Diffusion in Multicomponent Solids

Professor Kaustubh Kulkarni
Department of Material Science and Engineering
Indian Institute of Technology. Kanpur

Lecture 21

Solution to Diffusion Equation for Semi-Infinite Slab and Its Application in Carburizing of Steel

Welcome back, I hope you all are enjoying the lecture so far in this open course on Diffusion in Multicomponent Solids. In the last class, we went through the solution for diffusion equation for instantaneous planar source boundary conditions and we saw it has applications in doping of semiconductors and also in determination of impurity diffusion coefficients in metals and alloys.

Today we will solve the diffusion equation for another set of boundary conditions which is again industrially very important. It is encountered in one of the most commonly used industrial processes called carburizing and hardening. In many applications, it is required that the steel has a very hard surface and tough core. I has a very good wear resistance as well as it can withstand the high impacts.

Some of the examples are all the transmission components that they use in a vehicle like gears and shafts. These components undergo what is called as surface hardening processes, carburizing and hardening. There are various ways in which surface hardening can be carried out and one of the most commonly used way is carburizing and hardening. In this process we start with a steel component which is made in low carbon steel. So, to start with the steel has low carbon content around 0.2 weight % throughout the component. Then it is exposed to an atmosphere which is rich in carbon and it is heated to a high temperature. As a result there is a carbon concentration gradient from the atmosphere in the furnace to the steel component, so the carbon diffuses into the steel.

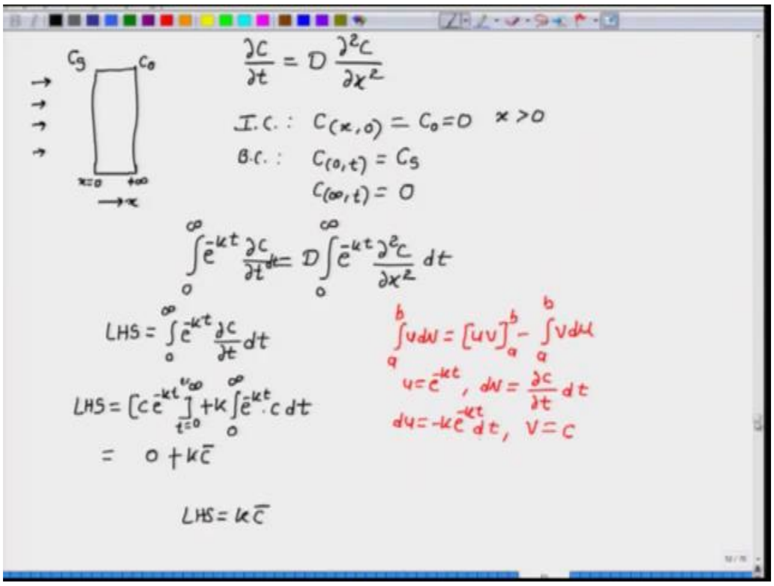
Now, this is a diffusion-based process. The depth up to which a particular carbon concentration can penetrate depends upon time and temperature and also the diffusivity of the material. In this case it is carbon in steel and it is very important to know to what extent a particular carbon content has penetrated or to what depth we have achieved a particular carbon content for a given time.

Or we need to know how much time we need to do the carburizing at a given temperature to achieve the desire case depth. Usually the depth up to which the desired hardness is achieved on the surface is referred to as case depth.

There are various ways the manufacturers characterize their case depth, it may be in terms of hardness or it may be in terms of the minimum required carbon concentration achieved at that particular depth. Obviously, this depends upon the diffusion. So, if we want to design the treatment parameters for this particular treatment, we should have the knowledge of diffusion of carbon in steel.

And then we need to solve the diffusion equation for this particular boundary condition. Let us talk about this problem here.

(Refer Time Slide: 04:20)



$$\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2}$$

I.C. : $C(x,0) = C_0 = 0 \quad x > 0$

B.C. : $C(0,t) = C_s$

$C(\infty,t) = 0$

$$\int_0^\infty e^{-kt}\frac{\partial C}{\partial t}dt = D\int_0^\infty e^{-kt}\frac{\partial^2 C}{\partial x^2}dt$$

$$LHS = \int_0^\infty e^{-kt}\frac{\partial C}{\partial t}dt$$

$$\int_a^b u\,dv = [uv]_a^b - \int_a^b v\,du$$

$u = e^{-kt}$, $dv = \frac{\partial C}{\partial t}dt$

$du = -ke^{-kt}dt$, $v = C$

$$LHS = [Ce^{-kt}]_{t=0}^{t=\infty} + k\int_0^\infty e^{-kt}\cdot C\,dt$$

$$= 0 + k\bar{C}$$

$$LHS = k\bar{C}$$

Let us consider a carbon component in the form of a slab, on the left side is the carbon atmosphere. And we have thickness of the slab in the x direction. At the surface, we have $x = 0$ and the components usually have large thickness such that during the carburizing treatment, the carbon does not penetrate all the way up to the other surface. Hence we can maintain the infinite boundary condition.

In this case x varies from 0 to $+\infty$. This is called semi-infinite slab boundary condition. The heat treatment is usually carried out in an atmosphere such that there is a constant carbon concentration at the surface. At the surface let us denote the concentration by:

$$C(0,t) = C_S$$

and typically steel will have certain carbon concentration to start with to make the problem simple initially. Let us assume the carbon concentration in the steel before carburizing is 0:

$$C(x,0) = C_o = 0 \quad for \;\; x > 0$$

and since we are maintaining infinite boundary conditions at the other end, the carbon concentration will always remain $C_o = 0$.

$$C(\infty, t) = 0$$

Now we have to solve the diffusion equation:

$$\frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2}$$

with the initial condition that:

$$C(x,0) = C_o = 0 \quad for \;\; x > 0$$

And what are the boundary conditions? At the surface, carbon concentration is always maintained as:

$$C(0,t) = C_S$$

and the second boundary condition is at the other end the original concentration of steel remains, in this case we are assuming it is 0:

$$C(\infty, t) = 0$$

We have to solve this diffusion equation with respect to these initial and boundary conditions. Let us use the Laplace transform just like we used it last time. If in the diffusion equation, we multiply both sides by e^{-kt}, and integrate from 0 to ∞, D is constant:

$$\int_0^\infty e^{-kt} \frac{\partial C}{\partial t} dt = D \int_0^\infty e^{-kt} \frac{\partial^2 C}{\partial x^2} dt$$

