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

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Module No.8
Lecture No.34
Diffusion equation: Error function solution II

Welcome we are trying to solve this equation $\delta\eta/\delta\tau = \delta^2\eta/\delta z$ and I have made the assumption that η is going to be only a f $(z/\sqrt{\tau})$ and now I am going to define that $z/\sqrt{\tau}$ as y I'm also going to define $d\eta/dy$ as some p these are just some definition so I am going to say y is $z/\sqrt{\tau}$. So in other words we are saying that $\eta = f(y)$ and $d\eta/dy$, we are going to call it as p, now let us take $\delta\eta/\delta\tau$ and try to find out what it is.

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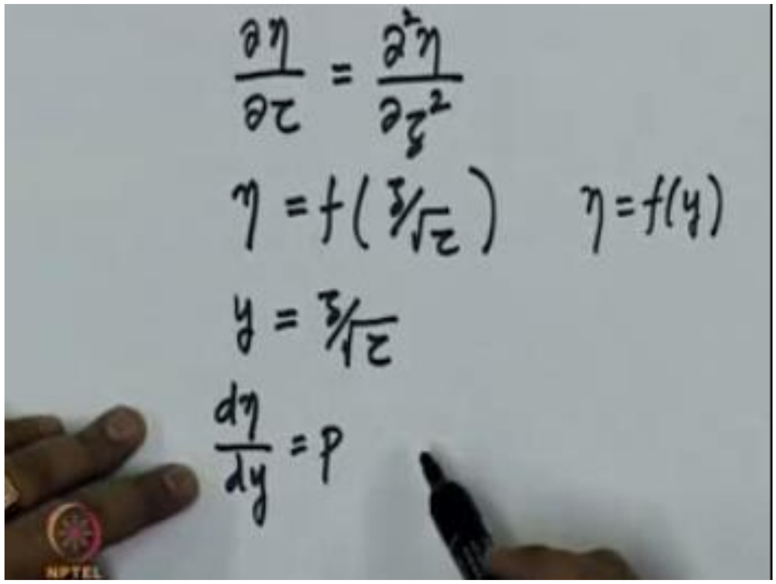

Okay so I want to take δη/δτ and I want to find out what that quantity is, so what is δη/δτ to me, we are going to the partial derivative means that the other quantity other variable that you have namely the z which are going to keep us a constant so I am going to write this δη/δτ as follows dη/dy and δy/δτ right, because I want to get the variation of η with respect to τ but, η is only a function of y but y is a function of τ, the way we have derived, we have defined right.

Now because we have defined y as z/√τ, so if you take δy/δτ will be minus right, because z τ power half minus half will be there ½ will come and z and then $\tau^{-3/2}$ so, it will become τ, so this is nothing but - z/√τ is nothing but y itself so y /2τ ,so let us put it back here so is δη/δτ nothing but dη/dy –y/2τ okay, so let us let us for now let us keep it as δη/δy. So I am going to say that and z is kept a constant δη/δy and δy/δτ is what δη/δy is.

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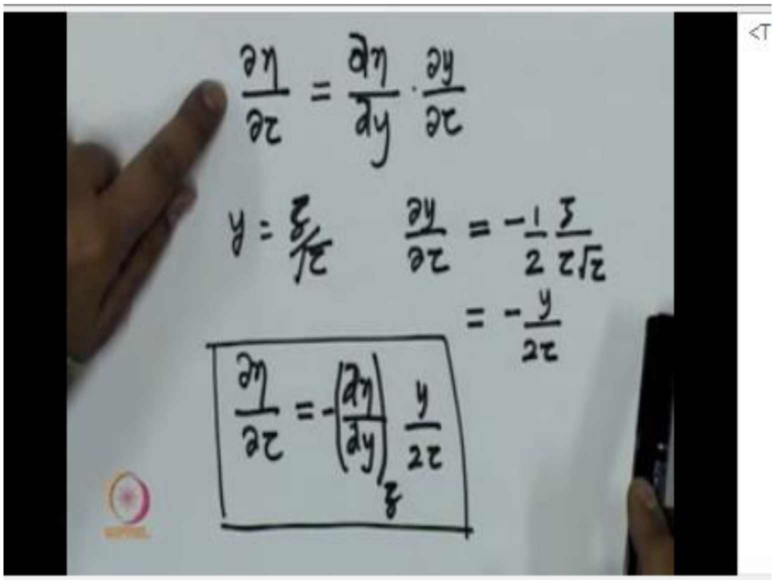

