Fundamentals of Transport Processes
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Lecture No. # 29
Diffusion Equation Apherical co-ordinates Separation of Variables

This is lecture number twenty nine in our course on fundamentals of transport processes and we were looking at conservation equations in three dimensions. First we looked at a Cartesian coordinate system and then at spherical and then at cylindrical. So, the basic idea is as follows; we have some concentration or temperature field for mass or heat transfer system and initially when we did shell balances we used to write down a shell specifically for the particular problem and then solve and then obtain a difference equation for the balances across the shell and then convert that into a differential equation and then solve it.

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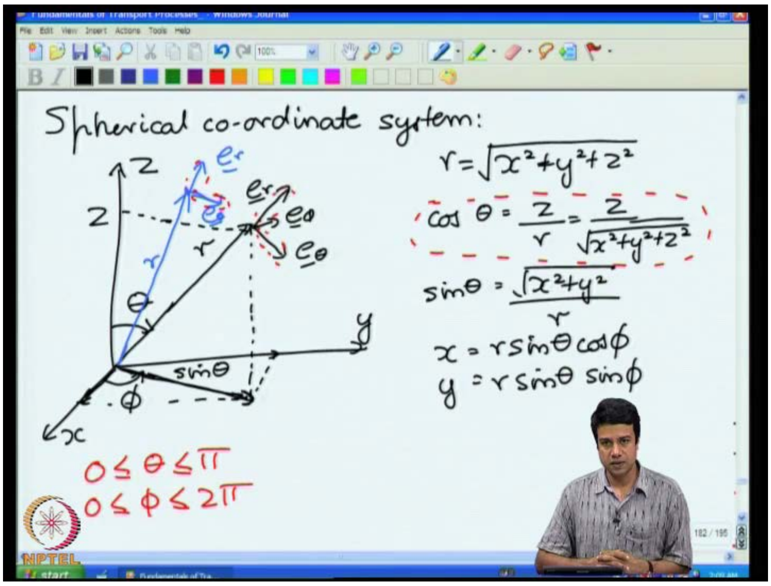

However, if we could write down equations that are general for the particular coordinate system that we are considering; then it is now necessary only to straight away use those equations and write down boundary conditions and go about solving them. And that was the basic strategy that we were following for transport problems. We had identified a three different types of coordinate systems the Carstesian coordinate system, the spherical and the cylindrical coordinate systems and we went about writing balance equations for each of these coordinate systems.

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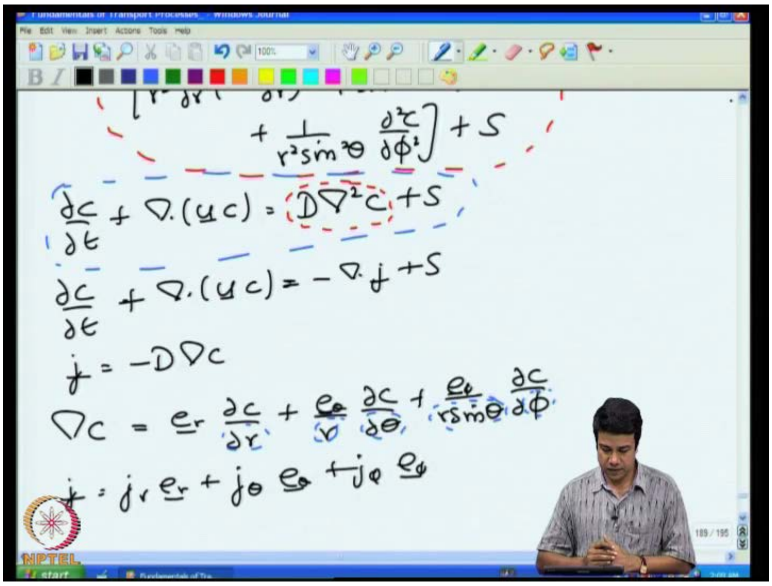

As we saw in all the coordinate systems the balance equations could be reduced to the form given here in the circled in the blue. Partial C by partial t plus diversions of u vector u is the mean velocity u vector times concentration is equal to D times the Laplacian of C plus any sources or sinks.

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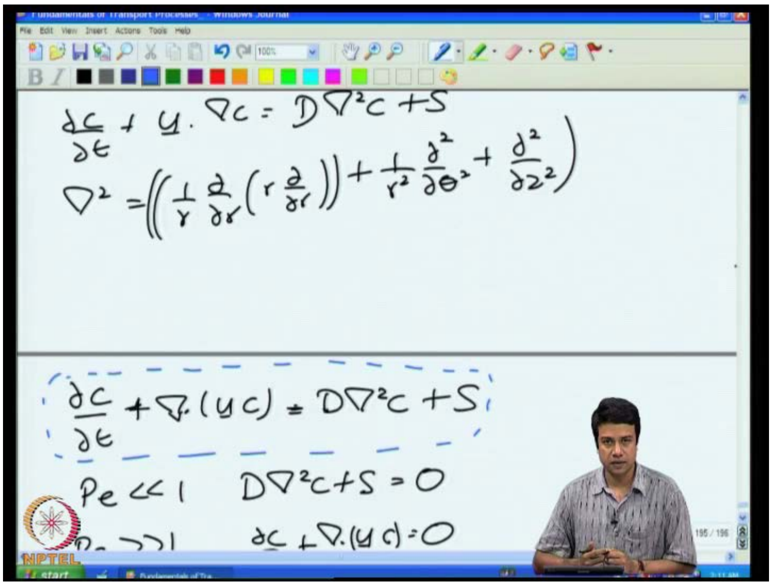

So in any coordinate system the conservation equation can be reduced to this particular form. Whether is it is for mass or heat transfer the terms on the left have the general form of diversions of velocity times concentration or diversions of velocity times temperature. The term on the right is a diffusion coefficient times the laplacian of the concentration or temperature fields. Note the dimensions here; the first term is concentration divided by time. The second is del q c u is a velocity length per time.

So, this also has dimensions of concentration per time. The term on the right hand side is a diffusion coefficient times del square C diffusion coefficient has dimensions of length square per unit time. So, this also has dimensions of concentration per time. Therefore, this equation dimensionally it just contains the first derivative specially as a concentration field as per as the second derivative contains a time derivative second order in space first order in time. Generally you require two special boundary conditions along each coordinate and one initial condition in time. These operators the divergence operator and the Laplacian operator have different forms in different coordinate systems as we saw in a spherical coordinate system, this one was a laplacian operator had this was the gradient operator in spherical coordinate system.

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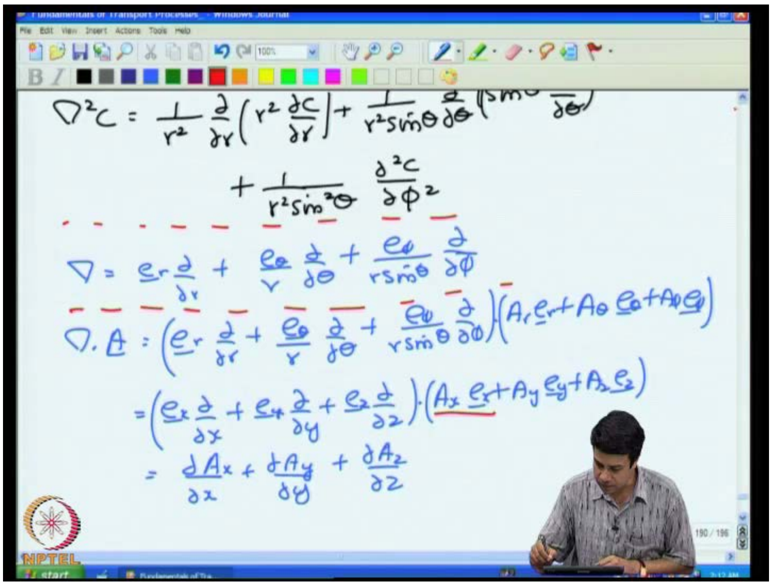

And this one was the laplacian operator in a spherical coordinate system and the divergence. So this was the gradient and this here was the divergence.

