Mathematical Modelling and Stimulation of Chemical Engineering Process
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Lecture 22
Modelling transport phenomena problems - part 2

Hello everyone, in this lecture we are going to see how does the mass transport coupled with chemical reaction can be modelled based on the idea that if we have already solved for the problem where we dealt with the scenario of mass transfer exclusively by diffusion, and now in the same problem we have chemical reaction.

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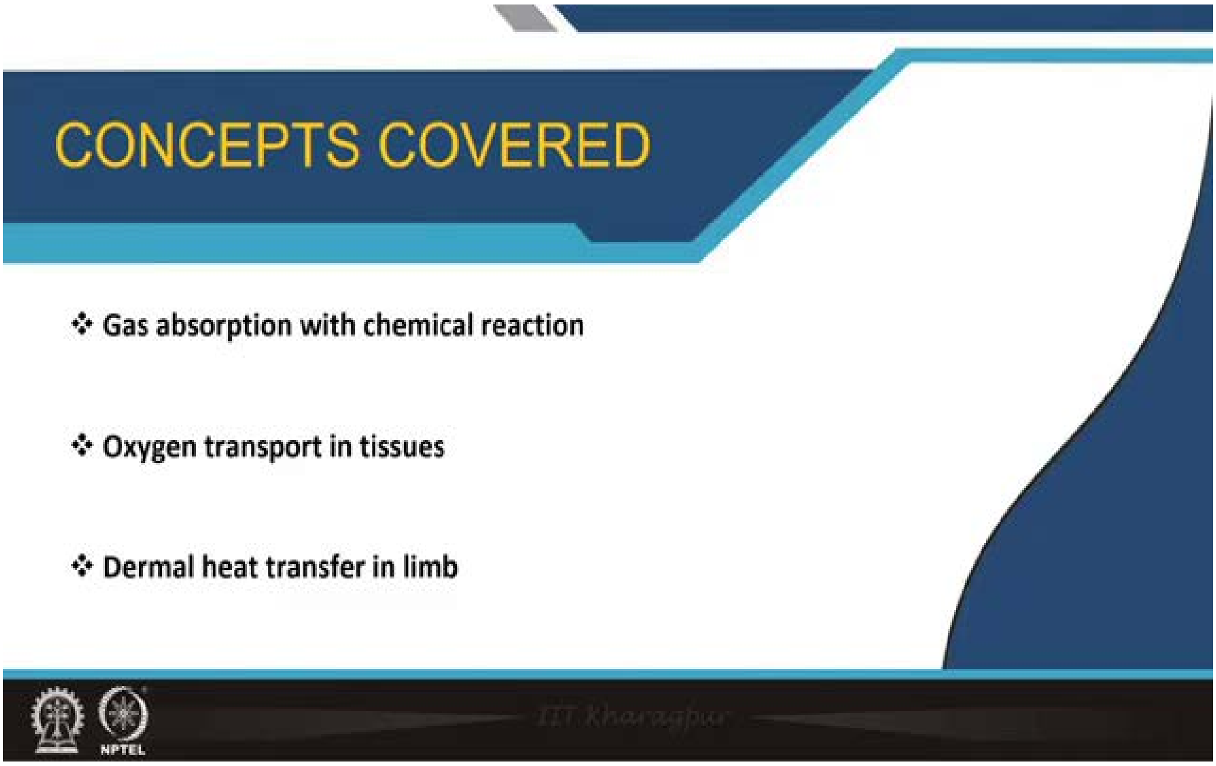

Together with this we are also going to study some more, are trying to model some more physical situations related to mass transfer port, let us say the this oxygen transport in tissues as well as heat transfer in a lump which are very relevant physiological problems. So, first let us talk about the scenario when we have chemical reaction along with absorption.

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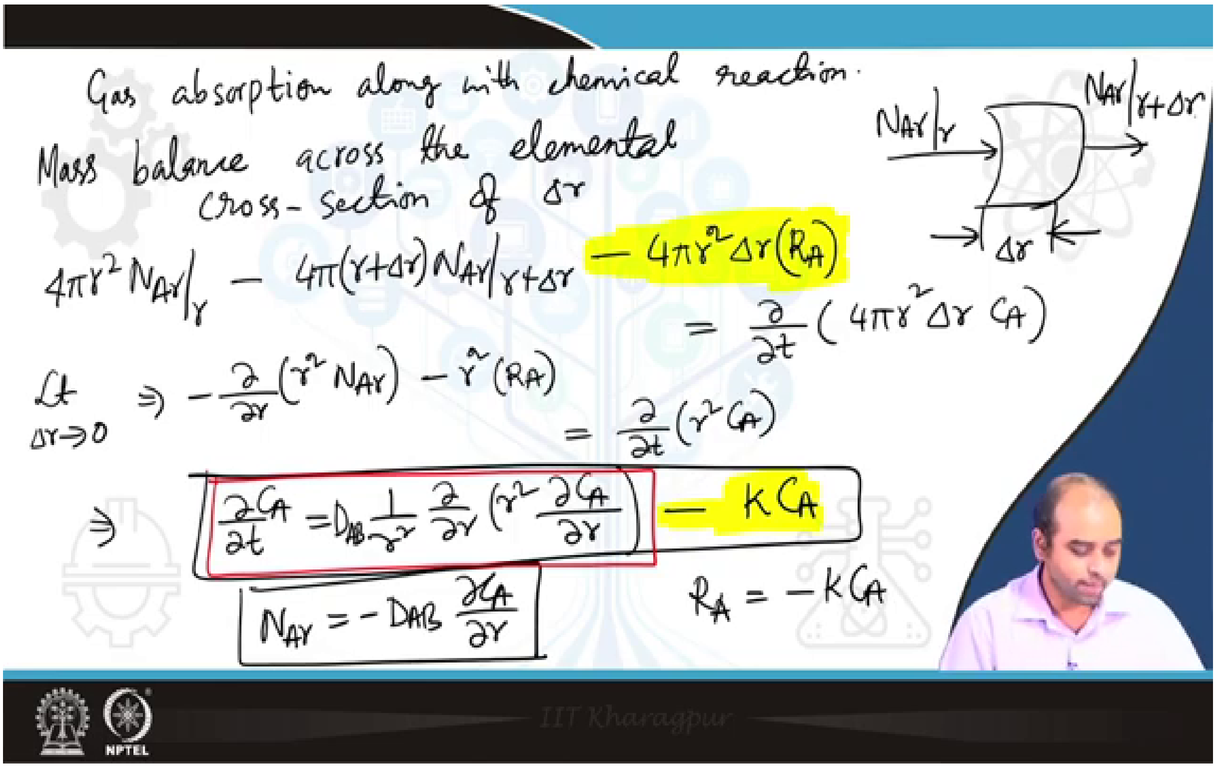

