Diffusion in Multicomponent Solids
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Lecture 19
Error Function and its Laplace Transform

Welcome back, to the class on Diffusion in Multicomponent Solids. In next few lectures, we will go over solutions of diffusion equation for various boundary conditions and Laplace transform will be an important tool in solving this diffusion equations. Last lecture, we went through the properties of Laplace transforms and we also solved some examples wherein we evaluated Laplace transforms for some simple functions. Today, we will evaluate the Laplace transforms for some of the important functions that we will encounter while solving diffusion equation.

When I say that, one of the important function that we will encounter in solutions of diffusion equation is error function. Let us first go over some of the properties of error function the definition first and it will be sufficient for this class to just know the definition and some of the properties of error functions. We do not need to go over in detail into this error function. The error function is defined as follows.

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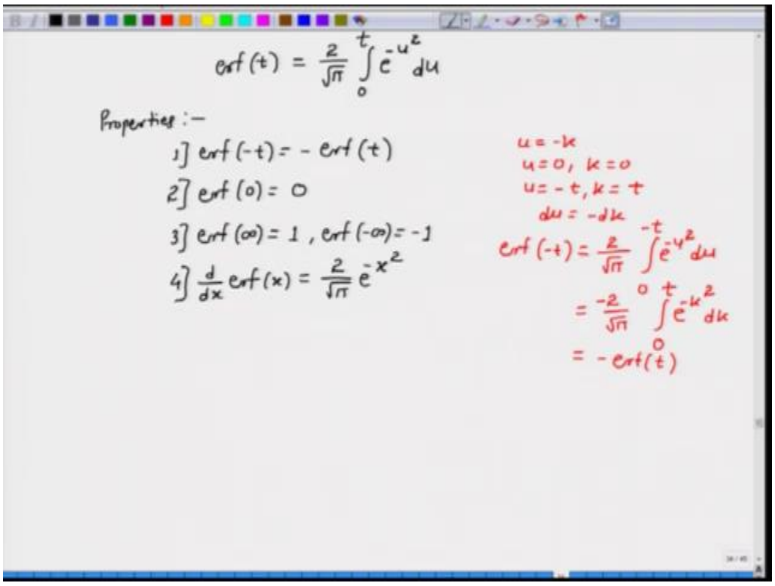

$$\text{erf}(t) = \frac{2}{\sqrt{\pi}} \int_0^t e^{-u^2} du$$

The factor $\frac{2}{\sqrt{\pi}}$ is the normalizing factor so that the error function of infinity turns out to be unity and this is an important function. Many of the solutions will have this error function form. Let us see some of the properties of error function.

First one is:

$$\operatorname{erf}(-t) = -\operatorname{erf}(t)$$

It is easy to show this. For example if we make a substitution for:

$$u = -k, \quad then \qquad u = 0 \quad for \qquad k = 0$$

$$for \quad u = -t, \qquad k = t$$

$$du = -dk$$

If we define $\operatorname{erf}(-t)$ it should be:

$$\operatorname{erf}(-t) = \frac{2}{\sqrt{\pi}} \int_0^{-t} e^{-u^2} du$$

Now, if we substitute $u = -k$ this turns out to be:

$$\operatorname{erf}(-t) = \frac{2}{\sqrt{\pi}} \int_0^{-t} e^{-u^2} du = -\frac{2}{\sqrt{\pi}} \int_0^{t} e^{-k^2} dk = -\operatorname{erf}(t)$$

Hence we have proved $\operatorname{erf}(-t) = -\operatorname{erf}(t)$. Similarly, the second property isL

$$\operatorname{erf}(0) = 0$$

It is very easy to see here, because integral from 0 to 0 should be 0. Third property is:

$$\operatorname{erf}(\infty) = 1$$

and from the first property it will turn out that:

$$\operatorname{erf}(-\infty) = -1$$

And then the fourth and one of the important property is:

$$\frac{d}{dx}\operatorname{erf}(x) = \frac{2}{\sqrt{\pi}} e^{-x^2}$$

These are some of the properties of error function. With that now let us try to evaluate the Laplace transform for error function. $\operatorname{erf}\left(\frac{a}{\sqrt{t}}\right)$ is an important function which we will encounter in the solutions for diffusion equation. So let us try to evaluate the Laplace transform for $\operatorname{erf}\left(\frac{a}{\sqrt{t}}\right)$.