So if I know the form for that specific coordinate system I can then go ahead and write down the equations for that particular coordinate system. In a similar manner I had got for you the operators in a cylindrical coordinate system.

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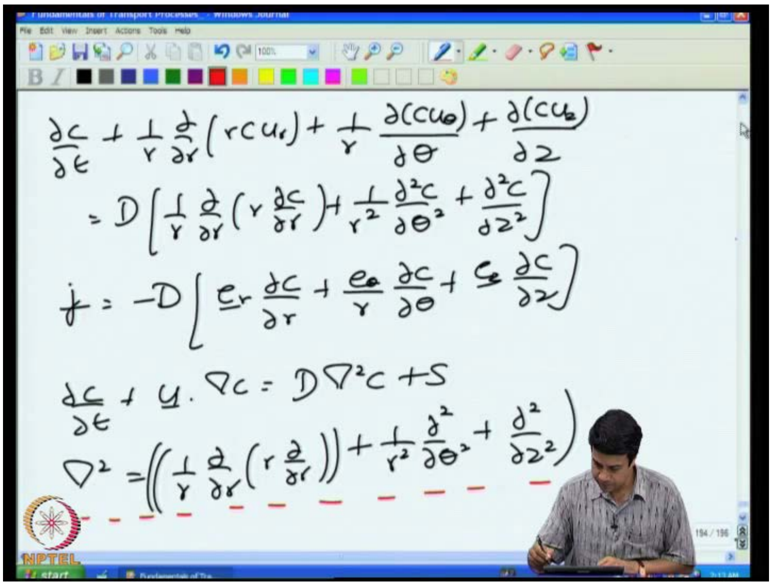

So this is the laplacian operator. The gradient is given right here and the divergence is given by these three terms.

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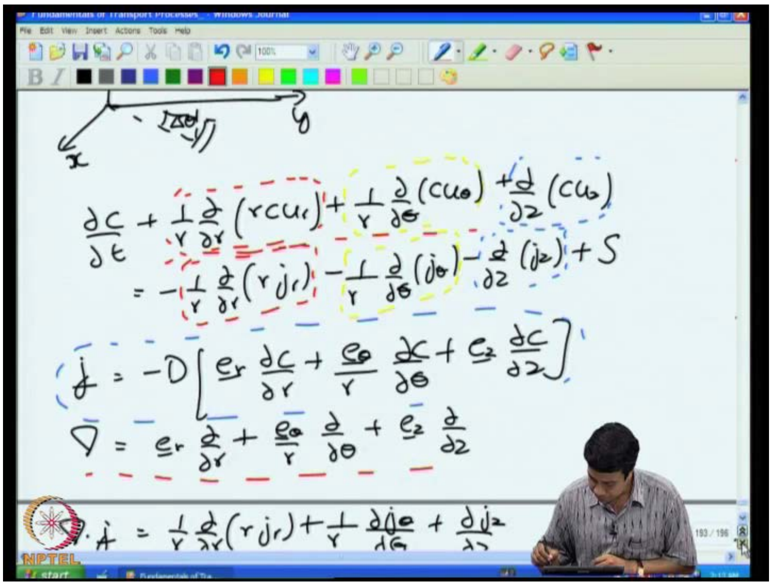

So this is the form of the operator in that particular coordinate system. One could work this out for other coordinate systems. For example, if you are solving an equation around an electrical particle you might want to choose an electrical coordinate system and standard expressions are are are available for these in each of these coordinate systems.

So, one would just write down the conservation equation in that particular coordinate system and then write down what are the boundary conditions for the particular system being considered.

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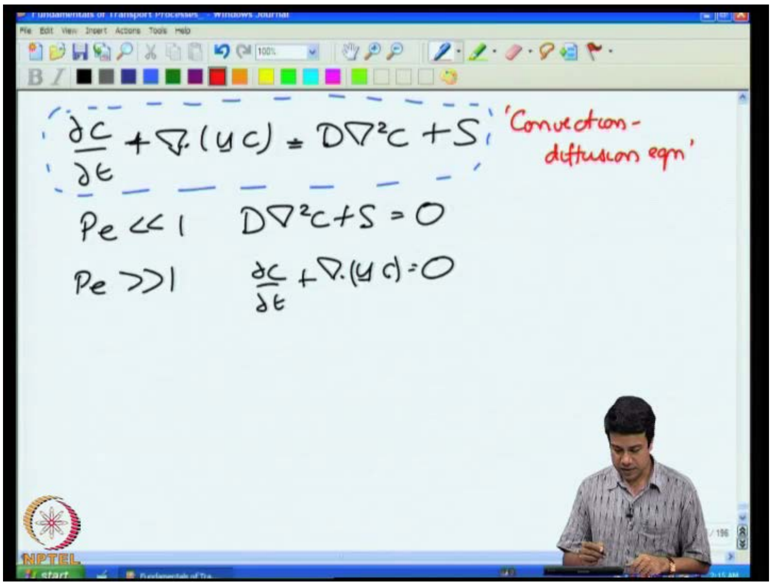

So, the next question is how do we go about solving these equations? This is the mass diffusion equation, the convection diffusion equation. This is a linear equation in the concentration field or the temperature field. So, provided the velocity is known this equation is linear in the concentration or temperature field. So, I can solve this in order to obtain concentration or temperature fields. However, it is a partial differential equation. It contains derivatives both in all three special dimensions as well as in time. Even if we considered a system at steady state, there would still be a partial differential equation with derivatives in all three spacial coordinates. Therefore, there are no general methods to solve this.

In order to solve this equation one has to have some physical insight into the nature of the problem. That physical insight is obtained as I said in the very first lecture by looking at the balance between convection and diffusion. Two processes for transport; convection due to the mean flow of the fluid, diffusion due to random molecular motion and a balance between these two is basically what determines the transport rates.

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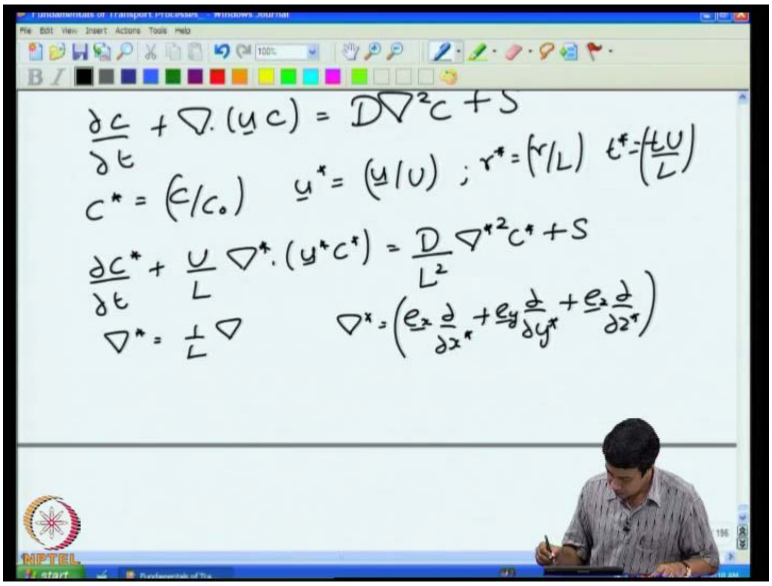

In this equation if I for example, scale I have an equation partial C by partial t plus del dot u C is equal to D del square C plus some sources or sinks; I can define a dimensionless concentration C by C naught where C naught is some characteristic concentration in the system. I can define a dimensionless velocity vector that is u by capital U. U is a characteristic velocity scale. If I had a flow in a pipe this could be the mean velocity or the maximum velocity. If I had a sphere moving in a fluid, this would be this sphere velocity the characteristic velocity and I can define the characteristic length scale r star is equal to r by capital L. Similarly, x y and z were all be scaled by this characteristic length scale and if I express this in terms of the differential equation in terms of this; I would get partial c star by partial t plus U by L del dot is equal to D by L square plus S where the scaled diversions the gradient operator is equal to 1 over L times grad where grad is the gradient operator.

