Diffusion in Multicomponent Solids
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Lecture 25
Numerical Problems

Welcome back, now that we have gone over derivation of some of the solutions to different boundary conditions. Today, we will go over couple of numerical problems. The first one deals with Carburizing of Steels and evaluating the case depths or carburizing time required. the second one deals with evolution of concentration profiles in a multicomponent diffusion couple.

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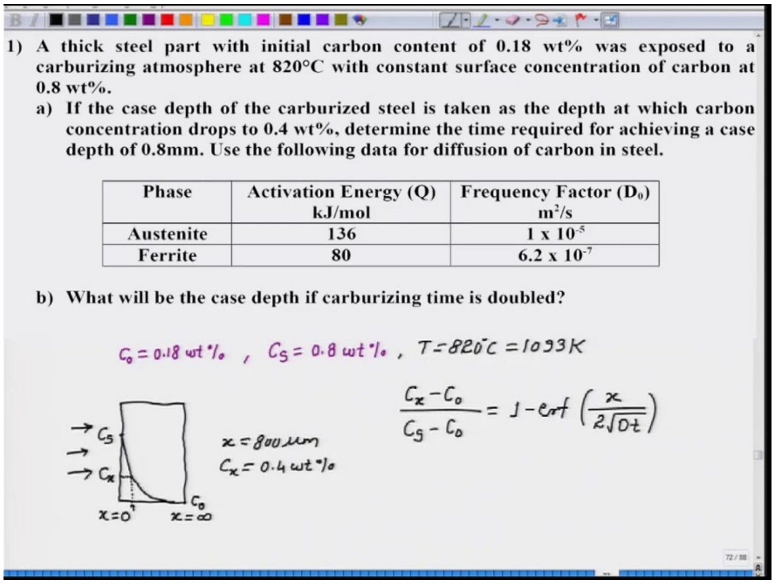


1) A thick steel part with initial carbon content of 0.18 wt% was exposed to a carburizing atmosphere at 820°C with constant surface concentration of carbon at 0.8 wt%.

a) If the case depth of the carburized steel is taken as the depth at which carbon concentration drops to 0.4 wt%, determine the time required for achieving a case depth of 0.8mm. Use the following data for diffusion of carbon in steel.

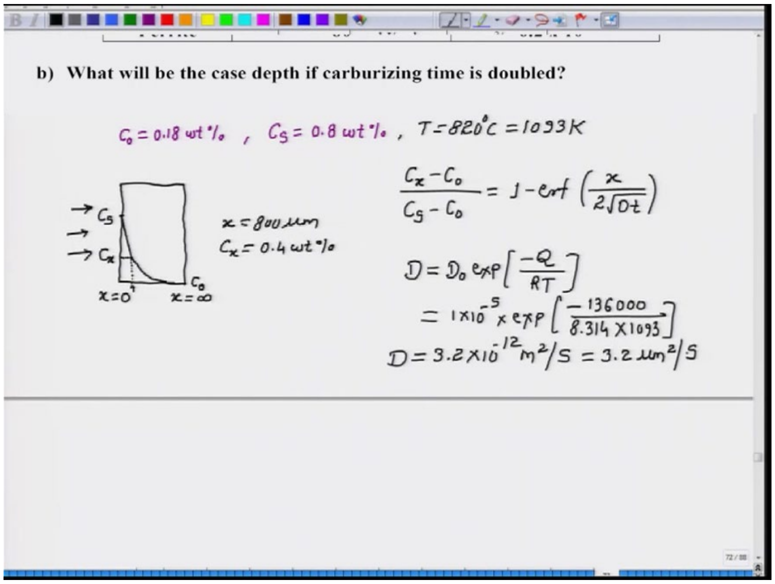
Phase	Activation Energy (Q) kJ/mol	Frequency Factor (D_0) m^2/s
Austenite	136	1×10^{-5}
Ferrite	80	6.2×10^{-7}

b) What will be the case depth if carburizing time is doubled?

