Transport Processes I: Heat and Mass Transfer Prof. V. Kumaran Department of Chemical Engineering Indian Institute of Science, Bangalore

Lecture – 56 Diffusion equation: Spherical harmonic solutions

We continue our discussion on how to solve the diffusion equation welcome. We had previously solved it in a Cartesian coordinate system using separation of variables in that case the basis functions in the homogeneous direction were the sin functions if you have 0 temperature conditions at there, homogeneous boundary conditions. Equivalently if you had 0 flux condition it would be the cos functions those who satisfy the boundary conditions in the homogeneous direction. You then have to obtain the solution in the inhomogeneous direction and then solve in order to find out what are the coefficients from the boundary conditions in the inhomogeneous direction or the integral or the initial condition in the inhomogeneous direction.

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We had done that in a spherical coordinate system first I had done it for you for a very simple example of a simple spherical coordinate system, where there was a variation only in the radial direction and we had got the temperature fields. If you recall from this we had found that the Nusselt number has to be two in the limit as for the diffusion problem and then we had taken a slightly more complicated problem, which was the

effective conductivity of a composite which consisted of spherical inclusions. The fact that the thermal conductivity of the inclusion is in general different from that for the matrix implies that there is going to be a disturbance to the temperature field around the inclusions.

If there were no inclusions, the temperature field would just have been a linear function of position, but since there are inclusions the temperature field is disturbed around the particles that is going to cause a disturbance to their flux lines which were just vertical lines in the absence of any inclusions and therefore, change in the average flux; this calculation had two components: the first was to calculate the average flux in terms of the temperature distributions and then the second was to calculate the temperature distribution itself around a single particle. We had considered this in the non interacting limit, where the temperature field around one particle does not affect the temperature disturbance around another particle.

The fact that disturbing the temperature at one location that disturbance decays sufficiently fast that it does not affect the temperature at another location. So, we had written the flux as a volume averaged flux over the matrix and the particles, it is more convenient if you write this flux in terms of an integral of the matrix conductivity times the temperature gradient over the entire system, plus over the particles alone since the conductivity is different, the difference in conductivity times the temperature gradient on the particles alone.

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Effective conductivity of a composite: $\langle q_2 \rangle = \frac{1}{\sqrt{\int}} \int_{V} dV \left(-\frac{k_m \delta T}{\delta \lambda} \right)$

The advantage of doing it in this manner is that the first term just reduces to an average of the gradient over the entire volume that has to be of course, equal to the applied temperature gradient; because the average subsequent over the entire volume has to reduce to the applied temperature gradient.

The second part was an integral over the particles alone, the difference in conductivity times the temperature gradient within the particles alone. Since these are non interacting, the temperature disturbance of one particle does not affect the other particle this integral consists of n identical contributions over a single particle, where n is the total number of particles and I reduced it to the integral over one particle. Now we had to find out the temperature gradient within a single particle, which was placed in a temperature field which had the linear temperature gradient far from the particle.

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Temperature of particle in lineon 0.0 temperature graduint: -200 At r= (sin 0 JT Y2sm0

So, that was our next task how do you find the temperature gradient in one particle, which is placed in the temperature field which is a linear temperature gradient far from the particle and which also satisfies the temperature and the flux boundary conditions at the interface between the particle and the matrix; at the interface the temperature has to be the same on both sides because temperature has a unique value at each position.

Similarly, the flux leaving the particle has to enter the matrix therefore, the temp flux is perpendicular to the surface, the flux is perpendicular to the surface have to be equal for both the particle and the matrix and then we have the differential equation in this case there is no variation around the z axis it is ax symmetric, there is no variation of the phi direction and therefore, this is the differential equation.

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 $\frac{1}{r^{2}}\frac{\partial}{\partial r}\left(r^{2}\frac{\partial T}{\partial r}\right)+\frac{1}{r^{2}sm\theta}\frac{\partial}{\partial \theta}\left(sm\theta\frac{\partial T}{\partial \theta}\right)=O\left[\left(l-r^{2}\right)\frac{d^{2}H}{dr^{2}}\right]$ - 2x dH -- n(n+1) H $T = F(x) H(\theta)$ 2E 90 Sim ean

We had solved this using separation of variables, we had solved this using separation of variables by writing the temperature is some function of r times some function of theta. In the theta direction there are no physical boundaries, there is a coordinate boundary at theta is equal to 0 and theta is equal to phi.