So this is the left-hand side of the equation so we have calculated $\delta\eta/\delta y$ in terms of y okay $\delta\eta/\delta y$ $y/2\tau$ with a minus sign is nothing but $\delta\eta/\delta y$. Now let us calculate the right hand side of the equation the right hand side of the equation is what it is $\delta^2\eta/\delta z^2$, I'm going to use the same trick I am going to say that δy and $\delta y/\delta z^{\text{right}}$, so that is going to be my trick so let us first split it $\delta/\delta z$ of $\delta\eta/\delta z$ this is what it is so let me keep this $\delta/\delta z$ and this I am going to write it as $\delta\eta/\delta y$ and $\delta y/\delta z$.

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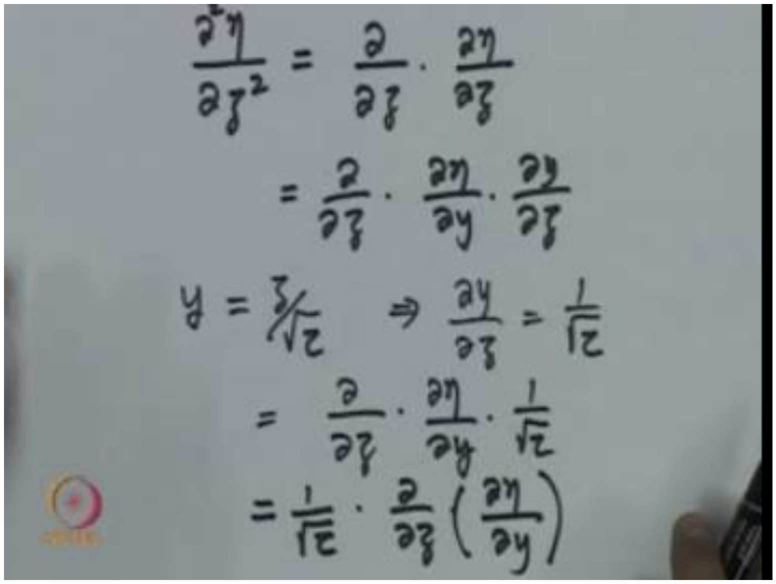

δy/δz again we go back to our definition y is z/√τ which means δy/δz is nothing but 1/√τ, so 1/√τ so we have C acting on δη/δy and 1/√τ ,so 1/√τ is this is a partial derivative with respect to z. So 1/√τ now can be pulled so you have 1/√τ δ/δz acting on δη/δy right, so this δ/δz that I am going to use the same trick once more, so what am I going to say same δ/δz is nothing but δ/δy δy/δz right, so I have now so I have $\delta^2\eta/\delta z^2$ is equal to 1/√τ δ/δz(δη/δy) so, I am going to use the same trick 1/√τ δ/δz is going to become δ/δy acting on δη/δy multiplied by δy/δz.

So δy/δz again we know is and that is 1/√τ going to come here and it is going to become 1/τ, this is going to become $\delta^2\eta/\delta y^2$ and in all this process we have kept power as constant right, so we know δη/δτ was obtained as this quantity we obtained it as –y/2τ δη/δy okay? So now let us equate these quantities and we get so - y/2τ δη/δy is equal to, we have derived the other quantity which is 1/τ $\delta^2\eta/\delta y^2$ and remember we said that δη/δy = P so the τ, τ goes away.