$C_0 = 0.18$ wt%, $C_S = 0.8$ wt%, $T = 820°C = 1093 K$

$$\frac{C_x - C_0}{C_S - C_0} = 1 - erf\left(\frac{x}{2\sqrt{Dt}}\right)$$

$x = 800 \mu m$
$C_x = 0.4$ wt%



b) **What will be the case depth if carburizing time is doubled?**

$C_o = 0.18\ wt\ \%$, $C_s = 0.8\ wt\ \%$, $T = 820^\circ C = 1093 K$

$x = 800\ \mu m$

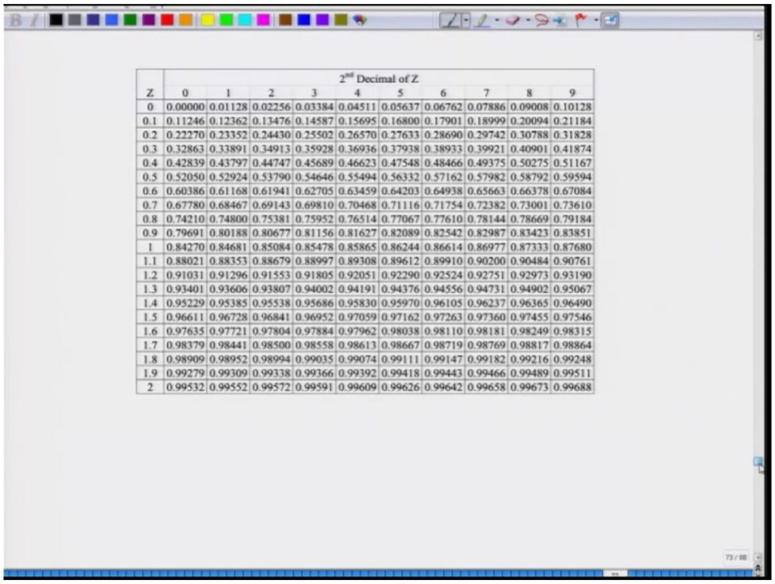
$C_x = 0.4\ wt\ \%$

$$\frac{C_x - C_o}{C_s - C_o} = 1 - \text{erf}\left(\frac{x}{2\sqrt{Dt}}\right)$$

