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

# Lecture – 55 Diffusion equation: Effective conductivity of a composite

In the last lecture, we were discussing the effective conductivity of a composite material which consists of spherical particles embedded in a matrix, this we had taken up as an illustration of the solution of the diffusion equation, diffusion dominated transport in A spherical coordinate system and I was using this to illustrate for you how we can do the separation of variables procedure in a spherical coordinate system for this particular problem.

So, we had spherical particles of radius r in the matrix in which there was an imposed temperature gradient in the z direction. This imposed temperature gradient if there were no particles, the flux would just be equal to the matrix conductivity times the temperature gradient; however, since we do have particles here. The conductivity is going to be different from just the matrix conductivity because the presence of the particles distorts the heat flux lines. If the particles are not present, the flux would just be along the z direction; however, since there are particles present there is going to be a distortion of the flux.

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As I showed you in the previous lecture, if the matrix particles had a higher conductivity, the flux lines would come in towards the particles whereas, if it had a lower conductivity it would go out. We had written the average flux as a volume average of the flux over the entire volume, which basically includes the matrix and the particles. So, we have to take the flux over the matrix and the flux over the particles. Over the matrix, we know that the matrix conductivity is just equal to k m whereas particle conductivity is equal to k p that has to be multiplied by in individual temperature gradients within the matrix and within the particle in the z direction.

I had rewritten this as 2 contributions one over the entire volume of the matrix conductivity times a temperature gradient. The other over the particles alone of the difference in conductivity between particles and matrix times the temperature gradient. This makes sense because the matrix part is what would have been there if there were no particles present and the particle part is the additional contribution either positive, if the particles are more conductive or negative whose particles are less conducting in comparison to the matrix.

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The matrix part of course, is I mean the volume average over the entire volume of course, gives me back the temperature gradient that was imposed because the volume average of the temperature grade has to be equal to be imposed temperature gradient and then I was reduced to finding out the integral over the particles of the change in

conductivity times the temperature gradient within the particle, if the difference between the particle and the matrix conductivities. Since you are considering the non interacting limit where the temperature around one particle is not affected by all the other particles, I wrote this as the total number of particles times the integral over one particle of the temperature gradient in the z direction in that particle and this final term is what we were trying to evaluate in a spherical coordinate system in the previous lecture.

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Temperature of particle in linear 0.0 24 temperature graduint: T= T'2:= T'r (0)0 At r= Smost 3

So, we have to solve the conservation equation in a spherical coordinate system with the boundary condition that the temperature far from the particles is a linear gradient in the z direction, at the particle surface the temperatures are equal in both the particles and the matrix and the fluxes perpendicular to the surface are equal because what leaves the particles has to invariably go into the matrix and outs line for you.

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 $\frac{1}{r^{2}}\frac{\partial}{\partial r}\left(r^{2}\frac{\partial T}{\partial r}\right) + \frac{1}{r^{2}sm}\frac{\partial}{\partial \theta}\left(sm\theta\frac{\partial T}{\partial \theta}\right) = O\left[\left(1-r^{2}\right)\frac{d^{2}H}{dr^{2}} - 2x\frac{dH}{dr} = -nhH\right]H$ 1241 T= F(+) H(0 p'(x) P (r 67 2ntl Sint 90 sinodo -x2) 2H )x XH Legendet ean

The separation of variables procedure for solving this problem, you separate variables into a function of the radius times a function of theta theta in a spherical coordinate system goes from 0 along the plus z axis to pi along the minus z axis. For the theta coordinate alone after doing the separation of variables we got an equation in which there were two terms, one is only a function of r and the other is only a function of theta both have to be constant. In the theta direction we get an equation which is in the form of a Legendre equation. This equation has finite solutions at the coordinate boundaries at theta is equal to 0 and theta is equal to pi that finite solutions at those coordinate boundary only if this constant is equal to minus n into n plus 1 where n is an integer.

You can show that I will not go through because it is a subject applied mathematics, but you can show analytically by serious solution that these solutions exist only if n is an integer and the solutions are of the form P n 0 of cos theta, the superscript 0; I will come to a little later. I wrote down for you the first few of these P 0, P 1, P 2 etcetera these are all polynomials P n is a polynomial for an n; P 0 is just 1, P 1 is equal to x itself or cos theta itself P 2 these three cos square theta minus 1 by 2 and so on and these satisfies the orthogonality relations that if you multiply any 2 of these and integrate over the domain in x from minus 1 to 1, you get a non zero value only when n is equal to n.

