

Fundamentals of Transport Processes
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Lecture No: # 31

Diffusion Equation Spherical Co-ordinates Effective Conductivity of a composite

So, welcome to lecture number 31 of our course on fundamentals of transport processes, where we were looking at ways to solve the diffusion equation. If you recall in the beginning of the class we had started out solving shell balances, for transport in one direction. And there we had chosen the shell over which the balance equation was written in such a way that it was it confirmed to the geometry that was being considered. Now, we made a step forward we have derived equations which are general in nature in the sense that, they are they can be used for any system for any configuration that is consistent with the coordination system under consideration.

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$$\frac{\partial c}{\partial t} + \nabla \cdot (uc) = D \nabla^2 c + S \quad \text{'Convection-diffusion eqn'}$$

$$Pe \ll 1 \quad D \nabla^2 c + S = 0$$

$$Pe \gg 1 \quad \frac{\partial c}{\partial t} + \nabla \cdot (uc) = 0$$

$$\frac{\partial c}{\partial t} + \nabla \cdot (uc) = D \nabla^2 c + S$$

$$c^* = (c/c_0) \quad u^* = (u/U) ; r^* = (r/L) \quad t^* = \left(\frac{tU}{L}\right)$$

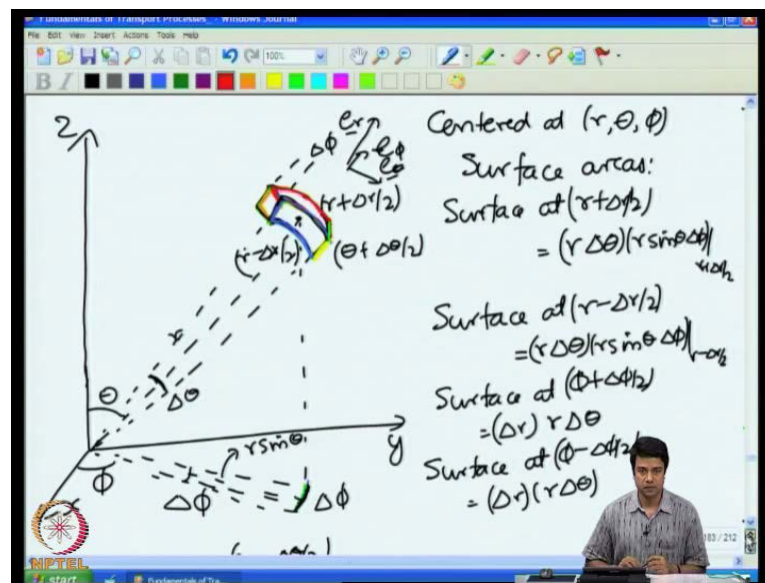
$$\frac{\partial c^*}{\partial t^*} + \frac{U}{L} \nabla^* \cdot (u^* c^*) = \frac{D}{L^2} \nabla^{*2} c^* + S$$

So, we derived a set of balance equations for a Cartesian coordinate system we derived one for a cylindrical as well as for a spherical coordinate system. In all of these equations had a specific form, the form of the equation was the derivative of the concentration with respect to temperature plus the divergence of u times c is equal to d del square c plus some source or sink term. These symbols the divergence and laplacian have different

interpretations in different coordinate systems however the equation can always be written in this form.

So, this is a general convection diffusion equation and the equation the actual the form of the divergence and the laplacian do change they do depend upon coordinate systems. And I showed you how we can derive these we derived these by writing a shell balance over a shell whose surfaces are surfaces of constant coordinate.

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So, when we looked at for example a spherical coordinate system,(no voice 02:31 to 02:37) we looked at surfaces of a shell whose surfaces are surfaces where the coordinates is a constant. There were three coordinates in a spherical coordinate system they are theta and phi coordinates. So, I chose two surfaces on which r is a constant where r is the distance from the origin, two surfaces on which the azimuthal angle theta is a constant, and two surfaces on which the meridional angle phi is a constant.

And of course, the total change in mass within this differential volume is equal to the change in concentration within a time divided by the **volume**- multiplied by the volume itself this is equal to what comes in minus what goes out plus any sources or sinks. The amount of mass coming in or going out of the surfaces is equal to the flux, times the surface area. Times the time interval and so all you need to know is, what are the expressions for a surface area on each of these surfaces and from that one can write down the flux balance.

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$$\begin{aligned}
 & + \frac{1}{r \sin \theta} \frac{\partial}{\partial \theta} (c u_{\theta} \sin \theta) - c u_{\theta} \sin \theta \left(\frac{1}{r} \frac{\partial}{\partial r} \right) \\
 & + \frac{1}{r \sin \theta} \frac{\partial}{\partial \phi} (c u_{\phi} \sin \theta) - c u_{\phi} \sin \theta \left(\frac{1}{r} \frac{\partial}{\partial r} \right) \\
 & + S \\
 \frac{\partial c}{\partial t} & = - \frac{1}{r^2} \frac{\partial}{\partial r} (r^2 j_r) - \frac{1}{r \sin \theta} \frac{\partial}{\partial \theta} (\sin \theta j_{\theta}) - \frac{1}{r \sin \theta} \frac{\partial}{\partial \phi} (\sin \theta j_{\phi}) \\
 & - \frac{1}{r^2} \frac{\partial}{\partial r} (r^2 c u_r) - \frac{1}{r \sin \theta} \frac{\partial}{\partial \theta} (\sin \theta c u_{\theta}) - \frac{1}{r \sin \theta} \frac{\partial}{\partial \phi} (\sin \theta c u_{\phi}) \\
 & + S \\
 \frac{\partial c}{\partial t} & + \frac{1}{r^2} \frac{\partial}{\partial r} (r^2 c u_r) + \frac{1}{r \sin \theta} \frac{\partial}{\partial \theta} (\sin \theta c u_{\theta}) + \frac{1}{r \sin \theta} \frac{\partial}{\partial \phi} (\sin \theta c u_{\phi}) + S = 0
 \end{aligned}$$

So, we did all this and we finally ended up with an equation of this kind. The change in the concentration with respect to time it contained terms due to diffusion, the diffusive fluxes due to the fluctuating motion of the molecules as well as the convective fluxes due to the mean flow of the fluid. So, you get terms that are of the form the derivatives of the flux with respect to position where j is the diffusive flux. And then there are terms which contain derivatives of the concentration times the components of the velocity.

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$$\begin{aligned}
 j_r & = -D \frac{\Delta c}{\Delta r} = -D \frac{\partial c}{\partial r} \\
 j_{\theta} & = -D \left(\frac{c(\theta + \Delta \theta) - c(\theta)}{r \Delta \theta} \right) \\
 & = -D \frac{1}{r} \frac{\partial c}{\partial \theta} \\
 j_{\phi} & = -D \left(\frac{c(\phi + \Delta \phi) - c(\phi)}{r \sin \theta \Delta \phi} \right) \\
 & = -D \frac{1}{r \sin \theta} \frac{\partial c}{\partial \phi}
 \end{aligned}$$

$$\frac{\partial c}{\partial t} + \frac{1}{r^2} \frac{\partial}{\partial r} (r^2 c u_r) + \frac{1}{r \sin \theta} \frac{\partial}{\partial \theta} (\sin \theta c u_{\theta}) + \frac{1}{r \sin \theta} \frac{\partial}{\partial \phi} (\sin \theta c u_{\phi}) + S = 0$$

And then we expressed the flux in terms of the change in concentration with position one has to be careful here in curvilinear coordinate systems. Because the coordinates themselves do not have dimensions of length therefore, when one takes the **the** flux the flux has to be written as minus of a diffusion coefficient times. The difference in concentration divided by the actual distance mode the actual distance mode is not just the change in coordinate, because the coordinate does not necessarily have dimensions of length.

