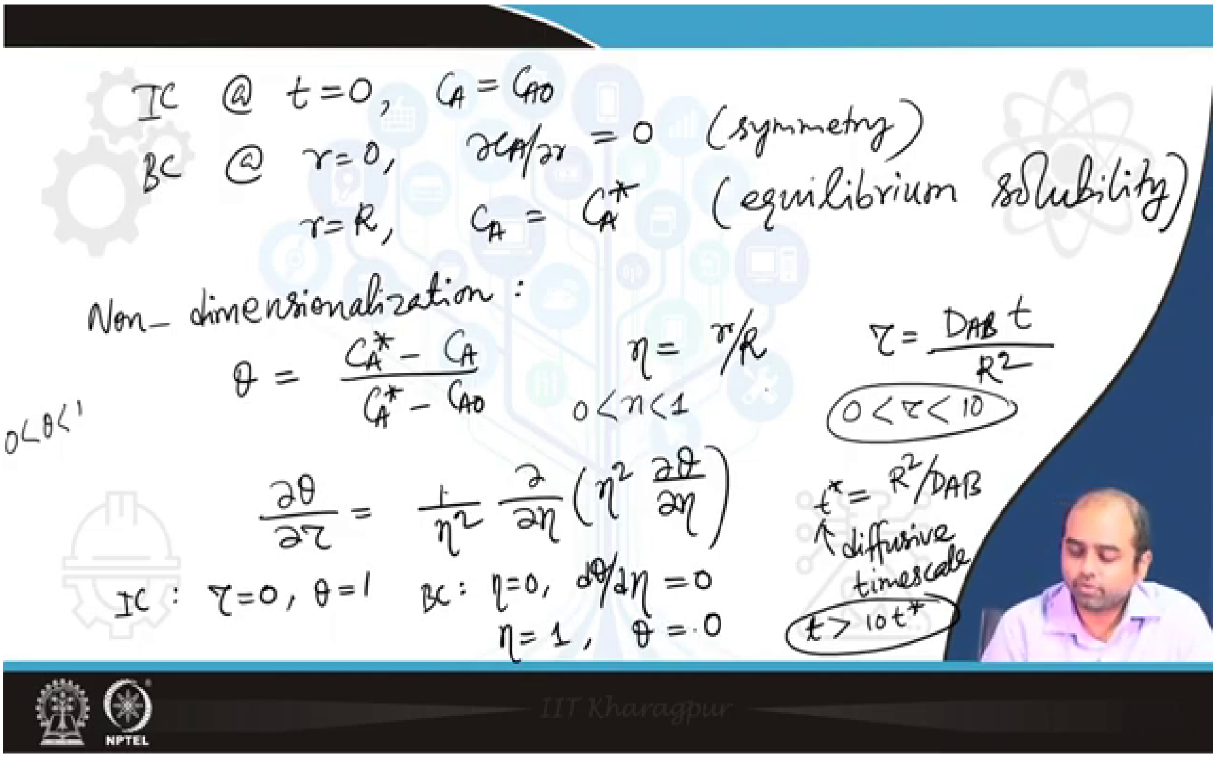

IC @ $t=0$, $C_A = C_{A0}$

BC @ $r=0$, $\partial C_A/\partial r = 0$ (symmetry)

$r=R$, $C_A = C_A^*$ (equilibrium solubility)

Non-dimensionalization :

$$\theta = \frac{C_A^* - C_A}{C_A^* - C_{A0}} \qquad \eta = r/R \qquad \tau = \frac{D_{AB}\, t}{R^2}$$

$0<\theta<1$ $\quad$ $0<\eta<1$ $\quad$ $\boxed{0<\tau<10}$

$$\frac{\partial \theta}{\partial \tau} = \frac{1}{\eta^2}\frac{\partial}{\partial \eta}\left(\eta^2 \frac{\partial \theta}{\partial \eta}\right)$$

$t^* = R^2/D_{AB}$

↑ diffusive timescale

$\boxed{t > 10t^*}$

IC : $\tau=0$, $\theta=1$ $\quad$ BC : $\eta=0$, $d\theta/d\eta = 0$

$\eta=1$, $\theta=0$

So, the initial condition at t is equal to 0 we have CA is equal to CA naught, there are two boundary condition at r is equal to 0 you have d CA d r to be equal to 0, this is the symmetry condition. And at r is equal to capital R which is the surface of the droplet or the sphere we say CA is equal to CA star, and this CA star can be related or can be considered to the equilibrium solubility limit.