So for example, in the Cartesian coordinate system del star will be equal to e x d by dx star plus e y d by dy star plus e z d by dz star where x star y star and z star are x by l y by l and z by l. Now, if I take this equation I have not scaled t yet. The natural scale for t is actually is equal to t times U by L because from the velocity u and the length scale l there is only one time dimension that I can get and that is L by U.

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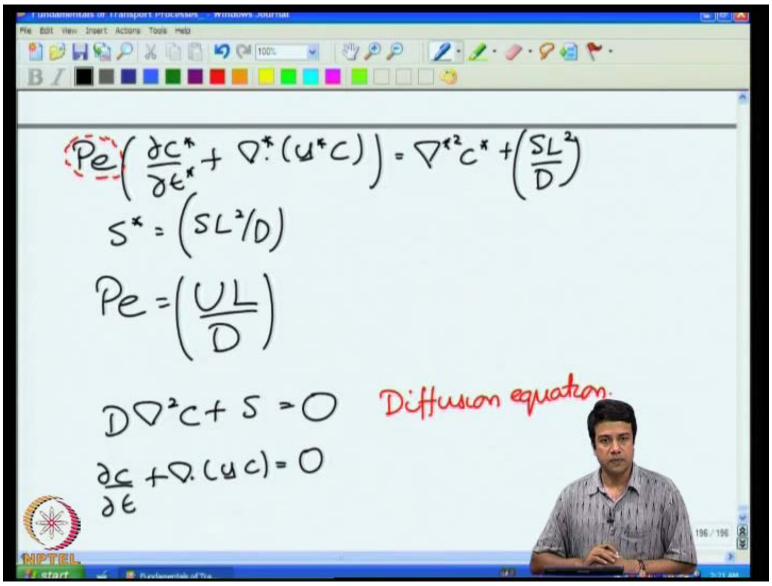

So if I express it in terms of this and divide throughout by L square by D what I will get is p e times dc by dt plus del dot u c is equal to del square plus S L square by D where this dimensionless source term is now S star is equal to S L square by D. So, I have an equation, a dimensionless equation now in which the left hand side has this dimensionless number where this dimensionless number p e is equal to U L by D.

So, this is the ratio of convection and diffusion in this equation. When this number is small then convective effects are small and the system is diffusion dominated. Locally there is a balance on every differential volume between the fluxes in and out due to diffusion or molecular motion. In that case you would expect that I can the the equations that I need to solve will be of the form D del square C plus S is equal to 0. In other words one can neglect convection in comparison to diffusion.

So this is the diffusion equation. On the other hand in the limit of high peclet number; one might think that one could just solve dc by dt plus del, del dot u c is equal to 0. One might think that this equation can now be solved it turns out not to be so. Especially near surfaces because ultimately when whenever transport takes place from a surface, the velocity at the surface itself has to be equal to 0 because of the no slip condition. There can be no velocity fluid, mean velocity perpendicular to the surface. That means that transport from the surface cannot take place by convection. Transport from the surface has to take place by diffusion alone and therefore, there has to be some small length scale over which there is a balance between convection and diffusion. Therefore, one cannot just solve this equation in the limit of high peclet number; one has to use more sophisticated technique where one takes into account the effect of diffusion very close to a surface. We will see a little later how one does that. The technique used there is called boundary layer theory.

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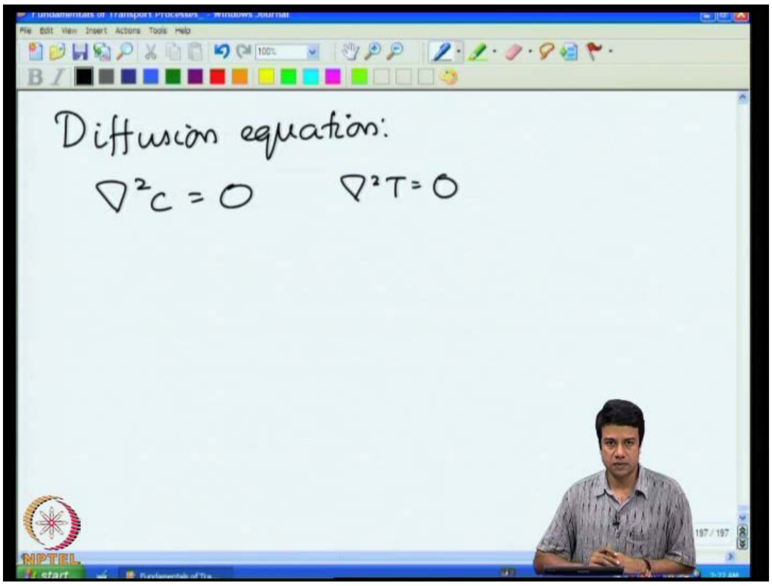

So first we will start solving the diffusion equation. The simplest equation del square C is equal to 0. If there are no sources or syncs within the field alternatively for heat transfer equivalent is del square T is equal to 0. So, the Laplacian of the concentration or the temperature field has to be equal to 0 in case there are no sources or sinks. We looked at how to solve this equation for a Cartesian coordinate system. If you recall we already did it the transport due to the heated cubic surface.

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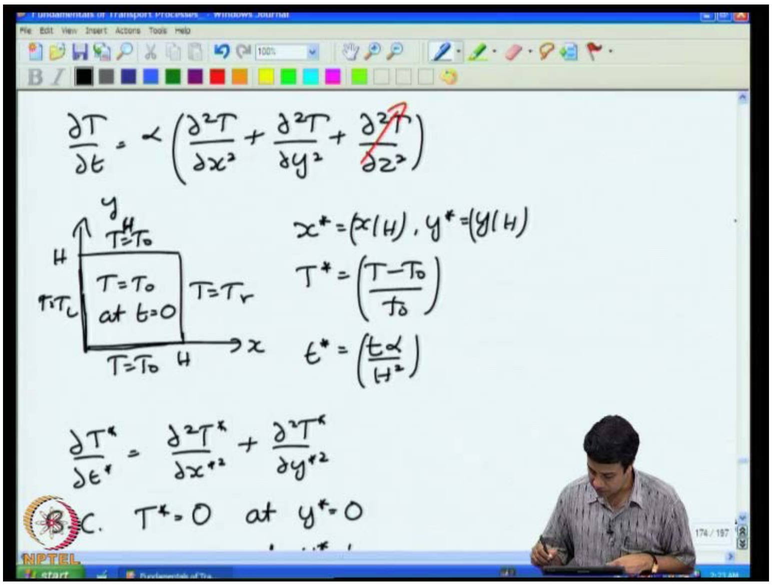

So, we had solved this problem of a heated cubic surface, unsteady problem partial T by partial T is equal to alpha times partial square T by partial x square plus partial square T by partial y square and first we had solved the steady state problem and the solution of the steady state problem was obtained by separation of variables.