Let us first solve the last left-hand side by integration by parts, LHS is equal to:

$$LHS = \int_0^\infty e^{-kt} \frac{\partial C}{\partial t} dt$$

We can solve this integral by integration by parts, and we know the formula for integration by parts:

$$\int_a^b u dv = [uv]_a^b - \int_a^b v du$$

If we look at the integrand here, we can assume:

$$u = e^{-kt}, \quad dv = \frac{\partial C}{\partial t} dt$$

$$du = -ke^{-kt} dt, \quad v = C$$

By solving integration by part, we get LHS:

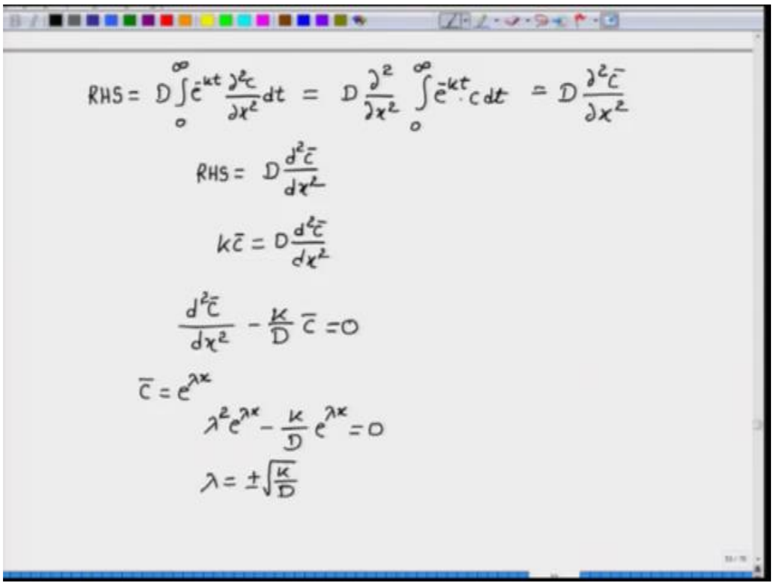
$$LHS = [Ce^{-kt}]_{t=0}^{y=\infty} + k \int_0^\infty e^{-kt} C dt$$

K is outside the integral because it is constant, not dependent on time. If we evaluate, remember these limits are for time, $t = 0$ to $t = \infty$. At $t = \infty$, e^{-kt} will be 0 and C will have a finite value. In this case it is 0. So:

$$LHS = [Ce^{-kt}]_{t=0}^{y=\infty} + k \int_0^\infty e^{-kt} C dt = 0 + k\bar{C} = k\bar{C}$$

The second integral is nothing but the Laplace transform of $C(x, t)$which is $\bar{C}$.

(Refer Time Slide: 11:02)



$$RHS = D\int_0^\infty e^{-kt}\frac{\partial^2 c}{\partial x^2}dt = D\frac{\partial^2}{\partial x^2}\int_0^\infty e^{-kt} c\,dt = D\frac{\partial^2 \bar{c}}{\partial x^2}$$

$$RHS = D\frac{d^2\bar{c}}{dx^2}$$

$$k\bar{c} = D\frac{d^2\bar{c}}{dx^2}$$

$$\frac{d^2\bar{c}}{dx^2} - \frac{K}{D}\bar{c} = 0$$

$$\bar{c} = e^{\lambda x}$$

$$\lambda^2 e^{\lambda x} - \frac{K}{D}e^{\lambda x} = 0$$

$$\lambda = \pm\sqrt{\frac{K}{D}}$$

Now, let us look at RHS which is equal to:

$$RHS = D\int_{0}^{\infty} e^{-kt}\frac{\partial^2 C}{\partial x^2}dt$$

Just like we did for the previous problem, e^{-kt} is independent of x, we can take it inside the differential. And then we can change the order of differential and integration, which would yield:

$$RHS = D\int_{0}^{\infty} e^{-kt}\frac{\partial^2 C}{\partial x^2}dt = D\frac{\partial^2}{\partial x^2}\int_{0}^{\infty} e^{-kt}Cdt$$

And again, this integral is Laplace transform of C, we can write RHS is equal to:

$$RHS = D\frac{\partial^2 \bar{C}}{\partial x^2}$$

And $\bar{C}$ is now not dependent on time and we can replace partial derivative with ordinary derivative. RHS becomes:

$$RHS = D\frac{d^2 \bar{C}}{dx^2}$$

So, we get:

$$k\bar{C} = D\frac{\partial^2 \bar{C}}{\partial x^2}$$

And if we rearrange, we get the ordinary differential equation in $\bar{C}$:

$$\frac{d^2 \bar{C}}{dx^2} - \frac{k\bar{C}}{D} = 0$$

Again, we have seen just like the last problem we solved, Laplace transform has helped us to convert the partial differential equation into an ordinary differential equation, which we can easily solve here. And the solution for this may be:

$$\bar{C} = e^{\lambda x}$$

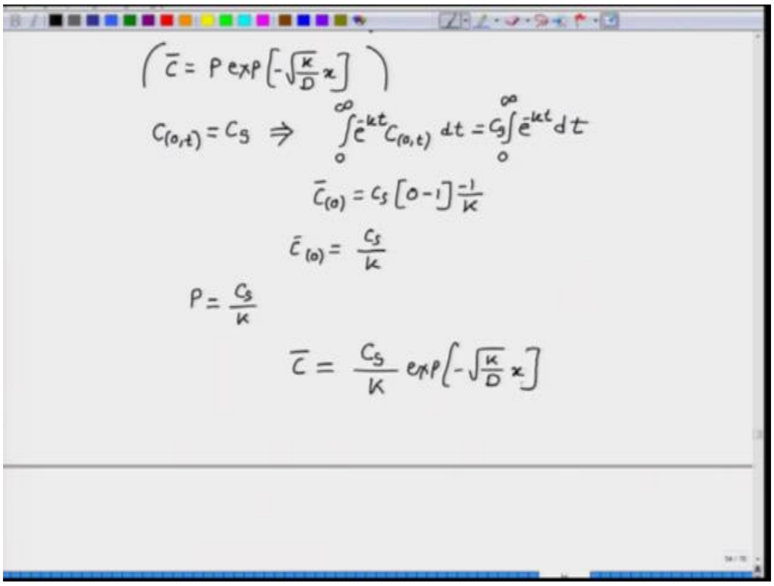
If you substitute back, we get:

$$\lambda^2 e^{\lambda x} - \frac{ke^{\lambda x}}{D} = 0$$

And then:

$$\lambda = \pm\sqrt{\frac{k}{D}}$$

(Refer Time Slide: 13:45)



$$\left(\bar{C} = P\exp\left[-\sqrt{\frac{K}{D}}x\right]\right)$$

$$C_{(0,t)} = C_S \Rightarrow \int_0^\infty e^{-kt} C_{(0,t)}\,dt = C_S\int_0^\infty e^{-kt}\,dt$$

$$\bar{C}_{(0)} = C_S\left[0-1\right]\frac{-1}{K}$$

$$\bar{C}_{(0)} = \frac{C_S}{K}$$

$$P = \frac{C_S}{K}$$

$$\bar{C} = \frac{C_S}{K}\exp\left[-\sqrt{\frac{K}{D}}x\right]$$

And if we have multiple solutions, the linear combination of the solutions is also a solution. So we can write:

$$\bar{C} = Pexp\left(-\sqrt{\frac{k}{D}}x\right) + Qexp\left(\sqrt{\frac{k}{D}}x\right)$$

We have to find out these constants P and Q, one constant we can straight away eliminate, which one is that? Q. Because our x is varying from 0 to ∞ and we want the concentration field to behave at all x, including at $x = \infty$, which is possible only if Q is . So, Q is 0 and now we are left with only one term giving:

$$\bar{C} = Pexp\left(-\sqrt{\frac{k}{D}}x\right)$$

Now, to get the value of constant P, let us use the boundary condition which is:

$$C(0,t) = C_S$$

And if we take the Laplace transform again on both sides;

$$\int_0^\infty e^{-kt} C_{(0,t)} dt = C_S \int_0^\infty e^{-kt} dt$$

As C_S is constant and LHS is Laplace transform of $C_{(0,t)}$. So on substituting in last equation:

$$\bar{C}_o = C_S[0-1] \times \frac{-1}{k} = \frac{C_S}{k}$$

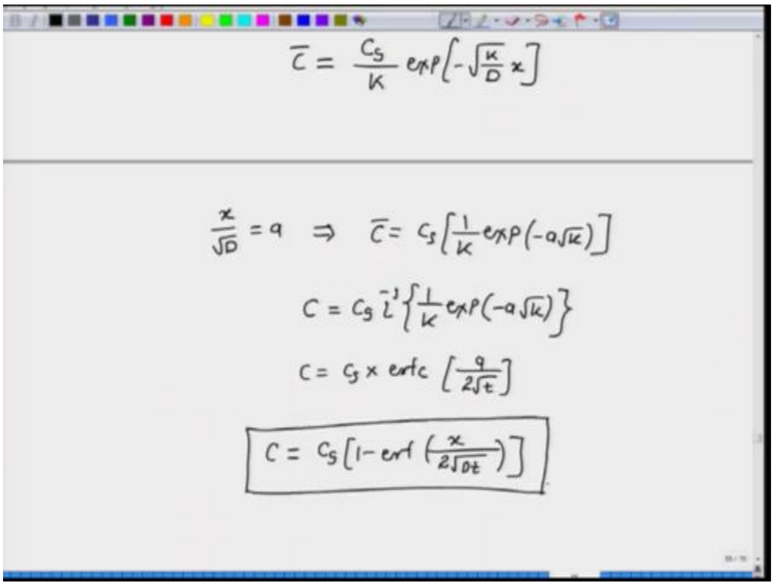
If we substitute in the equation that we got for $\bar{C}$, we get the value of P as:

$$P = \frac{C_S}{k}$$

And the solution for $\bar{C}$ is:

$$\bar{C} = \frac{C_S}{k} exp\left(-\sqrt{\frac{k}{D}}x\right)$$

(Refer Time Slide: 16:30)



$$\bar{C} = \frac{C_S}{K} exp\left[-\sqrt{\frac{K}{D}} x\right]$$

$$\frac{x}{\sqrt{D}} = a \Rightarrow \bar{C} = C_S\left[\frac{1}{K} exp(-a\sqrt{K})\right]$$

$$C = C_S L^{-1}\left\{\frac{1}{K} exp(-a\sqrt{K})\right\}$$

$$C = C_S \times erfc\left[\frac{a}{2\sqrt{t}}\right]$$

$$\boxed{C = C_S\left[1 - erf\left(\frac{x}{2\sqrt{Dt}}\right)\right]}$$

Now, if we take:

$$a = \frac{x}{\sqrt{D}}$$

we can write:

$$\bar{C} = C_S\left[\frac{1}{k} exp\left(-a\sqrt{k}\right)\right]$$

and this looks familiar, we solve this Laplace transform. If we take the inverse Laplace on both sides, we get to our concentration field:

$$C = C_S L^{-1}\left\{\left[\frac{1}{k} exp\left(-a\sqrt{k}\right)\right]\right\}$$

And if we look at Laplace transform table and we solve this in a previous class, the Laplace transform of this term is $erfc\left[\frac{a}{2\sqrt{t}}\right]$. So, we get the solution for concentration as:

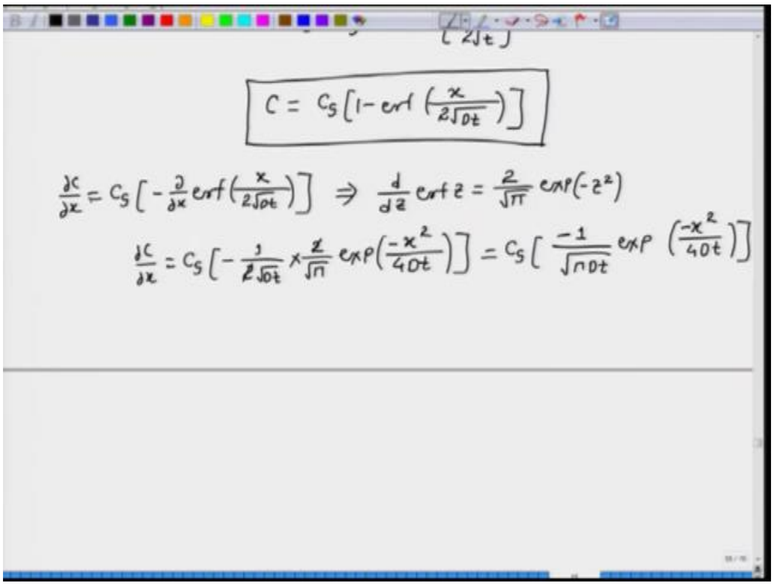
$$C = C_S erfc\left[\frac{a}{2\sqrt{t}}\right]$$

$$C = C_S\left(1 - erf\left[\frac{x}{2\sqrt{Dt}}\right]\right)$$

This is the solution that we have obtained for the semi-infinite slab with constant surface concentration, which is typically encountered for example in carburizing of steel.