So, in the same context from where we left off in the last class that you have a spherical droplet and the mass transfer takes place by diffusion it is a gas or a liquid droplet dispersed in a liquid or a gas. So, let us try to write this balance equation for the case when we have absorption along with reaction, along with chemical reaction.

So, it is the same kind of a small elemental section we are considering, flux is N Ar since we are considering only the situation in the radial direction, so we assume theta and phi symmetries, the rest of the assumptions that we talked about in the last lecture also holds true. Like for example, isothermal state then diffusivity is constant, the shape is also constant, size is also constant. I mean these are the properties that will stay constant and they form the list of assumptions in this problem, except for the case that there is no chemical reaction, we include it now, so we relax that one more assumption to this problem.

So, let us have a mass balance, so if you try to do a mass balance across this elemental section of delta r and elemental cross section of delta r. So, we write down this is the inlet flux, so it is mass conservation, then we have the outlet flux, then we have the term due to disappearance or the conservation, sorry consumption or generation due to chemical reaction.

So, in this case we are considering the chemical reaction is consuming the species that is a product A, and then on the right hand side we have the accumulation term which is same like the previous one. So, except for this, except for the term related to the chemical reaction, rest of the terms remains the same as to the previous problem.

So, if you try to write down, I mean taking the limit, taking the limit of delta r tending to 0 will be having minus d dr of, de del r minus r square, reaction term and is equal to del del t of r square C A. So, this is what we get. So, till this part it was the same because we considered that N Ar is equal to minus, sorry, minus D AB del C del r. So, this was the ficks law of diffusion.

And we consider here to be a first order chemical reaction, so this RA is written down as minus k CA, so this is the equation that we are getting here. So, let me write D AB on the right hand side so not to confuse you. So, this is the equation we are getting. So, the entire equation is same except this additional term that we get in this case is here.

So, now there we will use, so to solve this problem we can understand that we cannot solve it by separation of variables because in the right hand side now we have an additional term, of course, the equation is not non-linear, it is still linear because of the first order reaction criteria, but it cannot be solved by separation of variables.

Of course, you can try the other methods like Laplace or Fourier transform, but there is something known as the Danckwert's solution. So, the Danckwert's solution tells us that if the solution to this problem, this problem with the chemical reaction unsteady gas absorption with chemical reaction can be found out if we have knowledge or if we have the information or the solution of the unsteady gas absorption without reaction, if that is known. So, what essentially it means if we know the solution to this part of the equation, the Danckwert's formula can help us to calculate with this equation with the chemical reaction.