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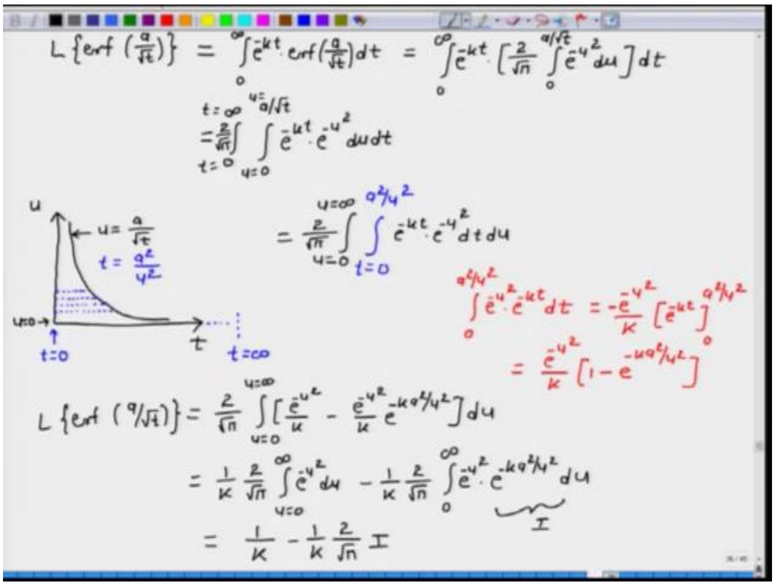


$$I_{(k)} = \int_0^\infty e^{-u^2}\cdot e^{-ka^2/u^2}\,du$$

$$\frac{dI_{(k)}}{dk} = \int_0^\infty e^{-u^2}\cdot\frac{d}{dk}e^{-ka^2/u^2}\cdot du = \int_0^\infty e^{-u^2}\cdot\frac{-a^2}{u^2}\,e^{-ka^2/u^2}\,du$$

$$\frac{dI}{dk} = -a^2\int_0^\infty e^{-u^2}\cdot\frac{1}{u^2}\cdot e^{-ka^2/u^2}\,du$$

$$\sqrt{k}\,a/u = x \qquad dx = \frac{-\sqrt{k}\,a}{u^2}\,du \quad \text{or} \quad du = \frac{-u^2}{\sqrt{k}\,a}\,dx$$

$$\frac{dI}{dk} = -a^2\int_\infty^0 e^{-ka^2/x^2}\cdot\frac{1}{u^2}\,e^{-x^2}\cdot\frac{-u^2}{\sqrt{k}\cdot a}\,dx$$

$$= \frac{-a}{\sqrt{k}}\int_0^\infty e^{-x^2}\cdot e^{-ka^2/x^2}\,dx$$

$$\frac{dI}{dk} = \frac{-a}{\sqrt{k}}\,I \;\Rightarrow\; \text{Solution } I = C\exp(-2a\sqrt{k})$$

$$I_{(0)} = C = \int_0^\infty e^{-x^2}\,dx = \frac{\sqrt{\pi}}{2}$$

$$I = \frac{\sqrt{\pi}}{2}\exp(-2a\sqrt{k})$$

$$= \frac{-a}{\sqrt{k}}\int_0^\infty e^{-x^2}\cdot e^{\ldots}\,dx$$

$$\frac{dI}{dk} = \frac{-a}{\sqrt{k}}\,I \;\Rightarrow\; \text{Solution } I = C\exp(-2a\sqrt{k})$$

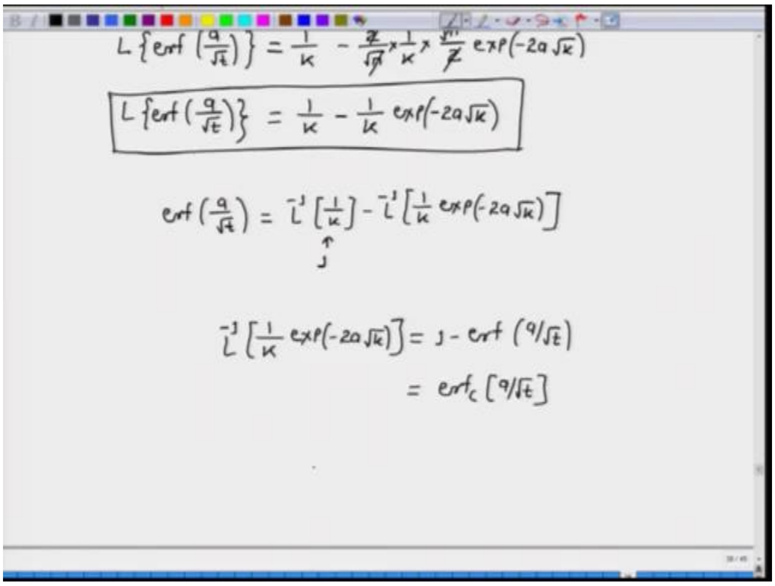
$$I_{(0)} = C = \int_0^\infty e^{-x^2}\,dx = \frac{\sqrt{\pi}}{2}$$