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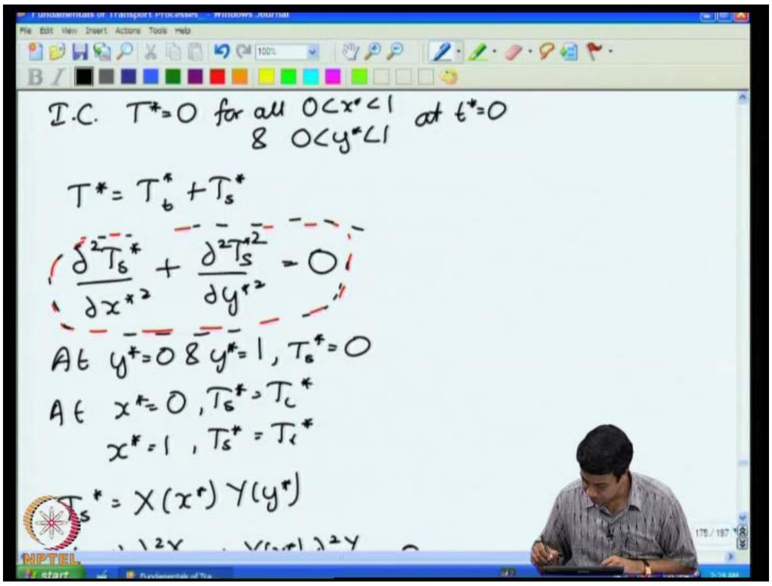

So, this was the steady state problem and we had obtained the solution by separation of variables. We had we had identified the homogeneous direction that was the y direction because there were homogeneous boundary conditions in that direction and the x direction was the inhomogeneous direction where they are boundary conditions were not homogeneous. So, in this case in the homogeneous direction, in the y direction we had got the solution in the form of basis functions sine n pi y star with Eigen values beta n is equal to n times pi.

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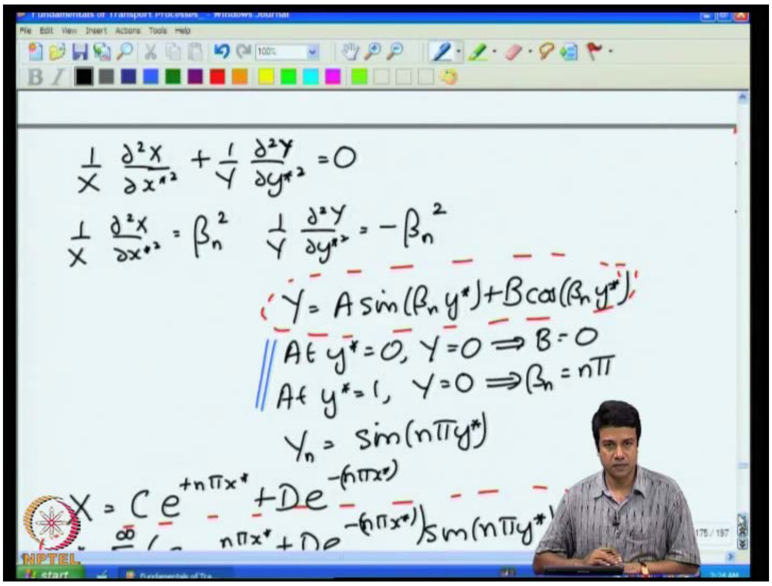

So, the homogeneous boundary conditions in the y direction had given us the values of the Eigen value in this direction and in homogeneous direction was the x direction. The coefficients in that x direction were subsequently determined from the boundary conditions using the orthogonality orthogonality relations here.

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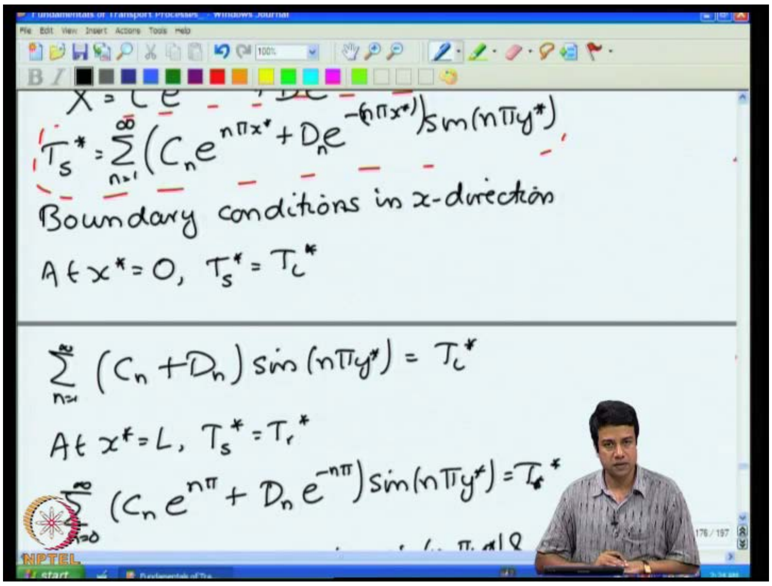

Now we will look at how to solve this in a spherical coordinate system. The procedure will be much the same. You will have to use separation of variables in a spherical coordinate system and we will look at what kind of solutions the separation of variables procedure provides us with.

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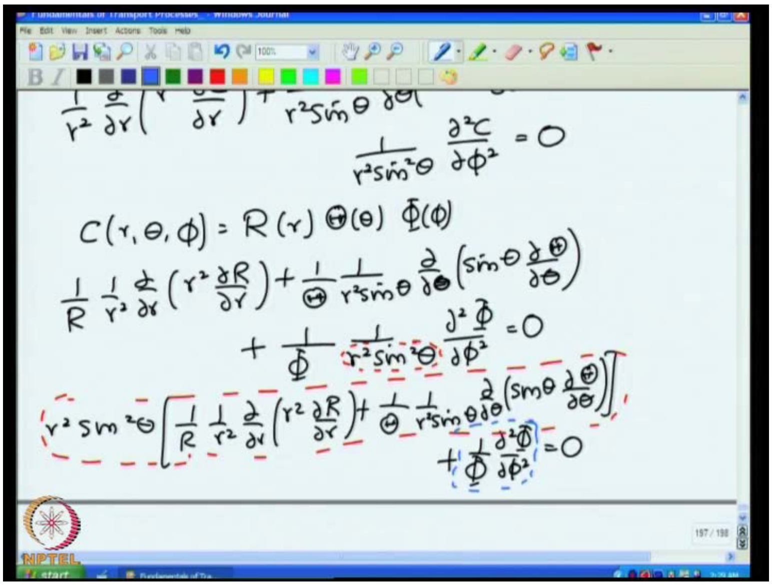

So, the conservation equation del square C is equal to 0 in spherical coordinates is given by 1 by r square d by dr r square partial c by partial r plus 1 over r square sine theta d by d theta sine theta partial c by partial theta plus 1 over r square sine square theta partial square c by partial phi square is equal to 0. So this is the equation. I would not specify boundary conditions for a specific configuration right now. But, rather I will look at what kinds of boundary conditions arise naturally from symmetry considerations.

So, I can use separation of variables and write concentration which is a function of r theta phi is equal to some function r of r, some function theta of theta, some function phi of phi. Separating the variables into their dependences on r theta and phi; insert this into the concentration equation and divide throughout by r times theta times phi. I will get 1 by R, 1 by r square d by dr of r square partial R ((no audio 19:22 to 20:08)).

So this is the conservation equation that we get in terms of r theta and phi a little more complicated than the equation that we got in terms of x y and z. That is it is not obvious from this equation how one would do a separation of variables. However it can be done. So, first thing is I multiply everything by r square sine square theta. Multiply all terms by r square times sine square theta. Then I will get r square sine square theta to 1 by R 1 by r square ((no audio 20:54 to 21:25)) is equal to 0.

So that is the final equation that I get and if we look at these terms here; this first term is only a function of r and theta. This first term here is only a function of r and theta the second term here is only a function of phi. The second term is only a function of phi. That means that both of these terms individually have to be equal to constants.