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$$\frac{\partial c}{\partial t} + \frac{1}{r^2} \frac{\partial}{\partial r} (r^2 u_r) + \frac{1}{r \sin \theta} \frac{\partial}{\partial \theta} (\sin \theta u_\theta) + \frac{1}{r \sin \theta} \frac{\partial}{\partial \phi} (\sin \theta u_\phi) = D \left[\frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial c}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial c}{\partial \theta} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial^2 c}{\partial \phi^2} \right] + S$$

$$\frac{\partial c}{\partial t} + \nabla \cdot (u c) = D \nabla^2 c + S$$

$$\frac{\partial c}{\partial t} + \nabla \cdot (u c) = -\nabla \cdot j + S$$

$$j = -D \nabla c$$

$$c = e_r \frac{\partial c}{\partial r} + e_\theta \frac{\partial c}{\partial \theta} + \frac{e_\phi}{r \sin \theta} \frac{\partial c}{\partial \phi}$$

So, once you write that correctly, you end up with an equation the equation on top there which contains the convective as well as the diffusive terms. And I showed you how to express that in the form of a convection diffusion equation, where we define the gradient operator as well as the laplacian, del square for the specific coordinate system that we consider. So, that gave us a differential equation. We see we obtained or I briefly showed you how to get a differential equation for a cylindrical coordinate system as well we can do the same thing for any coordinate system.

There are in fact more complicated coordinate systems that can be used for example, if you are solving the problem of the transport from an elliptical particle there are elliptical coordinate systems. Similarly, one can have bispherical coordinates for if you want to solve the problem around two particles. And so, on in each of these cases one has to identify the correctly the coordinates the surfaces of constant coordinate and their surface

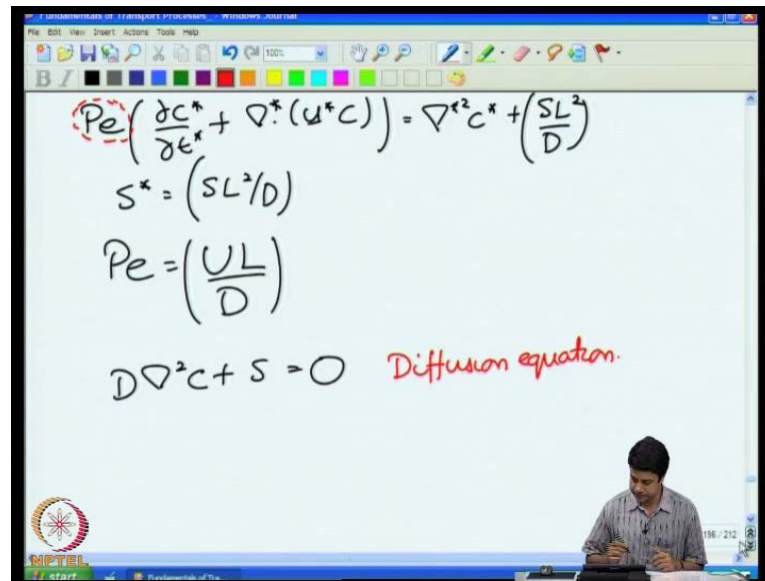
areas. And once that is done one can then obtain all of the differential equations for the concentration field.

As I told you in the last lecture it is little more complicated for momentum transfer and that is why we will look at that at a later date. So, we will restrict attention here to just the mass and heat transfer equations. The two equations are exactly the same except that in the energy balance equation, one has to replace the concentration by temperature and the mass diffusivity by the thermal diffusivity that is the only difference. Once that replacement is done the form of the equations are exactly the same provided that thermal conductivity or diffusivity and the mass diffusivity are independent of position. So, that is an important qualification here.

So, this equation contains convective term as well as time derivative on the left the convection diffusion equation diffusion terms on the right hand side. So, in that sense this convection diffusion equation balances convection and diffusion processes. One can scale this equation if one were considering a problem with a characteristic velocity and a characteristic length scale. For example, if we were trying to solve the problem of thermal diffusion from a catalyst surface in the presence of flow that is if the particle were moving with a velocity u with respect to the fluid. The characteristic velocity would be the particle velocity, itself characteristic length would be the particle radius.

So, one can scale the spatial coordinates by the particle radius, the velocity by the particle velocity and once that is done one gets a dimensionless equation. And this equation has a dimensionless number in it which is the Peclet number the ratio of convection and diffusion.

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$$Pe \left(\frac{\partial C^*}{\partial t^*} + \nabla^* \cdot (u^* C^*) \right) = \nabla^{*2} C^* + \left(\frac{SL^2}{D} \right)$$
$$S^* = (SL^2/D)$$
$$Pe = \left(\frac{UL}{D} \right)$$
$$D \nabla^2 C + S = 0 \quad \text{Diffusion equation.}$$

So, the speckle number is $U L$ by D or $U L$ by α for heat transfer problems U is a velocity length per unit time, L is a length and D is a diffusivity length square per time. So, this is a dimensionless number, In the limit where the speckle number is small one would expect diffusion to be dominant and therefore, one can solve just the diffusion equation $D \nabla^2 C$ plus sources and sinks is equal to zero. In the opposite limit when convection when the speckle number is large one might simplistically think that we can just neglect diffusion completely.

And solve only the convection part of the equation turns out not to be the case because when we neglect the diffusion term, we converted the second order differential equation to a first order. And we will not be able to satisfy all boundary conditions that is the mathematical reason. Physical reason is that when one takes only convection into account convective transport, transports heat or mass only in the direction of flow, there can be no transport in the direction perpendicular to the flow. Whenever we have flows near surfaces at the surface the fluid velocity has to be zero.

Therefore, the velocity perpendicular to the surface has to be equal to zero at the surface that means, there can be no transport due to diffusion due to convection at the surface itself, the only transport that can take place perpendicular to the surface is diffusion. Therefore, as one goes very close to the surface diffusion will still become important. We will see that in our next section on high speckle number flows will use techniques

similar to the similarity solutions that we have been using successfully all this while in that case. For now let us focus on the diffusion equation where we set the speckle number to zero.

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$$\nabla^2 C = 0 \quad \nabla^2 T = 0$$

$$\frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial C}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial C}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2 C}{\partial \phi^2} = 0$$

$$C(r, \theta, \phi) = R(r) \Theta(\theta) \Phi(\phi)$$

$$\frac{1}{R} \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial R}{\partial r} \right) + \frac{1}{\Theta} \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial \Theta}{\partial \theta} \right) + \frac{1}{\Phi} \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2 \Phi}{\partial \phi^2} = 0$$

So, that the convective terms are no longer important. I was solving for U the convection equation in a spherical coordinate system procedure is exactly the same in any coordinate system, whenever we have a function which is a function of multiple coordinates. If we can do a similarity transform based upon the scaling of the coordinates in the boundary conditions. That is best, because we can get a solution in terms of just one similarity variable, when that is not possible we try to use the separation of variables technique. And here we separate out the dependence of the concentration on r theta and phi in terms of a function of r alone of theta alone and of phi alone and we attempt to get a separate equations for each one of these. That was where we left off in the last class.

We expressed C as a product of r theta and phi substituted that into the differential equation divided throughout by r theta and phi, we had to multiply by this additional factor of r square sin square theta. In this case because this operator is little more complicated, but none other less when you multiply it by that you get an equation in which there are two terms one of which is only a function of r. And the other is only a function I am sorry, the first term here is only a function of r and theta. The term in red the term in blue is only a function of phi therefore, both of these have to be constants.

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The whiteboard contains the following mathematical content:

$$\frac{1}{R} \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial R}{\partial r} \right) + \frac{1}{\Theta} \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial \Theta}{\partial \theta} \right) + \frac{1}{\Phi} \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2 \Phi}{\partial \phi^2} = 0$$

$$r^2 \sin^2 \theta \left[\frac{1}{R} \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial R}{\partial r} \right) + \frac{1}{\Theta} \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial \Theta}{\partial \theta} \right) \right] + \frac{1}{\Phi} \frac{\partial^2 \Phi}{\partial \phi^2} = 0$$

$$\frac{1}{\Phi} \frac{\partial^2 \Phi}{\partial \phi^2} = -m^2 \quad \text{If } C = +m^2, \Phi = Ae^{m\phi} + Be^{-m\phi}$$

If $C = -m^2$, $\Phi = A \sin(m\phi) + B \cos(m\phi)$

$$\Phi(\phi + 2\pi) = \Phi(\phi)$$

$m = \text{Integer}$

What are the constant values, I solve the equation for phi and I showed you that if the constant is $(+)$ the solutions are exponentials. If the constant is negative the solution are sin and cosine functions which one should it be here. We use the symmetric condition, in the phi coordinate as we go from phi we go we keep increasing phi from some initial value. When you increase it by a value of two pi we come back to the exact same physical point in space therefore, the value of this function at angle phi has to be exactly equal to the value at angle phi plus two pi. The exponential functions will not satisfy this condition, the sin and cosine functions will satisfy this condition only if m is an integer.