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So, that is a solution the theta direction; this direction by default was the homogenous direction because even though there was no physical boundary there are coordinate boundaries and along those coordinate boundaries, you require that the solution has to be finite so that the homogenous direction in this case alternatively the derivative of the solution with respect to theta has to be 0. We solved in the other direction, in the r direction because we know from the theta equation that this constant is n into n plus 1. So, we put that in the r direction and we got the solution as power loss, so the total temperature field was equal to A n times r power n plus B n by r power n plus 1 P n 0 of cos theta.

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Now, the solution of the temperature field it is actually 0, so that was the solution that I had got. What are the boundary conditions, boundary conditions first one is that as r goes to infinity, T is equal to T prime z which is T prime r cos theta and since I told you that I had written down should make a slight correction here, I should drag this as P 0; 0, P; 1 0 and P 2, 0 in this case I told you that P 0; 0 of cos theta is equal to 1; P 1 0 of cos theta P 1 0 of x was x itself. So, P 1 0 of cos theta was cos theta P 2 0 of cos theta is equal to 3 cos squared theta minus 1 by 2 and so on. So, therefore, I can write this equivalent as T prime r into P 1 of cos theta because we know that P 1 of cos theta is equal to cos theta P 2 and P 3 and so on, you can extend the series by solving that equation by a series solution.

So, therefore, as at r goes to infinity the driving term, the inhomogeneous term is of the form P 1 of cos theta. Then at r is equal to r; you have T matrix is equal to T particle and k matrix times partial T matrix by partial r is equal to k particle times partial T particle by partial r and the solution is of this whole . So, now, I can separate out the solution into different components for n is equal to 0, n is equal to 1, n is equal to 2 etcetera and solve using boundary conditions for each one of them. If you look at the solutions for n is equal to 0, n is equal to 0, n is equal to 0; I have A 0 plus B 0 by r into P 0, 0 of cos theta; it is the solution.

As r goes to infinity right, the temperature T is equal to T prime r P 1; T prime r times P 1 0. So if actually what to calculate the boundary condition for P 0 that would be 0 because this forcing at infinity is of the form P 1, if you have P 1 and P 0 are orthogonal to each other. So, therefore, the forcing in the P 1 Legendre polynomial does not result in any contribution to the 0 Legendre polynomial because these are orthogonal polynomials, the forcing has to be equal to 0 therefore, for P 0; far from the surface.

And then I have the boundary conditions that T m is equal to T p and k m partial T m by partial r is equal to k p, partial T p by partial r. These boundary conditions are effectively they do not; they are homogeneous, there is no forcing in these boundaries it just states the temperature on both sides is equal and the flux on both sides is equal. The disturbance to the temperature field which results in a non zero temperatures around the particle comes from the forcing far from the surface, that forcing this is the form P 1 of cos theta, that forcing does not appear in the equation at n is equal to 0. So, the forcing does not appear in the equation at n is equal to 0 is identically equal to 0, it satisfies all the boundary conditions because there is no forcing as r goes to infinity and 0 temperature actually satisfies these two conditions.

If I assume n is equal to 0, for the first term in the expansion. As I said all of these Legendre polynomials are all orthogonal to each other. So, therefore, I can always decompose these; for n is equal to 0, n is equal to 1, n is equal to 2 and so on, decompose the boundary conditions also for n is equal to 0, n is equal to 1, n is equal to 2 and so on; solve each of those individually and then add them out to get the solutions.

Because each 1 of these is orthogonal, if I integrate multiply one solution by the Legendre polynomial of some other order and then integrate I will get 0 as a result. So, for n is equal to 0, so if the forcing is 0 as r goes to infinity and these boundary conditions just relate the temperature and the flux at the surface, if the temperature were 0 all of these conditions would be satisfied, this is a linear equation. Therefore, there should be only one solution and that solution is the 0 solution because there is no forcing in the equation and n is equal to 0.

Let us take n is equal to 1, the solution is of the form A 1 r plus B 1 by r square, P 1 0 of cos theta. This is the solution in both the matrix and the particle; the constants will be different of course, in the particle and matrix, but the solution will be of this form. As r

goes to infinity, I have T is equal to T prime; r P 1 of cos theta and then I have T m is equal to T p, k m partial T m by partial r is equal to k p, partial T p by partial r. Now this has a non trivial solution because I have a non trivial forcing in the P 1 Legendre polynomial, therefore, this will have a non trivial solution.

