Diffusion in Multicomponent Solids
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Lecture 22
Solution to Diffusion Equation for Binary Diffusion Couple

Welcome back, today we are going to solve diffusion equation for another set of boundary conditions. It is called diffusion couple. A diffusion couple is formed when you have two blocks of different compositions which come into contact of each other at an elevated temperature. At the elevated temperature the components diffuse from one block into the other and the interdiffusion process occurs.

Now we will talk about infinite diffusion couple which means the thickness of the two blocks in the diffusion couple that we are going to consider are large enough such that the diffusing species will not diffuse all the way to the other ends or all the way to the terminal ends of the two blocks.

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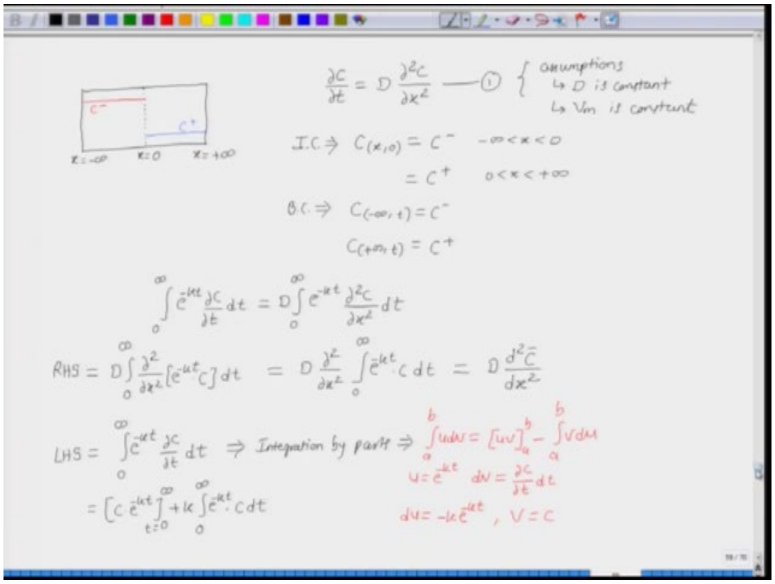

$$\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2} \quad \text{—①} \quad \left\{ \begin{array}{l} \text{assumptions} \\ \hookrightarrow D \text{ is constant} \\ \hookrightarrow V_m \text{ is constant} \end{array} \right.$$

$$\text{I.C.} \Rightarrow C_{(x,0)} = C^- \quad -\infty < x < 0$$

$$= C^+ \quad 0 < x < +\infty$$

$$\text{B.C.} \Rightarrow C_{(-\infty,t)} = C^-$$

$$C_{(+\infty,t)} = C^+$$

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

$$RHS = D\int_0^\infty \frac{\partial^2}{\partial x^2}[e^{-kt}C]dt = D\frac{\partial^2}{\partial x^2}\int_0^\infty e^{-kt}\cdot C\,dt = D\frac{d^2\bar{C}}{dx^2}$$

$$LHS = \int_0^\infty e^{-kt}\frac{\partial C}{\partial t}dt \Rightarrow \text{Integration by parts} \Rightarrow \int_a^b u\,dv = [uv]_a^b - \int_a^b v\,du$$

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

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

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

The problem is like this. We have two alloy blocks. The initial contact plane is denoted as $x = 0$ and let us denote the starting concentration of left side alloy by C^- and the starting concentration of the right side terminal alloy as C^+.

We will first consider binary diffusion couples which means there are two components and the composition of each of the block can be specified by just one concentration variable. So, we have to solve the diffusion equation:

$$\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2} \qquad (1)$$

And it has to be noted that we are making two assumptions here when we write this equation. First one is that D is constant or independent of composition and secondly the molar volume is also assumed constant. Since we are dealing with infinite diffusion couples, the two terminal ends we denote as $-\infty$ and $+\infty$.

We have on the left terminal $x = -\infty$, right terminal is at $x = +\infty$. The initial condition is:

$$C(x,0) = C^- \quad for \quad -\infty < x < 0$$

Now we have a step function here, the left terminal alloy initial concentration is C^-, for all $x < 0$. And in the right terminal alloy the concentration:

$$C(x,0) = C^+ \ for \quad 0 < x < +\infty$$

And the boundary conditions are:

$$C(-\infty, t) = C^-$$

$$C(\infty, t) = C^+$$

Now we have to solve the equation (1) with respect to this initial and boundary conditions. We will derive the solution for this with two different approaches. First we will use what we have been using so far, the Laplace transform approach. For Laplace transform we start with taking Laplace transform on both sides of equation (1) which means we multiply by e^{-kt} and integrate from $t = 0$ to $t = \infty$:

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

Here D is constant. So, we take D outside the integral. Since e^{-kt} is independent of x, we can take this term inside the partial derivative, then right hand side becomes:

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

If we solve the RHS we can change the order of differentiation:

$$RHS = D\int_0^\infty \frac{\partial^2}{\partial x^2}(e^{-kt}C)dt = D\frac{\partial^2}{\partial x^2}\int_0^\infty e^{-kt}Cdt$$

and this integral is again familiar as it is nothing but the Laplace transform of $C(x,t)$ which we denote as $\bar{C}$. And the Laplace transform is independent of time. So, we can replace the partial derivative with ordinary derivative. This becomes:

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

Now let us solve the left hand side:

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

Now let us use integration by parts here and we know the formula for integration by parts:

$$\int_a^b udv = [uv]_a^b - \int_a^b vdu$$

If you look at this integral here we can write:

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

We substitute here these functions and we get:

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

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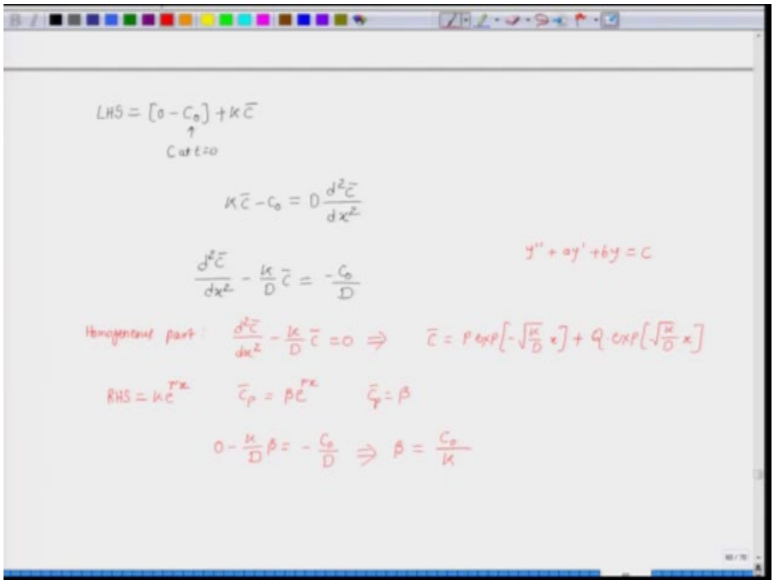

$$LHS = [0 - C_0] + k\bar{C}$$

$$\underset{C \text{ at } t=0}{\uparrow}$$

$$k\bar{C} - C_0 = D\frac{d^2\bar{C}}{dx^2}$$

$$\frac{d^2\bar{C}}{dx^2} - \frac{k}{D}\bar{C} = -\frac{C_0}{D}$$

$$y'' + ay' + by = c$$

Homogeneous part: $\frac{d^2\bar{C}}{dx^2} - \frac{k}{D}\bar{C} = 0 \Rightarrow \bar{C} = P\exp\left[-\sqrt{\frac{k}{D}}x\right] + Q\cdot\exp\left[\sqrt{\frac{k}{D}}x\right]$

$RHS = ke^{rx}$ $\quad \bar{C}_p = \beta e^{rx}$ $\quad \bar{C}_p = \beta$

$$0 - \frac{k}{D}\beta = -\frac{C_0}{D} \Rightarrow \beta = \frac{C_0}{k}$$

In LHS is you know C at $t = \infty$ will have a finite value and $e^{-kt} = 0$ and C at $t = 0$ let us call it as C_o plus this integral is the Laplace transform of C:

$$LHS = 0 - C_o + k\bar{C} = k\bar{C}$$

If we equate LHS and RHS we find:

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

Or

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

We could convert using Laplace transform the partial differential equation in x and t to an ordinary differential equation. Now, this is a non-homogenous ordinary differential equation which is of the form:

$$y'' + ay' + by = c$$

Here a, b, c are constants. Obviously a is 0 in this case, $b = -\frac{k}{D}$ and $c = -\frac{C_o}{D}$. Now to solve a non-homogeneous equation or to obtain the general solution for a non-homogeneous equation, we need to first obtain the general solution for the corresponding homogenous equation which in this case is:

$$Homogeneous\,part\colon\quad \frac{d^2\bar{C}}{dx^2} - \frac{k\bar{C}}{D} = 0$$

and one particular solution for the non-homogeneous equation. So, the sum of the two will give us the general solution for this non-homogeneous equation. Let us first consider the homogenous part and it has a general solution which we have seen last time when we solved for the semi-infinite slab boundary conditions.

The general solution for this is:

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

Now we need to know the particular solution for this. If you look at the right hand side of this non-homogenous equation:

$$\frac{d^2\bar{C}}{dx^2} - \frac{k\bar{C}}{D} = -\frac{C_o}{D} \qquad (2)$$

it is a constant $-\frac{C_o}{D}$. The RHS can be expressed in the form:

$$RHS = ke^{\gamma x}$$

In this case γ is 0 and we can start with the particular solution of the type $\bar{C}$:

$$\bar{C_P} = \beta e^{\gamma x}$$

As γ is 0,:

$$\bar{C_P} = \beta$$

If we substitute this value of $\bar{C}$ in the LHS of non-homogeneous equation we get:

$$0 - \frac{k}{D}\beta = -\frac{C_o}{D}$$

This gives the value of β as:

$$\beta = \frac{C_o}{k}$$

the sum of the general solution of homogenous part and the particular solution of the non-homogeneous ODE is the general solution of the non-homogenous ODE.

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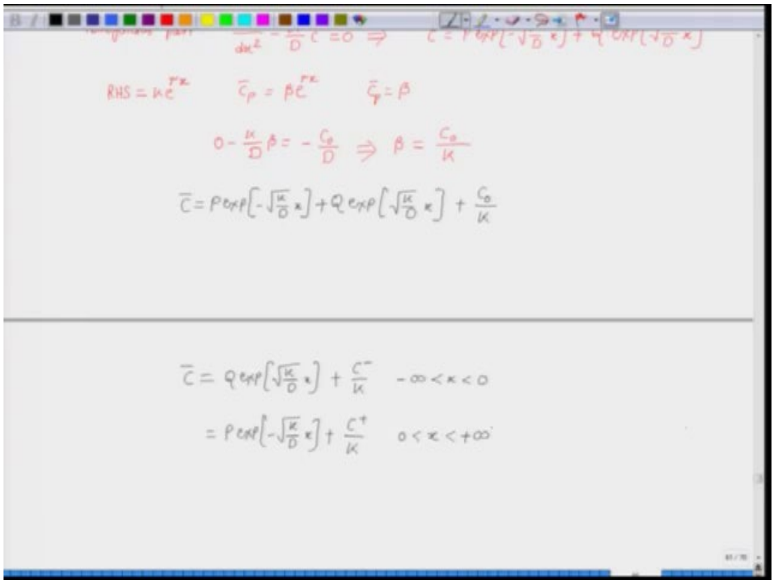