$$I = \frac{\sqrt{\pi}}{2}\exp(-2a\sqrt{k})$$

$$L\left\{\operatorname{erf}\left(\frac{a}{\sqrt{t}}\right)\right\} = \frac{1}{k} - \frac{2}{\sqrt{\pi}}\times\frac{1}{k}\times\frac{\sqrt{\pi}}{2}\exp(-2a\sqrt{k})$$

$$\boxed{L\left\{\operatorname{erf}\left(\frac{a}{\sqrt{t}}\right)\right\} = \frac{1}{k} - \frac{1}{k}\exp(-2a\sqrt{k})}$$

$$\operatorname{erf}\left(\frac{a}{\sqrt{t}}\right) = L^{-1}\left[\frac{1}{k}\right] - L^{-1}\left[\frac{1}{k}\exp(-2a\sqrt{k})\right]$$



The problem is to evaluate $L\left\{\text{erf}(\frac{a}{\sqrt{t}})\right\}$ and by definition the Laplace transform is:

$$L\left\{\text{erf}\left(\frac{a}{\sqrt{t}}\right)\right\} = \int_0^\infty e^{-kt}\,\text{erf}\left(\frac{a}{\sqrt{t}}\right)dt$$

And, if you substitute for error function from its definition, you will get:

$$L\left\{\text{erf}(\frac{a}{\sqrt{t}})\right\} = \int_0^\infty e^{-kt}\text{erf}(\frac{a}{\sqrt{t}})dt = \int_0^\infty e^{-kt}\left[\frac{2}{\sqrt{\pi}}\int_0^{\frac{a}{\sqrt{t}}} e^{-u^2}du\right]dt$$

There are two integrals involved here, let us try to rearrange them:

$$L\left\{\text{erf}(\frac{a}{\sqrt{t}})\right\} = \frac{2}{\sqrt{\pi}}\int_{t=0}^{t=\infty}\int_{u=0}^{u=\frac{a}{\sqrt{t}}} e^{-kt}e^{-u^2}du\,dt$$

Now we have to evaluate this double integral in this case. The first integral is with respect to du and then with respect to dt. Let us try to change the order of integration, so that it becomes convenient to solve. In this case the inner integral is with respect to u. Limits are defined for u as equal to 0 to $\frac{a}{\sqrt{t}}$ and the outer integral is for t, so the limit of outer integral are defined as $t = 0$ to $t = \infty$. How do we change the order of integration if there are two variables here u and t?

Let us draw a plot of u versus t. First let us discuss the inner integral limits: u equal to 0 is basically this t axis at $u = 0$ to u equal to $\frac{a}{\sqrt{t}}$. This upper limit is defined by the curve of $u =$

$\frac{a}{\sqrt{t}}$. So, iff you draw a plot of u versus t, such that u equal to $\frac{a}{\sqrt{t}}$ we will get a plot something like this and this plot defines the upper limit for u. For the outer integral, the limits of t are from t equal to 0 which is basically the u axis to $t = \infty$ as the upper limit for t is infinity.

If we try to change the order of integration, which means if we first want to evaluate the integral with respect to t and then with respect to u, we first have to take the limits of t. Now, in this case the limits of t will go from t equal to 0: so if we draw these horizontal lines, the t is bound by 0 on left side and by this plot on the right side.