You can also calculate that concentration, you can also have like the from the idea of the interface mass transfer you can also calculate out the balance of the fluxes. So, there are two possible conditions at the surface, one is the continuity of the concentration or you have continuity of the flux. So, in this case we are having this concentration as to be the equilibrium concentration and we are assuming that the outside concentration is same, so there is the concentration outside the droplet is constant.

So, let us try to non-dimensionalize this equation and how do we try to solve. So, see the, if you recall when, in the first week we talked about the steps of modelling a problem, the first thing we should try to do is to write down the assumptions because our model is based and is dependent on the assumptions that we make and assumptions should try to simplify the problem. So, that is the first thing that we should try to do.

The next step is of course try to make this non dimensionalizations because non dimensional helps in proper scaling of the terms and to find out that which term is having different orders of magnitude or not. So, based on this idea I try to scale the different terms or the different components here, so concentration is scaled in this way the form of theta, eta is r by r, tau is the diffusive time scale.

So, if you see here both theta varies in between 0 and 1, eta also varies in between 0 and 1. And similarly, tau is something that if it is too large then the problem becomes steady state. So, tau also varies to a positive value and in the same order of magnitude we can also get a fair idea about what is the order of magnitude beyond which the effects or the time effects are not important. So, if tau is too large then it means that, I mean you are you are achieving a steady state scenario or the dependence at that longer time scale is not important.

So, if you try to do this the equation that you get is will look something like this. And here please note that each of these term not only they lose the dimensionality but they are also scaled appropriately of order 1. So, if tau is not of order 1, but let us say of order 2 or order 3, then it simply means that the time dependent term is insignificant compared to the right hand side.

So, this will also give you a fair idea about the time scale of the problem beyond which the transient effects are not important. So, typically if tau is more than 10, you will see that d theta d tau term is order of magnitude less compared to the right hand side because the right hand side all of the terms are of order 1, eta is of order 1, theta is the order 1, so everything is the order 1 on the right hand side.

So, now if tau becomes of order 2, then this term on the, temporal term on the left right hand side is having one order less in comparison. So, then we mean that this problem achieves a steady state, so this will give you a physical idea of the time of the problem beyond which the transient effects are not important, and tau is the, I mean r square by d is essentially the diffusive time scale to the problem.

So, I can write t star as R square by D AB, so this t square is the diffusive time scale or the time scale to this problem. So, if t is greater than 10 t star you do expect that the transient effects are insignificant. What about the boundary conditions? So, the initial conditions also transformed by this scaling and the boundary condition we have eta is equal to 0, d theta, d eta to be equal to 0 and for eta is equal to 1 you have theta is equal to 0.

So, of course this problem can be solved with the help of the legendary polynomials, but there is one more transformation you can make to make this problem look much simpler.

