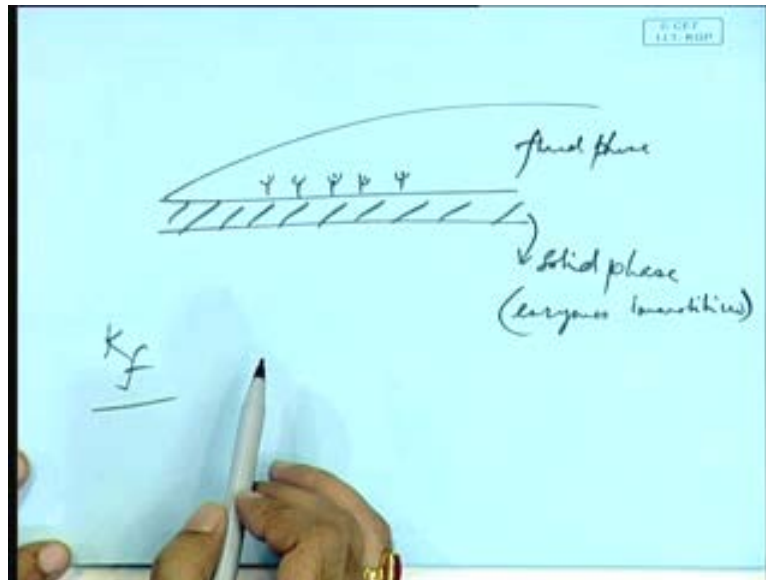


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**Lecture No. # 15**  
**Interphase Mass Transfer and Reaction in Immobilized Enzymes**

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So, in today's lecture in biochemical engineering we are going to continue looking at the immobilized enzymes. We will start from where we left in the last class, which was the mass transfer coefficient. So, what we were looking at in the last class, if you remember is intraphase mass transfer with reaction. There was a flat plate so, if I am to remind you. So, we had a flat plate like this and there is a boundary layer set and there these enzymes are receptor. You know under the receptors that are on bound to the surface and, because this is fluid phase and this is the solid phase in which the enzymes are immobilized. So, the enzymes are enzymes immobilized.

So, what happens is there is transfer between the fluid and the solid phase and that mass transfer coefficient was referred to as  $k_f$ . Now what we did not or do get the time do it

in the last class look how this  $k_f$  varies. How do you evaluate this  $k_f$  it turns out there lot of empirical relations to evaluate the  $k_f$  of the mass transfer co-efficient. Now what we looked at in the last class was flat plate, but if what if it were in the flat plate what it was circular tube or sphere or any other kind of things.

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**Mass transfer coefficients for laminar flows**

- Flat plate  $\frac{k_{obs}Z}{D_m} = .323 Re^{0.5} Sc^{.333}$
- Circular pipe  $\frac{k_f D}{D_m} = 1.86 Re^{0.5} Sc^{.333}$
- Forced convection around solid spheres:  
 $\frac{k_f D}{D_m} = 2 + 0.6 Re^{0.5} Sc^{.333}$
- Falling film  
 $\frac{k_{obs}Z^{.5}}{D_m} = .69 Re^{0.5} Sc^{.333}$

So, we what I wanted to show you on the screen today are these relations for mass transfer co-efficient these for laminar flows. So, different kind of geometry, first one is flat plate then circular tube then solid spheres and then finally, falling film. So, it is not the first relationship is  $k$ ,  $k$  observed time that is  $k$  observed is mass transfer co-efficient time's  $z$  over  $D_m$   $Z$  being the distance. So, this is the flat plate, depending on where are on the flat plate that goes as Reynolds to the power half and Schmidt number to the power one third.

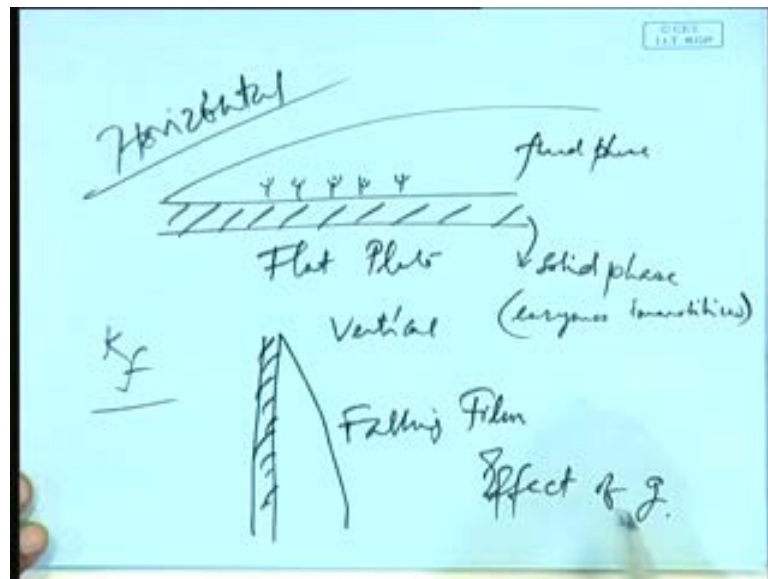
For A circular pipe you it the  $k_f$ , which is the mass transfer co-efficient is given by  $k_f D$  over  $D_m$ ,  $d$  being the diameter of the pipe over  $D_m$ . The molecular diffusivity that again goes as Reynolds to the half and Schmidt to the one third, but the co-efficient is different. So, co-efficient in the last one there is like 0.3 and here it is 1.8 so, it is like 6 times. So, what you see is that one important similarity is that that  $k$  observed  $k Z$  over  $D_m$  or  $k_f D$  over  $D_m$ . Whatever it is Sherwood number actually goes as Reynolds to the half and Schmidt to the one third.

So, how does it look when we have forced convection around solid spheres, this is

something probably. Have you read in the mass transfer classes again it goes as the same it again goes as Reynolds to the half and Schmidt to the one third, but there is little  $(C)$  attached is that there is a constant. Because the shape of the sphere is the constant with that and if you go to the screen, let what you will see the Sherwood number goes as  $2 + 0.6 \text{ Reynolds to the half Schmidt to the third}$ . So, that co-efficient those two co-efficient are there Reynolds to the half and Schmidt to the third, but you have the  $2(C)$ .

Finally, the scene that we want to look at is the falling film. So, the falling film turns out similar, to the flat plate in the sense that if the geometry. Similar also is the flat kind of thing and it goes again as Reynolds to the half and Schmidt to the one third and the co-efficient then the 0.7, which is not to different from 0.3.

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So, it is around twice that of the flat plate so, the difference that you know what would be the difference between the falling film and the flat plate? So, this is for this is if I go to this thing this is the flat plate what would be a falling film line. So, this is again a solid surface and this is how this going this is the falling film. So, what is different over here is the effect of...

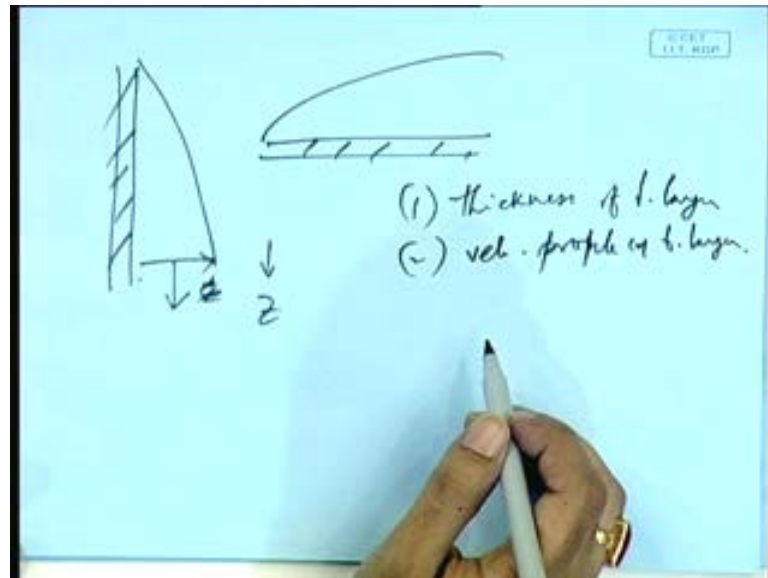
Gravity

Effect of gravity here

$(C)$

So, this is the vertical this is the horizontal. So, the gravity is going to affect the size of the boundary layer and also the velocity profile in the boundary layer, the thickness of the boundary layer and the velocity profile in the boundary layer.