So, the requirement physical requirement that you have to have the exact same value for the function at phi as well as at phi plus two pi restricts this constant to be minus m square where m is an integer.

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$$\frac{1}{\sin \theta} \frac{\partial^2 \Phi}{\partial \phi^2} = -m^2 \quad \text{If } C = +m^2, \Phi = A e^{m\phi} + B e^{-m\phi}$$

$$\boxed{\text{If } C = -m^2, \Phi = A \sin(m\phi) + B \cos(m\phi)}$$

$$\Phi(\phi + 2\pi) = \Phi(\phi)$$

$$m = \text{Integer}$$

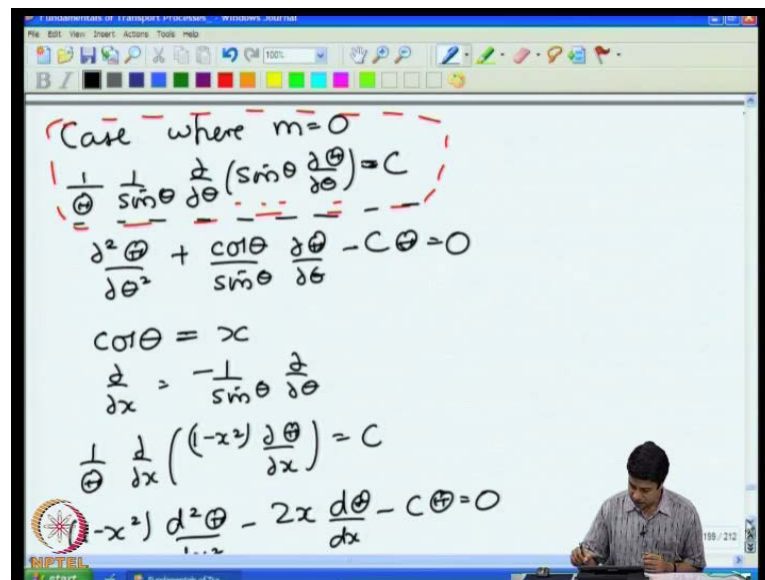
$$r^2 \sin \theta \left[\frac{1}{R^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial R}{\partial r} \right) + \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial \Theta}{\partial \theta} \right) \right] - m^2 = 0$$

$$\left[\frac{1}{R^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial R}{\partial r} \right) \right] + \left[\frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial \Theta}{\partial \theta} \right) - \frac{m^2}{\sin \theta} \right] = 0$$

Recall that when we did the heat conduction in a cube we similarly, got the value of the constant to be n times π where n was an integer. That came out with a homogenous boundary conditions on the two surfaces in the homogenous direction therefore, we got a discrete spectrum of Eigen values. In that case we get a discrete spectrum of Eigen values m , in this case as well just from the symmetric condition that when you go around. When angle of two π you have to come to the exact same location in space and then we looked at the other part of the equation the part that dependent upon θ and r .

Once again I was able to separate out separate it out into two parts one of which depended only upon r and the other depended only upon θ for the part that depends only upon θ .

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Case where $m=0$

$$\frac{1}{\Theta} \frac{1}{\sin \theta} \frac{d}{d\theta} \left(\sin \theta \frac{d\Theta}{d\theta} \right) = C$$

$$\frac{d^2 \Theta}{d\theta^2} + \frac{\cos \theta}{\sin \theta} \frac{d\Theta}{d\theta} - C \Theta = 0$$

$$\cos \theta = x$$

$$\frac{d}{d\theta} = -\frac{1}{\sin \theta} \frac{d}{dx}$$

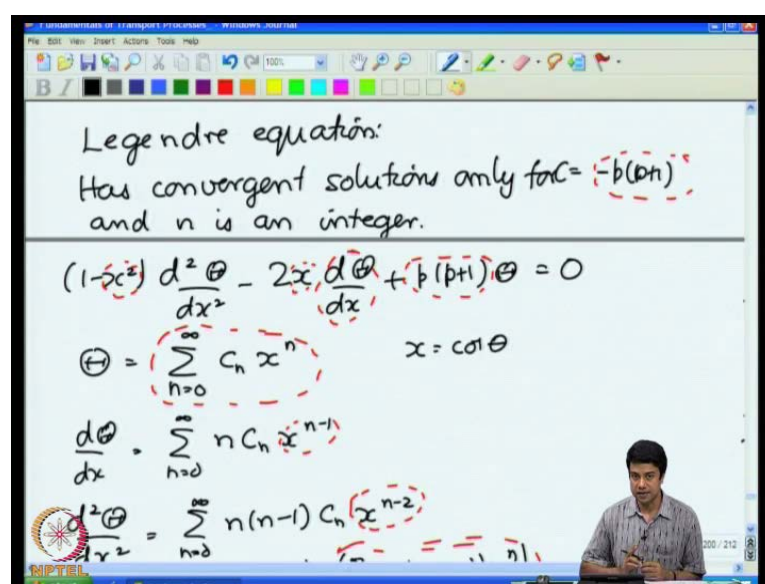
$$\frac{1}{\Theta} \frac{d}{dx} \left((1-x^2) \frac{d\Theta}{dx} \right) = C$$

$$(1-x^2) \frac{d^2 \Theta}{dx^2} - 2x \frac{d\Theta}{dx} - C \Theta = 0$$

I showed you that the solutions are in the form of functions called Legendre polynomials. In the case of the function of the meridional angle phi the discrete Eigen value came out of the fact that when you go around by an angle two pi you have to come to the same point in space.

There is a similar consideration for the theta angle as well, I substituted $\cos \theta$ is equal to x and I got the Legendre equation.

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Legendre equation:
Has convergent solutions only for $C = -b(b+1)$
and n is an integer.

$$(1-x^2) \frac{d^2 \Theta}{dx^2} - 2x \frac{d\Theta}{dx} + b(b+1) \Theta = 0$$

$$\Theta = \sum_{n=0}^{\infty} C_n x^n \quad x = \cos \theta$$

$$\frac{d\Theta}{dx} = \sum_{n=0}^{\infty} n C_n x^{n-1}$$

$$\frac{d^2 \Theta}{dx^2} = \sum_{n=0}^{\infty} n(n-1) C_n x^{n-2}$$

And I showed you that the Legendre equation has solutions only if the constant has a very specific form, only this constant in the equation has a very specific form since I have already used n in the previous case. I will write this as minus p into p plus one so, this becomes (no voice 16:26 to 16:36) so, what I had done was I had expanded this solution in a series in x is $\cos \theta$ varies between minus one and plus one. Therefore, this series is always convergent provided the coefficients decrease as n becomes large. This was p and p plus one.

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$$\frac{d^2x}{dx^2} = \sum_{n=0}^{\infty} C_n n(n-1) x^{n-2} - \left(\sum_{n=0}^{\infty} C_n n(n-1) x^n \right)$$

$$- 2 \sum_{n=0}^{\infty} C_n n x^n + p(p+1) \sum_{n=0}^{\infty} C_n x^n = 0$$

$$\sum_{n=2}^{\infty} [C_{n+2} n(n+1) x^n] - \sum_{n=0}^{\infty} C_n n(n+1) x^n + p(p+1) \sum_{n=0}^{\infty} C_n x^n = 0$$

$$C_{n+2} = \frac{[n(n+1) - p(p+1)] C_n}{(n+2)(n+1)}$$

In the limit $n \gg 1$; $C_{n+2} \approx C_n$

And I showed you that this series will converge only if, (no voice 17:21 to 17:34)

In the limit of n becoming large the series expansion will converge only if this coefficient is of the form minus of p into p plus one. Only if this coefficient is of this specific form will I get a convergence for the series solution. And the solutions for which this is of this p is an integer are what are called Legendre polynomial functions for a given value of p this function is p th order Legendre polynomial. And I showed you p naught p one and p two for this case one $\cos \theta$ and three $\cos^2 \theta$ minus one, and for the more general case I there is an orthogonality relation for these Legendre polynomial functions.