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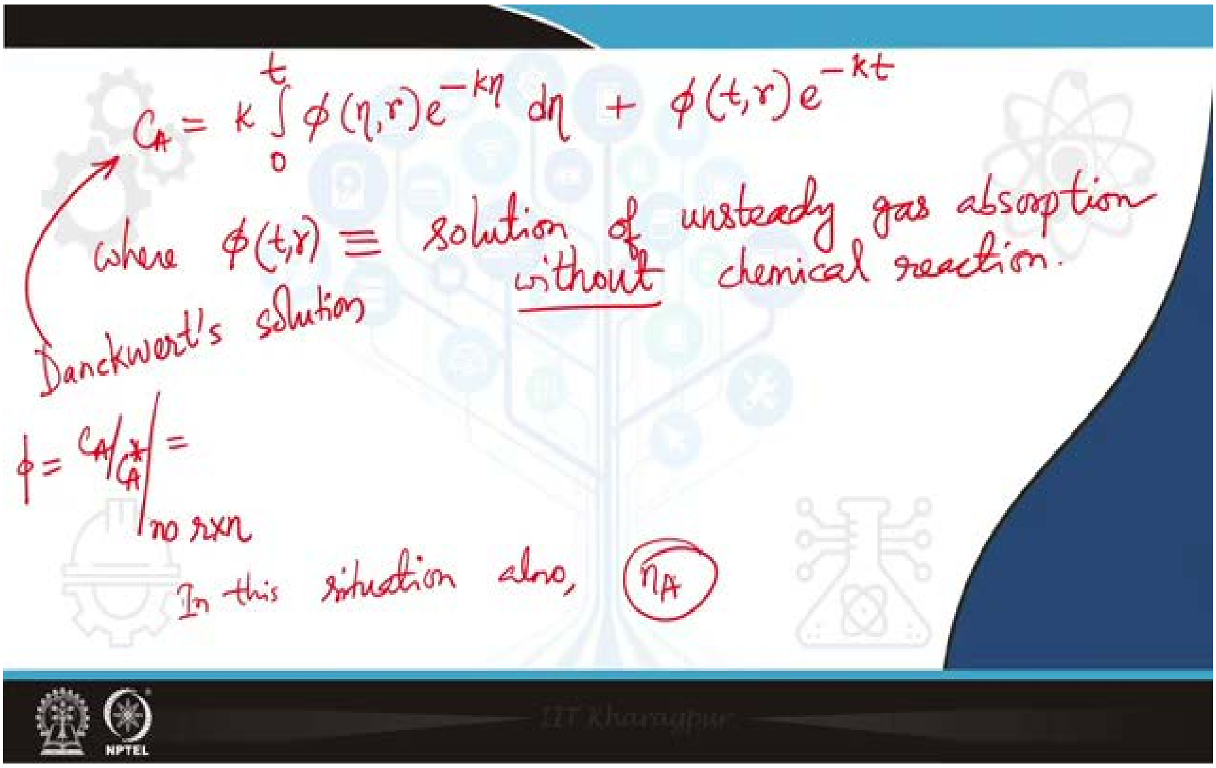

So, let us assume, I mean let us consider that we know the this Danckwert's solution. So, how does it looks like, let me just write you. So, the solution to this case can be written down as this where this phi t comma r is the solution of unsteady gas absorption without chemical reaction and this is something which we have done in the last lecture, we got a detailed solution from the idea of the separation of the variables. So, this is the Danckwert's formula that works in this case.

And of course this is the solution of the phi is something already known to you that CA by CA star, you can, I mean in the case of no reaction is something which is already known to you and I am not going to write it again here. But you can easily calculate it out that what would be the solution.

So, phi, essentially phi is nothing but, so this is phi CA by CA star and this is something we can also, we can, which you can also calculate it out based on the knowledge that this profile of the CA is already known. So, this theta that we have considered already is nothing but CA star minus CA by CA star minus CA naught. So, you know the profile of theta and from there you can easily write it out what is your CA. And you feed this solution here to get the solution for the problem with the chemical reaction.

So, similarly, in this case also you can also, in this situation also you can calculate out what is the net mass transfer rate or the gas absorption rate that is n A, that is also something that can be found out in this case. So, this is something for you to work it out yourself. So, next we move to another problem which is related to the problem on oxygen transport to tissues this is a different problem, again a mass transport problem but in a different context.

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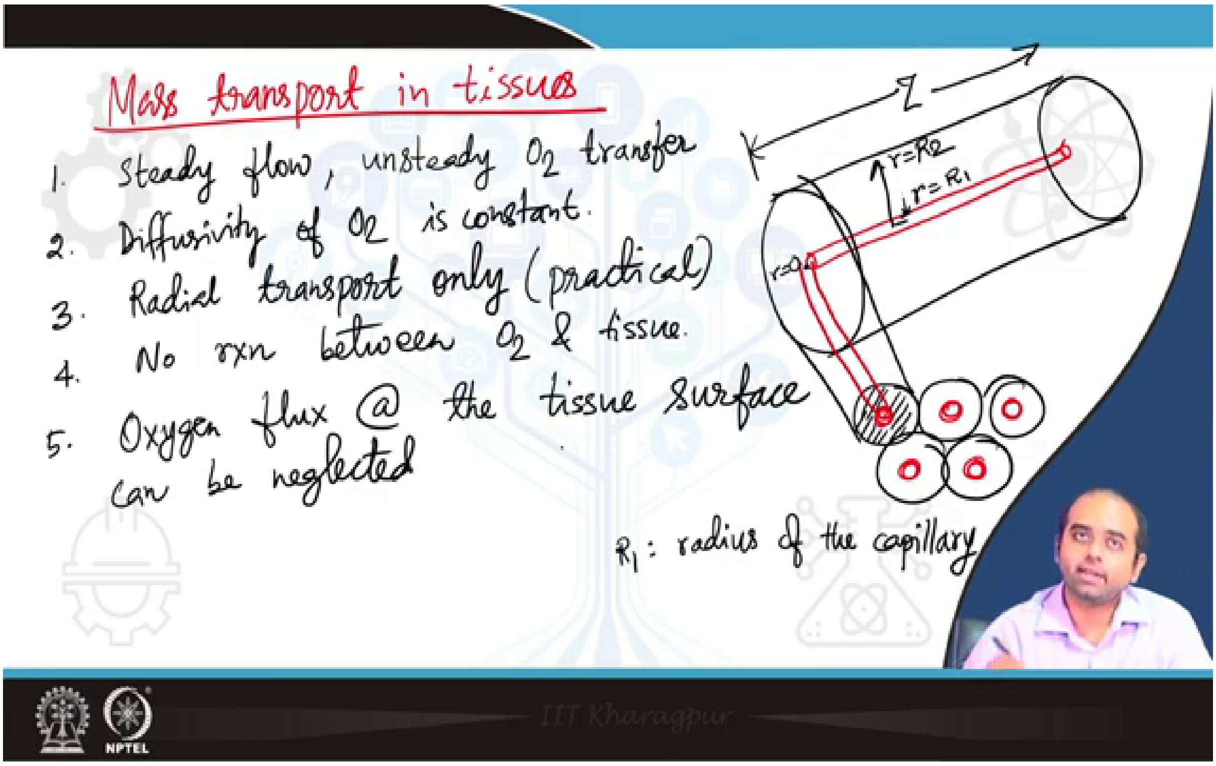

