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Phase field modeling; the materials science, mathematics and computational aspects

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Module No.8
Lecture No.33
Diffusion equation: Error function solution I

Welcome we are looking at analytical solutions to the diffusion equation, so yesterday we saw one solution in the in the last lecture we saw one solution where we had a sinusoidal variation and the time dependent part was exponentially decaying we found that solution by using variable separable method and we basically reduce the given PDE which is the diffusion equation 2 to 0 DE's and we solve them one after another.

And putting the solutions together we have kind that solution, this is a solution which we also use to discuss what happens to the classical diffusion equation when the diffusivity becomes negative, now I want to show another solution which is also very commonly seen but the derivation of this solution is not typically shown and I am going to try and derive this solution which is known as the error function solution.

And let us derive this solution and for doing that I am going to again non-dimensionalize the diffusion equation, the reason why I am doing it for the second time is that this non-dimensionalization is slightly different from what we did earlier that is one reason, the second reason is if I do more than once it will become much more clearer to you and the error function solution is also obtained under some boundary conditions. So we will also have a discussion on what type of boundary conditions we use in deriving this solution, so the equation that we are trying to solve.

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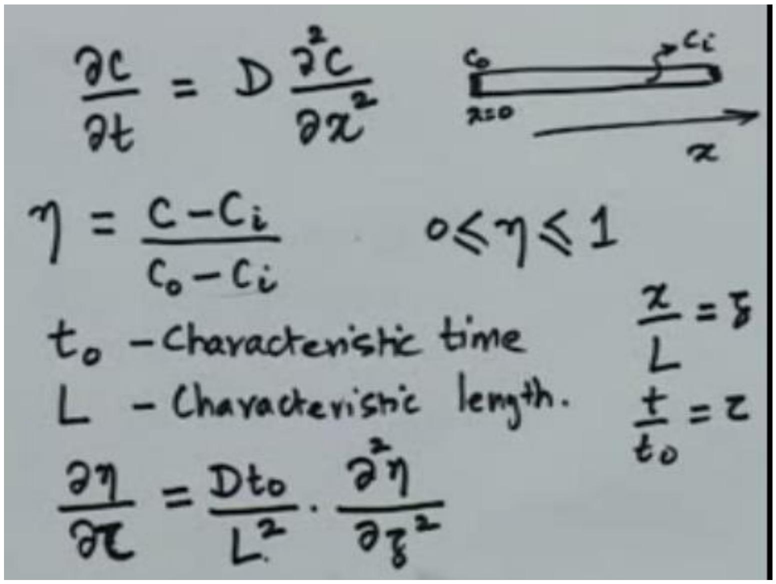

Is the diffusion equation so the rate of change of concentration is dependent on the curvature of the concentration with respect to the position the condition for which we are trying to solve this equation is as follows so I have so this is the domain and this goes up to infinity, okay and so this is the X and that X and the rod continues and at position this x = 0 I am going to have a concentration of C0.

A rest of the domain as a concentration Ci okay, this c0 and Ci could be very small numbers right 0 could be some 0.02 for example and the Ci could be some parts per million for example so we want to non-dimensionalize this is the reason why this non-dimensionalization that I am going to carry out a slightly different from what we did earlier so I am going to first define a parameter η.

Which is defined as follows the C at any point minus CI/ c0 – Ci right this is c0 this is Ci and c0 – Ci is basically the difference so I am going to normalize everything by that so you can see the advantage of for doing this is that at $x = 0$ when C is C0, η is going to become one and everywhere else where it is Ci η has going to become zero, so η is a variable that now runs between 0 and 1,right the range of η becomes 0 and 1,right it could be equal to 0 equal to 1 by anywhere in between it will be between 0 and 1 and of course we are going to non-dimensionalize.

So I am going to choose a time T0 as the characteristic time but for now I am not going to tell what that T0 is okay we will choose it later in such a way that some non-dimensional quantity becomes unity so T0 is the characteristic time and let us say that this rod which is very large right nothing physically is infinite mathematically it could be infinite so we are going to choose a Las the characteristic length.

And this L happens to be the length of this rod and the diffusion distances over which we are going to look at diffusion that is the normalized so X/L that I will call as z and T/T0 that I will call as τ, okay so this the x over which we are trying to look at diffusion compared to that the L is very large so that is going to be a small number okay but L is the characteristic length typically it is the length of the domain itself.

Now if we put it here we get $\partial \eta / \partial t = Dt0$ so $\partial \eta / \partial \tau$, $Dt0/L^2$, $\partial^2 \eta / \partial z^2$ okay so this is my non dimensional equation so it differs from the earlier non-dimensionalization in it that we did not non dimensionalize or scale C but even if it is a numbered this scaling is still useful because this makes the variable go from 0 to 1 whereas if you just take concentration the concentration would be anything.