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$$C_{n+2} = \frac{[n(n+1) - b(b+1)]C_n}{(n+2)(n+1)}$$

In the limit $n \gg 1$; $C_{n+2} \approx C_n$

$$n(n+1) - b(b+1) = 0$$

$$C = -b(b+1)$$

$$\Theta = P_n(\cos \theta)$$

where P_n = Legendre polynomial.

$$(1-x^2) \frac{d^2 \Theta}{dx^2} - 2x \frac{d\Theta}{dx} + n(n+1)\Theta = 0$$

They are orthogonal to each other over the domain theta going from zero to pi. P_n of course, theta P_m of course, theta sin theta d theta integrated from zero to pi is equal to delta n m. It is non zero only if n is equal to m times two n by two n plus one and for the more general case where m is non zero we got the Legendre polynomial solutions as P_n m of cos theta. These satisfy the orthogonality relations integral sin theta d theta d n m of cos theta $P_n P_m$ (0) n plus m n plus times delta m P.

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$$\Theta = P_n^m(\cos \theta) \int \sin \theta d\theta P_n^m(\cos \theta) P_l^m(\cos \theta)$$

$$|m| \leq n$$

$$\Theta \Phi = \sum_{n=0}^{\infty} \sum_{m=-n}^n Y_n^m(\theta, \phi)$$

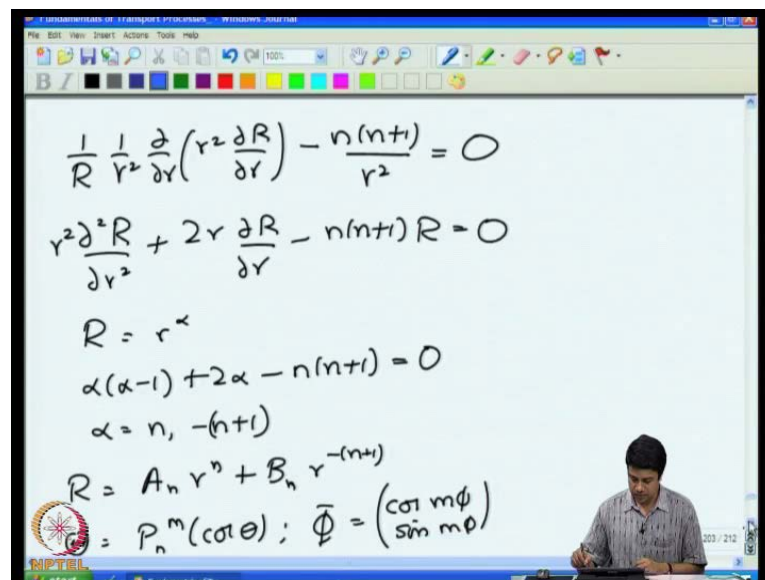
$$Y_n^m(\theta, \phi) = P_n^m(\cos \theta) \left(\frac{\sin(m\phi)}{\cos(m\phi)} \right)$$

$$\int_0^{2\pi} d\phi \int_0^\pi \sin \theta d\theta Y_n^m(\theta, \phi) Y_l^q(\theta, \phi) = \frac{2n}{2n+1} \frac{(n+m)!}{(n-m)!} \delta_n l \delta_m q$$

So, even if m is non zero the orthogonality relation still holds except it has a slightly more complicated form the product of two Legendre polynomials of order m and of order p turn out to be non zero only if n is equal to p so, of p and m times P_n is non zero only if n is equal to p . I told you that the product of the two $Y_{n,m}$ and the product θ times ϕ can be written in the form of the function Y_n and n of θ and ϕ . Where these $Y_{n,m}$ s are products of P_n of $\cos \theta$ and either $\sin$ or $\cos n\phi$ these are once again defined all to be orthogonal to each other.

The orthogonality relation involves an integral over both θ as well as ϕ in this case and so, these are the orthogonality relations for the θ and ϕ . Coordinates the basis functions and the orthogonality relation for the θ and ϕ coordinates.

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$$\frac{1}{R} \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial R}{\partial r} \right) - \frac{n(n+1)}{r^2} = 0$$

$$r^2 \frac{\partial^2 R}{\partial r^2} + 2r \frac{\partial R}{\partial r} - n(n+1)R = 0$$

$$R = r^\alpha$$

$$\alpha(\alpha-1) + 2\alpha - n(n+1) = 0$$

$$\alpha = n, -(n+1)$$

$$R = A_n r^n + B_n r^{-(n+1)}$$

$$\Theta = P_n^m(\cos \theta); \Phi = \begin{pmatrix} \cos m\phi \\ \sin m\phi \end{pmatrix}$$

So, multiplying the solutions for θ and ϕ that we obtained from this spherical harmonic expansion we get a set of basis functions $Y_{n,m}$ eigen values n and m both of which have to be integers. basis functions $Y_{n,m}$ they satisfy an orthogonality relation and this can be used for solving problems in a manner similar to the solutions that we had in the Cartesian coordinate system. what is left is the solution with respect to the radial coordinate and I showed you that in this case the solution was of the form r power plus n and r power minus of n plus one. So, A_n times r power plus n B_n times r power minus of n plus one.

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Handwritten notes on a whiteboard:

$$\Theta = P_n(\cos\theta), \quad \Psi = \sin m\phi$$

$$\Theta \Phi = Y_n^m(\theta, \phi)$$

$$C = \sum_{n=0}^{\infty} \sum_{m=-n}^{+n} \left(A_n r^n + \frac{B_n}{r^{n+1}} \right) Y_n^m(\theta, \phi)$$

Below the expansion, a circle is drawn with ΔT_0 inside. To the right, the following equations are written:

$$T = T_{\infty} + \frac{(T_0 - T_{\infty})R}{r}$$

$n=0 \text{ \& } m=0$

$$T = A_0 + \frac{B_0}{r}$$

$$T = T_{\infty} + \frac{Q}{4\pi k r}$$

So, with that we get finally, the spherical harmonic expansions shown in red in that equation for n is equal to zero Y_n^m is just one I showed you that the solution is identical to heat conduction from a spherical particle. The temperature field that you get is just the solution for n is equal to zero with the constants chosen in such a way that the boundary conditions both at zero and at infinity are satisfied. and then after that we solved the problem a slightly more complicated problem which did not have spherical symmetry and that was the effective conductivity of composite material.

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Handwritten notes on a whiteboard titled "Effective conductivity of a composite":

A diagram shows a cube with a grid of small circles representing inclusions. Labels include k_p (permeability of the matrix), k_m (permeability of the inclusions), and $q_z = ?$. A vertical arrow is labeled $(\Delta T/L)$.

To the right, a diagram labeled "Dilute" shows two circular inclusions with arrows indicating flow paths around them.

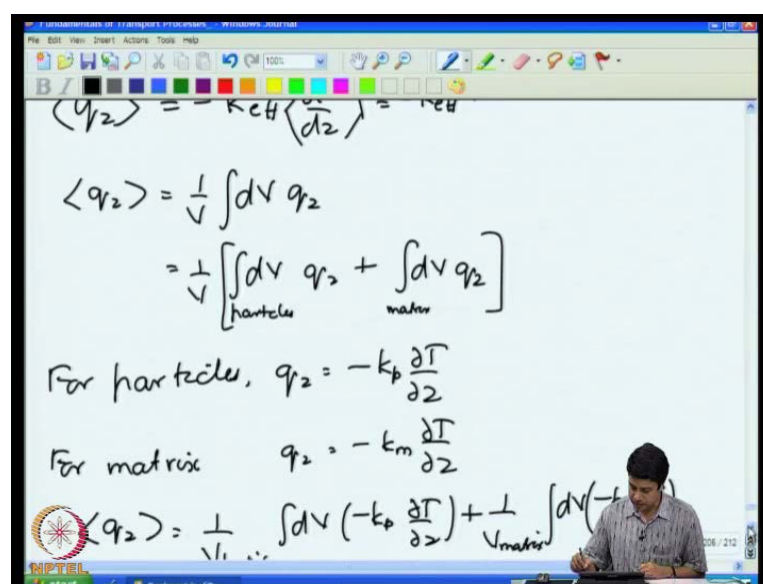
At the bottom, a coordinate system is shown with a vertical axis labeled z and a horizontal axis labeled x . A temperature profile is indicated by the equation $T = T_c + T'z$.

So, we have a composite material which consisted of a matrix and spherical particles in it. The matrix had conductivity k_m and the particles had conductivity k_p . The question we were asking was what is the conductivity of the entire composite due to these spherical particles as well as the matrix. We used the dilute assumption: the number of particles or the spacing between particles is large compared to the diameter of a particle. Since the particle and the matrix are of different conductivities, you would expect the heat flux lines to be curved near the particle surface.