RHS $= \kappa e^{rx}$ $\quad \bar{C}_p = \beta e^{rx} \quad \bar{C}_p = \beta$

$$0 - \frac{k}{D}\beta = -\frac{C_o}{D} \Rightarrow \beta = \frac{C_o}{k}$$

$$\bar{C} = P\exp\left[-\sqrt{\frac{k}{D}}x\right] + Q\exp\left[\sqrt{\frac{k}{D}}x\right] + \frac{C_o}{k}$$

$$\bar{C} = Q\exp\left[\sqrt{\frac{k}{D}}x\right] + \frac{C^-}{k} \quad -\infty < x < 0$$

$$= P\exp\left[-\sqrt{\frac{k}{D}}x\right] + \frac{C^+}{k} \quad 0 < x < +\infty$$

The general solution of this equation (2) becomes:

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

Now this C_o is the initial condition C at t=0 and it has different values for different ranges of x right because initial concentration profile was a step function.

Now if we look at the form of the solution and we know that the concentration field should behave at all values of x including x equal to $\pm\infty$, we can straight away say that for negative values of x, P should be 0 otherwise $\bar{C}$ will tend to infinity. Similarly for positive values of x, Q should be 0 and then C_o is also different for negative and positive x. We can write the solution as:

$$\bar{C} = Qexp\left(\sqrt{\frac{k}{D}}x\right) + \frac{C^-}{k} \qquad -\infty < x < 0$$

$$\bar{C} = Pexp\left(-\sqrt{\frac{k}{D}}x\right) + \frac{C^+}{k} \qquad 0 < x < +\infty$$

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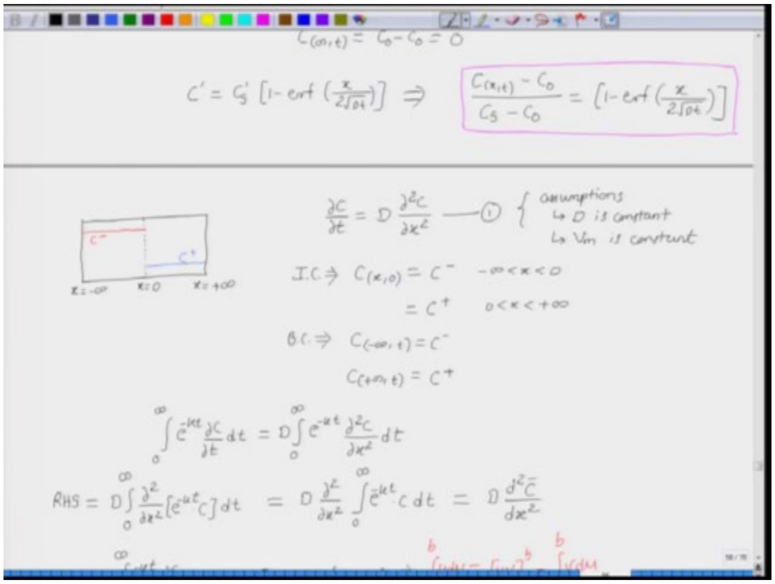

$$C_{(\infty,t)} = C_0 - C_0 = 0$$

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

$$\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2} \quad —① \quad \left\{ \begin{array}{l} \text{assumptions} \\ \hookrightarrow D \text{ is constant} \\ \hookrightarrow V_m \text{ is constant} \end{array} \right.$$

$$I.C. \Rightarrow C_{(x,0)} = C^- \quad -\infty < x < 0$$
$$= C^+ \quad 0 < x < +\infty$$

$$B.C. \Rightarrow C_{(-\infty,t)} = C^-$$
$$C_{(+\infty,t)} = C^+$$

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

$$RHS = D\int_0^\infty \frac{\partial^2}{\partial x^2}[e^{-kt}C]dt = D\frac{\partial^2}{\partial x^2}\int_0^\infty e^{-kt}C\,dt = D\frac{d^2\bar{C}}{dx^2}$$

Now we need to find the values of P and Q. If you look at the initial concentration profile and we know that D is constant or it is independent of composition here, obviously at x=0, the concentration should be constant and it should be equal to the average:

$$C_{(0,t)} = \frac{C^- + C^+}{2}$$

The profile should be symmetric about x=0 because D is constant, it is not varying with composition.

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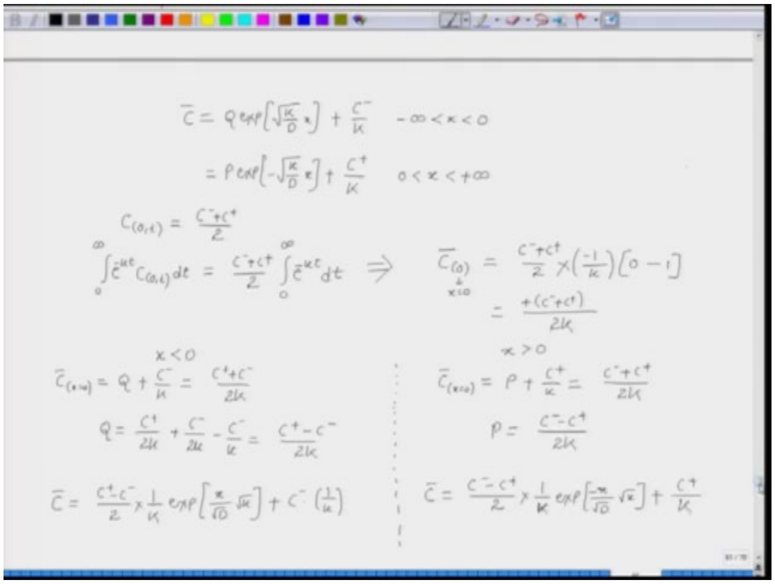