Let us look at some of the features of this solution. If we draw the plot of carbon concentration versus x or verses depth into the surface, how should it look like? So, if we know the curvature and slope, we can get an idea of the plot.

(Refer Time Slide: 18:58)



$$\boxed{C = C_S\left[1 - erf\left(\frac{x}{2\sqrt{Dt}}\right)\right]}$$

$$\frac{\partial C}{\partial x} = C_S\left[-\frac{\partial}{\partial x} erf\left(\frac{x}{2\sqrt{Dt}}\right)\right] \Rightarrow \frac{d}{dz} erf\, z = \frac{2}{\sqrt{\pi}} exp(-z^2)$$

$$\frac{\partial C}{\partial x} = C_S\left[-\frac{1}{\cancel{2}\sqrt{Dt}} \times \frac{\cancel{2}}{\sqrt{\pi}} exp\left(\frac{-x^2}{4Dt}\right)\right] = C_S\left[\frac{-1}{\sqrt{\pi Dt}} exp\left(\frac{-x^2}{4Dt}\right)\right]$$

If we evaluate the slope, which is nothing but the derivative $\frac{\partial C}{\partial x}$:

$$\frac{\partial C}{\partial x} = -C_S\frac{\partial}{\partial x}\left(erf\left[\frac{x}{2\sqrt{Dt}}\right]\right)$$

C_S is constant and we know the derivative of error function, what is it?

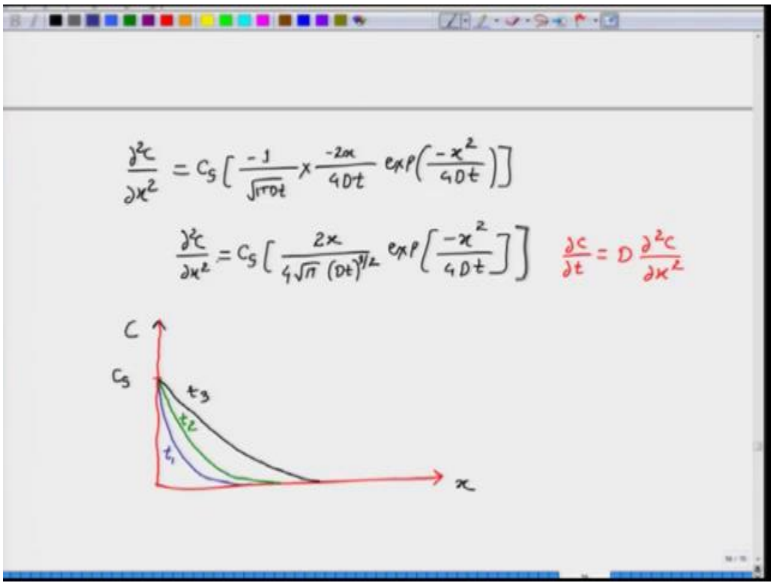
$$\frac{\partial}{\partial z} erf[z] = \frac{2}{\sqrt{\pi}} \exp(-z^2)$$

So, in this case:

$$\frac{\partial C}{\partial x} = -C_S\left[\frac{1}{2\sqrt{Dt}} \times \frac{2}{\sqrt{\pi}} exp\left[-\frac{x^2}{4Dt}\right]\right] = -C_S\left[\frac{1}{\sqrt{\pi Dt}} exp\left[-\frac{x^2}{4Dt}\right]\right]$$

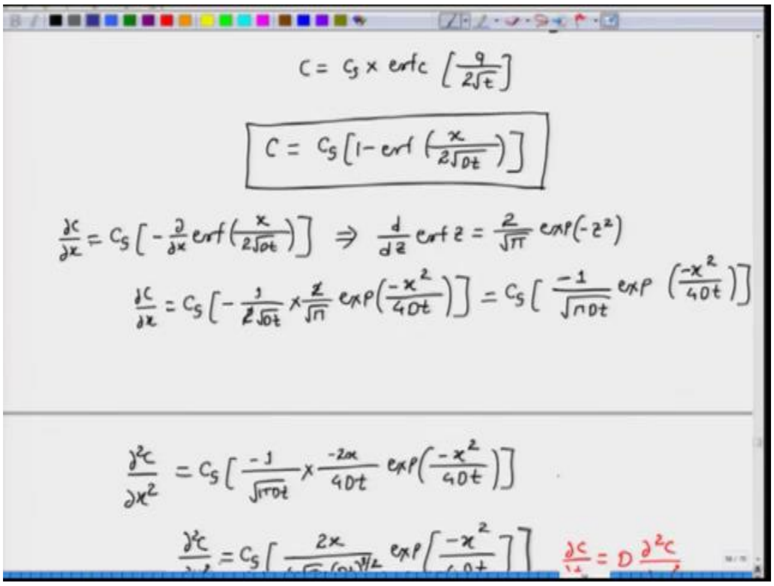
The slope will be negative because the exponential term will always be positive.