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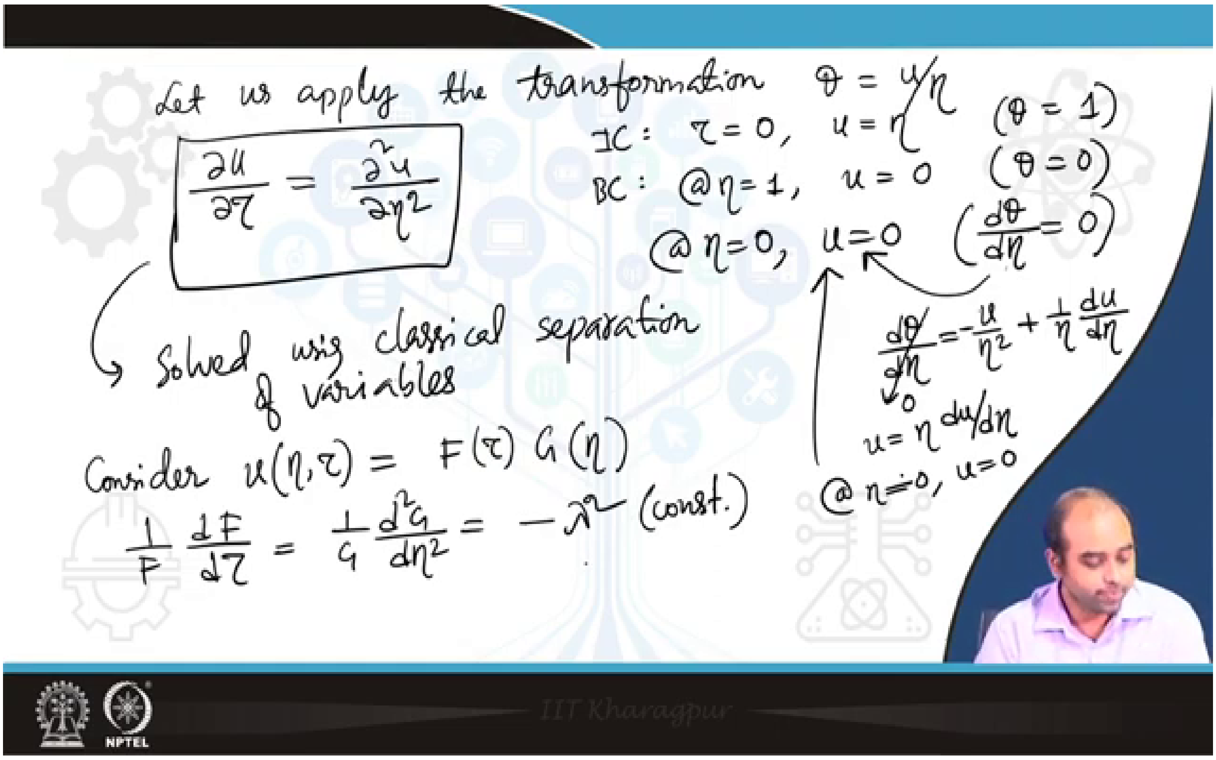


Let us apply the transformation $\theta = u/\eta$

$$\boxed{\frac{\partial u}{\partial \tau} = \frac{\partial^2 u}{\partial \eta^2}}$$