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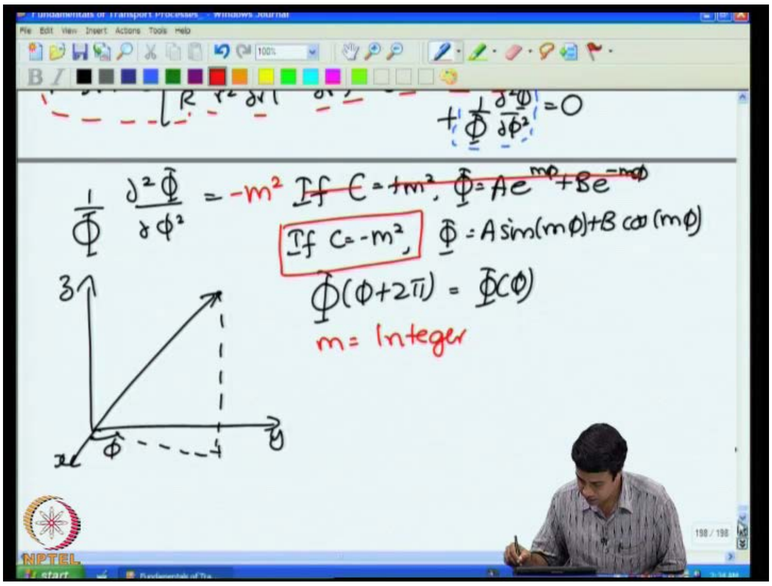

Now, the last term which is the function of phi is equal to a constant. 1 over phi d square phi by d phi square is equal to 0 is equal to a constant some constant C. As usual the question is the constant positive or negative. If the constant is positive then capital phi; if the constant is positive capital phi is equal to.

If the constant C is equal to plus m square; then capital phi is equal to A e power m phi plus B minus m phi. On the other hand the constant c is negative then phi is equal to A sine m phi plus B cos m phi. So, these are the two possibilities for the constant. Which one should it be? This is given by the physical consideration that in the phi coordinate. Note that phi is the angle made by the projection of the radius vector on the x y plane with the x axis when phi increases by an angle of 2 pi, we return to the same physical point in space. Therefore, I should get the exact same solution when phi increases by an angle of 2 pi because as far as the phi coordinate is concerned; it has increased by 2 pi when I have gone all the way around. However, the physical location in space is exactly the same when phi has increased by an angle of 2 pi. Therefore, we require that phi at theta at a physical boundary condition is that phi at phi plus 2 phi 2 pi is equal to value of capital phi at phi itself. And therefore, this is satisfied only if the solution if the constant is negative and if m is an integer.

So therefore, I get integer Eigen values in the phi direction just from the consideration that when I go around by an angle of 2 pi; I should return to the same physical location in space. That means that this one is the correct choice where m is an integer whereas this one is the wrong choice because if they are exponentially increasing or decreasing functions, the value will not be the same when you increase phi by 2 pi, an angle of 2 pi. So, just the, in this spherical coordinate system it is not the boundary condition that is giving me these integer Eigen values. It is the requirement that when I go around an angle of 2 pi I should return to exactly the same physical location in space. For that reason m has to be an integer and the constant has to be equal to minus m square where m is an integer.

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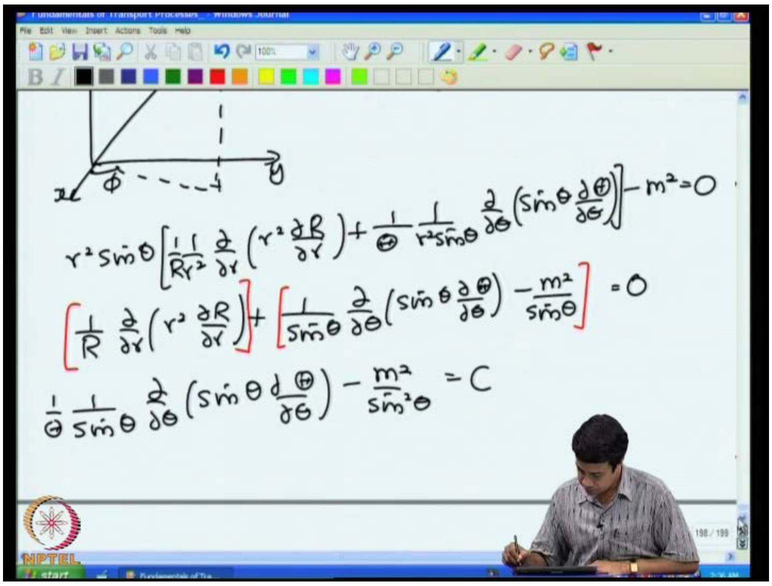

So, if I insert 1 over phi partial phi at partial phi is equal to minus m square in my equation what I will get is r square sine theta 1 by r square d by dr of r square dR by dr. There should be 1 over r there plus 1 over theta 1 over r square sine theta d by d theta of minus m square is equal to 0. I have inserted the value of 1 over phi d phi by d phi as m square. Once again this contains both r and theta in it but, however I can now divide throughout by sine theta. I can divide throughout by sine theta and I will get 1 over R d by dr of r square dR by dr plus 1 by sine theta minus m square by r square sine theta and now you can see that this term is a function of theta alone and this term is a function of r alone. That means that both of them individually have to be equal to constants.

Once again we will ask the question what should those constants be? Should they be positive or should they be negative? So, I should have 1 over sine theta d by d theta. Let me see is equal to some constant C. Now, in the phi direction, in the meridional of direction we have got the Eigen value from the consideration that if we go around by an angle of 2 pi, we should come back to the exact same location physically in space. In the theta direction there is a similar symmetry consideration which gives you discrete Eigen values and we will look at the reason for that as follows. First of all this is a little complicated.

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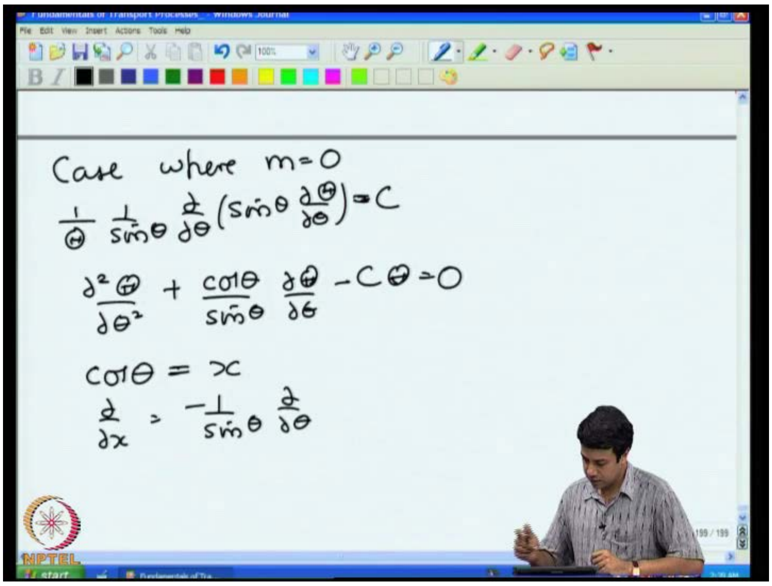

So I will just limit myself to consider the case where m equal to 0. Therefore, I get 1 over theta 1 by sine theta d by d theta of sine theta partial of theta by d theta is equal to C where C is a constant which is not known as yet and I can simplify this equation I will get partial square capital theta by partial theta square plus cos theta by sine theta partial theta by partial theta minus C times theta is equal to 0. I can simplify this equation a little by writing down cos theta is equal to some coordinate. Let me write cos theta is equal to x. This x is not the same as the coordinate x. It is just some variable that I am using. Cos theta is equal to x means that d by dx is equal to minus 1 by sine theta d by d theta.