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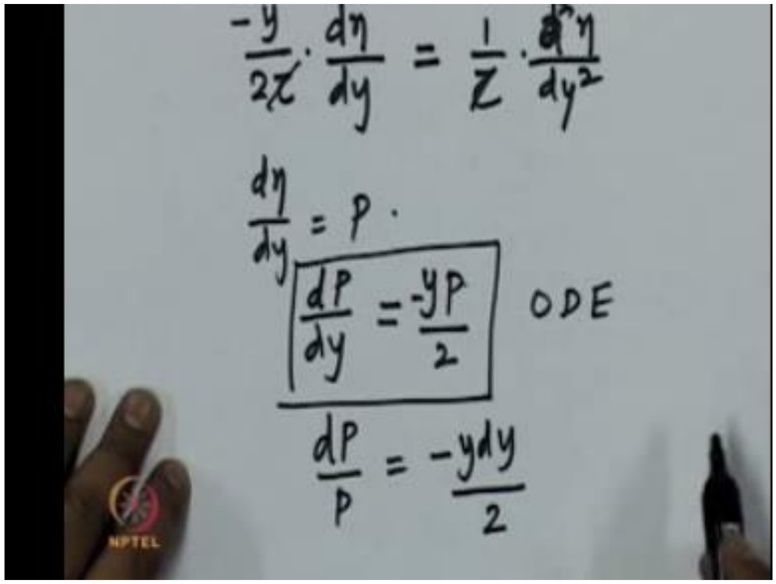

So you have what you have is as follows it is dP/dy – yp, is equal to –yp/2 right, dη/dy is P –y/2 is equal to d/dy(dη/dy) so that is dp/dy, so we have ended up with an ODE right, in from the PDE that we started with. This can be integrated so let us integrate it dp/p is equal to –ydy/2,so if you integrate that equation what do you get you get log(p) is equal to $–y^2/4$ + some logarithm of a that is a constant taking it as logarithm because now i am going to exponentiation so it will make it easy form, so then I get P as some A exponential ($–y^2/4$), but P is nothing but dη/dy let us integrate it one more η is nothing but integral A exp ($–y^2/4$) dy, this is the solution we have obtained.

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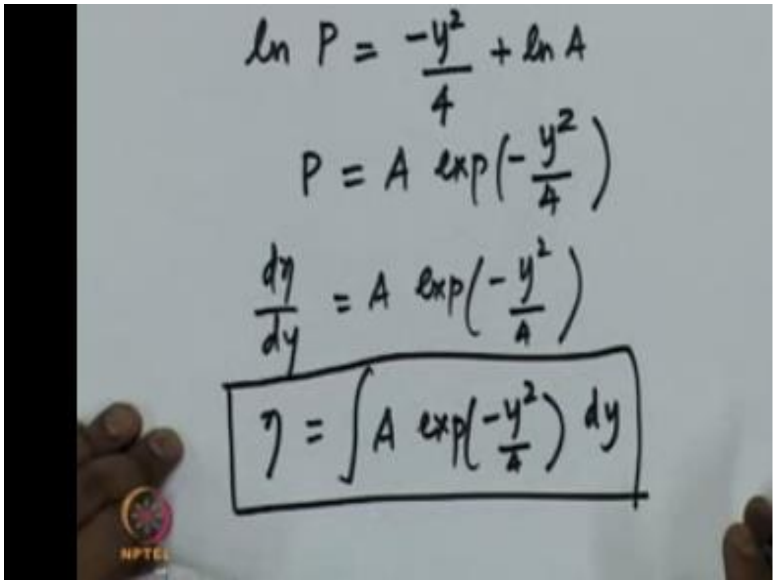

Remember η itself was a scale to quantity, so now I can go back and substitute for η and what do I get the η was nothing but C –Ci/ C0-Ci is equal to integral A exp $(-y^2/4)$ dy and let us recall what did we define as y, we defined this quantity $z/\sqrt{\tau}$ as y and y^2 is nothing but z^2/τ like I said the we took the normalized diffusivity to be 1, but that 1 is sitting somewhere here okay, so this is what I said in the other context I said x^2=Dt right, so this is z^2 / d time of τ, so it is the same quantity okay so this is the solution sometimes for example, if you look at a textbook like Porter and Easter link this solution is what is written it C = Ci + (C0 -Ci) ∫ A exp $(-y^2/4)$ dy.