IC: $\tau = 0,\ u = \eta$ $(\theta = 1)$

BC: @ $\eta = 1,\ u = 0$ $(\theta = 0)$

@ $\eta = 0,\ u = 0$ $\left(\frac{d\theta}{d\eta} = 0\right)$

Solved using classical separation of variables

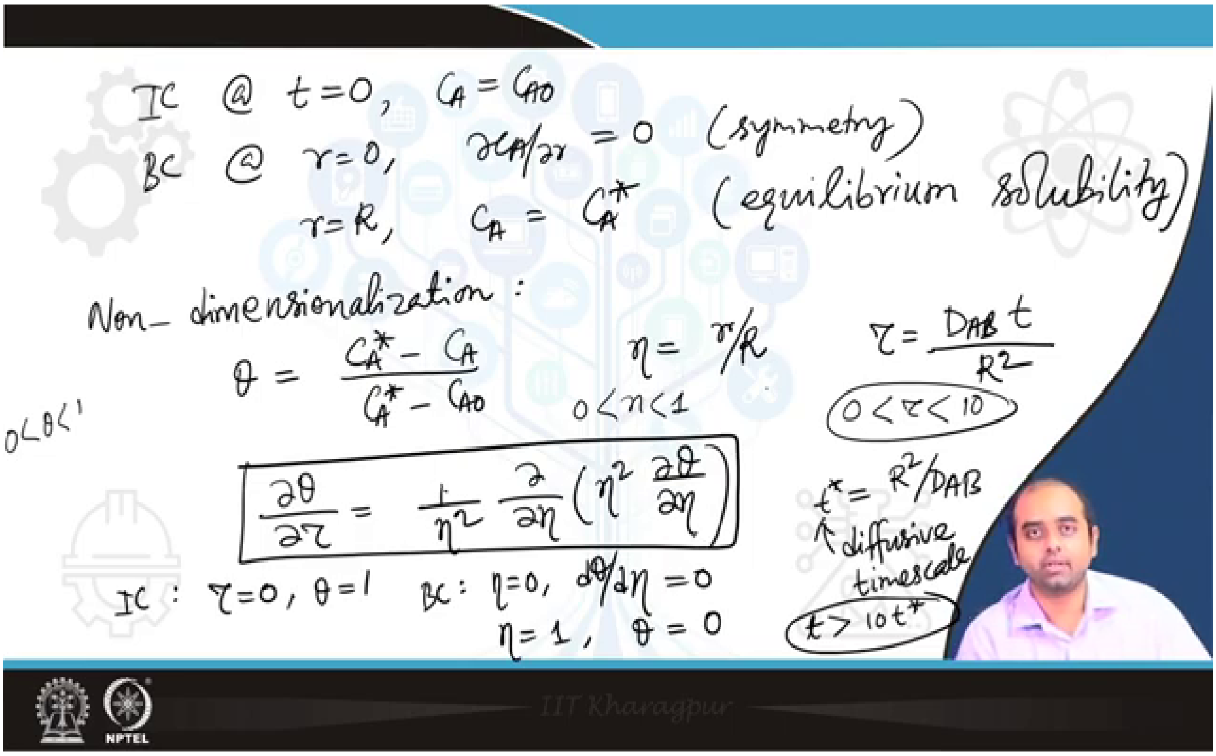
$$\underset{\downarrow 0}{\frac{d\theta}{d\eta}} = -\frac{u}{\eta^2} + \frac{1}{\eta}\frac{du}{d\eta}$$

$u = \eta\, du/d\eta$

@ $\eta = 0,\ u = 0$

Consider $u(\eta,\tau) = F(\tau)\, G(\eta)$

$$\frac{1}{F}\frac{dF}{d\tau} = \frac{1}{G}\frac{d^2G}{d\eta^2} = -\lambda^2 \text{ (const.)}$$



IC @ $t = 0,\ C_A = C_{A0}$

BC @ $r = 0,\ \partial C_A/\partial r = 0$ (symmetry)

$r = R,\ C_A = C_A^*$ (equilibrium solubility)

Non-dimensionalization:

$$\theta = \frac{C_A^* - C_A}{C_A^* - C_{A0}} \qquad \eta = r/R \qquad \tau = \frac{D_{AB}\, t}{R^2}$$

$0 < \theta < 1$ $\qquad 0 < \eta < 1$ $\qquad \boxed{0 < \tau < 10}$

$$\boxed{\frac{\partial \theta}{\partial \tau} = \frac{1}{\eta^2}\frac{\partial}{\partial \eta}\left(\eta^2 \frac{\partial \theta}{\partial \eta}\right)}$$

IC: $\tau = 0,\ \theta = 1$ $\quad$ BC: $\eta = 0,\ d\theta/d\eta = 0$

$\eta = 1,\ \theta = 0$

$t^* = R^2/D_{AB}$

↑ diffusive timescale

$\boxed{t > 10t^*}$

So, let us apply the transformation, theta is equal to u by eta. So, if you do this transformation you will find that this equation du d tau when converting it to I mean sorry d theta d tau getting converted to du d tau will look something like this. And the initial condition, so instead of theta we make a transformation in the dependent variable, instead of theta everything is represent in terms of u.

So, tau is equal to 0 you have u is equal to eta because theta was equal to 1, so u is equal to eta. Boundary condition at eta is equal to 1, you have u is equal to 0 because theta was equal to 0, here theta was equal to 1. And at eta is equal to 0 you will be having u is equal to 0 because d theta d eta was equal to 0. I think if you just try to think yourself you will realize that why d theta d eta is equal to 0 will lead to the condition that u is equal to 0. I mean it is very straight forward.