So for example this C0 could be 0.02 and Ci could be you know some parts per billion or parts per million so this kind of small numbers we do not want to deal with so concentration itself is going to be between 0 and 1 but it would be quite close to 0 or 1 number could be for example this would be like one and then that would be like 0.01 so that that is still about 100 difference in order.

So we do not want to do that so we are going to scale it in such a way it goes between 0 and 1 and this is the non dimensional equation that we have obtained.

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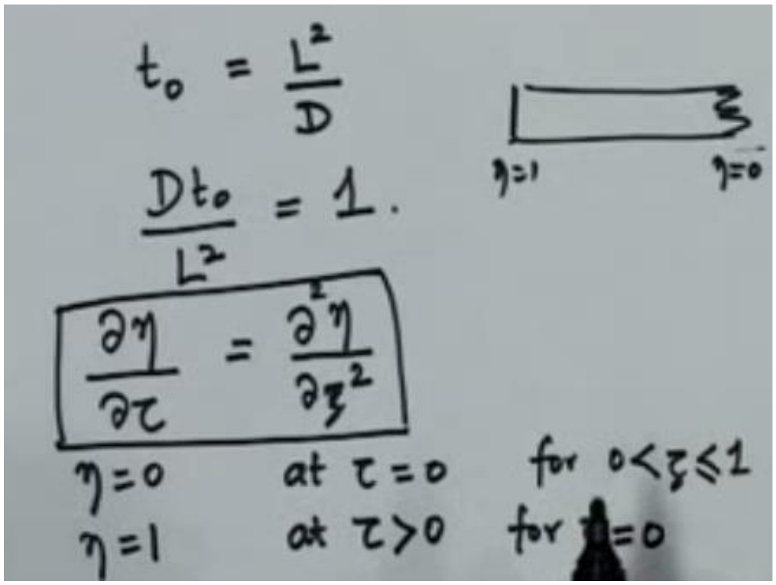

Now I am going to choose the characteristic time in such a way that $dt0/L^2$ becomes unity so that is what that is how I choose the characteristic time so what does that mean, so I want to choose t0 to be L_2 /D what does that mean, so you have some particular length and square the length divided by the diffusivity so that will give me the time that is probably it will take for the diffusion to happen over that entire length given that this is the difficulty.

So that is the T0 that we are going to choose if so then what happens to $dt0/L^2$ that becomes unity so our non dimensional equation now becomes $\partial \eta / \partial \tau = \partial^2 \eta / \partial z^2$ okay and we know that $\eta = 0$ at $\tau = 0$ for $0 < Z < 1$ right so this is the initial condition because at time $T = 0$ we are going to have this η to be 0 everywhere and then η becomes one at all $\tau > 0$ for $z = 0$ okay so here it is 0 > Z < = 1 we are excluding 0.

Because at that point we are always going to have a concentration okay, so this is the boundary condition you might think that you know there is only one initial condition now right because at time $T = 0$ I am telling you what η is and I am Telling one boundary condition for time greater than zero at one point what happens, what happens to the other boundary condition what to the other end that condition is already there okay.

That is not included explicitly because we are considering a system which is infinite, right we are only worried about $X = 0$ and what happens to the diffusion as far as we are concerned that the rod is extending to infinity that is the time scales that we are going to consider for looking at this solution the concentration still is going to remain at Ci at the extreme okay for far away from this point where we are looking at diffusion.

The concentration remains at Ci throughout so that is the reason why that other boundary condition is missing, so this solution error function solution is meant for as they call some semi infinite rod right so you have a point you know the origin $X = 0$ or $Z = 0$ but the length is so large and the Z for which we are looking for solutions is much smaller compared to L, so X/L which is the Z for which we are looking for solutions is much smaller.

So that is the condition under which we are looking at diffusion so we always assume though even though it is not explicitly put here that η remains at 0 far, far away from at this point so we have this where it is $\beta=1$and then this rod it continues and there is no end to it and that end wherever it is η remains 0 so that is the other boundary condition and that is why you do not see it explicitly mentioned here.

So we have now an equation which is non dimensionalize and which has a scale the composition variable we want to find a solution for this problem, the assumption that we are going to make or the way we are going to derive the solution is to say that this solution for concentration η is going to be like this.