$$\bar{C} = Q\exp\left[\sqrt{\frac{k}{D}}x\right] + \frac{C^-}{k} \quad -\infty < x < 0$$

$$= P\exp\left[-\sqrt{\frac{k}{D}}x\right] + \frac{C^+}{k} \quad 0 < x < +\infty$$

$$C_{(0,t)} = \frac{C^- + C^+}{2}$$

$$\int_0^\infty e^{-kt} C_{(0,t)}\,dt = \frac{C^- + C^+}{2}\int_0^\infty e^{-kt}\,dt \Rightarrow \underset{x=0}{\bar{C}_{(0)}} = \frac{C^- + C^+}{2} \times \left(\frac{-1}{k}\right)[0-1]$$

$$= \frac{+(C^- + C^+)}{2k}$$

$x < 0$

$$\bar{C}_{(x=0)} = Q + \frac{C^-}{k} = \frac{C^+ + C^-}{2k}$$

$$Q = \frac{C^+}{2k} + \frac{C^-}{2k} - \frac{C^-}{k} = \frac{C^+ - C^-}{2k}$$

$$\bar{C} = \frac{C^+ - C^-}{2} \times \frac{1}{k}\exp\left[\frac{x}{\sqrt{D}}\sqrt{k}\right] + C^-\left(\frac{1}{k}\right)$$

$x > 0$

$$\bar{C}_{(x=0)} = P + \frac{C^+}{k} = \frac{C^- + C^+}{2k}$$

$$P = \frac{C^- - C^+}{2k}$$

$$\bar{C} = \frac{C^- - C^+}{2} \times \frac{1}{k}\exp\left[\frac{-x}{\sqrt{D}}\sqrt{k}\right] + \frac{C^+}{k}$$

If we take the Laplace transform on both the side for this previous equation:

$$\int_0^\infty e^{-kt} C_{(0,t)}dt = \frac{C^- + C^+}{2}\int_0^\infty e^{-kt}dt$$

$\frac{C^- + C^+}{2}$ is a constant. Left hand side integral is nothing but the Laplace transform of $C_{(0,t)}$.

For $x = 0$ It should be equal to:

$$\bar{C}_o = \frac{C^- + C^+}{2} \times \frac{-1}{k} \times [0-1] = \frac{C^- + C^+}{2k}$$

For $x < 0$ condition if we substitute:

$$\bar{C}_o = Q + \frac{C^-}{k} = \frac{C^- + C^+}{2k}$$

and Q here comes out to be:

$$Q = \frac{C^+ - C^-}{2k}$$

Using the above expression $\bar{C}$ here becomes:

$$\bar{C} = \frac{C^+ - C^-}{2} \times \frac{1}{k} \times exp\left[\frac{x\sqrt{k}}{\sqrt{D}}\right] + C^-\left(\frac{1}{k}\right)$$

For $x > 0$ we substitute for $\bar{C}$ at x equal to 0, this should be:

$$\bar{C}_o = P + \frac{C^+}{k} = \frac{C^- + C^+}{2k}$$

And P here becomes:

$$P = \frac{C^- - C^+}{2k}$$

And $\bar{C}$ becomes:

$$\bar{C} = \frac{C^- - C^+}{2} \times \frac{1}{k} \times exp\left[\frac{-x\sqrt{k}}{\sqrt{D}}\right] + \left(\frac{C^+}{k}\right)$$

So we got the equation of $\bar{C}$ on both sides of $x = 0$.

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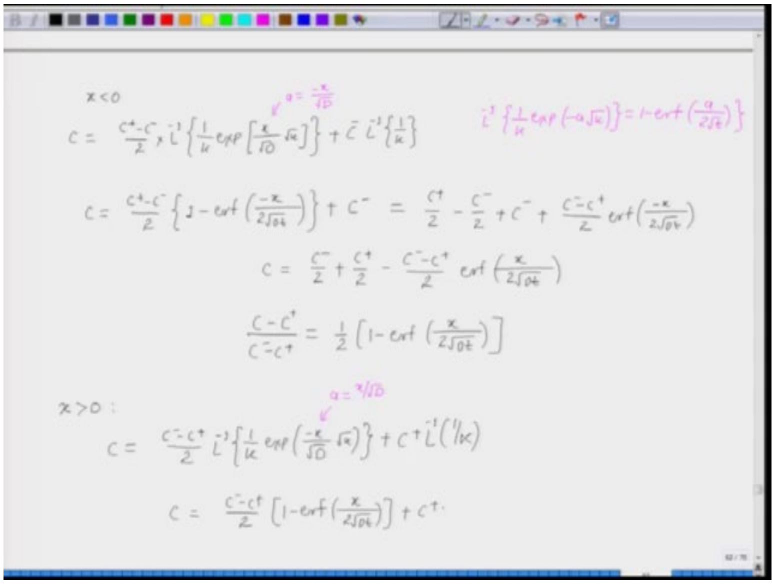


$x<0$

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

$$C = \frac{C^+ - C^-}{2} \times L^{-1}\left\{\frac{1}{k} exp\left[\frac{x}{\sqrt{D}}\sqrt{k}\right]\right\} + \bar{C}\, L^{-1}\left\{\frac{1}{k}\right\}$$

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

$$C = \frac{C^+ - C^-}{2}\left\{1 - erf\left(\frac{-x}{2\sqrt{Dt}}\right)\right\} + C^- = \frac{C^+}{2} - \frac{C^-}{2} + C^- + \frac{C^- - C^+}{2} erf\left(\frac{-x}{2\sqrt{Dt}}\right)$$

$$C = \frac{C^-}{2} + \frac{C^+}{2} - \frac{C^- - C^+}{2} erf\left(\frac{x}{2\sqrt{Dt}}\right)$$