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So, if you have taken a falling film like this and compared it with a flat plate, now the here what is going to happen here? Is that what you have at the bottom this is going to the liquid is going to drag. In this direction liquid is going to drag in this direction. So, as the liquid goes down the  $z$  or in other words as a length goes down, then the size of the boundary layer grows. So, as  $z$  goes high more and more you go down the size of the boundary layer is going to grow. Because it is dragging the fluid is dragging more in the in the vertical direction because of gravity.

So, as a result which in the two things that is different over here is the thickness of the boundary layer and the velocity profile and the boundary layer and therefore, the Sherwood number is slightly different from the flat plate. So, what we are looking at till now are these cases, if you remember all the examples. We did in the last couple of lectures are examples, where the enzyme is on the surface. The enzyme is on the surface and either it through diffusion or it is through convection that mass transfer is taking place.

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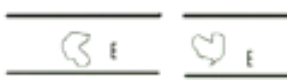
**Transport and reaction to enzyme encapsulated in tissue matrix:  
Intraphase Mass Transfer**

- Chemical reaction:  
Heterogeneous reaction that occurs within a tissue or porous matrix containing immobilized enzymes are called "intraphase" although the reaction occurs at the interphase between fluid and cell surface or at extracellular matrix the phases within the tissues is considered to be "pseudo homogeneous" if the reaction is macroscopically uniform.

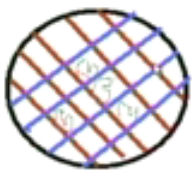
So, that is the whole idea of today's lecture is go the screen is intraphase mass transfer and reaction. So, what is different in this one is that is intraphase. So, let me see if I have picture I do not have picture here. Let see I have picture out here not let me go back and show you some so, I can use this picture.

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**Physical entrapments of enzymes**



Enzymes trapped in hollow fiber membrane



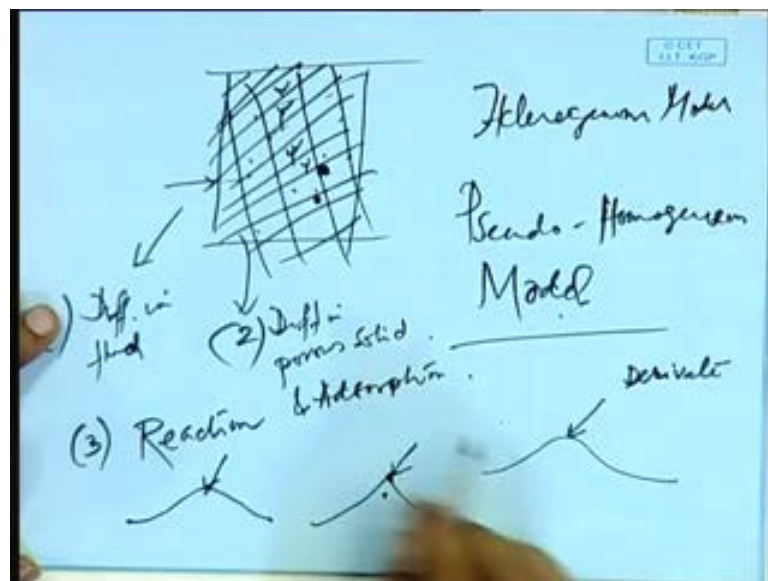
Enzyme entrapment within insoluble gel matrix

So, that is the difference you know. So, if for example, if you have intraphase mass transfer if the enzyme immobilized that is there is entrapment within the encapsulation within the gel of the matrix. Then there is no way for you to make it react with the

substrate without the substrate, actually diffusing into the enzymes. So, that is the different. So, intraphase is within the for phase the mass transfer should happen within the phase, and when you have the intraphase mass transfer? What happens is that the reaction occurs simultaneously. So, that is a major difference, this was an example, we had the only the intraphase mass transfer.

So, the solid (( )) the enzymes are encapsulate or on the surface of the solid and the fluid comes in and reacts. And then intraphase mass transfer then enzymes are on encapsulated within is this difference clear, the physical difference now in addition to this. You can what can you have you can have enzymes, which are on the surface in addition to which being entrap inside you can have enzymes on the surface. Now let us go and look at what the difference is and how to study this kind of models can we make. So, the first important thing that I want to discuss over here, is that the concept of pseudo homogeneous reaction and we did that before. So, if I can you know interact your attention to this.

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So, my enzymes are you know let us say these are my points of where the enzymes are... Now I can go and write homogeneous model for this heterogeneous model for this is something I had discussed, but I still want to go into details and try to see. If you can understand it completely so, if I am to do a heterogeneous modelling of this. What would I do, I would actually let the substrate diffuse to the surface then from the surface diffuse

then why do, I separate these two diffusion that diffusion over here. So, diffusion in fluid and then diffusion in this, because porous solid so, diffusion in the porous of diffusion co-efficient  $(D)$  for going to be different.

You know it could be  $(D)$  diffusion depending on if the porous is very small, if it not it could it would still be different the diffusion co-efficient still going to be different. So, if I am to do a heterogeneous model of this my step 1 is diffusion in fluid, step 2 is diffusion in porous solid then step 3 would be adsorption or you can just go straight to reaction. If you want reaction and adsorption you can say, but what is the challenge? That we face over there the challenge that we have to face over there is that we have to have a geographical. You know map of where these particular enzymes are located within the matrix, if we are to allow. So, because you are doing simulation, if you are doing simulation of the whole thing you need.

So, the material reception is defusing into the whole thing, but for you to figure out that for you to be able to quantify. That you need to know at which point this reacting what are these, because see what happens this within this matrix it become almost like point syncs for the substrate. These of points of reaction become point sync for this substrate and you need geographical, you need a map of where these points syncs out. So, if you want to do heterogeneous model is absolutely not impossible, but it is a little cumbersome in terms of the modelling. And then you have to do the diffusion out of the porous solid and out of the fluid that is not the problem the problem lies here.

So, what we do is we come up with what is known as a pseudo homogeneous model. What is the assumption of such a model? The assumption of pseudo homogeneous model, what is the assumption of pseudo homogeneous model? The assumption is that you homogeneous over the entire matrix. So, you assume that these receptors are present uniformly in the entire matrix. So, what you take? Is you take you figure out that, what is the total number of receptors? What is the reaction rate for each and multiply that and get the total amount of reaction rate for the receptors and then divided by volume together volume average reaction rate.

So, that would be once that is there, then it is assumed that though these reactions are in principal heterogeneous reaction and they are occurring at certain points. You assume that the whole thing occurs uniformly over the entire matrix so, this is the concept of

pseudo homogeneous reaction. Now is there any new concept for you studied this before know so, at least I hope, because we do not want to get over this again and again. Let us go back to what we have on the screen? So, there is a definition exactly what I have explained, but just to go through it the heterogeneous reaction that occurs within a tissue or porous matrix containing immobilized enzymes are called interphase.