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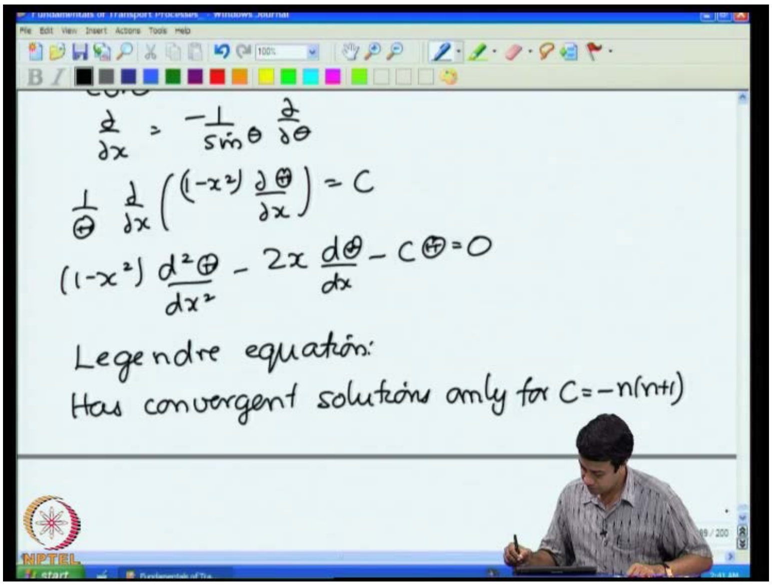

Therefore, in this equation I can write down one; I can rewrite this equation as 1 over theta d by dx of 1 minus x square d theta by dx is equal to C 1 over sine theta d by d theta is d by dx I have here sine theta times d by d theta which is sine square theta d by dx. Therefore, d I get d by dx of 1 minus x square d theta by dx is equal to a constant and if I expand this out I will get 1 minus x square d square theta by dx square minus 2x d theta by dx minus C theta is equal to 0. This equation is an equation for a special function called the Legendre equation and this equation has solutions which are convergent from minus 1 to plus 1 only if C has a specific form. That is only if C is of the form, only if C is equal to, has convergent solutions only for C is equal to minus n into n plus 1.

We will see how this particular convergent solution comes out and n is an integer. So, it has convergent solutions only if C is equal to minus n into n plus 1 and n is an integer. So, let us see how this convergence solution comes about. This case is (( )).

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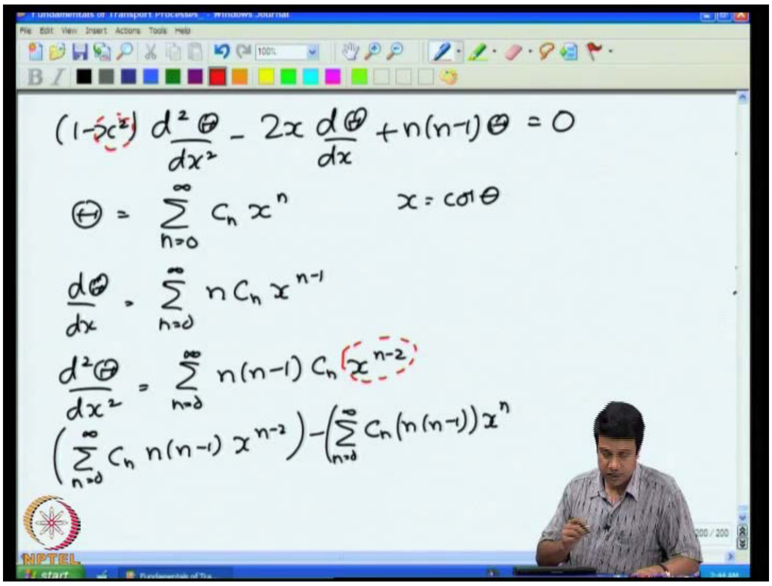

So let us take this equation 1 minus x square d square theta by dx square minus 2x d theta by dx plus n into into theta is equal to 0. Now, it is not possible to get an analytical solution of this equation but, one can get a good series solution by writing down theta of the form summation n is equal to 0 to infinity of some constant times x power n. Note that I have set x is equal to cos theta. In this particular coordinate system theta varies from 0 to pi.

Therefore, cos theta varies from minus 1 to plus 1. If I take a series of this form C n times x power n so long as x is smaller than 1 this will be a convergent series, so long as my coefficients do not diverge as n goes becomes large. So, because the modulus of x is less than 1 I can do this series expansion in this parameter x. Now, I then have d theta by dx is equal to summation n is equal to 0 to infinity, n C n x power n minus 1 and the second derivative is equal to summation n is equal to 0 to infinity, n into n minus 1 C n x power n minus 2.

So I substitute that into the differential equation. So, the first term is just d square theta by dx square. So, that is equal to summation n is equal to 0 to infinity C n n into n minus 1 x power n minus 2 minus x square into d square theta by dx square that is n is equal to 0 to infinity of C n n into n minus 1 x power n because the second derivative has x power n minus 2 here and for the second term I am multiplying this by x square.

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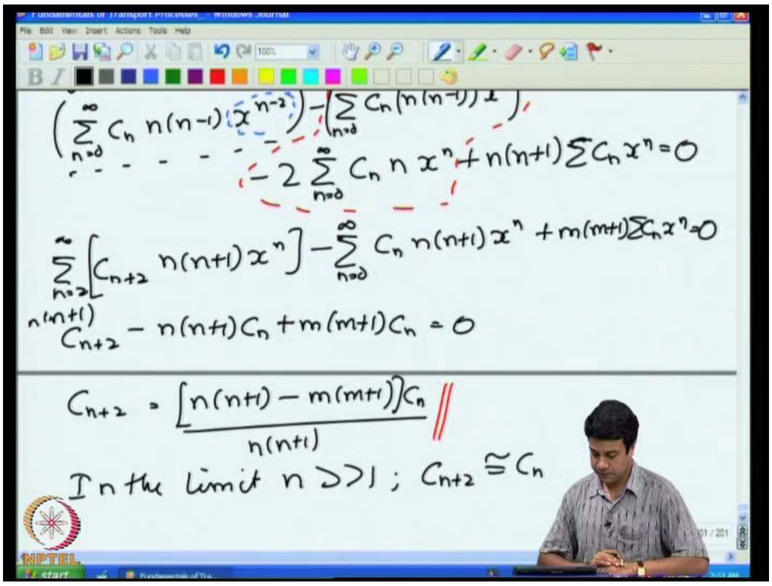

So I get back x power n and then I have with a third term here plus minus, minus 2 summation n is equal to 0 to infinity of C n into n into x power n because I have minus 2 x in 2 d theta by dx minus 2 x into d theta by dx and d theta by dx has C n x power n minus 1.

So I will get n into C n into x power n. Then I will get plus n into n plus 1 summation C n x power n this is equal to 0. Now, how do I get the coefficient C n? I get the coefficients by setting to 0 equal powers of x power n. You can see that all terms in this equation have power of x power n except for this first term here. This has a power of x power n minus 2. Therefore, what I need to do is to write down this as a series in x power n and you can do that of course, quiet easily. Summation n is equal to 2 to infinity C n n into n plus 1 I am sorry C n plus 2 n in this equation. I just set n is equal to n plus 2 n is an index that is being summed over in any case. Therefore, without loss of generality I can set n is equal to n plus 2 here in which case I had to have to some n n from 2 to infinity and in the other I just leave it as it is.