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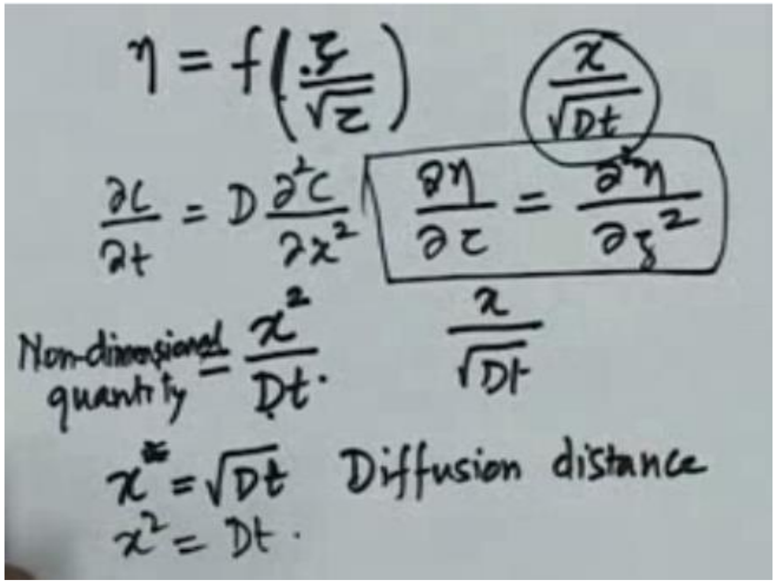

I am going to assume that η is only a function of z/ √ τ okay please remember we have assumed all of this as non dimensional so this is just a number dimensionally speaking if you are having a length as X then √DT is what will become non dimensional okay so because we have assumed this non-dimensional d to be one that is why it is not appearing otherwise there is a one here which is standing for the diffusivity, okay.

Now why is this true this is sometimes argued as follows so in the diffusion equation so let us take the diffusion equation only dimensional quantities are length and time and diffusivity has a derived units so if you try to form a non-dimensional number from these quantities that is of the type x^2 / Dt right because this is meter square per second and multiplied by time so it will become meter square meter square meter square will cancel.

So this is some non dimensional number right this is some non dimensional quantity right as X and T change this quantity value can change but it does not have any dimensions okay for a given diffusivity this quantity is a non-dimensional quantity so what we are saying basically when we are assuming that η is only a function of this quantity is to say that any solution for this equation will have only this quantity because I mean if you try to take the non dimensional version of this equation. Then this is the only non dimensional quantity that you can make so the solution should be in this form and this is nothing but a square root of this quantity right so $x/\sqrt{Dt}$ will also be non dimensional and this is what is being taken here is that $z/\sqrt{\tau}$ which is the quantity this quantity is very important by the way so this $x^{2} = \sqrt{Dt}$ is known as the diffusion distance okay and it is a very quick way of estimating how much diffusion will take place in a given time given a difficulty.

Suppose you want to throw something in a furnace and you want to know how long should you keep it in the furnace at that temperature for some amount of diffusion to take place if you know the diffusivity just to multiply by the time that you want to keep it and take the square root that will be the distance over which diffusion will take place in that particular time, now this is a very quick way of estimating it this is the answer will be scaled will be a factor of this distance.

But this is a very good first approximation for diffusion there are exercised problems probably we can have some tutorial problem where you can actually estimate it using the sorry X is D^3 Dt x^2 = DT, now so you can estimate this quantity and you can actually take the analytical solutions say let us say error function based solution and you can compare it and you will see that most of the times this predicts very nicely for most practical purposes okay.

And because there is also the analog there is a common exercise that I like to always give students that you can take a ceramic material for example and you can take its thermal diffusivity or you and you can take a metallic material for example and you can take its thermal diffusivity and you can assume that a cup made up of the ceramic material and a cup made up of this metallic material metal or alloy.

Let us say that they have the same thickness, okay and now you pour coffee in them coffee which is at say some 80^0 Celsius and you can hold the ceramic cup for longer than you can hold the metallic cup because the distance over which you will start feeling the heat or the heat conduction takes place and the temperature rises right for the same thickness you can assume that both of them for example 3 millimeter thick.

But the three millimeter thick metal how long will it take for you to start feeling the temperature on the outer wall if you pour hot coffee in the cup and three millimeter thick ceramic you can you can compare and basically it is the difference in thermal diffusivity in the two types of materials which decides that you know metallic material within a few seconds you will start feeling so you cannot hold the cup.

Whereas in ceramic material it is at least one order higher so maybe about a minute or so you will be able to hold so that is why it is preferable to drink coffee in ceramic cups it is always preferable to drink coffee and it is preferable to drink it then the ceramic cups okay, so this is an important quantity called the diffusion distance and here we are using some dimensional arguments to say why the solution should be of this type.

Please remember our aim is to take a PDE somehow convert it into OD because body is all we know how to solve so one way of converting into ODE is by variables separable method which we saw in the last lecture and this lecture we are going to see how to get a ODE from the PDE that is by using dimensional arguments, you say that there are two fundamental quantities and one derived quantity let us make a non-dimensional number out of it.

And that non-dimensional quantity is called the diffusion distance x^2 / DT and the solution should be a function of this quantity that is what we are claiming which is what going to help us to make a OD E out of this PDE so we will start from this point so we will take η to be just a function of Z by $\sqrt{\tau}$ and we are going to convert the diffusion equation not in this form so the non-dimensionalize diffusion equation, okay.

Using this we are going to convert this into an ordinary differential equation so which is what we will do in the next part of this lecture thank you.

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