Although the reaction occurs at the interphase between the fluid and the cell surface or at the cell extra cellular matrix the phases within the tissues is considered to be pseudo homogeneous. If the reaction is macroscopically uniform so, this is the term that we introduced here macroscopically uniform. What it means that as a microscopic level? It is occurring at different points inside the matrix, but at the microscopic level is uniform and when at the macroscopic level it is uniform. Then you can assume it to be pseudo homogeneous so, it is a matter of scale, if at the scale that you are looking your reaction is homogeneous. Then you can assume it to be pseudo homogeneous if, but as a microscopic scale it could be heterogeneous is the concept of scale.

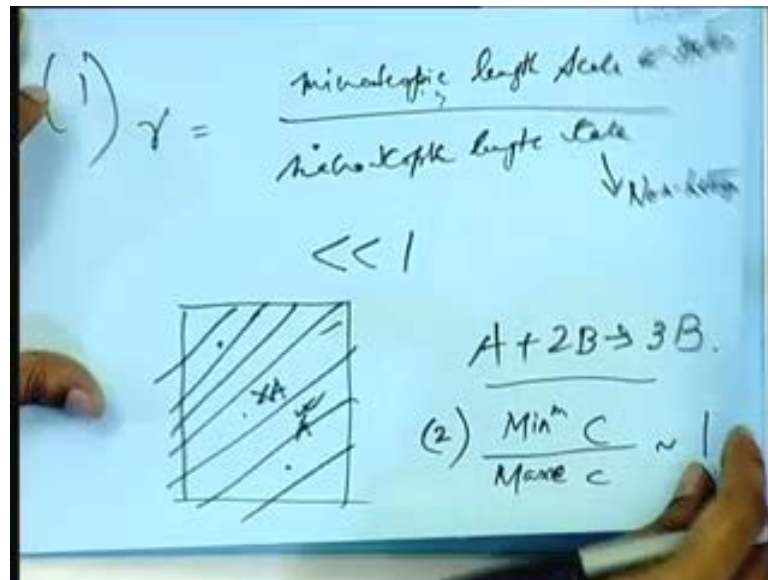
So, at the smallest of scale say for example, you know if you have surface **if you have a surface** like this and you are trying to take the derivative at this point. Which point you take the derivative? You never know or if you have surface like this. We can say that the microscopically at the microscopic scale, we can say that this is the singular point, because you cannot define the derivative here and this is a non-singular point. You can define the derivative here, but that the microscopic scale this is not singular. You see what I am saying, because when you go to the level of at the microscopic level this is no longer as sharp this peak is no longer as sharp.

Because when you go to the microscopic level this is not singular as a microscopic level. You can define the derivative at this point so, that is the matter of scale the manner of looking. So, the same thing happens here at the microscopic level, it is heterogeneous. Because these reaction happens at different point within the matrix, but at the macroscopic level you can average them out the macroscopically uniform, which means that you can average them out and the whole concept of averaging theory. You know the basic concept of averaging theory originate from this, where you can actually decide that. Whether the system is microscopically uniform or macroscopically uniform, that kind of things.



So, it is microscopically uniform, you know there is no question at all, but the whole concept of averaging comes in these certain issues or in these certain cases. Where the system is microscopically non-uniform, but at the macroscopic level, you can decide now what how do you decide, what is microscopic and macroscopic?

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You know that is the question that is important and what typically is done is that the let us call this  $r$ . So, is microscopic length scale versus macroscopic length scale, if this is much smaller than 1. Then you assume this is your criteria, typically you assume that it is microscopically uniform so, the length scale at which you see this heterogeneity. This is the heterogeneity length scale and this is the non-heterogeneity length scale. So, that the length scale you see at which you see heterogeneity over the length scale at which you do not see heterogeneity, the ratio of this two have to be much smaller than 1. So, if this is possible then what you do is you can average it out over the macroscopic length scale as soon as the average it out you gets the pseudo homogeneous model.

So, pseudo homogeneous model is not a matter of just intuition, it is a matter it evolves the out of you know averaging theory. Whether in the macroscopic once you have done the pseudo homogeneous got the pseudo homogeneous model. In the pseudo homogeneous model what happens? This assumption is that reaction and diffusion occurs simultaneously. In the real model in real life diffusion and reaction not occurring simultaneously, in the heterogeneous model diffuse reaction and not occurring

simultaneously remember. So, first diffusion followed by reaction, but in the pseudo homogeneous model diffusion and reaction is assumed to occur parallel.

So, if this is just you know corollary. So, to say if the reaction is too fast as compared to diffusion the concentration at some places becomes 0, because it is diffusion control. This is one of the interesting things that can happen in pseudo homogeneous model, I mean what pseudo homogeneous model cannot capture. So, if you have a system like this and say for example, you have a reaction like an autocatalytic reaction that we discussed in the last class. So, what can happen, because the reaction at some places can, if there is a small perturbation in the system? The reaction in some places could be much higher than the reaction in other places.

So, the concentration in some places the for example, the concentration of the substrate here could be 0 and next you know too far from that place the concentration could be high. So, what will happen in that case what would be the consequence of that there will be major difference, the large difference in concentrations, it could be next to each other depending on the kinetics, if you have kinetics of this type  $A + 2B \rightarrow 3B$ . Then A could be depleted in one place and A could be far from the depletion from another, it could be presented in large amount. So, what will happen in that case that is a real system I am talking about the heterogeneous system.

(C)

I am just talking of catalyst pellet here; you know it cannot be catalyst pellet. So, this is just catalyst pellet catalyst pellet or immobilized enzyme whatever you want to call it. So, what can happen what will happen is that the heterogeneous model is still finding, but you cannot average it anymore? So, there is no point in having an average when one part of that has a very large concentration and another part of that very small concentration, because the average value would not give sense of the distribution. So, when you want to average the criteria number 1 is that the ratio of the smallest through the largest length scale is much lesser than 1.

The criteria number 2 would be that the minimum over maximum concentration minimum C over maximum C should be of the order 1. This should not be a huge difference it could be 0.1 they still order 1, but it could be it cannot be that cannot be 10 to the minus 3 or 10 to the minus 4 within the matrix. So, which means that the variation

within the matrix has to be reasonable they cannot be very large variation. So, having set these things I think now that and it does not make sense to go and write a model. Unless we understand what are the constraints? What are the boundaries between which we writing that model so, having met that...

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• For drugs, biomolecules, therapeutic molecules, if the diffusion is too slow reaction rate could decrease significantly

$$D_{eff} \nabla^2 C = -R_v$$

Macroscopic rxn rate  $\bar{R}_v =$

$$\bar{R}_v = \frac{1}{V} \int R_v dv$$

$$= -\frac{1}{V} \int D_{eff} \nabla^2 C dv$$

$$= -\frac{1}{V} \int D_{eff} n \nabla C ds$$

$$\eta = \frac{\bar{R}_v}{\bar{R}_v(C_s)}$$

Let us we can you know try and write a model of A. So, what we do is these are for drug bio molecules, therapeutic molecules and so on. If the diffusion is slow then reaction rate could decrease significantly the reason is, because this is diffusion and reaction occur parallely, but in real life diffusion decrease reaction. So, if diffusion is very slow then reaction; obviously, would be hamper straightforward. So, what we do is that in the pseudo homogeneous model what we write over here is d effective Laplacian C minus R of v. Do you all remember by the way how to write Laplacian in spherical and cylindrical and all these coordinates, because you know they will be in (( )). So, why D is effective? Because this is not the real diffusion.