If they are at the same conductivity, then of course, the flux lines would all be parallel to each other; the temperature would be just a linear function of position. However, since the conductivities are different, in the two cases the flux lines are curved. This distortion due to one particle could affect the temperature field due to another particle. If we had just a particle in an infinite medium, one would expect that this disturbance would be significant over a distance comparable to the particle radius itself. Therefore, if the distance between particles becomes large compared to the radius of a particle, the disturbance in the temperature field due to one particle will not significantly influence the temperature field around another particle.

And therefore, we can solve for the temperature field due to a single particle alone and then use statistical averaging to get the effective conductivity of the composite. That was the procedure that we used in the last lecture.

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$$\langle q_z \rangle = -k_{eff} \langle \frac{\partial T}{\partial z} \rangle = -k_{eff} \frac{\partial T}{\partial z}$$

$$\langle q_z \rangle = \frac{1}{V} \int dV q_z$$

$$= \frac{1}{V} \left[\int_{particle} dV q_z + \int_{matrix} dV q_z \right]$$

For particle, $q_z = -k_p \frac{\partial T}{\partial z}$

For matrix, $q_z = -k_m \frac{\partial T}{\partial z}$

$$\langle q_z \rangle = \frac{1}{V} \int dV (-k_p \frac{\partial T}{\partial z}) + \frac{1}{V} \int dV (-k_m \frac{\partial T}{\partial z})$$

I defined an effective heat flux as the effective conductivity times the average temperature gradient, averages here defined over volume. So, the effective heat flux is one over the volume times the integral over the entire volume of the local heat flux. The volume of course, consists of two parts one is the particle and the other is the matrix. For the particles the flux is minus k of the particle times the temperature gradient and similarly, for the matrix it is equal to minus k of the matrix times the temperature gradient. And I wrote in a slightly different form for you, where I said I expressed it as minus k m times dt dz over the entire volume plus the integral over the particles alone of the difference in conductivity times dt by dz.

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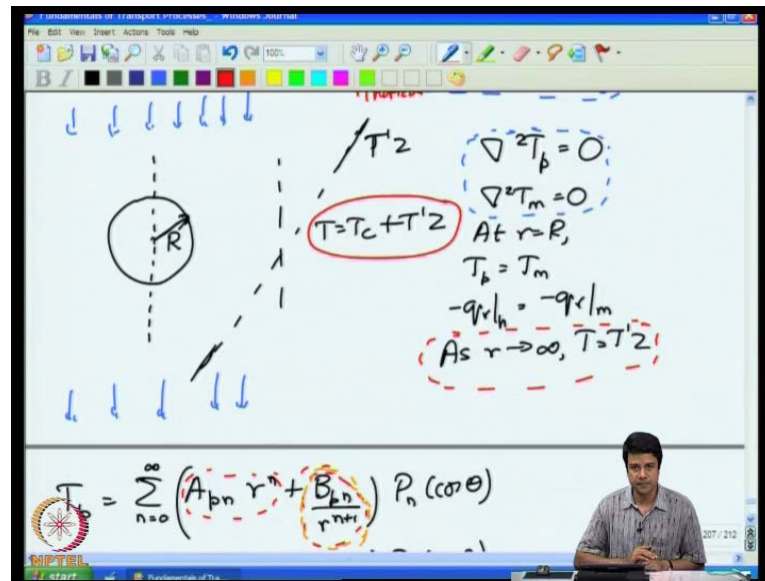
$$\begin{aligned}
 &= \frac{1}{V} \int_{\text{volume}} (-k_m \frac{dT}{dz}) + \frac{1}{V_{\text{particle}}} \int_{\text{particle}} (-k_p - k_m) \frac{dT}{dz} \\
 &= -k_m \left(\frac{dT}{dz} \right) + \frac{1}{V_{\text{particle}}} \int_{\text{particle}} (-k_p - k_m) \frac{dT}{dz} \\
 &= -k_m T' + \frac{N}{V_{\text{particle}}} \int_{\text{particle}} (-k_p - k_m) \frac{dT}{dz}
 \end{aligned}$$

$\nabla^2 T_p = 0$
 $\nabla^2 T_m = 0$
 At $r=R$,
 $T_p = T_m$
 $-\alpha_p \frac{dT_p}{dr} = -\alpha_m \frac{dT_m}{dr}$

$T = T_c + T'z$

This difference in conductivity basically accounts for the departure of the heat flux from the uniform value it would have had if there were no particles within this matrix. The matrix contribution is just equal to minus k m times the temperature gradient and then we were left with trying to evaluate the particle contribution.

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The particle contribution was done as follows, if you go sufficiently far from the particle the temperature gradient is just a constant. The temperature is a linear function of position far from the particle, as you approach close to the particle there is going to be a distortion because the conductivity of the particle and the matrix are not the same. How does one determine this distortion we write down the governing equations for the temperature in the particle and the matrix. In this case there are no sources or sinks there is no convection so, the equations just say that the laplacian of the temperature has got to be equal to zero in both the particle and the matrix. If you go far from the particle you have to recover the linear temperature gradient.

So, the temperature is got to be equal to a constant plus $T'z$ when you go far away from the particle in the limit as r goes to infinity, if I use a spherical coordinate system with origin at the centre of the particle (no audio 27:05 to 27:13). In addition to this we have boundary conditions at the particle surface temperature of the particle is equal to temperature of the matrix and the flux is as the same at the surface.

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$$T_p = \sum_{n=0}^{\infty} \left(A_{pn} r^n + \frac{B_{pn}}{r^{n+1}} \right) P_n(\cos \theta)$$

$$T_m = \sum_{n=0}^{\infty} \left(A_{mn} r^n + \frac{B_{mn}}{r^{n+1}} \right) P_n(\cos \theta)$$

At $r=R$, $T_p = T_m$

$$\sum_{n=0}^{\infty} \left(A_{pn} R^n + \frac{B_{pn}}{R^n} \right) P_n(\cos \theta) = \sum_{n=0}^{\infty} \left(A_{mn} R^n + \frac{B_{mn}}{R^n} \right) P_n(\cos \theta)$$

$$\left[A_{pn} R^n + \frac{B_{pn}}{R^n} \right] = \left[A_{mn} R^n + \frac{B_{mn}}{R^n} \right]$$

$\lambda T_p \quad -k_m \frac{\partial T_m}{\partial r}$

So, we wrote down our general solutions for the temperature field for the particle and the matrix, for the particle there is one part that is proportional to r power n there is another part that goes as r power one, over r power n plus one. The latter goes to infinity at the centre of the particle at r is equal to zero. Therefore, if the temperature at the centre of the particle is to be finite all coefficients B_{pn} have to be identically equal to zero. Similarly in the matrix I have two contributions one of which is growing proportional to r power n , the other is decaying proportional to r one over r power n plus one.

The decaying contribution to the temperature of course, goes to zero far away, as you go large distance from the particle one would expect that the particle temperature has the temperature has to be equal to T_{∞} . In the sense that the temperature has to increase proportional to $r \cos \theta$ as r becomes large that means that all coefficients A_{mn} for n two or greater have to go to zero because for n is equal to two. The contribution increases as r square whereas, the maximum increase in the matrix when you go far away is proportional to z itself is proportional to r to the first power. And then we enforce the boundary conditions at the two surfaces used orthogonality.

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$$k_p \left[A_{pn} (n R^{n-1}) - \frac{B_{pn} (n+1)}{R^{n+2}} \right] = k_m \left[A_{mn} n R^{n-1} - \frac{B_{mn} (n+1)}{R^{n+2}} \right]$$

At $r=0$, $\frac{\partial T_b}{\partial r} = 0 \Rightarrow B_{pn} = 0$ for all n

As $r \rightarrow \infty$, $T = T' z = T' r \cos \theta = T' r P_1(\cos \theta)$

$$\sum_{n=0}^{\infty} \left(A_{mn} r^n + \frac{B_{mn}}{r^{n+1}} \right) P_n(\cos \theta) = T' r \cos \theta = T' r P_1(\cos \theta)$$

$$\Rightarrow A_{m1} = T' \text{ \& } A_{mn} = 0 \text{ for } n \neq 1$$

And found out that A_{m1} is equal to T' and A_{mn} is equal to zero for all n not equal to one. Because I have this inhomogeneous forcing with n is equal to one my solution also consists only of Legendre polynomials with n is equal to one it does not consist of Legendre polynomials n is equal to two three etcetera. And we saw that from the orthogonality relations that A_m for all other values of n A_{p1} and B_{m1} were non zero all other values A_{mn} and B_{mn} is equal to zero for n greater than one.