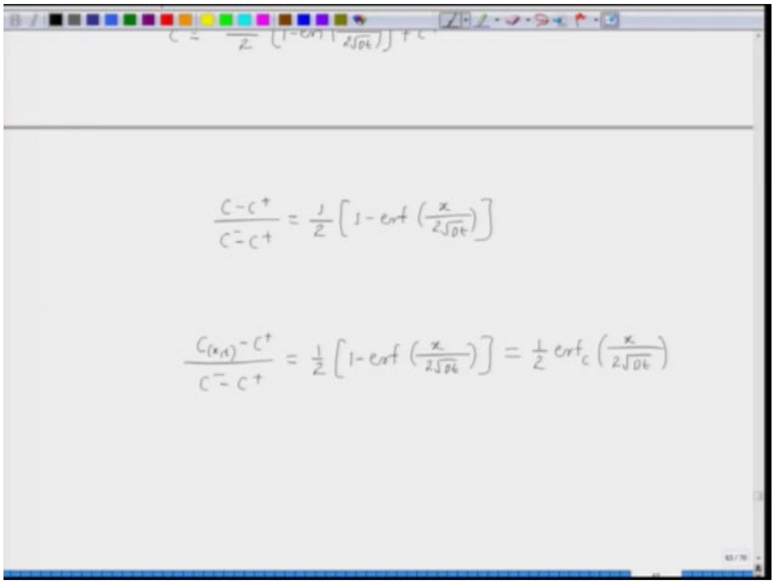
$$\frac{C - C^+}{C^- - C^+} = \frac{1}{2}\left[1 - erf\left(\frac{x}{2\sqrt{Dt}}\right)\right]$$

$x>0$:

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

$$C = \frac{C^- - C^+}{2} L^{-1}\left\{\frac{1}{k} exp\left(\frac{-x}{\sqrt{D}}\sqrt{k}\right)\right\} + C^+ L^{-1}(1/k)$$

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



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

$$\frac{C_{(x,t)}-C^+}{C^--C^+} = \frac{1}{2}\left[1-erf\left(\frac{x}{2\sqrt{Dt}}\right)\right] = \frac{1}{2}erf_c\left(\frac{x}{2\sqrt{Dt}}\right)$$

If we take the inverse Laplace transform for $x < 0$ we get back the function :

$$C = \frac{C^+ - C^-}{2} \times L^{-1}\left\{\frac{1}{k}\exp\left[\frac{x\sqrt{k}}{\sqrt{D}}\right]\right\} + C^- L^{-1}\left\{\frac{1}{k}\right\}$$

C^- is a constant. And the first function inside the inverse Laplace is familiar to us as :

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

If we try to bring our equation in the familiar form we know:

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

we can write:

$$C = \frac{C^+ - C^-}{2}\left\{1 - erf\left(\frac{a}{2\sqrt{t}}\right)\right\} + C^- = \frac{C^+}{2} - \frac{C^-}{2} + C^- + \frac{C^- - C^+}{2} erf\left(\frac{-x}{2\sqrt{Dt}}\right)$$

as $L^{-1}\left\{\frac{1}{k}\right\} = 1$. And we know:

$$erf(-z) = -erz(z)$$

This we can write in the form:

$$C = \frac{C^+}{2} + \frac{C^-}{2} - \frac{C^- - C^+}{2} erf\left(\frac{x}{2\sqrt{Dt}}\right)$$

And if we subtract C^+ from both the side and rearrange the term we get the familiar form for the diffusion couple equation:

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

Now for $x > 0$:

$$C = \frac{C^- - C^+}{2} \times L^{-1}\left\{\frac{1}{k}\exp\left[\frac{-x\sqrt{k}}{\sqrt{D}}\right]\right\} + C^+ L^{-1}\left\{\frac{1}{k}\right\}$$

And if we compare with the familiar expression for L^{-1} here:

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

and we can write:

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

and if we rearrange we get:

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

So, we get the same form for both $x < 0$as well as $x > 0$. We can write the solution in general as:

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

$1 - erf(z)$ is also called as complementary error function. It is denoted as erfc, we can write it as:

$$\frac{C_{(x,t)} - C^+}{C^- - C^+} = \frac{1}{2} erfc\left(\frac{x}{2\sqrt{Dt}}\right)$$

This is the solution that we obtain for a typical infinite diffusion couple. This we obtained by Laplace transform method.

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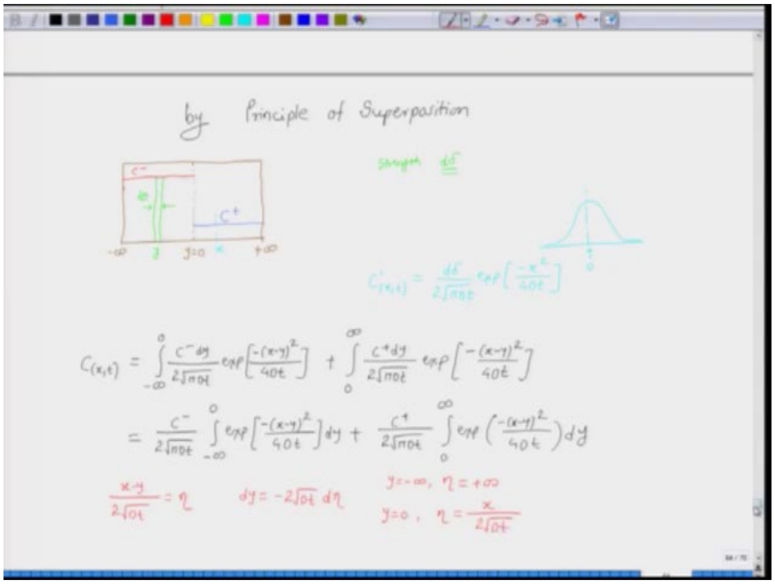