The differential equation for this reduces to this form; this satisfies the homogeneous boundary conditions at 0 and pi that the temperature has to be finite at the coordinate boundaries because there is no physical boundary there. So, therefore, it satisfies those conditions only if this value is minus of n into n plus 1; where n is an integer and the solutions for these I said are of the form P n 0 of cos theta and these have orthogonality relations, if you multiply P n 0 of cos theta, P n n 0 of cos theta times sin theta d theta the result is nonzero only when n is equal to n; that is the solution in the homogeneous direction.

In this case the homogeneous direction does not have a physical boundary, it has only coordinate boundaries at theta is equal to 0 and theta is equal to pi.

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 $\frac{1}{\gamma^{2}}\frac{d}{\partial r}\left(\gamma^{2}\frac{\partial T}{\partial r}\right)+\frac{1}{\gamma^{2}s_{HO}}\frac{d}{\partial \theta}\left(sm\theta\frac{\partial T}{\partial \theta}\right)=O; \ Te\ F(r)H(\theta)$ 0.0.0 -n(n+r) = 0 $\frac{1}{F}\frac{\partial}{\partial x}\left[r^{2}\frac{\partial F}{\partial r}\right] + \frac{1}{Hsin0}\frac{\partial}{\partial \theta}\left(sm0\frac{\partial H}{\partial \theta}\right) = 0,$ = -n(nti) $\frac{\partial x}{\partial x} \left[\left(1 - x_{5} \right) \frac{\partial x}{\partial H} \right]$ $-2x\frac{\partial H}{\partial x}$ + n(n+1)H = 0 $H = P_{n}^{o}(x) = P_{n}^{o}(cot\theta) \frac{Legendre}{Legendre} \frac{hdynomiali}{hdynomiali}$ $\int dx P_{n}^{o}(x) P_{m}^{o}(x) = \frac{2}{2nH} \int sim \theta d\theta P_{n}^{o}(cot\theta) P_{n}^{o}(cot\theta)$

Then we got the solution for the radial direction and the total solution for the temperature field was a summation of P n 0 of cos theta, times two functions in the radial direction one is increasing with r r power plus n; the other is decreasing with r 1 by r power n plus 1.

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rnei $= T' r c d \theta = T' r P'(c d \theta)$ T= T'2 As r -> 00, AtraR, T A. + B. P. (core); Asr n=1

Now, if you look at the boundary conditions, the boundary condition contains P 1 0 of cos theta. So, I have the solution it contains various terms P 0, P 2, P 3 etcetera; each of these is independent because each legendre polynomials orthogonal to each other

legendre polynomial therefore, what I can do is to solve what I can do is to first of all to expand the boundary conditions as well in the legendre polynomial expansion, the equation is a superposition of different legendre polynomials, in a similar manner I can expand out the boundary conditions in the legendre polynomial expansion as well. In that expansion there is a forcing function only for n is equal to one the forcing function for n is equal to 0 n is equal to 2, n is equal to 3 etcetera are all 0.

So, therefore, if this is the solution and I write down the solution individually in terms of each Legendre polynomial, only for n is equal to 1 will there be a nonzero value as r goes to infinity. So, all others for n is equal to 0 2 etcetera, the value of the temperature the component of the temperature which is the coefficient of P 0, P 2 etcetera that component will be 0 as r goes to infinity and at the surface we have these two boundary conditions: if the temperatures are equal and the fluxes are equal. If this forcing term is 0 if this forcing term is 0 then temperature is equal to 0 everywhere satisfies all the boundary conditions and that forcing term is equal to 0 for n is equal to 0, n is equal to 2, n is equal to 3 etcetera.