So this will become minus summation n is equal to 0 to infinity. These two terms can be combined, you can combine these two terms and once I combine those. What I will get is C n n into n plus 1 x power n. I am confusing here so let me just set this (( )). Since I have an index of addition n over here I do not want to confuse it with this constant. Therefore, I have set the coefficient is the constant to be equal to m instead of n because I do not want to confuse the index that I am adding over which is n in the series expansion with m which is the constant. Then here, I will get plus m into m plus 1 sigma C n x power n is equal to 0.

So, that is my differential, that is my equation for x and I can use this in order to determine the coefficient C n because I set each power of n in this expansion equal to 0. So, I have a series expansion if the entire series sums to 0 for all values of x then each power in that series has to sum to 0. Therefore, I will get C n plus 2 minus n into n plus 1 c n plus m into m plus 1 C n is equal to 0 or in other words C n plus 2 is equal to n into n plus 1 minus m into m plus 1 into C n.

So, this gives me C n plus 2 in terms of C n or for n going from 0 to infinity. In other words if I know what is C 0 and C 1 then I can determine C 2 C 3 C 4 etc all higher terms in the series. How about C 0 and C 1? Note that we were solving second order differential equation for x or for theta. Therefore, there are two constants which are determent from the boundary conditions. Those constants are C 0 and C 1.

So once those are known, then I can calculate all the higher constants C 2 C 3 etc. So, this should be, so this will give me total divided by n into n plus 1. So, note that as it is written down coefficient C n plus 2 is equal to n into n plus 1 minus m into m plus 1 divided by n into n plus 1 into C n. Please look at this equation. In the limit n large compared to 1; we find that in the limit n large compared to 1 note that the constant C is fixed and therefore, the constant m in this case is fixed in the limit as n becomes large compared to 1 what is going to happen is that C n plus 2, it is going to be approximately equal to C n because n is going to infinity m is finite.

So the higher coefficients all approximate to a constant value in the limit as n goes to infinity. So, I have a series solution I have a series solution and I find that as n becomes large; all the coefficients tend to a the same value. What is going to happen is that because this is a series solution in which all the higher constants they are not decreasing at x is equal to 1, this series is going to become infinite if C n is positive. If C n is negative at x is equal to minus 1 it will end up becoming infinite.

So, because I have a series solution in which the parameter x varies from minus 1 to plus 1 this entire summation and and I have the coefficient C n plus 2 by C n tending to 1 as n becomes large; this series will be will become infinite. So, there is no finite solution unless there is some value of n for which C n plus 2 is equal to 0. If C n plus 2 is equal to 0 for some value of n; then C n plus 4 is also equal to 0 C n plus 6 is also equal to 0 and the series terminates at that point.

So, the only way that the series will terminate at some value of n is if C n plus 2 is equal to 0 for that value of n and C n plus 2 will be equal to 0 only if n into n plus 1 minus m into m plus 1 is equal to 0 or m for some value.

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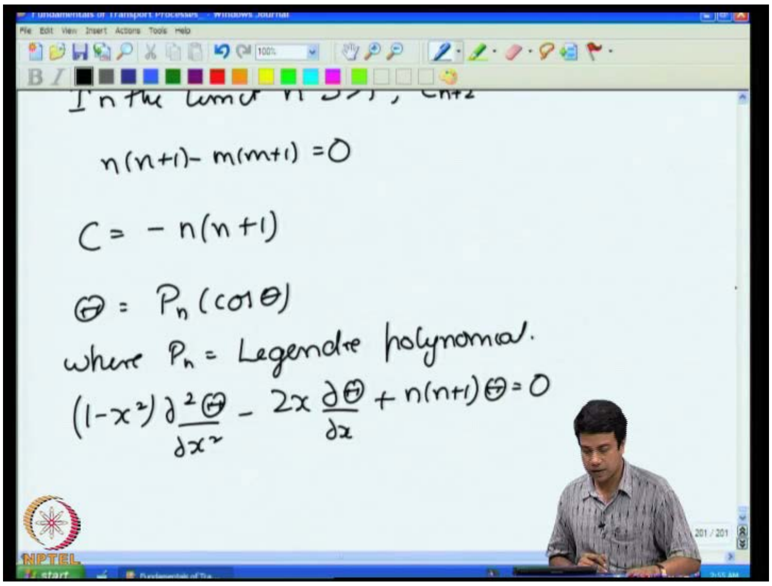

So, if I have some value for which n into n plus 1 is equal to m into m plus 1; at that point C n plus 2 is equal to 0 and automatically C n plus 4 is equal to 0 and all higher terms are 0 and the series truncates at that particular point. That can happen only if m is an integer. If m is not an integer, the series will not truncate. Therefore, the requirement that the series has to be finite itself gives you an integer value for the constant in the theta direction. The fact that the series has to terminate itself gives you an integer value for that constant in the theta direction.

Therefore, this implies that this constant that I had earlier C has to be equal to minus integer n into n plus 1 where n is an integer and for these integer values the solutions for the Legendre equations are of the form theta is equal to P n of cos theta where P n is equal to the Legendre (( )). So for for for this particular truncation of the series I will get an equation of the form 1 minus x square d square theta by dx square minus 2 x d theta by dx plus n into n plus 1 theta is equal to 0. This has a finite solution only if n is an integer and for this integer and this theta is in the form Legendre polynomials p n of cos theta.

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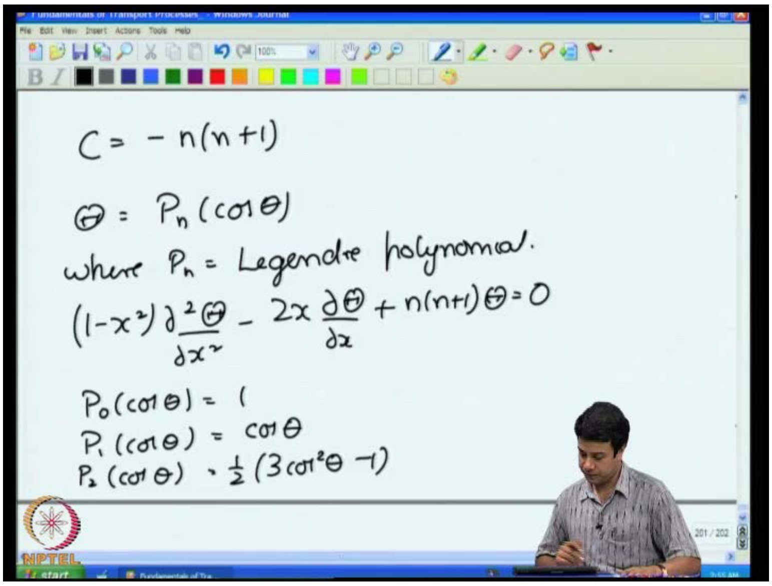

The first few terms are known. They are typically written as P 0 of cos theta is equal to 1, P 1 of cos theta is equal to cos theta itself, P 2 of cos theta is equal to half of 3 cos square theta minus 1 and so on.