by Principle of Superposition

$$C'_{(x,t)} = \frac{d\xi}{2\sqrt{\pi D t}}\exp\left[\frac{-x^2}{4Dt}\right]$$

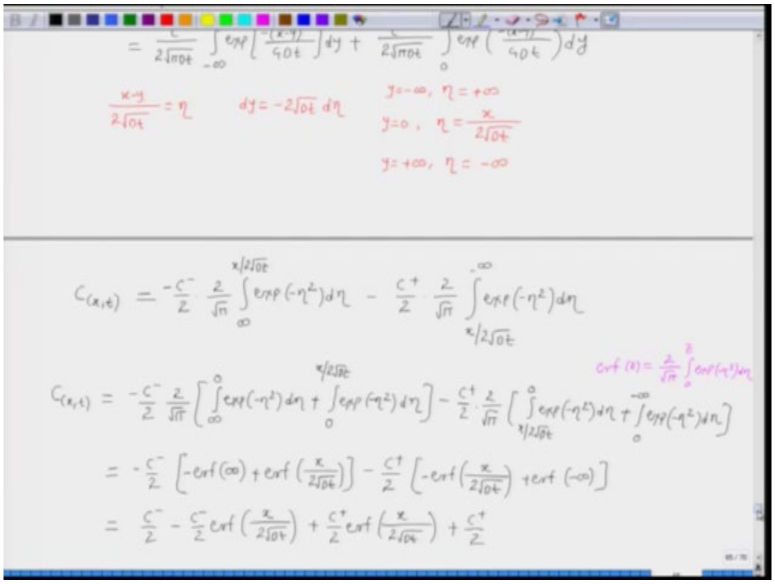
$$C_{(x,t)} = \int_{-\infty}^{0}\frac{C^- dy}{2\sqrt{\pi D t}}\exp\left[\frac{-(x-y)^2}{4Dt}\right] + \int_{0}^{\infty}\frac{C^+ dy}{2\sqrt{\pi D t}}\exp\left[-\frac{(x-y)^2}{4Dt}\right]$$

$$= \frac{C^-}{2\sqrt{\pi D t}}\int_{-\infty}^{0}\exp\left[\frac{-(x-y)^2}{4Dt}\right]dy + \frac{C^+}{2\sqrt{\pi D t}}\int_{0}^{\infty}\exp\left(\frac{-(x-y)^2}{4Dt}\right)dy$$

$\frac{x-y}{2\sqrt{Dt}} = \eta$ $\quad dy = -2\sqrt{Dt}\,d\eta$

$y=-\infty,\ \eta=+\infty$

$y=0,\ \eta=\frac{x}{2\sqrt{Dt}}$


$$= \frac{C^-}{2\sqrt{\pi D t}}\int_{-\infty}\exp\left[\frac{-(x-y)^2}{4Dt}\right]dy + \frac{C^+}{2\sqrt{\pi D t}}\int_{0}\exp\left(\frac{-(x-y)^2}{4Dt}\right)dy$$

$\frac{x-y}{2\sqrt{Dt}} = \eta$ $\quad dy = -2\sqrt{Dt}\,d\eta$

$y=-\infty,\ \eta=+\infty$

$y=0,\ \eta=\frac{x}{2\sqrt{Dt}}$

$y=+\infty,\ \eta=-\infty$

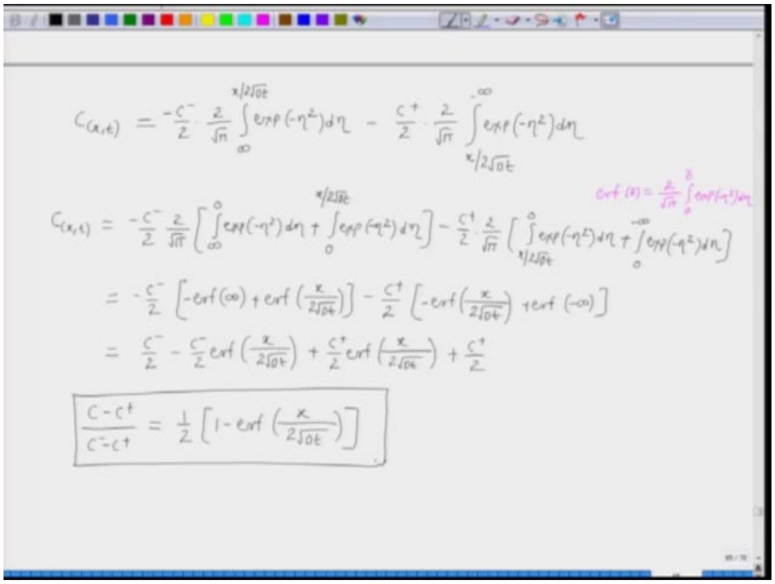
$$C_{(x,t)} = -\frac{C^-}{2}\cdot\frac{2}{\sqrt{\pi}}\int_{\infty}^{x/2\sqrt{Dt}}\exp(-\eta^2)d\eta - \frac{C^+}{2}\cdot\frac{2}{\sqrt{\pi}}\int_{x/2\sqrt{Dt}}^{-\infty}\exp(-\eta^2)d\eta$$