So, mass transport in tissues, tissue means biological tissues that we generally see in the human body or in any physiological in context. So, let us consider a capillary because mass transport the oxygen that is transported to the tissues is generally supplied by the capillaries. So, let us say I have a small capillary like this and surrounding the capillary, I have the tissue. So, this is the capillary where blood is flowing through the capillary and surrounding the capillary I have a tissue.

So, let me draw that by a different color, so you can consider the tissue to be something like this. So, this is a cylindrical region I am considering which encircles the capillary. So, the oxygen which is carried by the capillary transported to its surrounding tissue and you can also think of these, this arrangement of the capillaries and tissues in this way also, let us say these are tissues or tissue regions and I mean you can mark these tissue reasons encircling the small capillary or surrounded by the small capillaries.

So, these are the capillaries which contains or which carries the oxygenated blood which is to be transferred to the neighbouring tissue, so this is the tissue region, so this is the tissue region where the oxygen is getting supplied. So, this diagram I hope I can make some sense to you is trying to give a picture of how does this capillary actually looks like in this case and how the arrangement is there we are trying to consider.

So, we are trying to consider that let us say along a longitudinal length of the tissue how the oxygen is getting transferred radially from this capillary. So, what are the main assumptions in this problem? So, one of the assumptions is that let us consider it is a steady flow, so we take out any transient effects in this problem.

Let us consider, the flow effects are ignored, so we consider that there is no transience as far as the fluid flow is concerned or the blood flowing into these capillaries. But we are considering of course the unsteady nature of the mass transfer. So, unsteady O2 transfer. Next one is of course diffusivity of O2, let us say is constant. Third important thing we are considering or making an assumption here is that the radial transport only which means so the oxygen mole fraction in the tissue is assumed to be a function of time as well as radial coordinate.

So, we are ignoring any axial effects because axially this may be very long, so the diffusion along the axial direction is insignificant compared to the radial diffusion, by the time there is any axial diffusion so this entire central core that the oxygen or this capillary is clearing oxygenated blood the oxygen transfer would be dominated by radial diffusion rather than any lateral diffusion in the tissue.

So, oxygen transport, radial transport or transfer is the most dominant case here and this is also a practical scenario that you do not have any axial or a lateral transport. We do not consider no chemical reaction. So, no reaction between O2 and the tissue. There is also another important assumption that the oxygen flux at the tissue surface, at the tissue surface can be neglected. Why? Because it is the presence, due to the presence of the numerous neighbouring tissue regions which will also have the same amount of oxygen flux.

So, I mean at the surface, so we can consider that the oxygen flux at the periphery or at the surface of the tissue is negligibly small. So, by the time there is any this radially as the oxygen is transferred from the surface oxygen, I mean the oxygen concentration reaches almost minimum at the surface that is how the capillary points in the tissue are actually optimized and the rate of the oxygen transfer is optimized, so that this region of the tissue which is covered I mean the region of the tissue to be oxygenated which is covered by a capillary is almost at its optimum value.

So, that is how the capillary but the diameter, the blood flow in the capillary, everything is optimized such that it can oxygenate or oxygen can be transferred to the I mean, neighbouring tissues or to the tissue which encircles this capillary adequately. So, there is no shortage of oxygen supply to the tissue cells, that is how the capillaries are arranged in the body, that is a nice pattern actually.

So, now if you try to make a balance of the species, I mean the oxygen across an elemental section of delta r in this tissue region, so the centre is of course considered to be r is equal to 0 and then we have r is equal to this capital R2 that is the surface of the tissue and the radius of the capillary can be considered as r is equal to capital R1, so capital R1 is the radius of the capillary. So, we are considering a small elemental section of delta r in this case and let us consider that the length of this tissue region is Z and we are considering a small radial element of delta r.