You can also write the equation of this plot as:

$$t = \frac{a^2}{u^2}$$

If we define the inner integral limit as t equal to 0 to t equal to $\frac{a^2}{u^2}$ and the outer integral limit will now become u. The u in this case will be bound by u equal to 0 and all the way to infinity and the integrand is $e^{-kt}e^{-u^2}$:

$$L\left\{\text{erf}\left(\frac{a}{\sqrt{t}}\right)\right\} = \frac{2}{\sqrt{\pi}}\int_{u=0}^{u=\infty}\int_{t=0}^{t=\frac{a^2}{u^2}} e^{-kt}e^{-u^2}dt\,du$$

We have changed the order of integration and there is also a factor of $\frac{2}{\sqrt{\pi}}$ outside. Let us try to evaluate this inner integral now. The inner integral will be:

$$\int_{t=0}^{t=\frac{a^2}{u^2}} e^{-kt}e^{-u^2}dt = \frac{-e^{-u^2}}{k}[e^{-kt}]_0^{\frac{a^2}{u^2}} = \frac{e^{-u^2}}{k}\left[1 - e^{-\frac{ka^2}{u^2}}\right]$$

So, the Laplace transform of error function a by root t should be equal to:

$$L\left\{\text{erf}\left(\frac{a}{\sqrt{t}}\right)\right\} = \frac{2}{\sqrt{\pi}}\int_{u=0}^{u=\infty}\left[\frac{e^{-u^2}}{k} - \frac{e^{-u^2}}{k}e^{\frac{-ka^2}{u^2}}\right]du$$

If we evaluate this separately, this will be:

$$L\left\{\text{erf}\left(\frac{a}{\sqrt{t}}\right)\right\} = \frac{1}{k}\frac{2}{\sqrt{\pi}}\int_{u=0}^{u=\infty} e^{-u^2}du - \frac{1}{k}\frac{2}{\sqrt{\pi}}\int_{u=0}^{u=\infty} e^{-u^2}e^{\frac{-ka^2}{u^2}}du = \frac{1}{k} - \frac{1}{k}\frac{2}{\sqrt{\pi}}I$$

The first term here is $\frac{1}{k}$ and we have to evaluate this second integral here. Let us call this integral as I:

$$I = \int_{u=0}^{u=\infty} e^{-u^2} e^{\frac{-ka^2}{u^2}} du$$

and if you notice, the integration is with respect to u and it is a definite integral. I is a function of k, so we write $I(k)$. To evaluate this integral let us try to do a little bit of manipulation, if we take a derivative of I with respect to k:

$$\frac{dI}{dk} = \int_{u=0}^{u=\infty} e^{-u^2} \frac{d}{dk} e^{\frac{-ka^2}{u^2}} du$$

And if we evaluate the derivative of $e^{\frac{-ka^2}{u^2}}$ and substitute we get:

$$\frac{dI}{dk} = \int_{u=0}^{u=\infty} e^{-u^2} \frac{d}{du} e^{\frac{-ka^2}{u^2}} du = \int_{u=0}^{u=\infty} e^{-u^2} \frac{-a^2}{u^2} e^{\frac{-ka^2}{u^2}} du$$

$\frac{dI}{dk}$ in this case is:

$$\frac{dI}{dk} = -a^2 \int_0^\infty e^{-u^2} \frac{1}{u^2} e^{-\frac{ka^2}{u^2}} du$$

Now let us make a substitution here. If we define:

$$x = \frac{\sqrt{k}a}{u}$$

So,

$$dx = -\frac{\sqrt{k}a}{u^2} du \quad or\ du = -\frac{u^2}{\sqrt{k}a} dx$$

and we substitute this in $\frac{dI}{dk}$ which becomes:

$$\frac{dI}{dk} = -a^2 \int_{\infty}^{0} e^{\frac{-ka^2}{x^2}} \frac{1}{u^2} e^{-x^2} \frac{-u^2}{\sqrt{ka}} dx$$

and if we see the limits, when u is equal to 0 x will tend to ∞ and as u tends to ∞ x will tend to 0. These limits are reversed as ∞ to 0. Further the expression can be simplified as:

$$\frac{dI}{dk} = -\frac{a}{\sqrt{k}} \int_{0}^{\infty} e^{-x^2} e^{\frac{-ka^2}{x^2}} dx$$

and and if we closely look at this integral, it is basically the same as I of k. So what we get here:

$$\frac{dI}{dk} = -\frac{a}{\sqrt{k}} I$$

Now, if you solve this equation, the solution is:

$$I = Cexp\left(-2a\sqrt{k}\right)$$

Now, to evaluate C if you substitute for $k = 0$, then we know:

$$I_{(o)} = C$$

but if we substitute in the integral:

$$I_o = C = \int_{0}^{\infty} e^{-x^2} dx$$

As

$$\frac{2}{\sqrt{\pi}} \int_0^\infty e^{-x^2} dx = \mathrm{erf}(\infty) = 1$$

So:

$$I_o = C = \frac{\sqrt{\pi}}{2}$$

We have now got the value of I:

$$I = \frac{\sqrt{\pi}}{2} exp(-2a\sqrt{k})$$

If you substitute the expression for I back in the Laplace transform equation we get:

$$L\left\{erf(\frac{a}{\sqrt{t}})\right\} = \frac{1}{k} - \frac{2}{\sqrt{\pi}}\frac{1}{k}\frac{\sqrt{\pi}}{2} exp\left(-2a\sqrt{k}\right) = \frac{1}{k} - \frac{1}{k} exp\left(-2a\sqrt{k}\right)$$

We got the Laplace transform of one of the important function here. If we evaluate the inverse Laplace on both side here, then:

$$erf\left(\frac{a}{\sqrt{t}}\right) = L^{-1}\left[\frac{1}{k}\right] - L^{-1}\left[\frac{1}{k} exp\left(-2a\sqrt{k}\right)\right]$$

$L^{-1}\left[\frac{1}{k}\right]$ is nothing but 1 because the Laplace transform of 1 is $\frac{1}{k}$ and if you rearrange, we find $L^{-1}\left[\frac{1}{k} exp\left(-2a\sqrt{k}\right)\right]$ should be equal to:

$$L^{-1}\left[\frac{1}{k} exp\left(-2a\sqrt{k}\right)\right] = 1 - erf\left(\frac{a}{\sqrt{t}}\right)$$

This is an important result, because when we solve diffusion equation, we will do that Laplace transform and to get back the original solution when we take the inverse Laplace we will have to refer to this kind of solutions. And this is an important result here. $1 - erf(x)$ is also referred to as $erfc$ or complementary error function. So:

$$L^{-1}\left[\frac{1}{k} exp\left(-2a\sqrt{k}\right)\right] = erfc\left(\frac{a}{\sqrt{t}}\right)$$

This is one important formula that we have obtained.

We have now derived the formula for the Laplace transform of error function of $\frac{a}{\sqrt{t}}$ where a is a constant. Let us try to now use the property of Laplace transform of the derivative of functions and try to derive one more formula here. Let us say:

$$f(t) = erf\left(\frac{a}{\sqrt{t}}\right)$$

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$$f(t) = \mathrm{erf}\left(a/\sqrt{t}\right)$$

$$f'(t) = \frac{d}{dt}\mathrm{erf}\left(\frac{a}{\sqrt{t}}\right)$$

$$= \frac{-a}{2t^{3/2}} \times \frac{2}{\sqrt{\pi}} \exp\left[\frac{-a^2}{t}\right]$$

$$f'(t) = \frac{-a}{\sqrt{\pi}\, t^{3/2}} \exp\left[\frac{-a^2}{t}\right]$$

$$\frac{d}{dx}\mathrm{erf}(x) = \frac{2}{\sqrt{\pi}} e^{-x^2}$$

$$\frac{d}{dt}\left(\frac{a}{\sqrt{t}}\right) = \frac{-a}{2t^{3/2}}$$

$$L\{f'(t)\} = k\,L\{f(t)\} - f(0)$$

as $t \to 0$, $f(0) \to \mathrm{erf}(\infty) = 1$

$$= k\,L\{\mathrm{erf}(a/\sqrt{t})\} - 1$$

$$f(t) = \mathrm{erf}\left(a/\sqrt{t}\right)$$

$$f'(t) = \frac{d}{dt}\mathrm{erf}\left(\frac{a}{\sqrt{t}}\right)$$

$$= \frac{-a}{2t^{3/2}} \times \frac{2}{\sqrt{\pi}} \exp\left[\frac{-a^2}{t}\right]$$