(Refer Time Slide: 21:06)



$$\frac{\partial^2 c}{\partial x^2} = C_S\left[\frac{-1}{\sqrt{\pi Dt}} \times \frac{-2x}{4Dt} \exp\left(\frac{-x^2}{4Dt}\right)\right]$$

$$\frac{\partial^2 c}{\partial x^2} = C_S\left[\frac{2x}{4\sqrt{\pi}\,(Dt)^{3/2}} \exp\left[\frac{-x^2}{4Dt}\right]\right] \qquad \frac{\partial c}{\partial t} = D\frac{\partial^2 c}{\partial x^2}$$



$$C = C_S \times erfc\left[\frac{9}{2\sqrt{t}}\right]$$

$$\boxed{C = C_S\left[1 - erf\left(\frac{x}{2\sqrt{Dt}}\right)\right]}$$

$$\frac{\partial c}{\partial x} = C_S\left[-\frac{\partial}{\partial x} erf\left(\frac{x}{2\sqrt{Dt}}\right)\right] \Rightarrow \frac{d}{dz} erf\, z = \frac{2}{\sqrt{\pi}} \exp(-z^2)$$

$$\frac{\partial c}{\partial x} = C_S\left[-\frac{1}{2\sqrt{Dt}} \times \frac{2}{\sqrt{\pi}} \exp\left(\frac{-x^2}{4Dt}\right)\right] = C_S\left[\frac{-1}{\sqrt{\pi Dt}} \exp\left(\frac{-x^2}{4Dt}\right)\right]$$

$$\frac{\partial^2 c}{\partial x^2} = C_S\left[\frac{-1}{\sqrt{\pi Dt}} \times \frac{-2x}{4Dt} \exp\left(\frac{-x^2}{4Dt}\right)\right]$$

Now let us look at the curvature, which is the second derivative that should be:

$$\frac{\partial^2 C}{\partial x^2} = C_S\left[\frac{1}{\sqrt{\pi Dt}} \times \frac{2x}{4Dt} exp\left[-\frac{x^2}{4Dt}\right]\right] = C_S\left[\frac{2x}{4\sqrt{\pi}(Dt)^{\frac{3}{2}}} exp\left[-\frac{x^2}{4Dt}\right]\right]$$

So, the curvature is positive, what also means that if we look at the diffusion equation that $\frac{\partial C}{\partial t}$ is positive. The concentration at any x position should increase with time. Let us try to plot concentration versus x at any given time, if C_S is the start composition on the surface, slope is negative and curvature is positive.

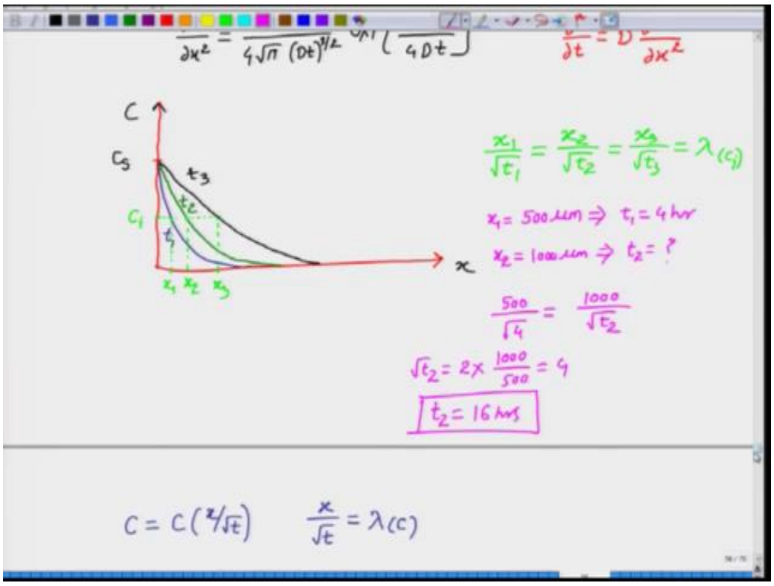
If you plot at different times we knew that surface concentration should always be constant and at other x the concentration should increase with time. Now again, if we look at the solution carefully:

$$C = C_S\left(1 - erf\left[\frac{x}{2\sqrt{Dt}}\right]\right)$$

C_S is constant and D is also constant. The concentration we can see is a function of $\frac{x}{\sqrt{t}}$.

$$C = C\left(\frac{x}{\sqrt{t}}\right)$$

(Refer Time Slide: 24:13)



What does this mean? Our concentration here is a function of $\frac{x}{\sqrt{t}}$. This $\frac{x}{\sqrt{t}}$ is usually referred to as Boltzmann parameter, $\lambda(C)$. Each concentration plane, here is a function of λ or $\frac{x}{\sqrt{t}}$. What does it mean physically if we track a particular concentration?

Let us see if we want to track the concentration C_i and the depth at which the concentration is C_i at different times,? Let us see then for times t_1, t_2 and t_3 here. And it denote the depth at which we see concentration at x_1, x_2 and x_3 at t_1, t_2 and t_3 respectively. What this relationship tells me is that:

$$\frac{x_1}{\sqrt{t_1}} = \frac{x_2}{\sqrt{t_2}} = \frac{x_3}{\sqrt{t_3}} = \lambda_{Ci}$$

It is a constant λ which is a function of C_i. This is a very important consequence.

Because, it helps us to roughly estimate the case depths once we design a process for a particular component for a given case depth. And suppose we want to change the case depth for that component, as let us say, required by the customer, then we do not have to again go back and do the redesign.

If we have the same steel component and we do the heat treatment at the same temperature (meaning basically D is constant) we can straightaway use this relation and decide the case depth. For example, if we had designed the process for case depth of $500\ \mu m$, and let us say:

$$x_1 = 500\ \mu m, \qquad t_1 = 4\ hr$$

and the carburizing heat treatment time for the attaining the $500\ \mu m$ case depth was let us say 4 hours. But now we want to design the process or we want the case depth of $1000\ \mu m$. What should be the heat treatment time? If we substitute here:

$$\frac{500}{\sqrt{4}} = \frac{1000}{\sqrt{t_2}}$$

$$t_2 = 16\ hrs$$

This is important because this tells me if I want to double the case depth and I have to increase the time to four times. This $\frac{x}{\sqrt{t}}$ is also called us parabolic relation:

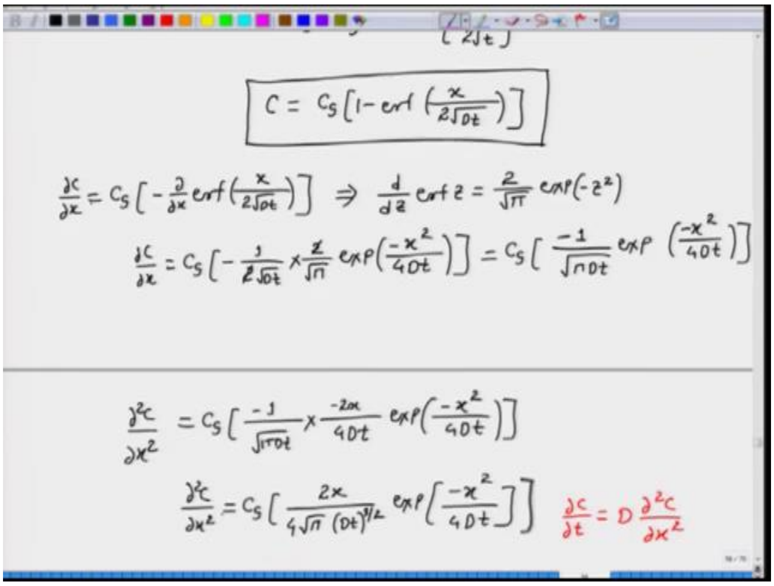
$$\frac{x}{\sqrt{t}} = \lambda_C$$

We say each concentration plane moves parabolically with time or has a parabolic relation with time:

$$C = C\left(\frac{x}{\sqrt{t}}\right)$$

Now, another point I would like to note here is we are maintaining infinite boundary condition which again means that the diffusing species is not penetrating all the way to the other surface. But is it really true in practice? Or can we estimate for the given thickness of the blade? Can we maintain the infinite boundary conditions?

(Refer Time Slide: 28:42)



$$\boxed{C = C_S\left[1 - erf\left(\frac{x}{2\sqrt{Dt}}\right)\right]}$$

$$\frac{\partial C}{\partial x} = C_S\left[-\frac{\partial}{\partial x} erf\left(\frac{x}{2\sqrt{Dt}}\right)\right] \Rightarrow \frac{d}{dz} erf\, z = \frac{2}{\sqrt{\pi}} \exp(-z^2)$$

$$\frac{\partial C}{\partial x} = C_S\left[-\frac{1}{2\sqrt{Dt}} \times \frac{2}{\sqrt{\pi}} \exp\left(\frac{-x^2}{4Dt}\right)\right] = C_S\left[\frac{-1}{\sqrt{\pi Dt}} \exp\left(\frac{-x^2}{4Dt}\right)\right]$$

$$\frac{\partial^2 C}{\partial x^2} = C_S\left[\frac{-1}{\sqrt{\pi Dt}} \times \frac{-2x}{4Dt} \exp\left(\frac{-x^2}{4Dt}\right)\right]$$

$$\frac{\partial^2 C}{\partial x^2} = C_S\left[\frac{2x}{4\sqrt{\pi}\,(Dt)^{3/2}} \exp\left[\frac{-x^2}{4Dt}\right]\right] \quad \frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2}$$

This is a typical error function solution:

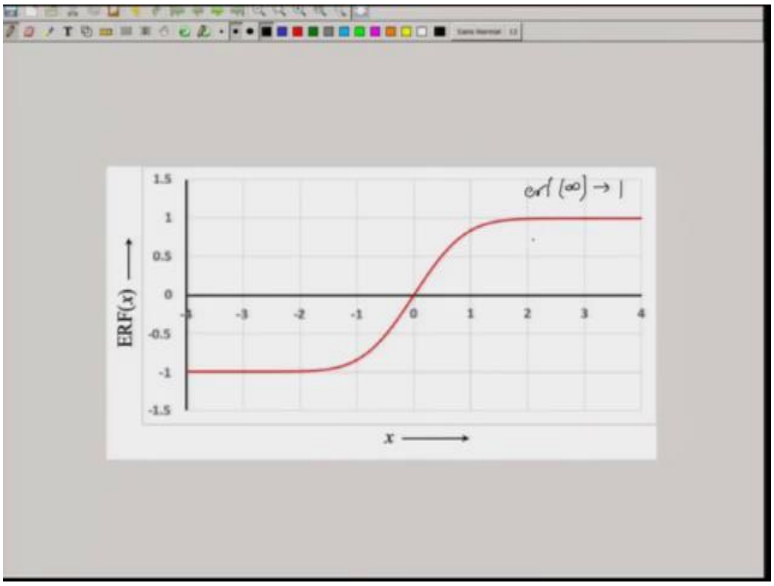
$$C = C_S\left(1 - erf\left[\frac{x}{2\sqrt{Dt}}\right]\right)$$

and we want basically the distance at which concentration drops to the original concentration that is 0. So, from this equation we will see that is where the error function tends to 1:

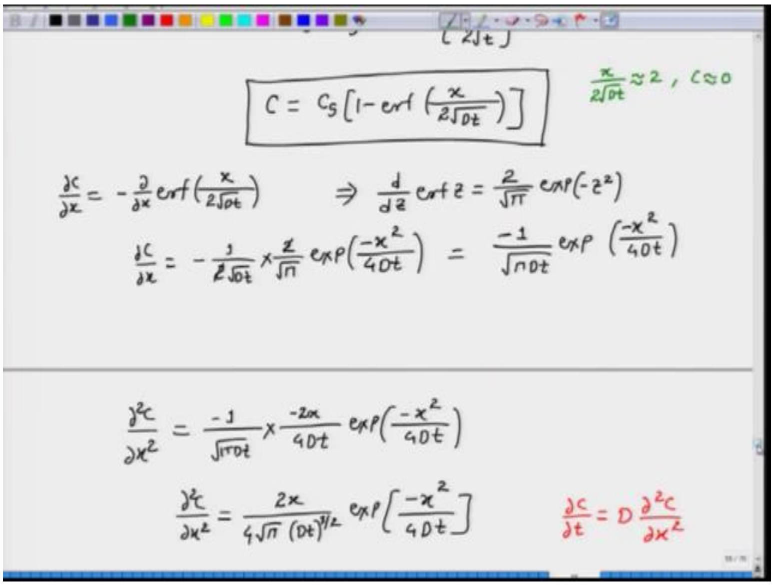
$$erf\left[\frac{x}{2\sqrt{Dt}}\right] = 1$$

Now mathematically, what is the value of Z for $erf[Z]$to be 1? Infinite and that is why it is infinite boundary condition.