So, if theta is equal to u by eta what you will get, so if I try to do d theta by d eta that will be equal to u by, minus u by eta square plus 1 by eta du d eta. So, this is equal to 0 so which means u is equal to eta du d eta. Now, at eta to be 0, it means u is equal to 0 and that is what we get this boundary condition.

So, now this equation can be solved very easily using classical separation of variables technique, I mean of course the previous version of the equation, separation of variables, I mean the previous equation can also, I mean this equation can also be solved by separation of variables and the auxiliary equation corresponding to the spatial part will give you legendary polynomials.

And in this case the auxiliary equation or the solution to the auxiliary equation or the auxiliary ODE using separation of variables will give you sine and cosine functions. So, let us just try to do this quickly so you consider, sorry, u eta tau is equal to two linearly independent functions. So, 1 by F dF, d tau is equal to 1 by G d2G d eta square and let us say we call this as minus lambda square which is a constant. So, this is based on the separation of principle which is, sorry separation of variable is something we have already done before.

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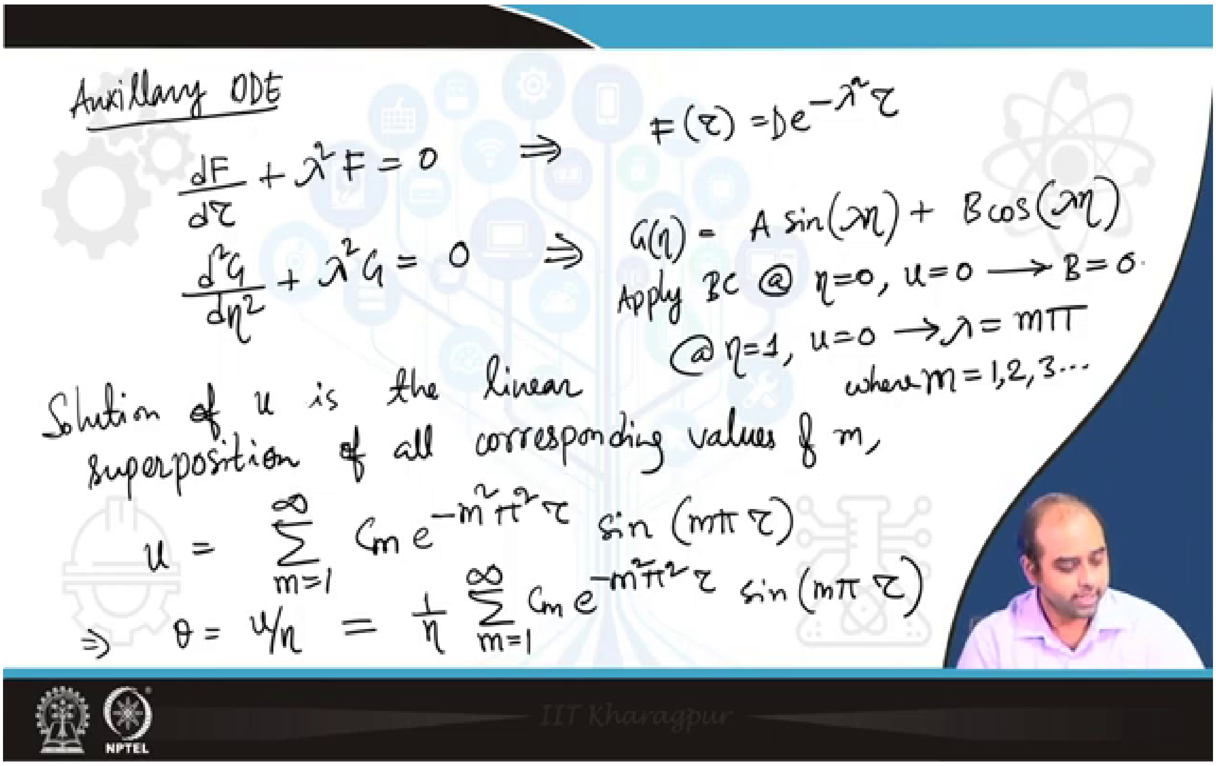