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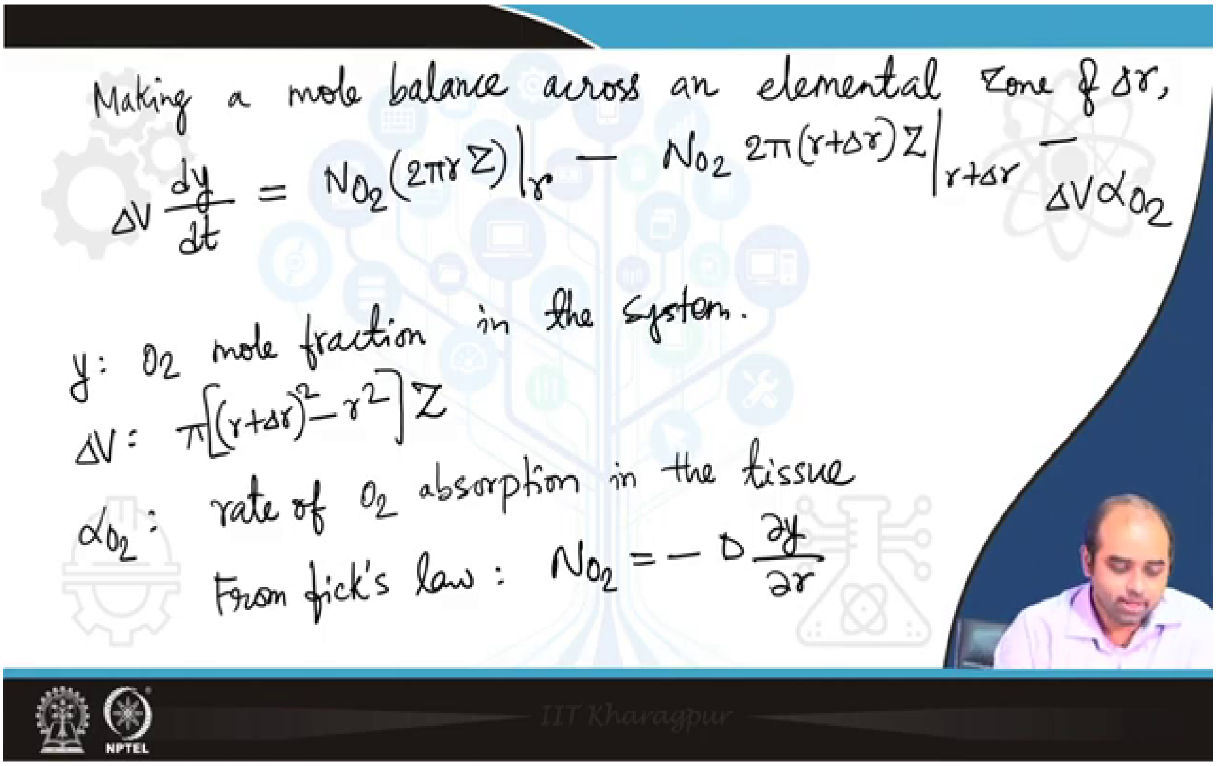

So, making a mole balance across an elemental zone of delta r, we write so this y is the mole fraction of O2, let me write it to you so O2 mole fraction. And delta V is the this elemental volume so which is pi r plus delta r square minus r square Z, of course Z is the length of the capillary that we are considering. This is equal to the flux in O2 2 pi r Z at r minus the flux at r plus delta r, sorry minus delta V alpha O2.

So, of course this alpha O2 means the rate of O2 absorption by the tissue. This to some extent can relate very similar to a chemical reaction because this leads to consumption of the species in the system. And you know that oxygen absorption or oxygen consumption is the tissue is very important, otherwise how the muscles will function or how the tissue will function. So, from Fick's law the you can write that this N O2 and we are only considering radial diffusion as delta r.

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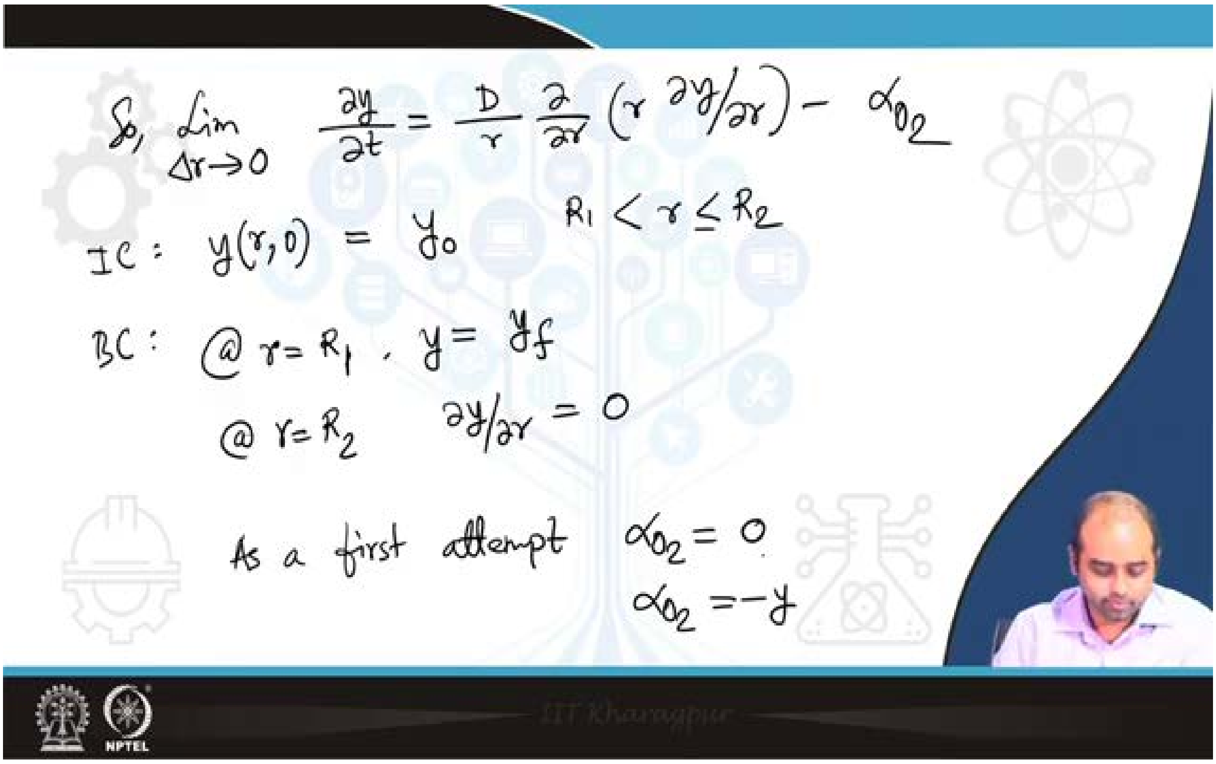