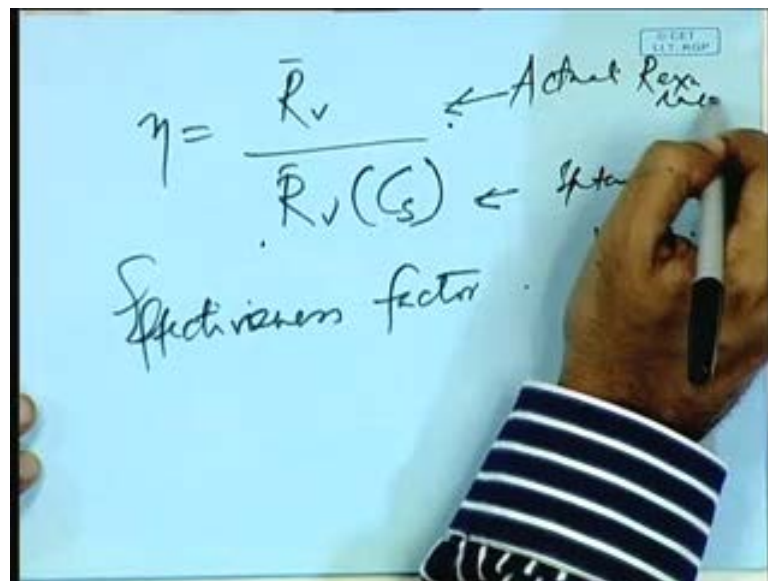
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Because this is not the real diffusion, the real diffusion occurs in the spaces between the porous. So, this is the effective diffusion co-efficient because you taken an average out of the whole thing, if the diffusion co-efficient also an also an average between the diffusion co-efficient of the solids through the solids and the spaces between the solids. So, R of v is let us defining R of R v average as the microscopic reaction rate. So, what

we would be the microscopic reaction rate as I just as I said before the summation of the all the microscopic reaction rates over the volume divided by the volume. So,  $R$  of  $v$  average is the summation of all the microscopic reaction rates divided by the volume fine. So, this is given by  $1$  over  $\int_V$ .

So, this is you know you can replace what you have over here the diffusion reaction problem from here to here and then what you do is you simply use the Stokes here. So, just change the Laplacian to the surface into this straightforward. I think you have done this before changing from the Laplacian to the surface integral. So, when you do that then this is all fine. So, you can write here  $R$  average in this way so, the advantage with this writing is that you just need to changing from the surface from the volume to the surface is that you just need to evaluate. What is going on to the surface? You really do not need to care about, what is going on in the volume?

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So, then we define this quantity  $\eta$  is my effectiveness factor and I think we did effectiveness factor in the lecture 1 of the lecture before also couple of lectures back know. So, this is something that we are going to do for the next couple of lectures. So, let us try and see what the effectiveness factor is essentially the reaction rate. When the reaction is occurring over the entire region over the reaction rate. If it were only occurring at the surface concentration or only occurring at the surface, if the entire concentration in other word if I am to explain little better. If the entire concentration if

the entire amount of material, where is the surface concentration.

So, that is my denominator entire material and  $C_s$  surface concentration over the actual reaction rate. That happens and this actual reaction rate you can obtain as I showed here on the screen, you see actual reaction rate you can obtain as the volume average fine. So, why is this important, because see for a material once you have evaluated. What is your effective reaction rate? If you want to know your actual reaction rate all you need to do is evaluate the actual rate at the surface and effectiveness and this is essentially effect on factor. This is very important thing that you know some of you are taking the advance reaction engineering course are you any of you.

(C)

Not taken. So, then you will study these things you know effectiveness factor. The effectiveness factor essentially measures that if reaction is occurring at if reaction were occurring at the surface concentration and if the actual rate of the reaction. The ratio between these two I am going to see how to how to incorporate that in the next few cases so, this is not important.

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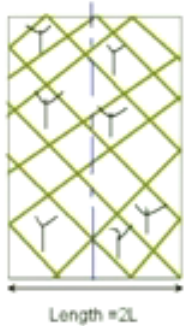
Intraphase Mass Transfer and Reaction in  
Tissue gel matrix (Rectangular Slab)

$$-R_v = k_v C$$

$$D_{\text{eff}} \nabla^2 C = k_v C$$

B.C.1:  $x = \pm L, C = k_m C_0$

B.C.2:  $x = 0, \frac{dC}{dx} = 0$



So, what we do now is now let us go and actually does A solve the problem. So, the first problem we look at the intraphase mass transfer and the reaction in a rectangular slab. We will look at the sphere and the rectangle. So, first thing we will look at today is this

problem in the rectangular slab. So, what is my what is my basic governing equation for the rectangular slab what is my governing equation for the rectangular slab in this case intraphase mass transfer? And reaction this you know there in the title if you look at here intraphase mass transfer and reaction in the rectangular slab. So, these are interrupt these receptors are interrupting inside. So, what would be my governing equation? So, what the basic phenomena let us talk about it for.

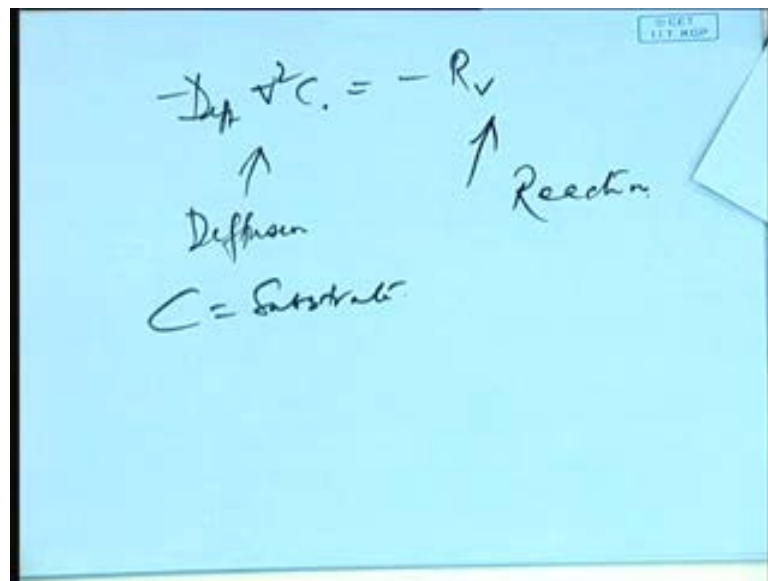
So, essentially the basic phenomenon is heterogeneous reaction, but we are going to use pseudo homogeneous model. So, let us make that clear first that we are essentially it is heterogeneous phenomena heterogeneous system, but we are going to use pseudo homogeneous model what is the basic assumption of pseudo homogeneous model? If reaction is uniform everywhere and you can use an average reaction rate A B is that, because use the average reaction rate diffusion and reaction occurs parallelly. So, what would be my model?