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$$k_p A_{pn} (R^{n-1}) = - \frac{k_m B_{mn} (n+1)}{R^{n+2}} //$$

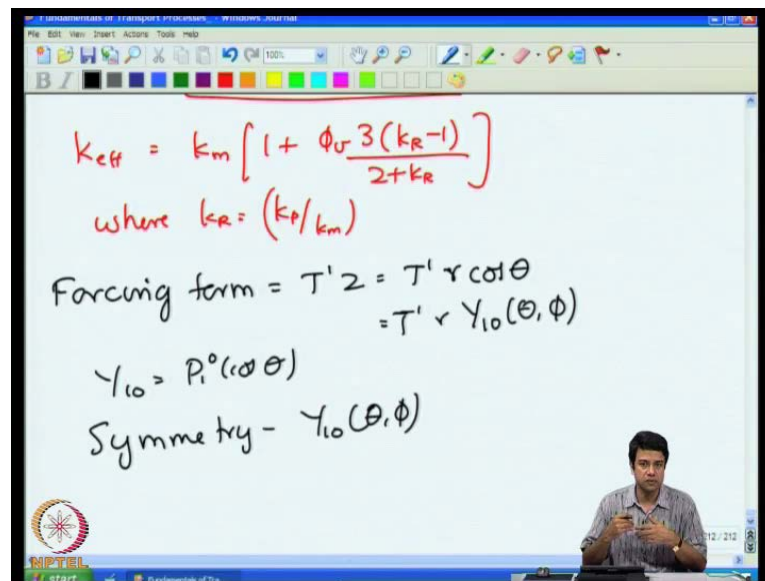
$A_{pn} = 0 \text{ \& } B_{mn} = 0 \text{ for } n > 1$

$$A_{p1} = \frac{3T'}{(2 + k_0/k_m)} \quad B_{m1} = \frac{(1 - k_0/k_m) R^3 T'}{(2 + k_0/k_m)}$$

$$T_b = \frac{3T' R r P_1(\cos \theta)}{(2 + k_0/k_m)} = \frac{3T' R z}{(2 + k_0/k_m)}$$

So, I got only one spherical harmonic solution whose coefficient was non zero from the orthogonality relations. That is because the forcing in this particular problem has a particular spherical symmetry the forcing they were homogenous boundary conditions at the surface T_p is equal to T_n . And the flux k_p times $d T_p$ by dr is equal to k_n times $d T_n$ by dr these are homogenous, they do not contain any forcing terms the only forcing term that was there was the term due to the temperature gradient far away that forcing was of the form $T' \text{ times } z$.

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$$k_{eff} = k_m \left[1 + \phi_0 \frac{3(k_R - 1)}{2 + k_R} \right]$$

where $k_R = (k_p / k_m)$

$$\text{Forcing term} = T' z = T' r \cos \theta = T' r Y_{10}(\theta, \phi)$$

$$Y_{10} = P_1^0(\cos \theta)$$

Symmetry - $Y_{10}(\theta, \phi)$

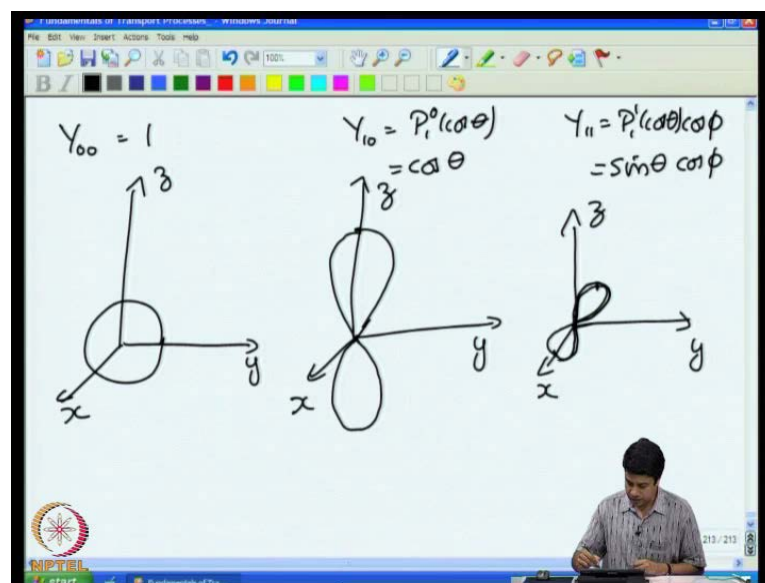
Which is $T' \text{ times } r \cos \theta$ this was what was causing the temperature distortion around the particle this I can write it as $T' r \text{ into } P_1^0 \text{ of } \cos \theta$. where Y_{10} is equal to $P_1^0 \text{ of } \cos \theta$ into $\cos$ or $\sin$ of $m \phi$ m is zero in this case so that is just a constant $\cos$ of that is just a constant. So, the forcing of course, of this form it had this symmetry from the orthogonality relations you will find that the solution also has the exact same symmetry. So, in this particular problem the symmetry was of the Y_{10} type of θ, ϕ .

And therefore, the solution that you get also has the exact same symmetry because if I did the expansion for all of those spherical harmonics. Included m and n all the way from zero zero zero to whatever large number that you decide put that into the equations do the orthogonality relations. The equations for all of those coefficients will all have zero constants except for the one with the forcing. So, the symmetry of the forcing is exactly

the same as the symmetry of the final solution that you get it is possible that you can have a forcing which has contributions due to two different symmetries.

In that case you can separate out those two, solve for each one separately and then add them all because this equation is linear one can always use superposition you separate out the solution into two parts. The boundaries have to be the same in other words the surfaces on which you apply the boundary conditions have to be the same in this case it is a spherical surface, but I have different kinds of forcing. For each forcing I can solve the equations to get one particular solution and then add up all those solutions if I if the sum of the equations gives you the equation for the final temperature. The sum of the boundary conditions gives you the boundary condition for the temperature that you want then the sum of the solutions will also give you the solution that you want.

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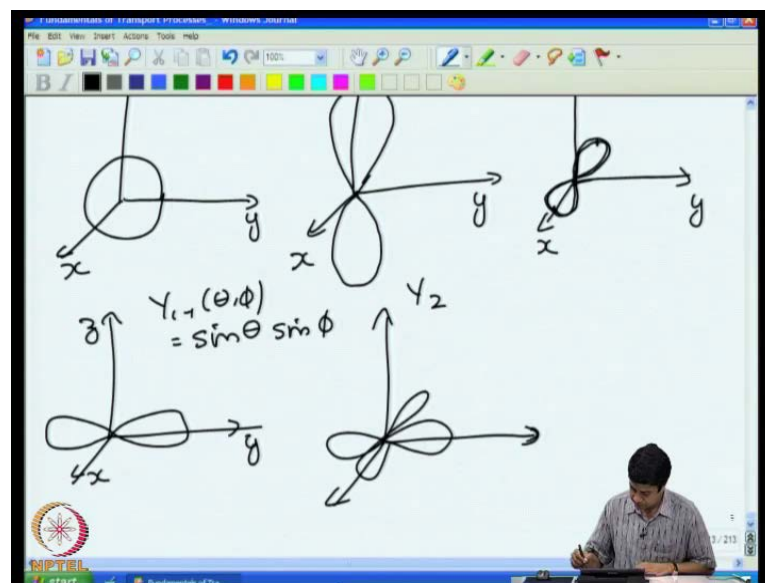


So, what are these symmetries? So, let us look at Y_{00} it is just equal to one. So, this is a spherical harmonic function which does not depend upon θ or ϕ , that means that surfaces of constant value of this are spherical shells. So, surfaces of constant which have the zero zero symmetry are basically surfaces, where are basically spherical shells. How about Y_{10} which is equal to $P_1^0(\cos \theta)$ so, this surface is proportional to $\cos \theta$. Therefore, if you actually plot out surfaces of constant P_1^0 zero will look something like this note that θ is the angle with respect to z , this is r and this is θ .