So, for this limit delta r tending to 0 you have dy dt so I can write this D as nothing but diffusivity of oxygen actually. What about the boundary condition? So, the initial condition y r comma 0, t is equal to 0 is let us say this is the initial level of oxygen inside the tissue region, so this of course please note that this r is in between R1 to R2, so it is not from 0 to R2, so it is from the surface of the capillary to the surface of the tissue.

And Boundary condition, so initial condition is actually valid for the initially at all r that is valid at all spatial locations, boundary conditions are valid at all times. So, at r is equal to capital R1 that is the surface of the capillary, let us say this is the feed concentration of O2 and at r is equal to capital R2 we say that del y del r to be equal to 0, so you can consider this to be the far field boundary condition, you can also consider that there is no effective oxygen transfer from the periphery.

So, this is the model formulation, of course, this model in this case looks very similar to the gas absorption problem in spherical coordinates. So, this is also something for the first attempt you can try to be consider as I mean as a first attempt you can try to consider this alpha and there is no absorption in the system, there is no absorption by the tissue, so it becomes a problem which you can easily solve by separation of variables.

Then in the second case you can consider alpha O2 to be something like minus y, just a first order variation with respect to the concentration. So, this will still make the problem linear and you can apply the similar kind of Danckwert's solution to this problem. So, now let us to the next problem of dermal heat transfer.

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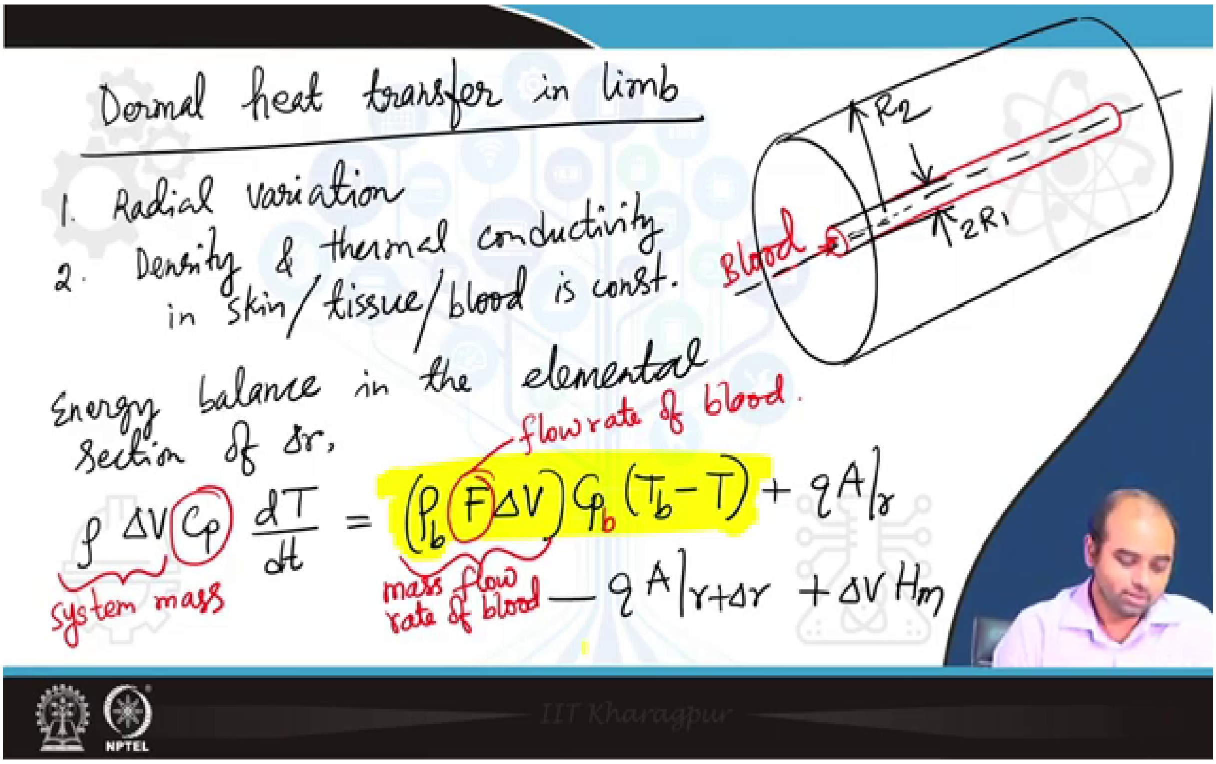

So, let us consider what happens when we try to, when there is heat transfer, so far we have been talking about mass transfer problems, let us consider the heat transfer problem now. Again, we take a similar this physiological context where we have a temperature to be or heat transfer from the capillary or from the blood flow to the neighbouring tissue or to the neighbouring bones or to the neighbouring skin region.