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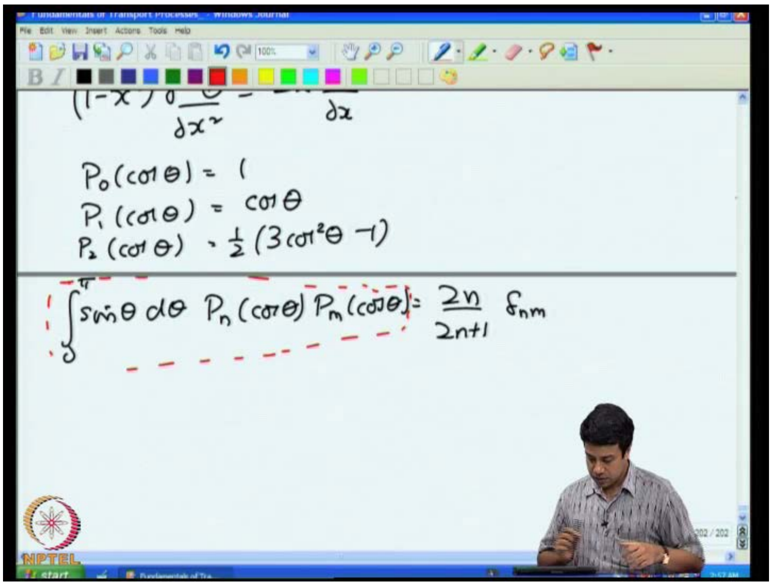

So P 2 is second order polynomial in cos theta, P 3 is a third order polynomial P 4 is a fourth order polynomial these are all chosen in such a way that P P n of cos theta is equal to 1 at theta is equal to 0 or cos theta is equal to 1. And these Legendre polynomials also satisfy orthogonality relations, integral sine theta d theta from 0 to pi, P n of cos theta into P n of cos theta is equal to 2 n by 2 n plus 1 times delta n m.

So, this enough product that is defined for the Legendre polynomials. This is the definition of the inner product for the Legendre polynomial expansions it is equal to 1 only if n is equal to m. That is you are multiplying two identical Legendre polynomials. If the Legendre polynomials are different then the product equal to is equal to 0 is non zero only if n is equal to m. So, they satisfy this orthogonality relation as well. This orthogonality relation can now be used to determine the boundary conditions when you solve the problem in a manner similar to the solution in Cartesian coordinates.

So, this I had solved only for the case where I did not have any dependence on phi for a particular case where m is equal to 0. For the particular case where m is equal to 0 I had solved this equation for you in order to get the value of the solution or the Legendre polynomials. What happens when m is not equal to 0?

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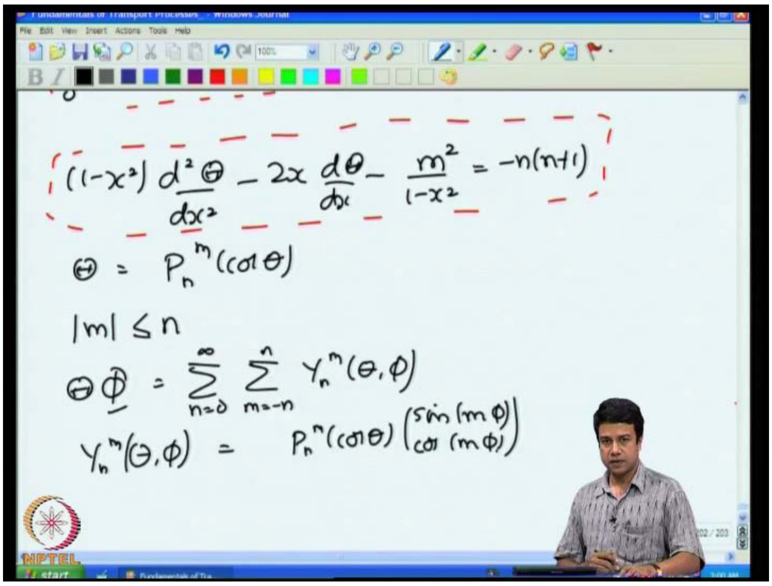

When m is not equal to 0; the equation becomes of the form 1 minus x square d square theta by dx square minus 2 x d theta by dx minus m by 1 minus x square is equal to 0. That is because I have an m by sin square theta here and I divide throughout by sin square theta I have m by sin square theta. This term, this has to equal to minus n into n plus 1 where n is an integer. The solution for this theta is equal to P n m of cos theta where solutions are convergent and exist only if the modulus of m is less than or equal to n. Therefore, m can vary only between minus n and plus n in this particular case.

So therefore, this additional restriction comes out of solving this entire equation this additional restriction comes out solving this entire equation in a manner similar a series solution similar to what we dealt further Legendre polynomials in the first case. Therefore, the solutions for theta and phi is often written as sum n is equal to 0 to infinity summation m is equal to minus n to plus n Y n m of theta phi where these spherical harmonics are combinations of P n m of cos theta as well as sin and cosine functions as well as sin and cosine functions.

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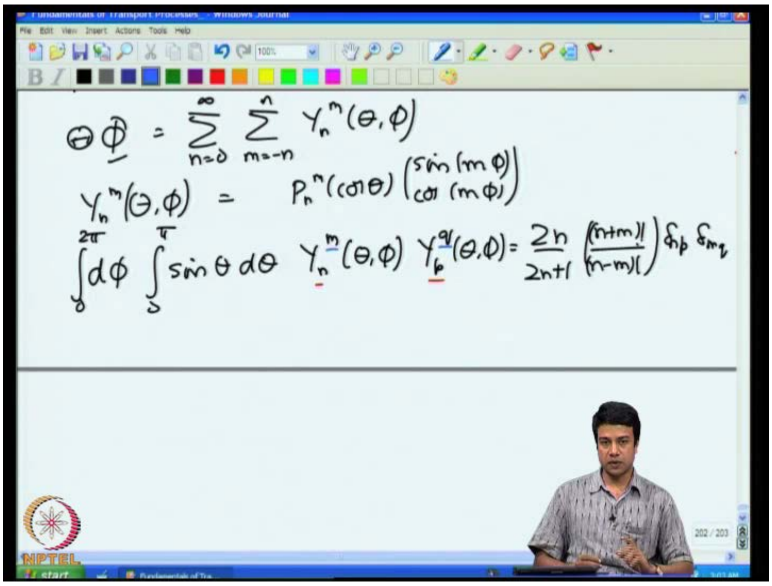

In such a way that these spherical harmonics also satisfy orthogonality relations integral d phi from 0 to 2 pi integral sin theta d theta from 0 to phi Y n m of theta phi Y p q of theta phi is equal to 2n by 2n plus 1 n plus m factorial by n minus m factorial times delta n p delta m q.

So, this integral is actually non zero only when n is equal to p and m is equal to q. So, this orthogonality relation basically tells you that two spherical harmonics are 0. The the inner product is 0 if both the coefficients n and m for the two are not the same and it is non zero only when both of those are the same. So, these spherical harmonics are defined as some combinations of P n m of cos theta times sine of m phi as well as cos of m phi.

So this is the orthogonality relation for the theta in the phi direction. As I told you in a spherical coordinate system in this particular problem I did not consider a specific value or specific boundary condition to apply. These, the the discrete Eigen values were determined primarily from the considerations of special symmetries in the phi direction if I go from 0 to 2 pi I should come back to the exact same location in space. That gave the coefficient as minus m square in the phi direction in the theta direction the requirement that the solutions have to be finite in the limit of theta going to 0 or cos theta is equal to 1 gave me discrete Eigen values n in the theta direction and solutions for the theta direction in the form of Legendre polynomial expansions. In the in the phi direction we got solutions in the form of cos and sine functions because when I go around by an angle of 2 pi I had to return to the exact same location in space.

So theta and phi solutions, the the orthogonal solutions in the theta and phi directions were obtained primarily from symmetric consideration not by specific reference to a particular problem with a particular set of boundary conditions. So, these are the solutions for the the Laplace equation obtained by separation of variables in a spherical coordinate system for the theta and phi coordinates. What about the radial coordinate? For the radial coordinate we still have to solve the operator form for the radial coordinate set at equal to 0 and find out what are the solutions in the radial coordinate.

So, we will start doing that in the next lecture and then I will try to solve a specific problem in order to give you a physical understanding how these spherical harmonic expansions work. So, we will continue with our solution of the Laplace equation for the temperature or concentration field in the next class and I will solve first for the radial coordinate and then we will look at a specific example. So, will see you in the next lecture.