So, theta is the angle with respect to the z axis so, when theta is equal to zero the surface the value will be one, and theta is equal to pi it will be minus one at theta is equal to zero along the x y plane this has zero value. So, if you plot surfaces of constant y one zero they will actually look something like this(no voice 35:38 to 35:46) it will be symmetric about the plane, but it will look something. It will be a maximum that is a surface of constant value of this function will be a maximum at theta is equal to zero, it will have a negative minimum at theta is equal to pi.

And it will vary it will be zero exactly in the plane so, this is just equal to cos theta. I can have the next harmonic expansion Y one one is equal to P one one of cos theta fine times cos phi, this is actually P one one is basically equal to sin theta, sin theta times cos phi. So, surfaces with constant value of this along the x axis let us the axis here(no voice 36:45 to 36:54) along the x axis at y and z is equal to zero you will find that theta is equal to pi by two phi is equal to zero so, it will have maximum value here and along the minus x axis it will have a minimum value.

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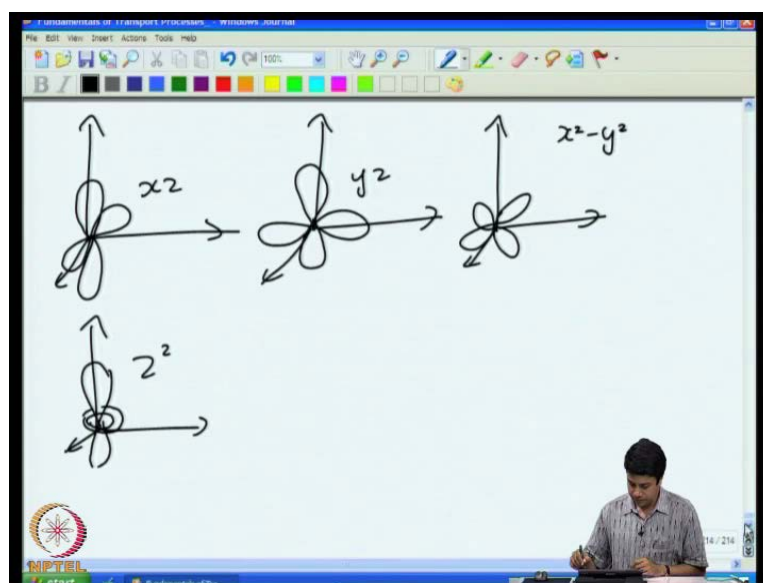


So, it will look something like this a surface of constant Y one one for the symmetry of Y one one will look something like this. That was along the x axis and the other one Y one minus one of theta and phi this is equal to sin theta times sin phi it is along the y axis so, this is x y z. So, that was for symmetries for zero zero one zero one one and minus one one minus one one can plot similarly, as I said there are functions for n going from

zero to infinity for each value of n the value of m goes from minus n to plus n . Where therefore, for n is equal to one there are three values of m minus one zero and plus one for n is equal to two there are five values of m and each one of those has its own symmetries.

And these are all orthogonal to each other in other words you take one of these functions multiplied by the other integrate over θ and ϕ you will get zero. So, in that sense these have their own unique symmetries the zero zero symmetry one zero, one one, one minus one, two zero, two one, two two, two minus one and two minus two and each of these are orthogonal. (no voice 31:01 to 31:13) the other functions Y_{20} , let me just plot them for Y_{20} for Y_{20} you have five functions there are two that are along the x and y axis, yz axis, zx axis then you have one that is $x^2 - y^2$ and the other is z^2 so, you have functions that look like this (no audio 39:45 to 40:56).

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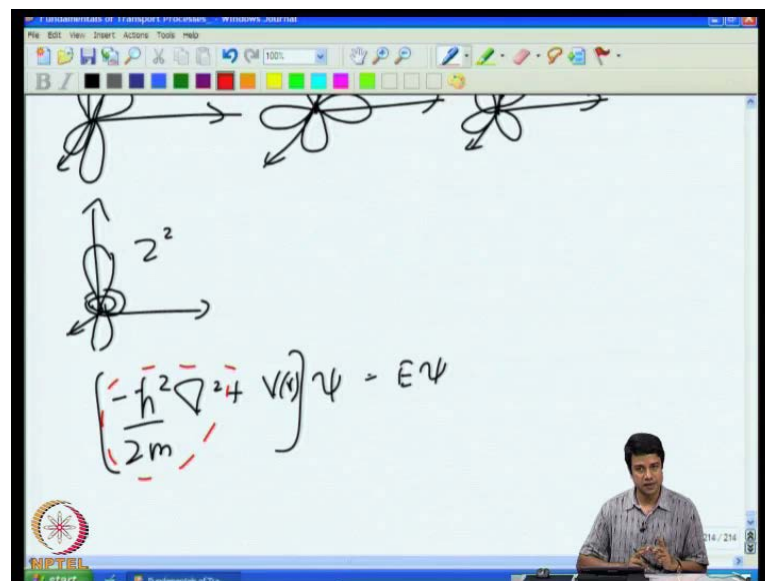
The ϕ functions at the two level this is z^2 this is $x^2 - y^2$ this is yz this is xz and this is (no voice 41:10 to 41:24) xy .

Most have you have seen these functions before molecular orbitals for the hydrogen atom the s shell is spherically symmetric that is the zero zero orbital. The P shells are one zero one one and one minus one, two zero two one two two two minus one and two minus two have the symmetry of x^2 , xy , yz , xz , $x^2 - y^2$ and z^2 . These surfaces that you have you are familiar from quantum mechanics are

surfaces of constant wave function the reason they are the same is because surfaces of constant wave function in that case the wave function is also a solution of the Laplace equation.

The equation **has** is of the form $\nabla^2 \psi - E \psi = 0$ and for an for a system with only electronic energies or electronic potential I have to solve an equation of the form $-\frac{\hbar^2}{2m} \nabla^2 \psi + V \psi = E \psi$.

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This v in the case of hydrogen atom is only a function of the distance between the nucleus and the electron. Therefore, for the θ and ϕ coordinates I am just solving $\nabla^2 \psi = 0$ for the θ and ϕ coordinates because V is only a function of radius. And that is the reason that I am getting the exact same solutions Y_n^m of θ and ϕ as I got for my diffusion equation, the laplacian these solutions are properties of the laplacian operator. Not of this particular this the, they are exactly the same whether one does it for the heat diffusion problem the electrostatic potential problem.

Where also $\nabla^2 \phi = 0$ where ϕ is the electrical potential or for the quantum mechanical problem where in that case we are solving for the laplacian acting on the wave function. Where the probability function is the part of the wave function and its complex conjugate. So, that is the reason that these solutions that we get from the spherical harmonic expansion are exactly the same as solutions that you have seen many

places before. These are all orthogonal solutions therefore, because of symmetries if I force the system with one particular kind of forcing whether spherically symmetric forcing or its forcing along one direction. The solution will have the exact same symmetry in the theta and the phi coordinates just from orthogonality alone.

So, these solutions have each one has its own symmetry and if I know what is the symmetry of the forcing I can then zero in on the solution the form of the solution. When I solve my heat conduction problem around a sphere I did not I knew that the forcing for the temperature field far away was of the form Y_{10} of theta and phi. At that point itself I could have said the forcing is of the form y_{10} therefore, the solution will also have that exact same symmetry and chosen only n is equal to 1 and m is equal to 0. The solutions for those values of n and m and proceeded, I did I used the complete expansion when I proceed it just to show you that all of the other coefficients will turn out to be equal to zero from orthogonal T and $E V$.

Because there is a forcing only due to this particular term, there is no forcing due to all other terms for n is greater than one. I have two equations with no inhomogeneous term in it these are two linear equations with no inhomogeneous term so, either you have to have no solutions or multiple solutions. In this case we have no solutions except the trivial one where A_{pn} is equal to zero and $V A_{mn}$ is equal to zero. So, that explains why we were able to get a solution just in terms of P_{10} of $\cos \theta$ and we actually solved for the thermal conductivity of spherical of composite with spherical inclusions.

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Source, dipole, . . .