So, the problem setup is more or less the same and this is also relevant physiological problem that you have this sort of the capillary which is carrying your blood. So, let us say blood is flowing through the capillary and it is surrounded by a region of you can consider this to be a region of tissue, skin layer, whatever.

So, heat is getting transferred by this capillary, of course, there is no mass transfer in this problem. So, it is the heat supplied by this blood which is getting conducted into the neighbouring tissue zone. Again, in this problem we consider only the radial variation so assumption is like the radial variation of the temperature because any diffusion, any conduction in the axial direction is too slow and by the time the axial conduction takes into effect the radial heat transfer from the blood will dominate the heat transfer.

So, there is radial heat transfer and we also consider that the density thermal conductivity, density thermal conductivity does not change or they remain constant in the skin as well or are the tissue region as well as in the blood region. In the skin or the tissue is constant, of course, skin, tissue, blood is constant.

So, let us try to write the energy balance across a small elemental section of delta r in this tissue region. So, please note that the surface or the capillary radius is R1 and consider that the radius of the tissue region is R2. So, if I take a elemental cross section of r, so I can write the energy balance or the enthalpy balance, energy balance in the elemental section of delta r or delta V.

So, that is rho del V Cp dT is equal to rho b F delta V Cp, there is actually a lot of terms here. So, this delta V is the volume of the elemental section. So, rho delta V gives you the, so this rho delta V gives you the system mass, this F is the flow rate of the blood, so this is the mass flow rate of blood and this is the specific heat capacity of blood and this is the specific heat capacity of the tissue.

So, this portion on the right hand side the first term on the right hand, this first term on the right hand side is the this term on the right hand side represent the heat transfer or the heat that is supplied by the blood, because the blood is at higher temperature so this is the heat supplied by the blood into this system. And the next part is qA r and r plus d r, this represents the conductive heat transfer and the last part del V Hm represents any if there is any metabolic heat generation.

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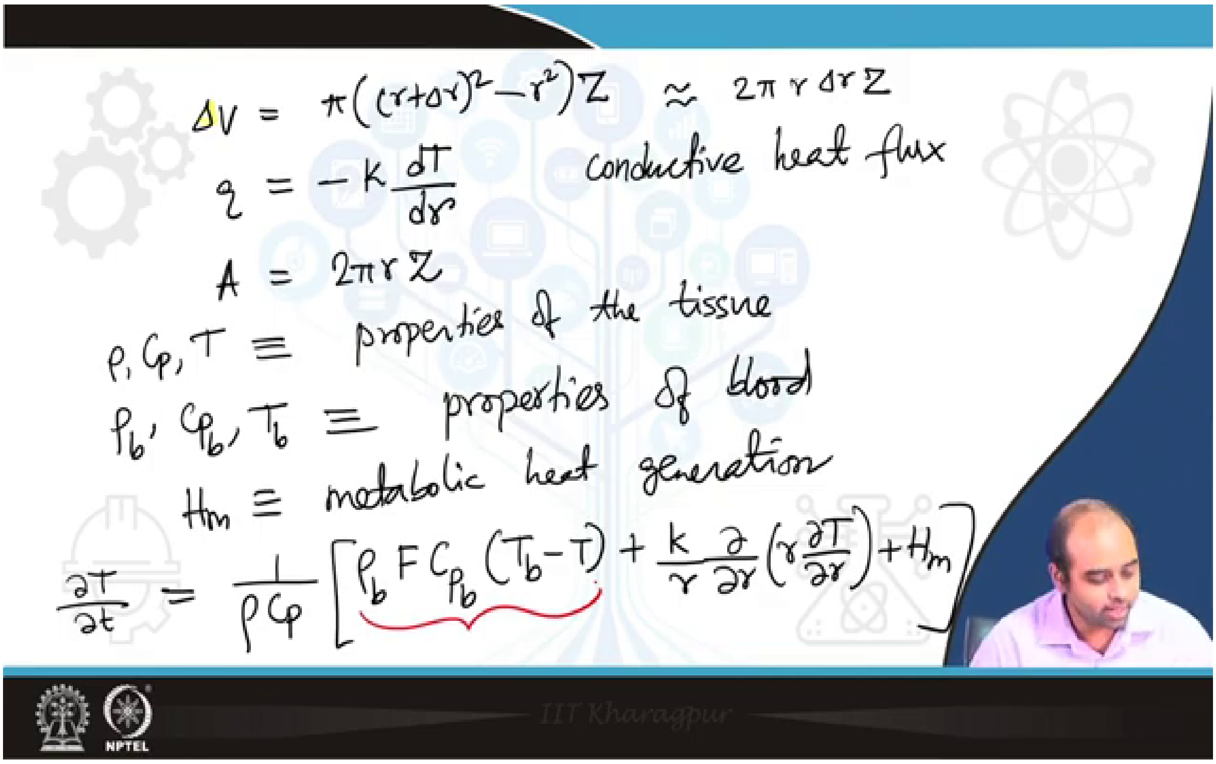

So, here this here delta V is pi r plus delta r so that is the elemental volume multiply with Z, so this is approximately 2 pi r delta r delta Z. q is the from the Fourier law of heat conduction we know that minus K dT dr and only this radial direction heat transfer is considered, so conductive heat flux.