$$f'(t) = \frac{-a}{\sqrt{\pi}\, t^{3/2}} \exp\left[\frac{-a^2}{t}\right]$$

$$\frac{d}{dx}\mathrm{erf}(x) = \frac{2}{\sqrt{\pi}} e^{-x^2}$$

$$\frac{d}{dt}\left(\frac{a}{\sqrt{t}}\right) = \frac{-a}{2t^{3/2}}$$

$$L\{f'(t)\} = k\,L\{f(t)\} - f(0)$$

as $t \to 0$, $f(0) \to \mathrm{erf}(\infty) = 1$

$$= k\,L\{\mathrm{erf}(a/\sqrt{t})\} - 1$$

$$= k\left[\frac{1}{k} - \frac{1}{k}\exp(-2a\sqrt{k})\right] - 1$$

$$= -\exp[-2a\sqrt{k}]$$

$$L\left\{\frac{a}{\sqrt{\pi}\, t^{3/2}} \exp\left(\frac{-a^2}{t}\right)\right\} = \exp[-2a\sqrt{k}]$$

$$L\{f'(t)\} = k\,L\{f(t)\} - f(0)$$

as $t \to 0$, $f(0) \to \mathrm{erf}(\infty) = 1$

$$= k\,L\{\mathrm{erf}(a/\sqrt{t})\} - 1$$

$$= k\left[\frac{1}{k} - \frac{1}{k}\exp(-2a\sqrt{k})\right] - 1$$

$$= -\exp[-2a\sqrt{k}]$$

$$L\left\{\frac{a}{\sqrt{\pi}\, t^{3/2}} \exp\left(\frac{-a^2}{t}\right)\right\} = \exp[-2a\sqrt{k}]$$

$$L^{-1}\left\{\exp[-2a\sqrt{k}]\right\} = \frac{a}{\sqrt{\pi}\, t^{3/2}} \exp\left(\frac{-a^2}{t}\right)$$

The derivative of $f(t)$ will be:

$$f'(t) = \frac{d}{dt} erf\left(\frac{a}{\sqrt{t}}\right) = -\frac{a}{2t\sqrt{t}}$$

and we know $\frac{d}{dx}$ of error function x is equal to:

$$\frac{d}{dx} erf(x) = \frac{2}{\sqrt{\pi}} e^{-x^2}$$

Here we will have to first evaluate $\frac{d}{dt}\left(\frac{a}{\sqrt{t}}\right)$ as:

$$f'(t) = \frac{d}{dt} erf\left(\frac{a}{\sqrt{t}}\right) = -\frac{a}{2t\sqrt{t}} \frac{2}{\sqrt{\pi}} exp\left[\frac{-a^2}{t}\right]$$

This should be:

$$f'(t) = -\frac{a}{\sqrt{\pi} t^{3/2}} exp\left[\frac{-a^2}{t}\right]$$

Now let us make use of formula for Laplace transform of derivative of a function. $L\{f'(t)\}$ should be equal to:

$$L\{f'(t)\} = kL\{f(t) - f(0)\}$$

Since, our $f(t)$ is $erf\left(\frac{a}{\sqrt{t}}\right)$ t, as t tends to 0 $f(0)$ tends to 1, the right hand side here will be:

$$L\{f'(t)\} = kL\{f(t) - f(0)\} = kL\left\{erf\left(\frac{a}{\sqrt{t}}\right)\right\} - 1$$

And, we just derived the formula for Laplace transform of error function of $\frac{a}{\sqrt{t}}$. If we substitute for the Laplace transform of $erf\left(\frac{a}{\sqrt{t}}\right)$, that should be equal to $\frac{1}{k} - \frac{1}{k} exp\left(-2a\sqrt{k}\right)$. So:

$$L\{f'(t)\} = kL\{f(t) - f(0)\} = kL\left\{erf\left(\frac{a}{\sqrt{t}}\right)\right\} - 1 = k\left[\frac{1}{k} - \frac{1}{k} exp\left(-2a\sqrt{k}\right)\right] - 1$$

$$L\{f'(t)\} = -exp\left(-2a\sqrt{k}\right)$$

If you substitute for $f'(t)$ here on the left hand side and get rid of the negative sign from both the sides, we find:

$$L\left\{\frac{a}{\sqrt{\pi}t^{3/2}}exp\left[\frac{-a^2}{t}\right]\right\} = exp(-2a\sqrt{k})$$

This is one more formula that we have derived.

If we take inverse on both the side, we can also write this as:

$$L^{-1}\{exp(-2a\sqrt{k})\} = \frac{a}{\sqrt{\pi}t^{3/2}}exp\left[\frac{-a^2}{t}\right]$$

This is another formula that is often used while solving the diffusion equation.

We have derived a couple of formula today, we will stop here for today, thank you.