So, for all of those these constants will both be 0, it will be nonzero only for n is equal to 1 because that is the only contribution for which I have a nonzero forcing term. Just from the symmetries I can straightaway say that the solution has to be of the form A 1 times r plus B 1 by r square P 1 0 of cos theta because the forcing for all other legendre polynomials are identically 0 because they are all orthogonal to each other. The forcing is of their form P 1and therefore, the forcing for all other Legendre polynomials has to be equal to 0 because they are all orthogonal to each.

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 $T_{p} = \begin{pmatrix} A_{p}r + i\underline{B}_{k} \\ r^{2} \end{pmatrix} P_{i}^{*}(col \theta) \qquad T_{m} = \begin{pmatrix} A_{m}r + \underline{B}_{m} \\ r^{2} \\ r^{2} \end{pmatrix} P_{i}^{*}(col \theta)$ $A\ell r = 0, T_{b} = finite \implies B_{p} = 0 \qquad As r \rightarrow \infty, T_{m} = T'r col \theta \Rightarrow A_{m} = T'$ $T_{m} = T'r col \theta + \begin{pmatrix} B_{m} \\ r^{2} \\ r$ At r=R, $k_{b}\frac{\partial T_{k}}{\partial Y} = k_{m}\frac{\partial T_{m}}{\partial Y} \Longrightarrow A_{b} = T' - \frac{2B_{m}}{R^{3}}$ $A_{b} = \frac{3T'}{2+K_{R}}$, $B_{m} = \frac{(1-K_{R})T'R^{3}}{2+K_{R}}$ where $K_{R} = \frac{(k_{b})}{k_{m}}$ $T_{p} = \frac{3T'rcd\theta}{2+K_{R}}$, $T_{m} = T'rcd\theta + \frac{(1-K_{R})T'R^{3}}{2+K_{R}}cd\theta$

So, just from the symmetry and the orthogonality of the legendre of polynomials, we have managed to reduce the solution to just P 1 0 of cos theta in both the matrix and the particle and then I impose the boundary conditions in order to find out what is the matrix temperature and what is the particle temperature and with that I had gone back.

Now, that I have the temperature field I know what is the gradient and from that I got this non trivial result for the effective thermal conductivity of a composite material, in this dilute limit it is proportional to the volume fraction of the particles times K R minus 1; where K R is the thermal conductivity times this coefficient here. So, that was the solution for an axis symmetric coordinate system for an axis symmetric problem, where there was no variation in the temperature in the meridional or phi direction

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12 smo de (smo dT)+ $\begin{pmatrix} r^2 \partial T \\ \partial r \end{pmatrix}$ 21 r25m20 20 F(x) H(O) AD

Now, what about the general case, how would I go about solving the equation for the general case? I will just outline it for you here equations of the form 1 by r square d by d r of r square d T by d r, plus1 by r square sin theta. So, that was the original equation and that was the coordinate system.

For any general coordinate system what I would do is to write down the temperature using separation of variables, how do I go about doing that? First thing is I can write the temperature first separate out the phi separation of variables, F of r H of theta and I have one more term which is P of phi. Insert it into this equation and divide throughout by F H P. So, first time I will get 1 by F r square. Now this is still not in a variable separable form so what I can do is multiply throughout by r square sin square theta. So, you have multiply it throughout by r square sin square theta, here I will get sin squared theta into 1 or F; in this equation the first term depends only upon r and theta the second term depends only upon phi therefore, each of these individually has to be a constant.

So, take the phi dependence first. This equation of the form 1 over P partial square P by partial phi square is equal to some constant alpha. Depending upon the sin of alpha you will either get P is equal to A e power e power alpha phi, plus B e power minus alpha phi if alpha is positive. If on the other hand alpha is negative if I write this as minus m square, P will be equal to A cos of m phi plus B sin of m phi, which of these should we choose? Should we choose a positive constant or a negative constant? That comes out of the symmetry of the problem.