$$D = D_o \exp\left[\frac{-Q}{RT}\right]$$

$$= 1 \times 10^{-5} \times \exp\left[\frac{-136000}{8.314 \times 1093}\right]$$

$$D = 3.2 \times 10^{-12}\ m^2/s = 3.2\ \mu m^2/s$$



Z	2nd Decimal of Z 0	1	2	3	4	5	6	7	8	9
0	0.00000	0.01128	0.02256	0.03384	0.04511	0.05637	0.06762	0.07886	0.09008	0.10128
0.1	0.11246	0.12362	0.13476	0.14587	0.15695	0.16800	0.17901	0.18999	0.20094	0.21184
0.2	0.22270	0.23352	0.24430	0.25502	0.26570	0.27633	0.28690	0.29742	0.30788	0.31828
0.3	0.32863	0.33891	0.34913	0.35928	0.36936	0.37938	0.38933	0.39921	0.40901	0.41874
0.4	0.42839	0.43797	0.44747	0.45689	0.46623	0.47548	0.48466	0.49375	0.50275	0.51167
0.5	0.52050	0.52924	0.53790	0.54646	0.55494	0.56332	0.57162	0.57982	0.58792	0.59594
0.6	0.60386	0.61168	0.61941	0.62705	0.63459	0.64203	0.64938	0.65663	0.66378	0.67084
0.7	0.67780	0.68467	0.69143	0.69810	0.70468	0.71116	0.71754	0.72382	0.73001	0.73610
0.8	0.74210	0.74800	0.75381	0.75952	0.76514	0.77067	0.77610	0.78144	0.78669	0.79184
0.9	0.79691	0.80188	0.80677	0.81156	0.81627	0.82089	0.82542	0.82987	0.83423	0.83851
1	0.84270	0.84681	0.85084	0.85478	0.85865	0.86244	0.86614	0.86977	0.87333	0.87680
1.1	0.88021	0.88353	0.88679	0.88997	0.89308	0.89612	0.89910	0.90200	0.90484	0.90761
1.2	0.91031	0.91296	0.91553	0.91805	0.92051	0.92290	0.92524	0.92751	0.92973	0.93190
1.3	0.93401	0.93606	0.93807	0.94002	0.94191	0.94376	0.94556	0.94731	0.94902	0.95067
1.4	0.95229	0.95385	0.95538	0.95686	0.95830	0.95970	0.96105	0.96237	0.96365	0.96490
1.5	0.96611	0.96728	0.96841	0.96952	0.97059	0.97162	0.97263	0.97360	0.97455	0.97546
1.6	0.97635	0.97721	0.97804	0.97884	0.97962	0.98038	0.98110	0.98181	0.98249	0.98315
1.7	0.98379	0.98441	0.98500	0.98558	0.98613	0.98667	0.98719	0.98769	0.98817	0.98864
1.8	0.98909	0.98952	0.98994	0.99035	0.99074	0.99111	0.99147	0.99182	0.99216	0.99248
1.9	0.99279	0.99309	0.99338	0.99366	0.99392	0.99418	0.99443	0.99466	0.99489	0.99511
2	0.99532	0.99552	0.99572	0.99591	0.99609	0.99626	0.99642	0.99658	0.99673	0.99688

Here is the first problem on carburizing. This is a thick steel part with initial carbon content of 0.18 weight percent which was exposed to a carburizing atmosphere at 820 °C with constant surface concentration of carbon at 0.8 weight percent. The original carbon content of steel is:

$$C_o = 0.18\ wt\ \%$$

and constant surface concentration maintained during carburizing is:

$$C_s = 0.8\ wt\ \%$$

Assume that molar volume and interdiffusivities are independent of composition (interdiffusivity of carbon in steel should be considered here) and since the interdiffusivity can be assumed constant we can use the solution that we have derived for the carburizing boundary conditions, that is, the semi-infinite boundary conditions. Since the problem states that steel part is thick, which means it obeys the semi-infinite boundary conditions. We can draw the schematic of the steel part carburizing surface: left side we can call as $x = 0$ and it is thick enough, so that the carbon does not diffuse all the way to the other side. The other surface can be considered as $x = \infty$. The concentration on the surface is $C_s = 0.8\ wt\ \%$. at the other end the original concentration is maintained at all times as C_o. At any time t, we have seen the diffusion profile will be something like this. Now the first problem is if the case depth of the carburized steel is taken as the depth at which carbon concentration drops to $0.4\ wt\ \%$, determine the time required for achieving a case depth of 0.8 mm. We want to find the time at which at x is equal to 0.8 mm, or 800 μm, the carbon concentration achieved at that distance is:

$$C_x = 0.4\ wt\ \% \quad at \quad x = 800\ \mu m$$

$$T = 820\ °\mathrm{C} = 1093\ K$$

We can use the solution that we have derived, which states that:

$$\frac{C_x - C_o}{C_s - C_o} = 1 - erf\left(\frac{x}{2\sqrt{Dt}}\right)$$

Now, we are considering the ratios of concentration here. Since the problem states that the molar volume can be assumed constant, it should not matter which unit of concentration we are using. We can straightaway use the weight percent as given and on the right hand side of above equation, we need to evaluate this error function term which contains $erf\left(\frac{x}{2\sqrt{Dt}}\right)$, x is given here which is 800 μm and for D we need to consider the interdiffusivity of carbon in steel. Now, in the given table, we see there are 2 phases austenite and ferrite in which activation energy and frequency factor for carbon diffusion are given. Now, which one we should use?