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So,

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$$-D_{eff} \nabla^2 C = -R_v$$

↑ Diffusion                      ↑ Reaction

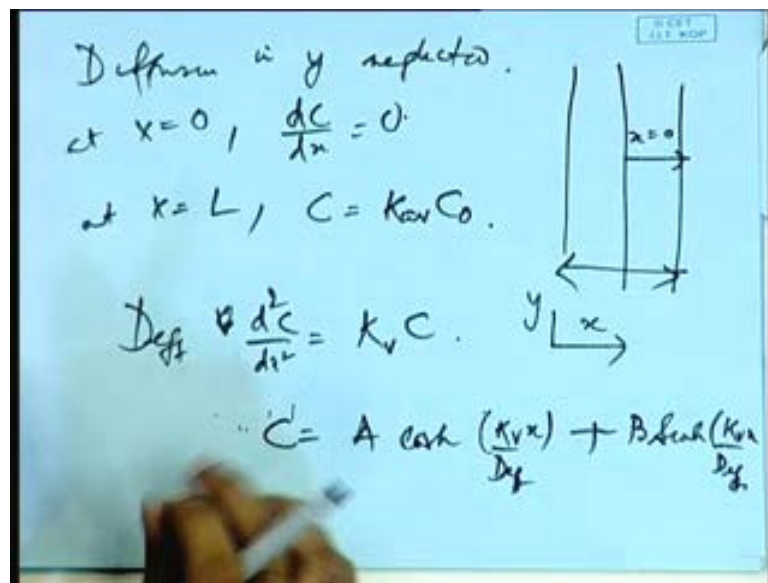
$C = \text{Substrate}$

So, minus the effective Laplacian of C should be equal to minus R of v. So, this is my diffusion reaction because this has been you know C is a substrate. So, C is a substrate

concentration. So, this reaction is A sync term, because it being consumed fine. So, this is my basic equation the reaction rate is here given as  $k_v$  times  $c$ . So, the Laplacian the effective transverse Laplacian of  $C$  equal  $k_v$  times  $C$ . Now, what would be my boundary conditions? Let us talk about that there is several possibilities with boundary conditions, but let us you know talk about boundary conditions. So, what are my two boundaries one would be at the centre, because we are going to this is the symmetric we have to assume.

So, depends on how what we assume, if we assume Laplacian to be A symmetric Laplacian means in the case what would do you have let us you know in think you do not really remember all the Laplacian things. So, this is the no this is the rectangular slab. So, there is not you know not too much of question still there is, but if it were cylindrical then there is A question of symmetric.

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Now what we assume over here, let us put this assumption very clearly, if this is my rectangular slab and I am going to consider diffusion in this region in this direction. Which is  $x$  and diffusion in the  $y$  direction is neglected why, because it is assumed to be too long fine. So, diffusion is neglected now if I am doing it, because of symmetry my condition at this my  $x$  equal says this  $x$  equal to 0. So, at I think that is my  $x$  equal to 0 my fine, now what will be the other condition?

(C)

Is equal to L what there several possibilities with this. So, you have to just pick one the let us talk about the simplest. Now we will do the little more complicated one in the next class.

(( ))

Continuity: is the simplest form. So, there could have A robin boundary condition, which is flux type flux with concentration or you can have simple continuity. So, let us assume the simple one which is continuity at this point I think this would be  $k v C_{naught}$ . So, what is  $k v$ ? So, this is my  $x$  equal plus minus  $1 x$  is dimensionless by the way here. So, how make dimensionless just by dividing by  $l$ . So,  $k C$  equals  $k A v$  times  $C_{naught}$  and rather boundary condition is the centre  $x$  equal to  $0 \Delta C \Delta x$  equal to  $0$  fine. So, can we go ahead and solve this why not you do that. So, what would be max Laplacian simply  $D$  effective time  $\Delta^2 C \Delta x^2$  equals  $k v C$ . So, again you know we are going to assume these two different limits of it  $1$  is the zeroth order and one of the first order like we had been doing all through.

So, the zeroth order is very easy why, because it is simply came  $k v$  and you can just go and straight integrate it. And then what the solution you know you have done the something time. So, the first order what is the solution of this?

(( ))

First order of this what is the solution of this?

(( ))

Problem

(( ))

No, look carefully first is you have to see what is physically meaning full  $A \sin x$  and  $B \cos$ .

(( )) into power minus...

$A \sin x B \cos x$  what is the problem with that you know one of them I dropped out. You will have **you will have** A sinusoidal wave of concentration inside the matrix is that



physically meaningful. So, whenever you write solution the thing it will figure out whether it is physically meaningful or not and that is not physically meaningful. So, the physically meaningful solution would be exponential and you, because you forgotten how to do these things which is A strange thing that you know. So, essential when you have a positive on this side you will have an exponential. If you have a negative out there then only you can have that and that is not possible, because you know that that is not possible out here.

So, the solution would be simple A cos hyperbolic, I think what is going to I am going to do this little differently later that is do dimensionless and all the stuff, but just to give you A sense. I think  $k_v$  over  $D$  effective I think why cosine hyperbolic  $x$  and sin hyperbolic  $x$  just from the plus  $x$  and minus  $x$  I get this. So, what we are going to do now is use a dimensionless form of this we can go ahead and solve this, but the advantage of making the system. Dimensionless is that you can just scale all the variables as you want and you will see that it is very easy to work with the dimensionless system.

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**Non dimensionalisation of Model Equation**

$$\phi = \frac{k_v L^2}{D_{eff} t_R} = \frac{t_D}{t_R} \qquad \bar{x} = \frac{x}{L}, \theta = \frac{C}{k_s C_0}$$

Dimensionless model

$$\frac{d^2 \theta}{d\bar{x}^2} = \phi^2 \theta$$

So, what we do is make it make the system non-dimensional and what will happen is, when we make the system non-dimensional it will come up with numbers dimensionless numbers. Which ratios of important time scales in system and that is one of the added advantages of making the system dimensionless, it comes out naturally and these are very important number. So, the first number we will get is in this case is A Thiele

modulus and I have already taught discussed A Thiele modulus. In the last class if I remember which the ratio of diffusion time is over reaction time and why is this important here, because these are the two dominant phenomena in the system diffusion and reaction.

So, it is very important to have the sense of the numbers ratios of these numbers why that important to have a sense, because if Thiele modulus is given as ratio of diffusion time to reaction time and Thiele modulus is very large. That means that diffusion is...

(( ))

If (( ))

Limiting

Limiting. So, that is something that you know we need to figure out here so, why do not you do it on your own little bit. So, let we all help you out now out with this.

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Handwritten mathematical derivation on a blue background:

$$\hat{x} = \frac{x}{L} \quad , \quad \theta = \frac{C}{K_v C_0}$$

$$D_{eff} \frac{d^2 C}{dx^2} = K_v C$$

$$\frac{D_{eff} L^2}{L^2} \frac{d^2 \theta}{dx^2} = K_v \theta$$

$$\frac{d^2 \theta}{dx^2} = \frac{K_v L^2}{D_{eff}} \theta = \phi^2 \theta$$

$$= \frac{L^2 / D_{eff}}{V / K_v} \theta = \frac{t_D}{t_R} \theta$$

So, say x that because we need to do this unless and otherwise (( )). So, this is all we need to go here so, D effective times Del 2 C Del x square equals k v into C. So, x is this is how define x. So, you get the d effective L square Del 2 theta Del x hat square equals k v into theta. So, k v

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(( )) So,  $k_v L^2$  over  $D_{eff}$  time's theta, now this is this could be written as  $L^2$  over  $D_{eff}$  divided by  $1$  over  $k_v$  time's theta. So, this is  $\phi^2$  over theta. So, this is term  $L^2$  over  $D_{eff}$  is the  $t_D$  transverse diffusion and this is the transverse reaction time so, you get theta  $\phi^2$ . So, this is your basic equation  $\Delta^2 \theta = \phi^2 \theta$  and that  $\phi^2$  is  $k_v L^2$  over  $D_{eff}$  and that is the ratio of the transverse diffusion time of reaction time.