In the meridional direction in the phi direction there is no physical boundary, when you go from phi if you increment phi by 2 pi, you come back to the same physical location in space. If you increment phi by 2 pi, you will go all the way around the axis and you will come to the same location physical location in space. So, the coordinate has been incremented by a value of 2 pi, the location in physical space is exactly the same therefore, the temperature at that location has to be exactly the same. You cannot enforce that that you can do the same physical location when phi increases by 2 pi, if you use exponential functions because we increase exponential by a value of 2 pi, it does not give you the same result; you can enforce it in the case of sin and cosine provided m is an integer.

So, the requirement that when you increment phi by 2 pi, you have to come to exactly the same physical location in space implies that these 1 by P times d square t by d phi square has to be negative and it has to be minus m square where m is an integer. So, just the fact that there is no physical boundary the coordinate boundaries at 0 and 2 pi have to be exactly the same means that phi has to have this form. So, this gives us the Eigen function for phi, you could write it when is equal to minus m square you could write it as I have said a sin m phi and b cos m phi, the simpler way to write it is some complex constant as e power i m phi. If I have some complex numbers times e power i m phi, the real part of that will be cos imaginable be part of the sin. So, both of those are included within this function ok.

Therefore the fact that you do not have a physical boundary in the meridional direction imposes discrete set of Eigen values minus m square where m is an integer. So, therefore, for the rest of the equation I now have to solve, I have got one Eigen value m and integer an Eigen function e power i m phi therefore, I can solve for the rest of it. I know that sin square theta into 1 over F d by d r of r square d F by d r, plus 1 over H sin theta d by d theta of sin theta d H by d theta, minus m square has to be equal to 0 because this was equal to minus m square where m is an integer.

How I solve this I divide throughout by sin square theta. So, first time I will get 1 over F d by d r of r square d F d r plus. So, now, in this equation this first term is only a function of r and these two terms it only a function of theta therefore, each of these individually has to be equal to a constant each of these individually has to be equal to a constant, what constant should it be? Let us first look at the theta equation, the theta equation has the

form d by d theta of minus m square by sin theta into H is equal to some constant is equal to some constant alpha into H.

So, I set this entire term equal to a constant and then multiply it throughout by H to get this equation. When m was equal to 0, I told you that this equation could be reduced to the form d by d x of 1 minus x square, partial H by partial x is equal to alpha times H that was when m was equal to 0 where x is cos theta, in this case when m is not equal to 0 I will get minus m square by 1 minus x square into H is equal to alpha times H. when m was equal to 0 when it was an axisymmetric problem, I told you that the solution is finite at theta is equal to 0 and theta is equal to pi only if this constant has the form minus n into n plus 1, that applies in this case as well with one modification.

I told you that one m was equal to 0, this was valid only when n was an integer when this term was not present previously for the axisymmetric case. In this case the condition that the solution has to be finite at theta is equal to 0 and theta is equal to pi the condition that the solution has to be finite, still implies that n has to be an integer n has to be an integer, but also that n is greater than or equal to the magnitude of n ok therefore, minus m less than n less than m. If n is an integer if it is a positive integer then m can only go from 0 to n.

So; that means, that if n is equal to 1 then m can be minus 1, 0 and plus 1. Where n is equal to 2 the m can be minus 2, minus 1, 0 plus 1, plus 2 etcetera with this the solution in the theta direction the solution in the theta direction will turn out to be.

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 $H(\theta) = P_n^m(cd\theta) P(\phi) = e^{im\phi} \int_{3\pi/\theta}^{3\pi/\theta} d\theta P_n^n(cd\theta) P_n^m(cd\theta) = \frac{2}{2n+1}$ $\frac{1}{1} \frac{\partial}{\partial t} \left(\frac{1}{2} \frac{\partial}{\partial t} \right) = -n(n+1)$ = -n(n+1) $\frac{1}{1} \frac{\partial}{\partial t} \left(\frac{1}{2} \frac{\partial}{\partial t} \right) = -n(n+1)$ = -n(n+1) = -n(n+1) = -n(n+1) = -n(n+1) $T = \sum_{n=0}^{\infty} \sum_{m=n}^{n} \left(A_n r^n + \frac{B_n}{r^{mr}} \right) \frac{Y_{nm}(\theta, \varphi)}{r}$ Heat conduction from a sphere: $T = T_0 + \frac{Q}{4T_0 r} \Rightarrow n = 0$ Sphere in Unior tomp gradient: $T = \left(A_1 + \frac{B}{r^2} \right) \frac{P_0^0(cd\theta)}{r^2}$