Since the temperature being considered is:

$$T = 820\ °\mathrm{C} = 1093\ K$$

Stable phase in this low carbon steel should be austenite. We should use diffusivity of carbon in austenite phase. If we evaluate:

$$D = D_o exp\left(\frac{-Q}{RT}\right) = 1 \times 10^{-5} \times exp\left(\frac{-136000}{8.314 \times 1093}\right)$$

we have to substitute for D_o and Q for austenite. Gas constant R is 8.314.

$$D = 3.2 \times 10^{-12}\frac{m^2}{s} = 3.2\ \frac{\mu m^2}{s}$$

Let us refer to this error function table in a moment. Now we need to substitute for concentrations.

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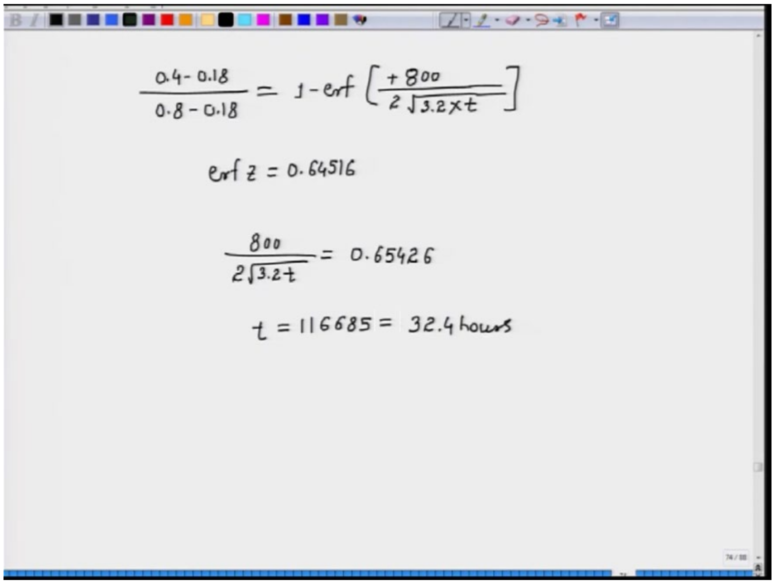

$$\frac{0.4-0.18}{0.8-0.18} = 1-\text{erf}\left[\frac{+800}{2\sqrt{3.2 \times t}}\right]$$

$$\text{erf}\ z = 0.64516$$

$$\frac{800}{2\sqrt{3.2t}} = 0.65426$$

$$t = 116685 = 32.4 \text{ hours}$$

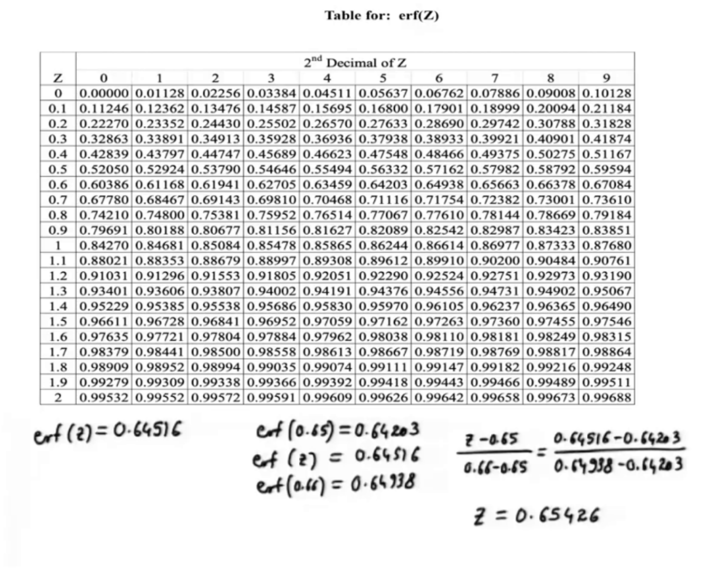

Table for: erf(Z)