$\operatorname{erf}(z) = \frac{2}{\sqrt{\pi}}\int_0^z \exp(-\eta^2)d\eta$

$$C_{(x,t)} = -\frac{C^-}{2}\frac{2}{\sqrt{\pi}}\left[\int_{\infty}^{0}\exp(-\eta^2)d\eta + \int_{0}^{x/2\sqrt{Dt}}\exp(-\eta^2)d\eta\right] - \frac{C^+}{2}\cdot\frac{2}{\sqrt{\pi}}\left(\int_{x/2\sqrt{Dt}}^{0}\exp(-\eta^2)d\eta + \int_{0}^{-\infty}\exp(-\eta^2)d\eta\right]$$

$$= -\frac{C^-}{2}\left[-\operatorname{erf}(\infty) + \operatorname{erf}\left(\frac{x}{2\sqrt{Dt}}\right)\right] - \frac{C^+}{2}\left[-\operatorname{erf}\left(\frac{x}{2\sqrt{Dt}}\right) + \operatorname{erf}(-\infty)\right]$$

$$= \frac{C^-}{2} - \frac{C^-}{2}\operatorname{erf}\left(\frac{x}{2\sqrt{Dt}}\right) + \frac{C^+}{2}\operatorname{erf}\left(\frac{x}{2\sqrt{Dt}}\right) + \frac{C^+}{2}$$



$$C_{(x,t)} = -\frac{C^-}{2}\cdot\frac{2}{\sqrt{\pi}}\int_{\infty}^{x/2\sqrt{Dt}}\exp(-\eta^2)\,d\eta - \frac{C^+}{2}\cdot\frac{2}{\sqrt{\pi}}\int_{x/2\sqrt{Dt}}^{-\infty}\exp(-\eta^2)\,d\eta$$

$$\mathrm{erf}(z) = \frac{2}{\sqrt{\pi}}\int_0^z \exp(-\eta^2)\,d\eta$$

$$C_{(x,t)} = -\frac{C^-}{2}\frac{2}{\sqrt{\pi}}\left[\int_{\infty}^{0}\exp(-\eta^2)\,d\eta + \int_{0}^{x/2\sqrt{Dt}}\exp(-\eta^2)\,d\eta\right] - \frac{C^+}{2}\cdot\frac{2}{\sqrt{\pi}}\left[\int_{x/2\sqrt{Dt}}^{0}\exp(-\eta^2)\,d\eta + \int_{0}^{-\infty}\exp(-\eta^2)\,d\eta\right]$$

$$= -\frac{C^-}{2}\left[-\mathrm{erf}(\infty) + \mathrm{erf}\left(\frac{x}{2\sqrt{Dt}}\right)\right] - \frac{C^+}{2}\left[-\mathrm{erf}\left(\frac{x}{2\sqrt{Dt}}\right) + \mathrm{erf}(-\infty)\right]$$

$$= \frac{C^-}{2} - \frac{C^-}{2}\mathrm{erf}\left(\frac{x}{2\sqrt{Dt}}\right) + \frac{C^+}{2}\mathrm{erf}\left(\frac{x}{2\sqrt{Dt}}\right) + \frac{C^+}{2}$$

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

Now we will derive the equation for concentration evolution in an infinite diffusion couple using another method called Principle of Superposition. Let us draw the initial concentration profile, let us denote the x coordinate with y. It will be clear soon why we are denoting it now by y.

$y = 0$ and then we have 2 terminals at $-\infty$ and $+\infty$. The initial concentration in the left terminal alloy is C^-, the initial concentration in the right terminal alloy is C^+. We already defined the initial and boundary conditions and we have to solve the diffusion equation.

Now let us consider a small volume element of very small width dy which is located at some coordinate y within the diffusion couple. Now this small element can be considered as an instantaneous planar source for the diffusing component, right and let us say it's strength is $d\delta$. Now we have seen the solution for instantaneous planar source which is sandwiched between two infinite blocks.

If you remember, you got concentration profile something like this, the instantaneous planar source was situated at this position 0. We have found the equation for evaluation concentration at any position $x = y$ because of the instantaneous planar source at $y = 0$.

And that we know is:

$$C_{(x,t)} = \frac{d\delta}{2\sqrt{\pi Dt}}\exp\left(\frac{-x^2}{4Dt}\right)$$

Now this whole diffusion couple can be thought of as composed of large number of such instantaneous planar sources and from the initial concentration profile we know what would be their strength. On the left hand side or for $y < 0$ the strength will be $C^- dy$ and for right hand side the strength would be $C^+ dy$ and if you want to find the total concentration at any position x there will the contribution from each of these instantaneous planar source. So, we can obtain the individual contribution by the solution for instantaneous planar source sandwiched between two infinite blocks. And if we sum the concentration field because of each of this instantaneous source we will get the total concentration at this position x at any time t. $C_{(x,t)}$ would be nothing but integral $-\infty$ to $+\infty$ for all the sources. Now from $-\infty$ to 0 we have a different strength and 0 to $+\infty$ we have different strength. Let us split this integral at 0, from $-\infty$ to 0 we know $d\delta$ for $y < 0$ is $C^- dy$. Similarly for the right side of the couple. Now we need to know the distance between the source and the plane at which we want to find the concentration field. That will be $x - y$. So we get finally:

$$C_{(x,t)} = \int_{-\infty}^{0} \frac{C^- dy}{2\sqrt{\pi Dt}}\exp\left[\frac{-(x-y)^2}{4Dt}\right] + \int_{0}^{\infty} \frac{C^+ dy}{2\sqrt{\pi Dt}}\exp\left[\frac{-(x-y)^2}{4Dt}\right]$$

Let us take the constants out:

$$C_{(x,t)} = \frac{C^-}{2\sqrt{\pi Dt}}\int_{-\infty}^{0} \exp\left[\frac{-(x-y)^2}{4Dt}\right] dy + \frac{C^+}{2\sqrt{\pi Dt}}\int_{0}^{\infty} \exp\left[\frac{-(x-y)^2}{4Dt}\right] dy$$

Now if we substitute:

$$\frac{x-y}{2\sqrt{Dt}} = \eta$$

then we can write:

$$dy = -2\sqrt{Dt}\,d\eta$$

and when:

$$y = -\infty, \qquad \eta = +\infty$$

$$y = 0, \qquad \eta = \frac{x}{2\sqrt{Dt}}$$

$$y = \infty, \qquad \eta = -\infty$$

If we substitute these, $C_{(x,t)}$ becomes:

$$C_{(x,t)} = -\frac{C^-}{2}\frac{2}{\sqrt{\pi}}\int_{\infty}^{\frac{x}{2\sqrt{Dt}}} \exp[-\eta^2]\,d\eta - \frac{C^+}{2}\frac{2}{\sqrt{\pi}}\int_{\frac{x}{2\sqrt{Dt}}}^{-\infty} \exp[-\eta^2]\,d\eta \qquad (3)$$