(Refer Time Slide: 29:33)



$\mathrm{erf}(\infty) \to 1$



$$\boxed{C = C_s\left[1 - \mathrm{erf}\left(\frac{x}{2\sqrt{Dt}}\right)\right]}$$

$\frac{x}{2\sqrt{Dt}} \approx 2\,,\ C \approx 0$

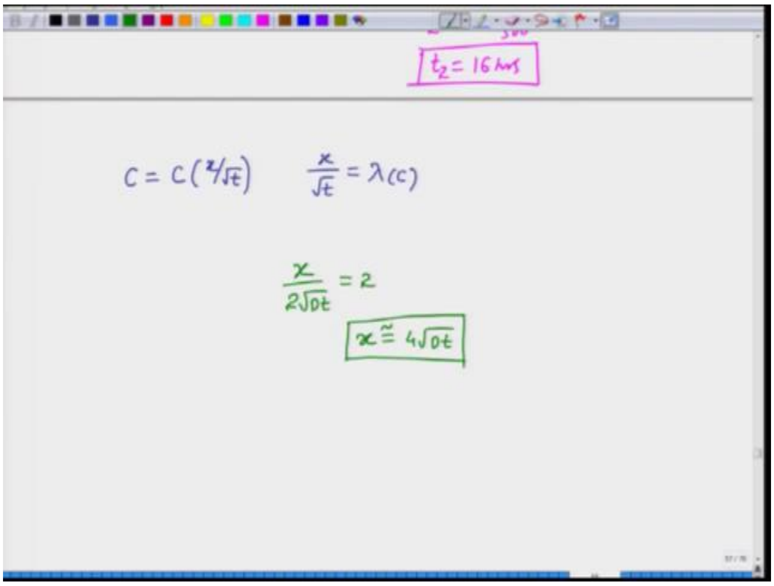
$$\frac{\partial c}{\partial x} = -\frac{\partial}{\partial x}\mathrm{erf}\left(\frac{x}{2\sqrt{Dt}}\right) \qquad \Rightarrow \frac{d}{dz}\mathrm{erf}\,z = \frac{2}{\sqrt{\pi}}\exp(-z^2)$$

$$\frac{\partial c}{\partial x} = -\frac{1}{2\sqrt{Dt}} \times \frac{2}{\sqrt{\pi}}\exp\left(\frac{-x^2}{4Dt}\right) = \frac{-1}{\sqrt{\pi Dt}}\exp\left(\frac{-x^2}{4Dt}\right)$$

$$\frac{\partial^2 c}{\partial x^2} = \frac{-1}{\sqrt{\pi Dt}} \times \frac{-2x}{4Dt}\exp\left(\frac{-x^2}{4Dt}\right)$$

$$\frac{\partial^2 c}{\partial x^2} = \frac{2x}{4\sqrt{\pi}\,(Dt)^{3/2}}\exp\left[\frac{-x^2}{4Dt}\right]$$

$$\frac{\partial c}{\partial t} = D\frac{\partial^2 c}{\partial x^2}$$



$$\boxed{t_2 = 16\ \mathrm{hrs}}$$

$$C = C(x/\sqrt{t}) \qquad \frac{x}{\sqrt{t}} = \lambda(c)$$

$$\frac{x}{2\sqrt{Dt}} = 2$$

$$\boxed{x \cong 4\sqrt{Dt}}$$

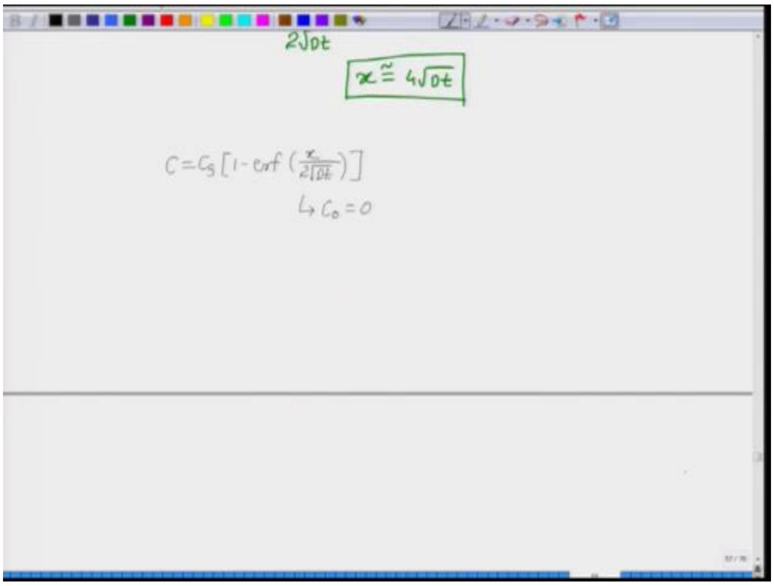
But physically, let us see, the plot of $\mathrm{erf}(x)$ versus x. And we know $\mathrm{erf}(\infty) \rightarrow 1$, but if you closely look at the plot, this plot kind of flattens out or levels approximately to 1 even at x=2.

We can approximate that even when:

$$\frac{x}{2\sqrt{Dt}} \sim 2 \quad or \quad x \sim 4\sqrt{Dt}$$

we will get the original composition. That is one rough measure to see if the given thickness of plate and time can satisfy the infinite boundary condition. So, the thickness has to be at least $4\sqrt{Dt}$ of course or more than that. To be safer, we take maybe $6\sqrt{Dt}$ or $8\sqrt{Dt}$ minimum thickness. And typically, the component thicknesses encountered are much larger than the case depth. Thus infinite boundary condition will always be satisfied.

(Refer Time Slide: 31:25)