H of theta is equal to P n m of cos theta and P of phi was equal to e power i m phi therefore, the product they call the spherical harmonics theta and phi, turns out to be of the form p n m of cos theta e power i m phi. Note that n is an integer and m goes from minus n. So, for n is equal to 0 m is equal to 0, for n is equal to 1, m is equal to minus 1 0 plus 1; for n is equal to 2, m is equal to minus 1 2; minus 1 0 plus 1, plus 2 etcetera.

So, those are the solutions in the theta and phi directions and finally, we have to come to the solution in the radial direction. That solution in the radial direction we know that this term here as got to be equal to minus n into n plus 1. So, solution in the radial direction is of the form and this we have already solved F is equal to A n r power n plus therefore, the most general solution for the temperature field is of the form sigma n is equal to 0 to infinity, sum over m is equal to minus n to plus n, A n r power n plus. Note that while we were solving these we had applied homogeneous boundary conditions in the theta and the phi directions, when we are solving this we had applied homogeneous boundary conditions in the theta and the phi directions.

Therefore these spherical harmonic solutions satisfy orthogonality relations; just in the previous case P 1 P n 0 in the previous case we had integral sin theta d theta P 1 0 of cos theta, P m 0 or cos theta is equal to 2 by 2 n plus 1, that was for the axis symmetric problem where m was equal to 0; when m is equal to 0 e power i m phi is 1 and therefore, there is no variation in the phi direction, this was from 0 to pi. Similarly the

spherical harmonics satisfy orthogonality relations as well, in this case you go from 0 to 2 pi in the phi direction; because in the meridional direction you go from 0 to pi, in the azimuthal direction you go from 0 to pi, plus z axis's theta is equal to 0 minus z axis is theta equals pi, sin theta d theta times if you take any two of these Y n m of theta phi, Y n prime m prime of theta phi, these are nonzero only when m is equal to n prime and when m is equal to m prime otherwise it is zero. So, it is nonzero only when n is equal to m prime and n is m is equal to n prime and the value is 2 by 2 n plus 1 into n plus m factorial by n minus m factorial. So, each of these spherical harmonic in the theta and phi directions is orthogonal to every other.

So, each value of n and m you have two solutions in the radial direction: one of which is increasing as a function of r and it is called the growing harmonic, the other one is decreasing as r goes to infinity that is called the decaying harmonic. So, this is the general solution for the conduction equation in a spherical coordinate system. I had explained to you what this spherical harmonic what the Legendre polynomial expansion means in the context of an axis symmetric problem in the previous lecture.

In the following lecture I will try to give you some physical insight into what these spherical harmonic expansions mean. If you recall when we did the problem of the heat conduction from a sphere, a heat conduction from a sphere T is equal to T infinity, plus Q by 4 pi k r; this corresponding to this solution for n is equal to 0, because for n is equal to 0 the growing harmonic is just a constant r power 0, the decaying harmonic goes as 1 over r and there is no dependence on theta and phi, p 0 was 1 and when m is equal to 0 there is no dependence on theta or phi therefore, this corresponded to the solution for n is equal to 0.

Similarly, for the case of the heat conduction for T was of the form A r plus B by r square, P 1 0 of cos theta, this corresponds to n is equal to 1, r power n is r and 1 over r power n plus 1 is one over r square; n was equal to 1 and m was equal to 0 for the second problem that we had solved.

So, these are all terms in this expansion. So, the first term corresponds to just the zeroth n is equal to 0 corresponds to just an isotropic problem spherically symmetric heat conduction, the T is equal to the n is equal to 1 corresponds to heat conduction with a linear gradient along the z direction, what do the other terms correspond to? I will give

you some physical insight into what these terms mean, when we continue with the next lecture I will see you then.