Now the integral limits I have changed corresponding to η. So these looks something similar to error function type and we know:

$$\operatorname{erf}(z) = \frac{2}{\sqrt{\pi}}\int_{0}^{z} \exp[-\eta^2]\,d\eta$$

So to bring to this from each of the integrals in Eq. (3) is split at 0. We can write:

$$C_{(x,t)} = -\frac{C^-}{2}\frac{2}{\sqrt{\pi}}\left[\int_{\infty}^{0} \exp[-\eta^2]\,d\eta + \int_{0}^{\frac{x}{2\sqrt{Dt}}} \exp[-\eta^2]\,d\eta\right]$$

$$-\frac{C^+}{2}\frac{2}{\sqrt{\pi}}\left[\int_{\frac{x}{2\sqrt{Dt}}}^{0} \exp[-\eta^2]\,d\eta + \int_{0}^{-\infty} \exp[-\eta^2]\,d\eta\right]$$

If we look at each of the integrals they are error functions. So I can write this as:

$$C_{(x,t)} = -\frac{C^-}{2}\left[-\operatorname{erf}(\infty) + \operatorname{erf}\left(\frac{x}{2\sqrt{Dt}}\right)\right] - \frac{C^+}{2}\left[-\operatorname{erf}\left(\frac{x}{2\sqrt{Dt}}\right) + \operatorname{erf}(-\infty)\right]$$

Again, we know erf(∞) is 1 and erf(−∞) is -1. We can write this as:

$$C_{(x,t)} = \frac{C^-}{2} - \frac{C^-}{2}\operatorname{erf}\left(\frac{x}{2\sqrt{Dt}}\right) + \frac{C^+}{2}\operatorname{erf}\left(\frac{x}{2\sqrt{Dt}}\right) + \frac{C^+}{2}$$

Again if we subtract C^+ from both side and rearrange we will get the solution:

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

So, we derived this equation with the principle of superposition. Basically each of the small element in these blocks of the diffusion couple can be assumed as an instantaneous planar source sandwiched between two infinite blocks and by summing all their concentration field at any given x we find the net concentration at that particular value of x.

Now let us quickly look at some of the features of this error function solution, this is a similar solution that we obtained for the carburizing problem, so similar properties will apply here. The solution is same except for this factor of $\frac{1}{2}$.

We will see that C^+, C^- and D are constants.

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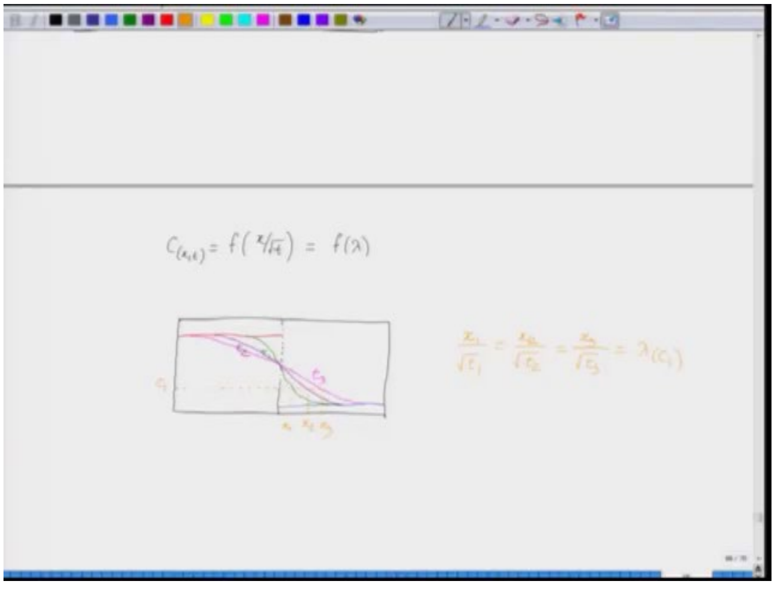

$C_{(x,t)} = f(x/\sqrt{t}) = f(\lambda)$

$\frac{x_1}{\sqrt{t_1}} = \frac{x_2}{\sqrt{t_2}} = \frac{x_3}{\sqrt{t_3}} = \lambda(C_1)$

Again we can say that C at any position x and t is a function of $\frac{x}{\sqrt{t}}$ and $\frac{x}{\sqrt{t}}$ is also called as Boltzmann parameter λ. What does this mean again? If we draw the schematic concentration profiles at different times for infinite diffusion couple, these are the initial profiles for three times, t_1, t_2 and t_3. If we consider any particular composition let say C_i here and track its x position at different times these will be x_1, x_2, and x_3.

What this relation tells me that:

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

Each composition plane in a diffusion couple moves parabolically with time, it is what we usually call it because $\frac{x}{\sqrt{t}}$ is equal to constant. This is a parabolic relation that each of the composition plane follows in a diffusion couple:

$$C_{(x,t)} = f\left(\frac{x}{\sqrt{t}}\right) = f(\lambda)$$

And this is an important property because this helps us in roughly estimating the penetration depths at different times if you know penetration depth at one time for a given composition plane.

Okay, this diffusion couple is very important for in our class, we will use this diffusion couple concept quite frequently because most of the experiments that we carry out to determine the interdiffusion and intrinsic diffusion coefficients are based on this infinite diffusion couples.

So, far we derived the expression for binary diffusion couple, but when it comes to multicomponent diffusion couple the problem becomes little more complicated but we will also derive the equation for a concentration profiles of multi-component diffusion couple. We will look into it in the next class. Thank you.