I cannot just use temperature is equal to 0 as the solution because it does not satisfy this boundary condition in the limit as r goes to infinity. Similarly if I were to do it for n is equal to 2 for example, and so on, I will get A 2 r square plus B 2 by r cubed, P 2 0 of cos theta. For this, once again the forcing is 0 because the forcing is of the form P 1 of cos theta, it is just orthogonal to P 2. So, as far as the P 2 symmetry is concerned, the forcing is 0, so basically I have T is equal to 0 as r goes to infinity.

Then I have the homogenous boundary conditions; T m is equal to T p, 0 temperature satisfies all of these conditions as well and so on for all other orders n. So, since the forcing has the symmetry P 1 0 of cos theta, it projects only onto the P 1 Legendre polynomial solution it projects onto the solution only for n is equal to 1; all of these harmonics are all orthogonal to each other this forcing projects only on to the solution at n is equal to 1 for n is equal to 0, 2, 3 etcetera this forcing is equal to 0.

Therefore, for 0, 2, 3 etcetera however forcing that is 0; I have boundary conditions which basically relate the temperature in the matrix and the particle and the flux in the matrix and particle. If the forcing is 0, all of these conditions are satisfied if the temperature or rather A 0 and B 0 here, if both of them are 0; all of these conditions are satisfied. Similarly if A 2 and B 2 are 0; all these conditions are satisfied that is because there is no forcing with symmetry of P 0, P 2 etcetera. The only forcing is with symmetry P 1 and since all of these Legendre polynomials are orthogonal to each other, the solution should also have the same symmetry.

So just based upon symmetries alone, we have to made the argument that only the term with n is equal to 1 has to be included in the solution because there is no forcing with symmetry of P 0, P 2 etcetera. All of these are all orthogonal to each other therefore, if the forcing the zone has a symmetry; P 1, all of the solutions also should have the same symmetry P 1, there is no forcing the symmetry P 2, P 0, P 2 etcetera because if I take the boundary condition and expand it out in a Legendre polynomial expansion, the only term that will be non zero is the one corresponding to P 1, the terms correspond because

they are all orthogonal the terms corresponding to P 0, P 2 etcetera will all be 0. Therefore, the solutions for the temperature 10 is equal to 0, 2 etcetera will all be 0 and that just comes out of this of the orthogonality of the Legendre polynomials.

 $T_{p} = \begin{pmatrix} A_{p}r + i \underbrace{B_{k}}_{r^{2}} \end{pmatrix} P_{i}^{*}(col \theta) \qquad T_{m} = \begin{pmatrix} A_{m}r + \underbrace{B_{m}}_{r^{2}} \end{pmatrix} P_{i}^{*}(col \theta)$  $Al r^{2}(r^{2}) T_{b} = finite \Rightarrow B_{b} = 0 \qquad As r \rightarrow \infty, T_{m} = T'r col \theta \Rightarrow A_{m} = T'$  $T_{m} = T'r col \theta + (\underbrace{B_{m}}_{r^{2}}) Col \theta$  $Al r^{2}(r^{2}) R_{b} = T_{m} \Rightarrow A_{b}R = T'R + \underbrace{B_{m}}_{R^{2}}$  $Al r^{2}(r^{2}) R_{b} = \underbrace{K_{m}}_{dr} \xrightarrow{dT_{m}} \Rightarrow A_{b} = T' - \frac{2B_{m}}{R^{3}}$  $Al r^{2}(r^{2}) R_{b} = \underbrace{K_{m}}_{dr} \xrightarrow{dT_{m}}_{dr} \Rightarrow A_{b} = T' - \frac{2B_{m}}{R^{3}}$  $A_{b} = \underbrace{3T'}_{2+K_{R}} ; \qquad B_{m} = \underbrace{(I-K_{k})T' R^{3}}_{2+K_{R}} \text{ where } K_{2} = (\underbrace{K_{b}|_{k_{m}}}_{r^{2}})$  $T_{b} = i\underbrace{3T' r col \theta}_{2+K_{R}} ; \qquad T_{m} = T'r col \theta + \underbrace{(irk_{a})T' R^{3}}_{2+K_{R}} \text{ of } \theta$ **9 11 19** 0.002.0

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What that means, is that the temperature in the particle has got to be equal to A particle times r plus B particle by r square; P 1; 0 of cos theta; for n is equal to 1 and the matrix temperature has to be equal to A matrix times r plus B matrix by r square. Now the boundary condition as r goes to infinity, the temperature in the matrix equal to T prime; r cos theta, as r goes to infinity you can see that this term goes to 0 because r goes to infinity 1 over r square goes to 0 and what that would imply is that A m is just equal to T prime, that satisfies the boundary condition as r goes to infinity are goes to infinity therefore, the matrix temperature is equal to; you note that P 1 of cos theta is just cos theta x 1. As far as the particle is concerned you require that at r is equal to 0, temperature has to be finite which means that this coefficient B p has to be equal to 0 because you have B p by r square and the B p by non zero then the temperature would go to infinity.