T_∞ as $r \rightarrow \infty$

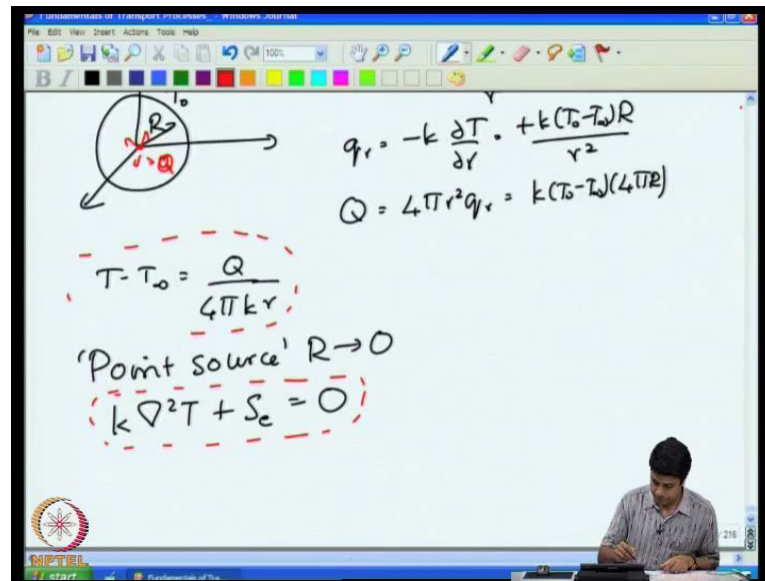
$T - T_\infty = \frac{(T_0 - T_\infty)R}{r}$

$q_r = -k \frac{\partial T}{\partial r} = \frac{k(T_0 - T_\infty)R}{r^2}$

$Q = 4\pi r^2 q_r = k(T_0 - T_\infty)(4\pi R)$

Now let us look at another interpretation of the spherical harmonic expansions in terms of, source dipole etcetera so, this is another interpretation of this spherical harmonic expansions. If you recall we had solved the problem for the heat conduction from a sphere of radius R with temperature T_0 at the surface T_∞ as r goes to infinity. The temperature turned out to be $T - T_\infty = (T_0 - T_\infty)R/r$, this was the solution we got for the temperature field. The heat flux q_r is equal to $-k \partial T / \partial r = k(T_0 - T_\infty)R/r^2$. This is the heat flux coming out of the surface the total heat coming out of the surface was equal to $4\pi r^2 q_r = k(T_0 - T_\infty)(4\pi R)$. Now if I express the temperature field in terms of the total heat coming out rather than the temperature at the surface and far away.

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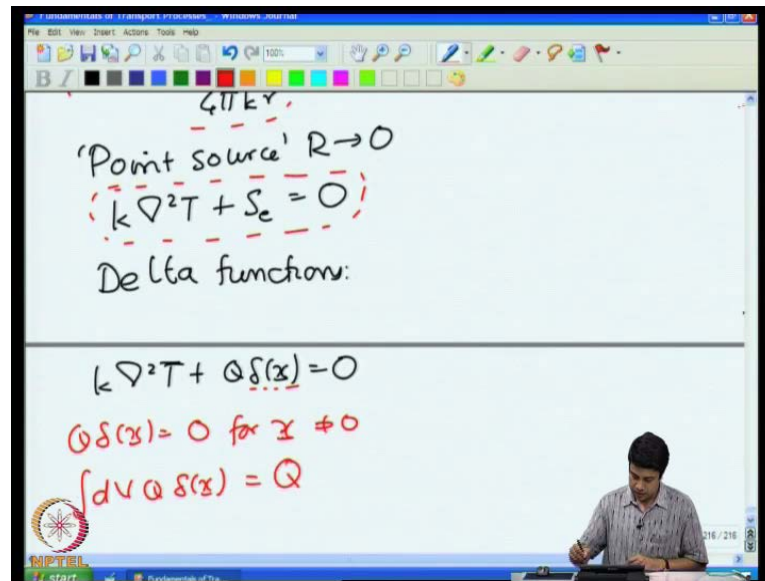
Then there the temperature field is of the form $T - T_\infty$ is equal to q by four pi k r as I told you this solution is actually independent of the radius of this spherical particle. Express in terms of the total heat coming out the solution is independent of the radius of the particle it decreases as r goes to infinity far away from the particle as one over r .

Therefore this solution is also valid in the limit as the radius of the particle goes to zero or it is also valid in the limit of the particle shrinking to a point the point source (no voice 48:54 to 49:02) provided you take the limit of R going to zero. While keeping q fixed therefore, if you should keep q fixed and take R going to zero, this solution is still valid what happens when we take R going to zero. This just shrinks to a point this and the heat coming out of this point source is basically q so, I can consider this as a source within the differential equation a source within the differential equation that is this point source is a solution of the differential equation $k \nabla^2 T + S_e = 0$.

Where this source of energy is non zero it has a value q only at the origin it is zero everywhere else. So, this source of energy is non zero only at the origin it is zero, everywhere else however note that in the conduction equation that we had defined earlier. The source was defined as the source per unit volume so, this S_e is actually a source per unit volume q in the solution is a the total amount of heat coming out not the

source per the amount of heat per unit volume. In contrast s is the amount of heat coming out per unit volume how do we define this source term for the energy conduction equation. In such a way that we can solve this equation in order to get a solution for the temperature field (no voice 51:06 to 51:13) this is done using by defining something called delta functions.

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So, if we can define a delta function in such a way that that delta function is non zero only for the point at the origin it is zero everywhere else the total amount of heat coming out is Q then we can define that as the source within this equation.

It is written as $k \nabla^2 T + Q \delta(x) = 0$ this source this point source is written as $k \nabla^2 T + Q \delta(x) = 0$. Where this delta of x is the delta function it has to be defined in such a way that the delta function, this source is non zero only at x is equal to zero this source is zero everywhere else. And the total amount of heat coming out from $Q \delta(x)$ has got to be equal to Q itself so, in other words is equal to zero for x naught is equal to zero. This and integral over the entire volume $Q \delta(x)$ this has to be equal to I am sorry this has to be equal to Q so I can do this representation then I can solve this equation $(())$.

And get temperature field and get this temperature field, but I can actually do more than that since I have a source at a single point. I find out the temperature field if I have a second source I can now add up solve for one source find the temperature field solve for

the other source find the temperature field at the two up. And I will get the total temperature field so, you can do more than that with these delta function definitions.

So, next lecture we will start of on how we express sources and sinks in terms of delta functions, and how we can use that to solve problems. In addition what is the relation between the solutions written in this form and the spherical harmonic expansions that we just derived.

So, to briefly recap what I did in this lecture I focused on the symmetries of the solution of the Laplace equation in spherical coordinates. I showed you that the solution for the theta and phi coordinates are both in the form of Eigen function solutions with discrete Eigen values in the phi coordinate the discrete Eigen value, comes about because when you go around π and angle 2π in the phi direction you return to the exact same position in space. Therefore, the solutions have to be of the form $\cos$ and $\sin$ and phi where m has to be an integer otherwise when it come back to the same location you will not get the exact same value similarly, in the theta direction also there is a constraint on the basis that at theta is equal to zero or $\cos$ theta is equal to one as well as theta is equal to one or $\cos$ theta is equal to minus one. The solutions are finite only if the constant in the equation is of the form p into p plus one where p is an integer this only if it is that form that the series solution in the theta direction gets truncated at a finite value. And one that is there you have a finite solution otherwise the solutions are all infinite.

So, these the these considerations in the theta and phi direction give you discrete Eigen values. And a set of bases functions in the theta and phi direction the theta bases functions and the form of Legendre polynomials and the phi direction the bases functions are in the form of $\cos$ and $\sin$ functions. The most general solution is the sum of all of these I can express the product of the theta and phi bases functions as Y_n^m of theta and phi these satisfy orthogonality relations. And therefore, whenever I solve a problem in a spherical coordinate system I can use this bases function along with either the growing or the decking part in the radial direction. If you recall when I solve the problem the radial direction I got two solutions one increasing as r power n the other decreasing as r power minus of n plus one.

So, the most general solution is the far out of these three and these are called the spherical harmonic expansions the equation in red there that is the most general solution.

since these spherical harmonics are orthogonal whenever there is a forcing, due to one spherical harmonic the solution will also have that exact same symmetry and that is what I tried to convey to you in this lecture. The symmetries of these spherical harmonics since they are orthogonal when you multiply two of them and integrate you get zero therefore, if you have one spherical harmonic function that is driving the heat or mass transfer problem the solution will be of that exact same form. Next lecture we will take up delta function solutions that is how do we what is the how do we express the sources a point source as a delta function. And how do we use that in order to solve problems what is the relation between the point source solutions and the spherical harmonics that is what we will continue in the next lecture we will see you then.