This a has to be determined so, this is part of the error function definition it is a 2/л or something like that but I have left it as A itself for now and you can look at so Porter for example you will know the exact value for this quantity and this is known as the error function without this constant exponential $(-y^2/4)$ dy so typically this quantity is tabulated and you look up the tables and you use the values and that is how you calculate composition as a function of position and time right ,so for any given any position you can calculate y which is a combination of position and time and you can put it here and then you will get the solution corresponding to that quantity.

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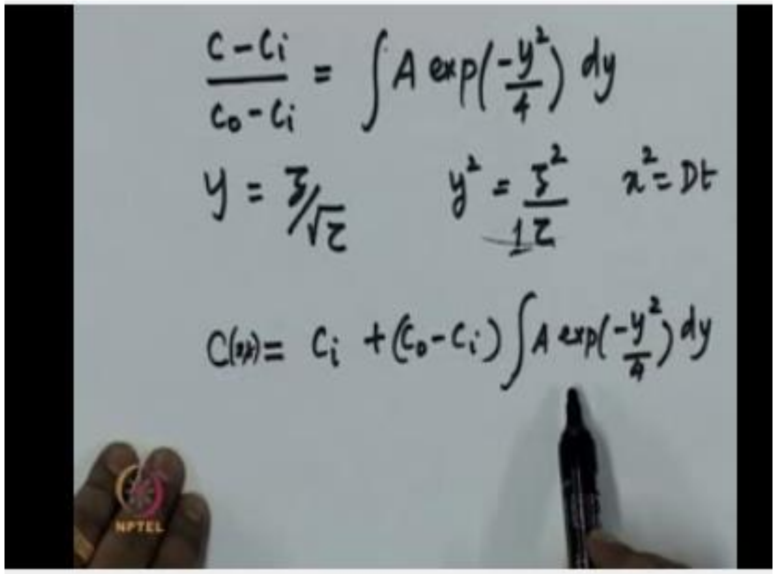

And this is plotted so we will do it we do not need to look up tables for getting error function octave has a function call called error function, I suppose so we will use that and we will try to plot this solution and so on. Okay so this is something that we will do later when we start going back to octave and doing some of these things numerically but the point that I'm trying to make is that there are two ways in which we have solved the diffusion equation it is a partial differential equation so you try to convert it into ordinary differential equations and solve.

Variable separable is one method using dimensional arguments and using some transformation of variables to reduce it to ordinary differential equation and solving it is the second approach, this approach gives us the error function solution which is meant for semi infinite case as they are described sometimes in the literature and the other solution that we sub variable separable is basically the homogenization solution that is what it is called.

So this solution that we have obtained is very important for example, if you are looking at the carburizing decarburizing or if you are looking at doping a semiconductor with some doped and those kinds of situations where you keep the one end of your material at some concentration.

For example carburization you keep it at some carbon concentration that your material is at some other carbon concentration and you carburized okay, or decarburization that happens because outside the carbon concentration is less than what you're still has, so from the surface it starts losing carbon and so these kind of solutions are obtained sometimes diffusivity is also measured by putting together like it is like a rod and then somewhere in between you put a radioactive material okay, very thin slice of radioactive material so it is like two semi-infinite rods put together so the error function solution on both sides that will give you the spread of the radioactive material into the into the material loop in which you are trying to measure the diffusivity.

So using then the error function solution you can back calculate the diffusivity for a given time, you take slices away from this source point and you look at the carbon whatever concentration of the radioactive material from that plot you try to calculate you know the distance you know the time for which it was thereat that temperature so, at that temperature what is the diffusivity can be obtained using similar experiments.

All this is explained the in Port Henry sterling for example so what we have done is to derive that solution, so important installing it is written this is the solution. So we have just tried to derive the solution and see how we get this solution in the first place okay, so the next step is of course to go and solve the classical diffusion equation numerically, so in the next part of this lecture I will do the leg work that is required to solve the equation numerically actually solving it numerically, we will do it in the next lecture. So thank you

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