Therefore the temperature on the particle is just equal to A particle; r times cos theta and then now you have the boundary conditions of the particle surface; at r is equal to R T p is equal to T m which implies that A p into R is equal to T prime R plus B m by r square just equating the temperatures at the surface. Also at r is equal to R; the fluxes have to be equal what this implies is that A p is equal to T prime, when I take the derivative of this term with respect to r, I will get minus 2 B m by R cube.

So, you can solve these two equations to find what is A p and B m to get the solutions for A p and B m. The solutions are quite straightforward, you just have to solve these two simultaneously and what you will get is that A p is equal to 3; T prime by 2 plus k r and B m is equal to 1 minus k r, T prime by 2 plus k r into I think it is r cube, where k r is equal to the ratio of the conductivities. You can solve this quite easily and with this the temperatures in the particle becomes T p is equal to 3 T prime r cos theta by 2 plus k r and the matrix temperature is equal to T prime; r cos theta plus 1 minus k r; T prime by 2 plus k r into R cube by r square into cos theta.

So, this has given us the temperatures in the matrix and in the particle; in particular the particle temperature actually is only a function of z. The particle temperatures I have written it here is only a function of z, I can rewrite in terms of z 3; T prime z by 2 plus k R, so that is the temperature within the particle.

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Now, we have to determine the effective thermal conductivity. Yes let us go back and get us the expression for the effective thermal conductivity. This is the expression for the average flux and we had written it in this form. So, this is equal to minus k m; T prime minus k p minus k m, N by V integral over the particle of partial T by partial z, within the particle, integral over the particle of partial T by partial z over the particle and now we have the temperature within the particle temperature is equal to 3 T prime z by 2 plus k R.

We just calculated that from the spherical harmonic expansion which means that the temperature gradient within the particle is going to be equal to 3 T prime by 2 plus k r. So, this is a constant, this temperature gradient within the particle is a constant, therefore, this is minus k m; T prime minus of k p minus k m; number of particles, the volume of one particle divided by the total volume, times partial T by partial z which is 3 T prime divided by 2 plus k R.

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So, this is the expression for the average flux within the particle. Now if I take divided by k m; alternatively I can write this as minus k m; T prime into 1 plus, I will take the k m and T prime outside and I will get here k p minus k m by k m into n V p by the total volume into 3 by 2 plus k r; we call that k r was the ratio of the thermal conductivities of the particle and the matrix.

So, I can write this as minus k m; T prime into 1 plus 3 k R minus 1 by 2 plus k R into n times, the volume of the particle strike by total volume; n is number of particles V is volume of 1 particle and V in the denominator is the total volume. So, it is basically the ratio of the volume occupied by the particles to the total volume that is what is called the volume fraction.

So, this gives me the effective thermal conductivity of a composite the effective thermal conductivity is effectively the matrix thermal conductivity times this additional factor due to the presence of the particles. So, k effective is effectively k matrix times 1 plus 3 into k R minus 1 by 2 plus k R into the volume fraction of the particles, where k R is equal to the particle conductivity divided by the matrix conductivity; that is the relative conductivity of the particles with respect to the matrix. So, that is the final solution for the effective thermal conductivity of a composite. If k R is greater than 1, the effective conductivity is greater than the matrix conductivity, if k r is less than 1 the effective conductivity is less than the matrix conductivity as we had expected.

It is important to note that this effective conductivity depends only upon the volume fraction of the particles, it does not depend on either the number of particles or the volume of each particle regardless of whether you have larger number of small particles of a smaller number of large particles, if the volume fraction is the same the effective thermal conductivity will be exactly the same. So, this completes our analysis of the effective thermal conductivity of a composite material, in the dilute limit, where the temperature field around one particle is not affected by the presence of the other particles.

I have shown you how to use separation of variables to obtain a solution for the temperature field around a spherical particle and use that in order to calculate the effective flux, this we did for an axis symmetric system because it was symmetric about the z axis; there was no phi dependence in this expansion. In general cases, you will have a phi dependence; in that case how does one solve the problem that I will continue in the next lecture; I briefly go through how this problem was solved and then show you how to solve it for in more general case. We will continue this in the next lecture; I will see you then.