Auxillary ODE

$$\frac{dF}{d\tau} + \lambda^2 F = 0 \Rightarrow F(\tau) = De^{-\lambda^2\tau}$$

$$\frac{d^2G}{d\eta^2} + \lambda^2 G = 0 \Rightarrow G(\eta) = A\sin(\lambda\eta) + B\cos(\lambda\eta)$$

Apply BC @ $\eta=0$, $u=0 \rightarrow B=0$

@ $\eta=1$, $u=0 \rightarrow \lambda = m\pi$ where $m=1,2,3\ldots$

Solution of u is the linear superposition of all corresponding values of m,

$$u = \sum_{m=1}^{\infty} C_m e^{-m^2\pi^2\tau} \sin(m\pi\tau)$$

$$\Rightarrow \theta = u/\eta = \frac{1}{\eta}\sum_{m=1}^{\infty} C_m e^{-m^2\pi^2\tau} \sin(m\pi\tau)$$

So, we frame the two auxiliary ODEs. So, the first auxiliary ODE is d F by d tau, so this will give you the solution that F of tau is equal to e to the power minus lambda square tau and another one was, okay. So, solution to this G eta will be in terms of sin and cosine functions. So, if we apply the boundary condition at eta is equal to 0 you have u is equal to 0, this gives you B should be equal to 0 and based on the condition that eta is equal to 1, u is equal to 0, this gives you that lambda is equal to n pi, where, so this is n, where n is equal to 1, 2, 3, so for simplicity not to confuse with eta, let us make it m pi.

So, this is just you are in the standard template of the separation of the variables. So, we know that the solution of u, solution of u is the linear superposition of all corresponding values of m. And we club the constant A and the constant that we have got, let us say I missed a constant here for the spatial part something like let us say C, C1, so I multiply A and C, let us mark this as C, on or something like D or something. So, multiply A and D as like Cm e to the power minus m square pi square tau sin m pi tau.

And next we try to I mean the immediate thing we can do is that since u, I mean theta is equal to u by eta, so I can write this as one in terms of eta, so it is eta. So, we have to also find this constant Cm and for that we use the principle of orthogonality.

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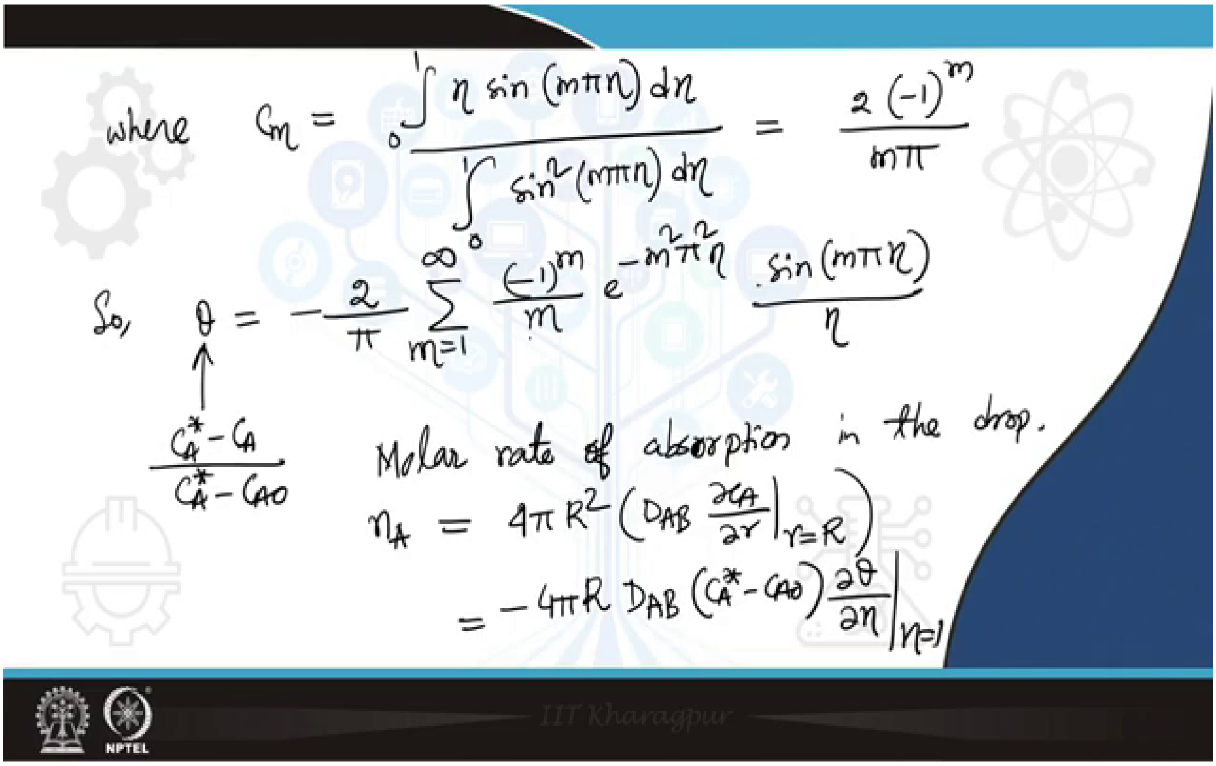