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**Non dimensionalisation of Model Equation**

$$\phi^2 = \frac{k_v L^2}{D_{eff}} = \frac{t_D}{t_R}$$
$$\hat{x} = \frac{x}{L}, \theta = \frac{C}{k_s C_0}$$

Dimensionless model

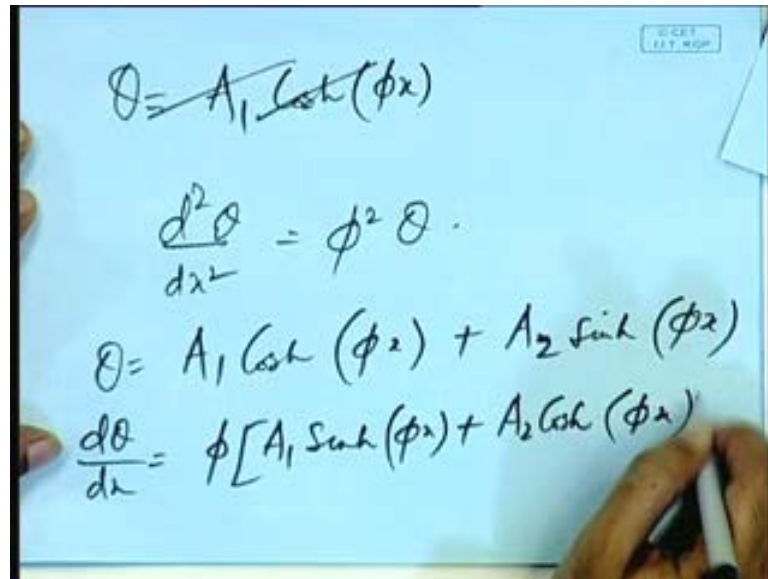
$$\frac{d^2 \theta}{d\hat{x}^2} = \phi^2 \theta$$

Solution

$$\theta = Ae^{\phi \hat{x}} + Be^{-\phi \hat{x}}$$
$$\theta = A(c^{\phi \hat{x}} + c^{-\phi \hat{x}})$$
$$= 2A \cosh(\phi \hat{x})$$
$$\hat{x} = \pm 1, \theta = 1$$
$$\hat{x} = 0, \frac{d\theta}{d\hat{x}} = 0$$
$$A = \frac{1}{2 \cosh(\phi)}$$

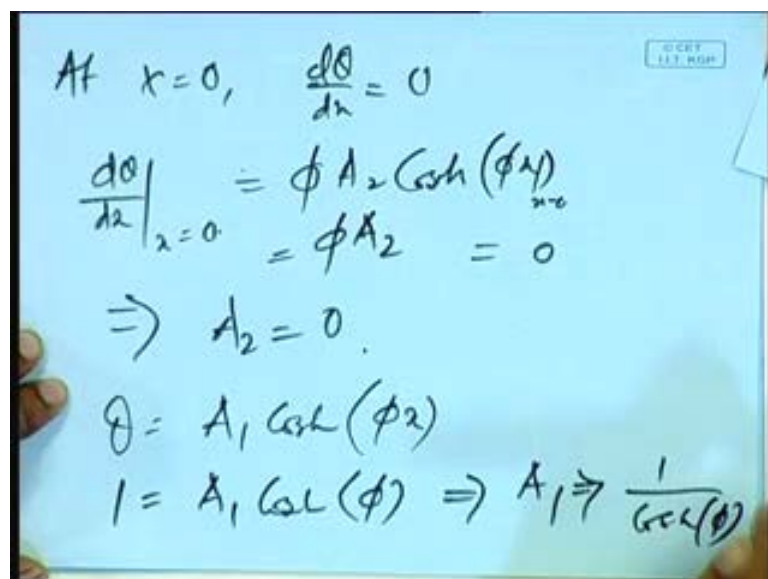
So, this is my dimensionless model and my dimensionless boundary conditions are very straightforward. So, at  $x$  equals plus minus 1 you get theta equals 1 and  $x$  equals 0  $\Delta \theta = 0$ . This is very straightforward and solution is also something I had discussed. So, this is the solution, but you should write it as so, but I know I think it is always best to write it as  $A \cosh$  and  $A \sinh$ , because it is much easier.

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$$\theta = A_1 \cosh(\phi x)$$
$$\frac{d^2 \theta}{dx^2} = \phi^2 \theta$$
$$\theta = A_1 \cosh(\phi x) + A_2 \sinh(\phi x)$$
$$\frac{d\theta}{dx} = \phi [A_1 \sinh(\phi x) + A_2 \cosh(\phi x)]$$

So, if you write theta as say A 1 cosine hyperbolic phi x, because if you look at your reaction equation over here it is Del 2 theta. So, equation over here is Del 2 theta Del x square equals phi square times theta. So, the solution is theta equals A 1 cosine hyperbolic phi x plus A 2 sin hyperbolic phi x. So, Del theta Del x equals phi times A 1 sin hyperbolic phi x plus A 2 cosine hyperbolic phi x.

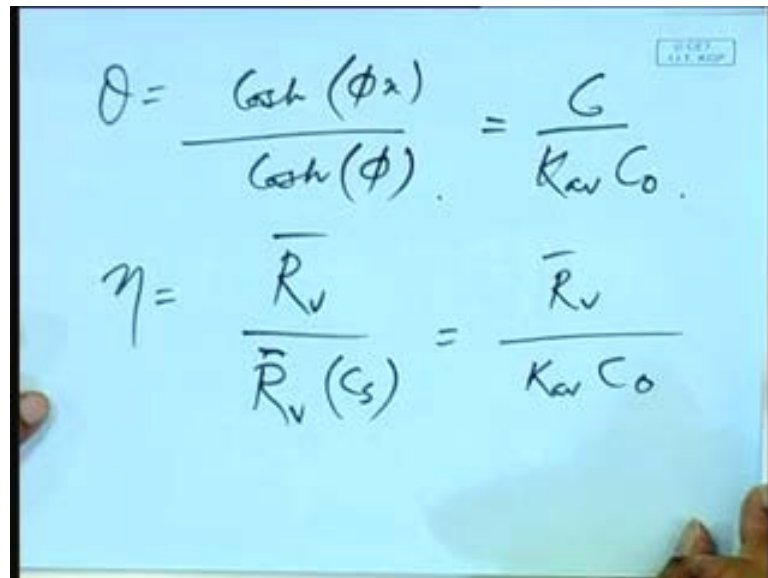
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$$\text{At } x=0, \frac{d\theta}{dx} = 0$$
$$\left. \frac{d\theta}{dx} \right|_{x=0} = \phi A_2 \cosh(\phi x)_{x=0} = \phi A_2 = 0$$
$$\Rightarrow A_2 = 0$$
$$\theta = A_1 \cosh(\phi x)$$
$$1 = A_1 \cosh(\phi) \Rightarrow A_1 = \frac{1}{\cosh(\phi)}$$

So, next step is that at X equal to 0 Del theta Del x equal to zero. So, Del theta Del x at x equals to 0 turns out to be phi times A 2 cosine hyperbolic phi x equals phi times x

equals  $0 \phi$  times  $A^2$  which is  $0$  which implies that  $A^2$  equals  $0$ . So, what you get is  $\theta$  equals  $A^1 \cosh \phi$  x now your other boundary condition is that  $x$  equals plus minus  $1$   $\theta$  equals one. So, equals  $A^1 \cosh \phi$  x. So, with my  $A^1$  becomes  $1$  over  $\cosh \phi$ .

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$$\theta = \frac{\cosh(\phi_2)}{\cosh(\phi)} = \frac{G}{k_a v C_0}$$

$$\eta = \frac{\bar{R}_v}{\bar{R}_v(C_s)} = \frac{\bar{R}_v}{k_a v C_0}$$

So, my solution is  $\theta$  equals  $\cosh \phi$  x divided by  $\cosh \phi$ . So, this is what I have which is which equals  $C$  over  $k_a v C_0$ . Now, what we intend to do now what we intend to do is find my effectiveness factor  $\eta$ . So,  $\eta$  if you remember was defined as  $R$  of the average over  $R$  of the average  $R$  of  $v$  evaluates with this  $C_s$ . So, my  $C_s$  is  $x$  at  $x$  equals  $1$ ,  $C_s$  is defined as  $x$  equals  $1$  which is given as  $k_a v C_0$ . So, the denominator is known only you have to do is evaluate the numerator  $k_a v C_0$  clear. So, how do you evaluate the numerator?