$2\sqrt{Dt}$

$\boxed{x \cong 4\sqrt{Dt}}$

$C = C_S\left[1 - erf\left(\frac{x}{2\sqrt{Dt}}\right)\right]$

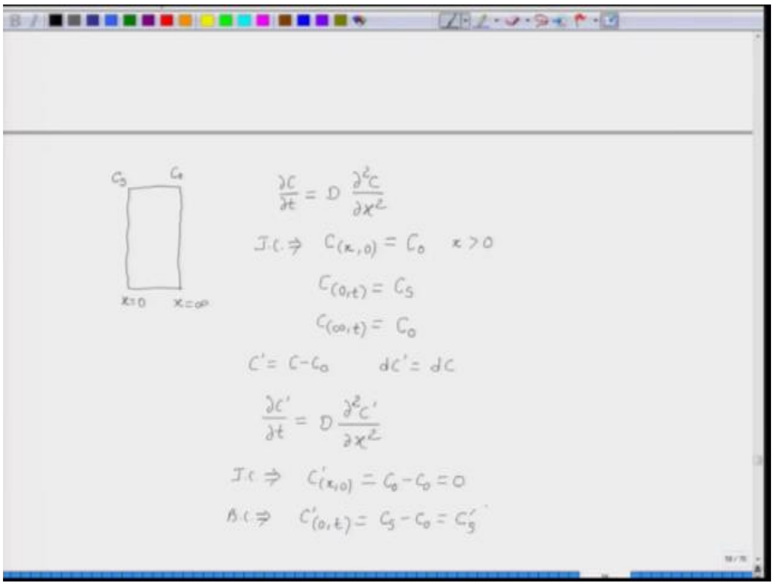
$\hookrightarrow C_o = 0$

So, we derived an equation for evolution of concentration profile in a semi-infinite slab boundary condition and which takes the form of:

$$C = C_S\left(1 - erf\left[\frac{x}{2\sqrt{Dt}}\right]\right)$$

Now, we derived this equation assuming that $C_o = 0$, that is, concentration of the species in the slab to start with was 0 or when we talk about carburizing the solution assumes that the initial concentration of steel that has been carburized is 0. However, this is not the case in practice as I said, the steel that is going to undergo carburizing heat treatment is a low carbon steel. So, it has some carbon concentration, typically around 0.2 weight % carbon. How do we solve the diffusion equation in this case, it is simple, we just need to rescale our concentration axis.

(Refer Time Slide: 32:48)



$$\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2}$$

I.C. ⇒ $C_{(x,0)} = C_0 \quad x>0$

$C_{(0,t)} = C_S$

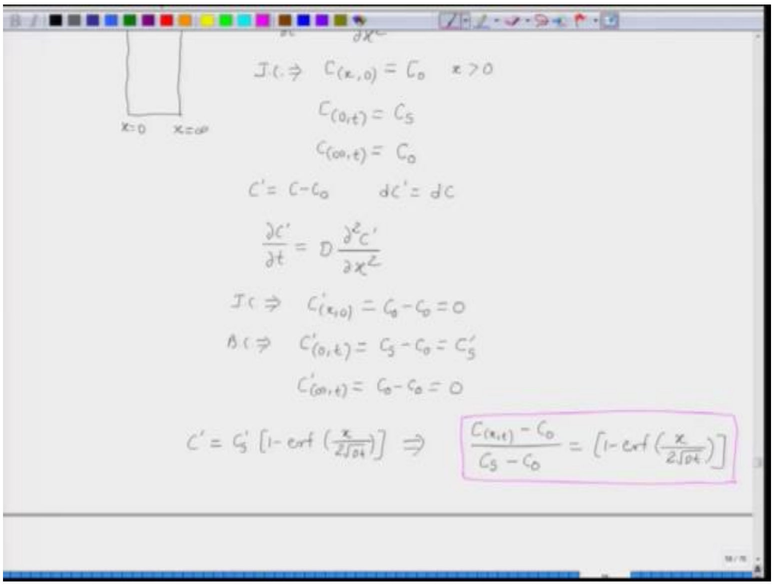
$C_{(\infty,t)} = C_0$

$C' = C - C_0 \qquad dC' = dC$

$$\frac{\partial C'}{\partial t} = D\frac{\partial^2 C'}{\partial x^2}$$

I.C ⇒ $C'_{(x,0)} = C_0 - C_0 = 0$

B.C ⇒ $C'_{(0,t)} = C_S - C_0 = C'_S$



I.C. ⇒ $C_{(x,0)} = C_0 \quad x>0$

$C_{(0,t)} = C_S$

$C_{(\infty,t)} = C_0$

$C' = C - C_0 \qquad dC' = dC$

$$\frac{\partial C'}{\partial t} = D\frac{\partial^2 C'}{\partial x^2}$$

I.C ⇒ $C'_{(x,0)} = C_0 - C_0 = 0$

B.C ⇒ $C'_{(0,t)} = C_S - C_0 = C'_S$

$C'_{(\infty,t)} = C_0 - C_0 = 0$

$$C' = C'_S\left[1 - \text{erf}\left(\frac{x}{2\sqrt{Dt}}\right)\right] \Rightarrow \boxed{\frac{C_{(x,t)} - C_0}{C_S - C_0} = \left[1 - \text{erf}\left(\frac{x}{2\sqrt{Dt}}\right)\right]}$$

To state the problem, we have a semi-infinite slab whose initial concentration is denoted by C_o and the surface concentration which is maintained constant during the process is C_S. Now we have to solve the diffusion equation:

$$\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2}$$

Now $C_o \neq 0$ in this case. The initial conditions are:

$$C(x,0) = C_o \;\; for \;\; x > 0$$

and the boundary conditions are:

$$C(0,t) = C_S$$

And since we are maintaining infinite boundary conditions here, $x = 0$. The other end we denote as $x = +\infty$. So:

$$C(\infty, t) = C_o$$

C_o is the original concentration. Now, we make a little bit of substitution here, let us call:

$$C' = C - C_o$$

C_o is a constant.

$$dC' = dC$$

Our diffusion equation with the new modified concentration variable becomes:

$$\frac{\partial C'}{\partial t} = D \frac{\partial^2 C'}{\partial x^2}$$

And the initial condition becomes:

$$I.C.\ :\quad C'(x, 0) = C_o - C_o = 0$$

And the boundary conditions becomes:

$$B.C.\ :\quad B.C.\ :\quad C'(0, t) = C_S - C_o = C'_S$$

$$B.C.\ :\quad C'(\infty, t) = C_o - C_o = 0$$

We got back the diffusion equation and the initial and boundary conditions in the form that we have already solved. And the equation for the concentration profile in terms of C' would be:

$$C' = C'_S \left(1 - erf\left[\frac{x}{2\sqrt{Dt}}\right]\right)$$

Then if we substitute for C' it takes the form:

$$\frac{C_{(x,t)} - C_o}{C_S - C_o} = \left(1 - erf\left[\frac{x}{2\sqrt{Dt}}\right]\right)$$

This is the more popular form that you will see in most of the textbooks, and this is applicable for a semi-infinite slab which has an initial concentration equal to C_o. And this is more practically applicable to the carburizing problem. With this we will stop here for today. Thank you.