where $C_m = \frac{\int_0^1 \eta \sin(m\pi\eta)\,d\eta}{\int_0^1 \sin^2(m\pi\eta)\,d\eta} = \frac{2(-1)^m}{m\pi}$

So, $\theta = -\frac{2}{\pi}\sum_{m=1}^{\infty} \frac{(-1)^m}{m} e^{-m^2\pi^2\eta} \frac{\sin(m\pi\eta)}{\eta}$

$\uparrow$

$\frac{C_A^* - C_A}{C_A^* - C_{A0}}$

Molar rate of absorption in the drop.

$$n_A = 4\pi R^2 \left(D_{AB} \frac{\partial C_A}{\partial r}\Big|_{r=R}\right)$$

$$= -4\pi R\, D_{AB} (C_A^* - C_{A0}) \frac{\partial \theta}{\partial \eta}\Big|_{\eta=1}$$

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So, if you just use them you will find out that Cm turns out to be eta sin m pi eta d eta by integration of sine square, m pi eta, so you will be getting 2 minus 1. So, theta is equal to minus 2 by pi and then we have minus 1 by m e to the power minus m square pi square eta sin m by eta and there will be one more eta. So, this is m, so I mean this theta is nothing but CA star minus CA divided by CA star minus CA naught.

So, the molar rate so the important parameter here is the molar rate of absorption in the droplet, I mean from the concentration profile this is an important parameter that we are interested to find out. So, what is this molar rate of absorption? It is nothing but 4 pi capital R square is the molar rate of absorption, that is the surface area multiplied with the diffusive flux at the surface.

So, this is D AB d CA by dr at r is equal to capital R. So, you all, since you already know the this molar, this function, sorry this concentration profile you can find out that this what would be the molar rate of adsorption, I mean absorption, I am just trying to convert this in terms of eta. So, this will give you a fair idea about, I mean from the concentration profile to estimate the molar rate of absorption in this drop or the effective mass transfer that is taking place in this drop.

I hope all of you got a fair idea about how this mass transfer effects can be computed or evaluated. Of course, it is subjected to the assumptions in this problem, but how these can be incorporated in the problem and still we get a fair idea of the concentration profile as well as the mass transport rate from the droplet or this mass transfer in the dispersed phase systems from each of the individual particle.

So, in the next class we will see that how this idea can be extended to the case of the problem when you have droplet mass transfer along with chemical reaction. And then, we will see some more Chemical Engineering problems related to mass transfer and heat transfer. I hope all of you have enjoyed today's class, we will see you in the next lecture. Thank you.