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$$\begin{aligned} -\bar{R}_v &= \frac{1}{V} \int R_v dV \\ &= \frac{1}{V} \int kC dV \\ &= \frac{1}{V} \int k k_{av} C_0 \theta dV \\ &= \frac{1}{2L} \int_{-L}^L k k_{av} C_0 \theta dx \\ &= \frac{1}{L} \int_0^L k k_{av} C_0 \theta dx \end{aligned}$$

I think you can use that, but I think one of the other ways that is also you can do you can, because we got the theta. You can just evaluate the surface and do that and another option is what I have on the screen over here just use this straight away calculation of eta this one. So, because you know what is the volume of your slab? So, and what you got over here is this there is A slight typo which should be R this 1 should be R v average you know this should be (( )) on the top of it. So, minus R v average is simply going to be 1 over V times R v times d v and that that equals what we got. So, k C time d v equals k times k a v times C naught into theta times d v and d v you can cancel out a v on both sides.

So, you will get 1 over I think 2 L this goes from minus L to plus L k a v C naught times theta into d x is it. So, then you can write this take this two out and write this as 1 over L going from 0 to L k a v C naught theta into d x fine . So, what would be the integral if I have A cos hyperbolic it will simply be sin hyperbolic integral.

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$$\begin{aligned}
 -\bar{R}_v &= \frac{k K_{av} C_0}{L \cosh \phi} \int_0^L \cosh\left(\frac{\phi x}{L}\right) dx \\
 &= \frac{k K_{av} C_0}{L \cosh \phi} \left[ \frac{L}{\phi} \sinh\left(\frac{\phi x}{L}\right) \right]_0^L \\
 &= \frac{k K_{av} C_0}{L} \left( \frac{\tanh \phi}{\phi} \right)
 \end{aligned}$$

So, know that is not minus  $R_v$  equal  $\frac{1}{L} \int_0^L k a v C_0 \cosh(\phi x / L) dx$  was what  $\cosh(\phi x / L)$  divided by  $\cosh \phi$  I think of  $dx$  not this  $(\phi)$   $k a v C_0$ . Now this integral turns out to be this whole thing turns out to be  $k a v C_0$  over  $L$  slightly complicated integral. This is comes out to be this  $\tanh \phi$  if this  $\cosh(\phi x / L)$  divided by  $\cosh \phi$  comes out be  $\tanh \phi$  over  $\phi$ . So, you can do that what you have to do is essentially, because you know this will be  $\sinh$ . So, you have  $A \cosh$ , but this  $1$  over  $\phi$  will come, because of the integral. So, this will be  $\sinh(\phi)$  over  $\phi$  over  $\cosh \phi$  in the denominator  $(\phi)$ . So, my  $\eta$  is going to be what? Does my  $\eta$  is going to be...

$(\phi)$

Let us go back here  $\eta$  is  $R$  this  $R_v$  is this and this is  $k$  actually here and I think the  $L$  should go from here, because there will be you know  $L$  and you know this. If you put this in the dimensionless coordinate, because  $x$  is in the dimensional coordinate. What do you used hat over here? So, if I convert this is a hat and if I convert this with the hat then you got  $L$  over here then the  $L$  would go. So, this is what you have.

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$$\begin{aligned}\eta &= \frac{\bar{R}_v}{R_v(G)} = \frac{\bar{R}_v}{K K_{av} C_0} \\ &= \frac{K K_{av} C_0}{K K_{av} C_0} \frac{\tanh \phi}{\phi} \\ &= \frac{\tanh(\phi)}{\phi}\end{aligned}$$

Then your eta is going to be  $R_v$  over  $R_v C_s$ , now it comes out be  $k_a v C$  naught over  $k_a v C$  naught tan hyperbolic phi over phi equal. So, this is what we get and this is a very important formula to remember for eta, because I will show you later may be in the couple of lectures. So, that this is something that you can use independent of geometry, because though you change the geometry and we will do in the little time. We have another geometry you will see it is difference, but what happened is that overall be it cylinder or sphere or A slab the effectiveness factor is more or less close to tan hyperbolic phi over phi more or less close to.

So, if you use this number you are not really very off. So, something this is something you might want to remember this formula. So, this is just going through what you have done over here the same thing you will get the tan hyperbolic phi over phi. So, what we do now is that in the next 10, 15 minutes we have lets quickly do this same thing and I want you to go take the lead on this is take exactly the same thing, but this. So, this is the typo over here this is not A rectangular slab. So, I want you to do this in A sphere. So, this is that example, we had before much before the picture I showed you where the enzymes are actually trapped here.

So, the enzymes are actually trapped and this is a very common example, because you know when you take some of your capsules. For example, enzymatic capsule they are the spherical (( )) like stuff and the enzymes entrap. So, this is very physical, very practical



example. So, this is the one that I want you to look at now. And I showed you how to do it. So, what I want you to do in the next few minutes are go and do it for the sphere. So, first write this is again your basic equation. All you have to do is write Laplacian in the in the spherical coordinate and then go and make it dimensionless and then go and solve it. So, just star doing it and I will help you (( )).

So, we have written the Laplacian I do not know some of you might have forgotten, but if you have not forgotten. Then this is what you have on the screen is Laplacian and the spherical coordinate. So, D effective again over R square d R of R square Del C Del R. Now what is your boundary conditions going to be?

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Because you have assumed symmetry so, the basic assumption I want here that this is a symmetric and once a symmetric if it is a non-symmetric. For example, let me ask you this for a spherical substance if this is non-symmetric. So, what would be the can you write 2 D model for a non-symmetric here for a cylinder for example, if it is symmetric?

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Def  $\nabla^2 C = KC$  Cylinder

Diff  $\left[ \frac{1}{r} \frac{d}{dr} \left( r \frac{dc}{dr} \right) + \frac{d^2 C}{dr^2} \right] = KC$   
Symmetric.

Symmetric Sphere 2-D Model

Diff  $\left[ \frac{1}{r^2} \frac{d}{dr} \left( r^2 \frac{dc}{dr} \right) + \dots \right]$

So, this is my D effective of Laplacian k C let say k c. So, for a cylinder what is my Laplacian? 2 D Laplacian is 1 over R d R of Del C Del R plus Del 2 C Del x square this is for a cylinder. Now this for a symmetric cylinder symmetric cylinder, now if I ask you for a symmetric sphere can you write the 2 D model what is (( )) 2 D model for

symmetric sphere. So, let me add that you know let me close my eyes and add the radial part plus. What is the other component be there comment?

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The theta and phi, but I asked you to write the 2 D model. So, which one you choose?

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Why is that?

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Think about it physically the sphere has you know cylinder, you have this access of symmetry and you are taking symmetric about the radial coordinate. But the physically you know how would you physically denote that about this access of symmetry you have a symmetry is it possible to do it. In a sphere it is not think about that in a cylinder you can do it, because in cylinder you can fix your access of symmetry. And you can say about this you can, but in a sphere theoretically it is possible, but physically is it possible to denote the system and say that there is an is an access of symmetry it is not possible.

Then what would be your answer? The answer is that it is not possible to write the symmetric 2 D model in sphere. For physical system theoretically mathematicians can write, but as a engineers you know there is no point. You know do you understand what I am trying to say that at what point how we are going to denote your access of symmetry and say that only around this. There is a symmetry, because if you there is a symmetry in this direction. Then if there is no physical demarcation of that and if you turn that sphere around then there is no symmetry. So, if you write have to write a symmetric model the way do it. Is actually gone and write a 3 D model you can have both in phi and theta.