And this area is the area of the elemental cross section is a cylindrical surface area at r. So, rho, Cp, temperature T are the properties of the tissue which is the system here and into which we are considering the heat transfer, these are the properties of blood and H m as I have said is could be some metabolic heat generation. So, what we get?

So, taking the limit of delta r tending to 0 and further simplification the delta r square and all those things will be equal to 0. We get the equation as like this, so this is the part, this is the part which is the heat supplied by the blood to the tissue region and this is a one dimensional parabolic PDE which is a linear PDE again but it is non homogeneous. So, anyway you will try to find out a technique to make it homogeneous and then possibly you can use one of the linear PDE solution techniques. Now, quickly learn about the boundary and the initial conditions.

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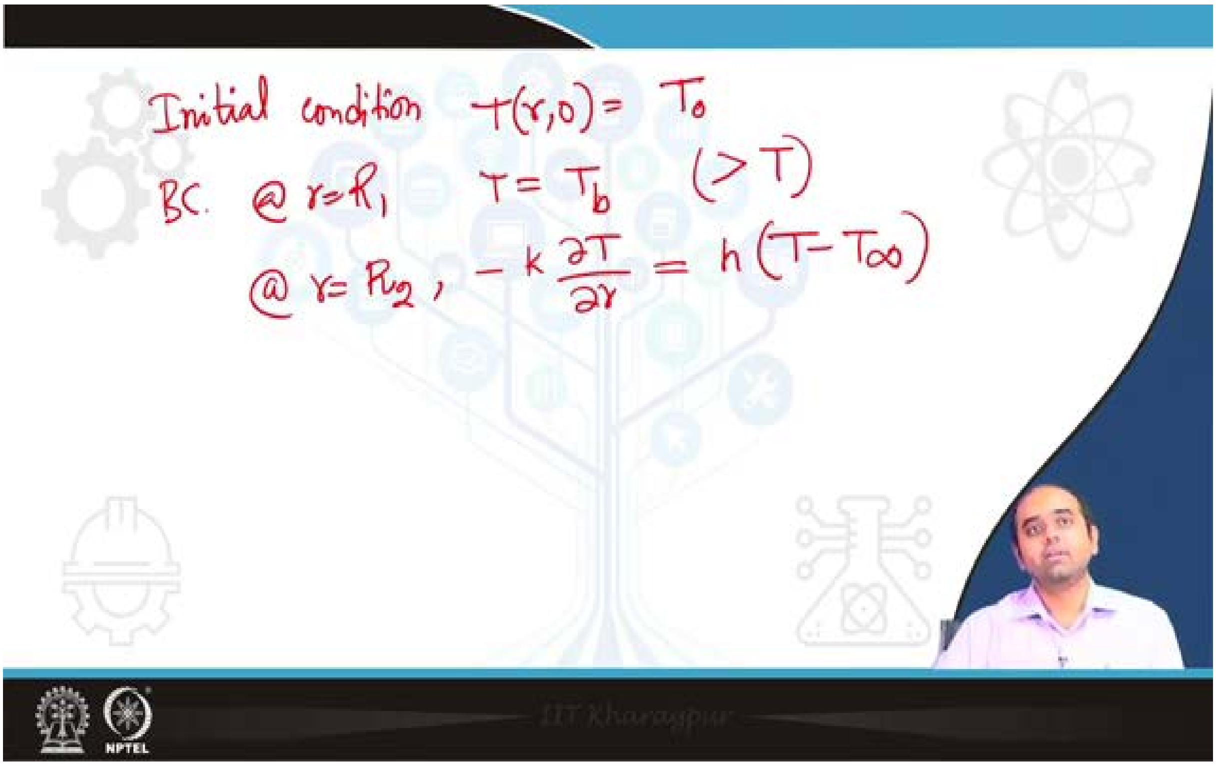

So, the initial condition T r, 0 let us say it has some certain temperature T0 and the boundary condition that r is equal to capital R1 let us say the temperature of course is having a temperature of Tc and Tc is of course higher than T always in the system. And at r is equal to capital R2 that is the surface of the tissue you can say that minus K del T del r the convective, conductive heat flux is equal to the heat flux with respect, I mean the convective heat flux with respect to the surroundings.

Sorry, this is not Tc, this is Tb that is the temperature of the blood and of course the temperature of the blood has to be higher than tissue temperature for the positive heat transfer. So, alternative boundary condition could be like at r is equal to 0 you can have the symmetry boundary condition but we are not interested at r is going to 0 that solution domain is from R1 to R2 and at the boundary please note that we are having a mixed boundary type condition where the conductive flux is equated to the convective flux from the surface to the neighbouring ambient region.

So, of course, you can try, I mean this is the, I mean in this part of the, and this week we are mostly focusing on trying to formulate the model or the model equations for different systems involving different types of transport phenomena processes. We have extensively covered the different solution techniques of mathematical equations of different levels of complexity, so we are not going to work more on the solution schemes for these type of partial differential equations. Okay. So, I hope all of you have liked the lecture today and we will see you again in the next class. Thank you.