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Intraphase Mass Transfer and Reaction in Tissue gel matrix (Rectangular Slab)

$$\frac{D_{\text{eff}}}{r^2} \frac{d}{dr} \left( r^2 \frac{dc}{dr} \right) = k_v c$$

$$r = 0, \frac{dc}{dr} = 0$$

$$r = R_M, c = k_{av} c_0$$

$$\xi = \frac{r}{R_M}$$

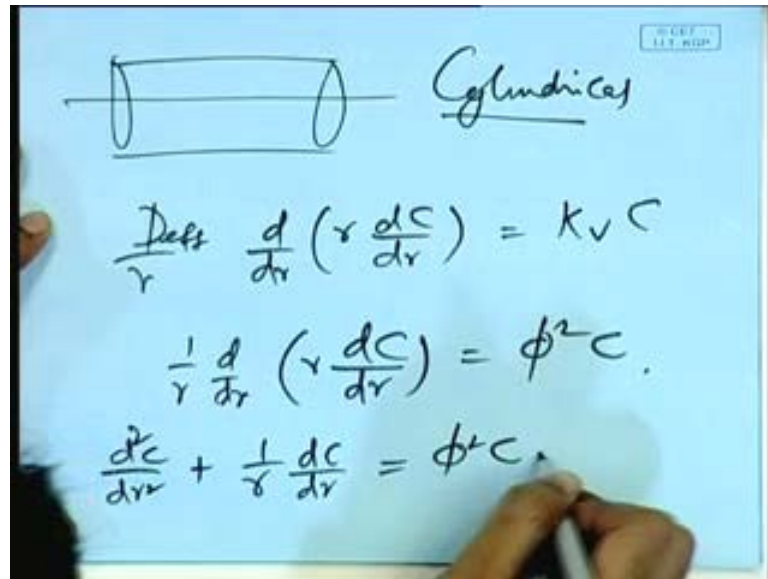
$$\frac{1}{\xi^2} \frac{d}{d\xi} \left( \xi^2 \frac{dc}{d\xi} \right) = \phi^2 c$$


So, let us go ahead with this I do not think we will have the time to finish this, but the boundary condition is such symmetric boundary conditions, because you have assumed symmetry  $r$  equals 0  $\Delta c / \Delta r$  equals 0. What will be the other boundary condition? Straightforward that at on the surface the concentration is given by  $k_v C_0$ . So, how do you solve this? So, the surface is given by  $r$  equals  $R_M$ . So, how do you solve this now? So, one thing that we can do is we can safely close our eyes and make the system dimensionless for the sake of simplicity my dimension is variable would be  $R_M$ . So, zeta is given by  $r$  over  $R_M$  then my governing equation is given by this  $1$  over  $\xi$  square  $\Delta d \xi$  of  $\xi$  square  $\Delta c / \Delta \xi$  equal  $\phi$  square times  $c$ .

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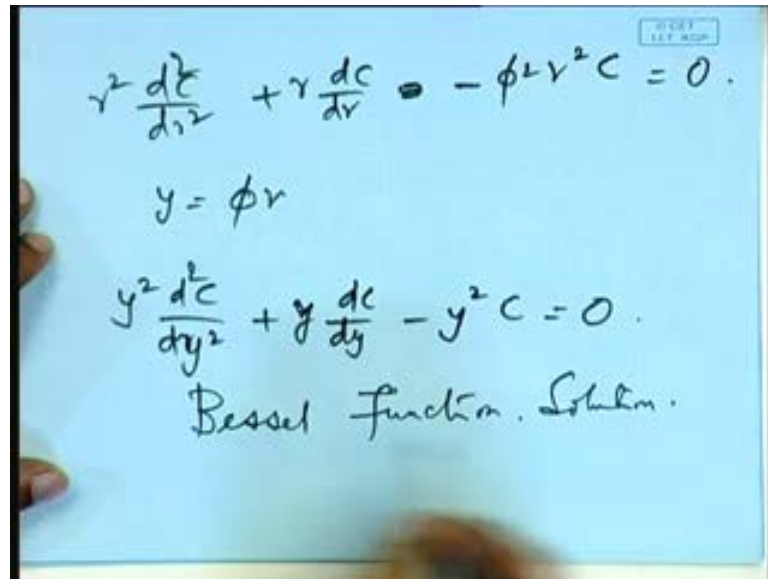
No, solution is not Bessel function you need to go and brush up your mathematics. So, let me go back a little bit we have complete run out of time, but because we have mentioned the Bessel function. So, what is the coordinate is a Bessel function is actually in the cylindrical coordinate.

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So, I did not do the cylinder, but that does not mean that I have to go back and do the cylinder now. So, this is my  $D_{effective} \frac{d}{dr} \left( r \frac{dc}{dr} \right) = k_v C$ . So, after making the dimensionless you get  $\frac{1}{r} \frac{d}{dr} \left( r \frac{dc}{dr} \right)$  this is the cylindrical coordinate by the way do not confuse its spherical. So, let us the spherical where we there, because the mentioned Bessel function that I am going back to  $\phi^2 C$  fine. So, what would be the solution of that the solution of this is going to Bessel function. So, this you can write as  $\frac{d^2c}{dr^2} + \frac{1}{r} \frac{dc}{dr} = \phi^2 C$  multiply this by  $r^2$  both sides.

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$$r^2 \frac{d^2 c}{dr^2} + r \frac{dc}{dr} - \phi^2 r^2 c = 0.$$
$$y = \phi r$$
$$y^2 \frac{d^2 c}{dy^2} + y \frac{dc}{dy} - y^2 c = 0.$$

Bessel function. Solution.

Then we will have  $r^2 \Delta^2 c + r \Delta c - \phi^2 r^2 c = 0$ . So, then your new variable you have to what is the next step you have to find a new variable  $y$ ?

$y = \phi r$ .

$y$  equals  $\phi$  times  $r$ . So, then equation becomes; now you can use the Bessel function solution. This is you know function solution what I want you to do I will stop it here today, but what I want you to do is to complete this Bessel function solution. Because these are things that you need to review on your own and I cannot review. This is not a maths class complete this Bessel function solution and come up with some clue and what would be the solution of the spherical thing. So, the cylinder the flat plate was very easy, it is cosine hyperbolic and sin hyperbolic this is the Bessel function solution. I gave you the solution, but all you have to do is figure out what kind of Bessel function first kind, second kind modified what kind of Bessel function is going to be and...

So, you figure that out and last thing that you have to do is, what would be your solution in the spherical coordinate? Which is the most pretty interesting thing to do? So, I will leave at that if there is any question on the part that we did today. So, what we essentially did with let me talk conceptually for 1 minute. About what we did we and the whole thing whole lecture kind of  $y = \phi r$  on this idea of the pseudo homogeneous model and the basic idea that we try to discussed is that for a pseudo homogeneous model. Pseudo

homogeneous model is really actually for a heterogeneous system, where these different points sources of sync of reaction and essentially. If the two conditions on which you can do an averaging one is that the microscopic scale length.

The microscopic scale over the length is much smaller than 1 and second is there is a large. There is no large variation in concentration over the entire domain; it should not be the concentration is very smaller at one place and very large. In another if these two conditions are satisfied then you can average it over the volume and come up with the pseudo homogeneous model. The main characteristic of the pseudo homogeneous model is that diffusion and reaction occur parallel in the pseudo homogeneous model, while it does not occurs parallelly in the heterogeneous model. And then you can just write the diffusion equation and solve this so, what are these are two things? I want to you to come up with one is the final Bessel function solution and second is how to solve it in the spherical coordinates. So, tomorrow I will start off with that what is that?

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No, not a function. So, just a trick you know you have to do this and it will come. So, we will stop here thanks.