Z	2nd Decimal of Z 0	1	2	3	4	5	6	7	8	9
0	0.00000	0.01128	0.02256	0.03384	0.04511	0.05637	0.06762	0.07886	0.09008	0.10128
0.1	0.11246	0.12362	0.13476	0.14587	0.15695	0.16800	0.17901	0.18999	0.20094	0.21184
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1.3	0.93401	0.93606	0.93807	0.94002	0.94191	0.94376	0.94556	0.94731	0.94902	0.95067
1.4	0.95229	0.95385	0.95538	0.95686	0.95830	0.95970	0.96105	0.96237	0.96365	0.96490
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$erf(z) = 0.64516$

$erf(0.65) = 0.64203$
$erf(z) = 0.64516$
$erf(0.66) = 0.64938$

$$\frac{z - 0.65}{0.66 - 0.65} = \frac{0.64516 - 0.64203}{0.64938 - 0.64203}$$

$z = 0.65426$

We can write:

$$\frac{0.4 - 0.18}{0.8 - 0.18} = 1 - erf\left(\frac{800}{2\sqrt{3.2t}}\right)$$

We need to find the carburizing time, okay. We can solve this left side. Let us call this quantity inside error function as z and it is obtained as:

$$erf(z) = 0.64516$$

We need to evaluate first value of z which will give error function z equal to 0.64516. We can refer to the standard error function tables which are available. The way we read this is on the leftmost column, you have the values of z up to one decimal place and on the right side on the topmost row are the values of z in the second decimal place

If we want the error function of 0.32 refer to 0.3 and the second decimal place is 2. The error function of 0.32 is 0.34913. Now, we need to find out z such that error function z is equal to 0.64516. Now exactly this value may not appear in the table, but we can assume the linear relation within the small range of z. Let us see one value which comes before 0.64516 and the other which is slightly greater than 0.64516 from this table. We have:

$$erf(z) = 0.64516$$

$$erf(0.65) = 0.64203$$

$$erf(0.66) = 0.64938$$

If we assume linear relation, we can find the value of z here, we can write:

$$\frac{z - 0.65}{0.66 - 0.65} = \frac{0.64516 - 0.64203}{0.64938 - 0.64203}$$

This will give me the value of z as:

$$z = 0.65426$$

If I substitute for z:

$$\frac{800}{2\sqrt{3.2t}} = 0.65426$$

This will give me the value of t, which comes out to be:

$$t = 116685 = 32.4\ hours$$

In this particular case, to achieve the case depth of 800 μm, the carburizing time should be 32.4 hours at 820 ℃ and the case depth in this case is defined as the depth at which carbon concentration becomes 0.4 weight percent.

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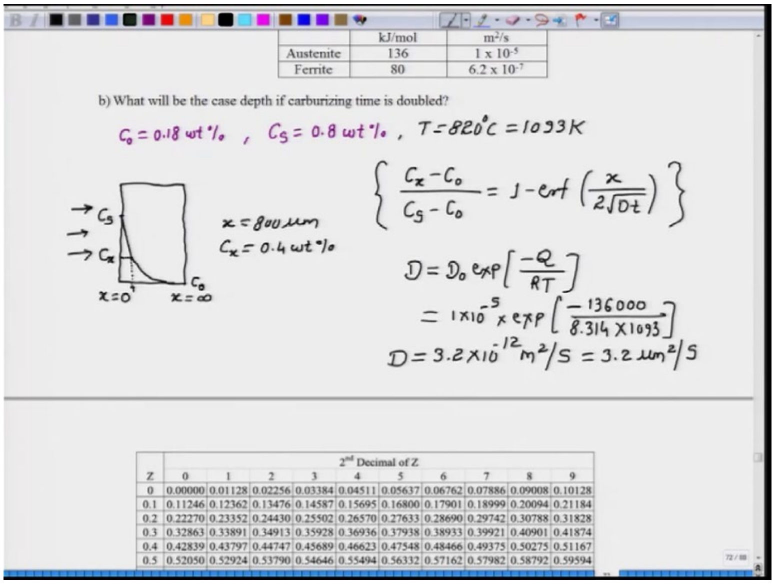

	kJ/mol	m²/s
Austenite	136	1×10^{-5}
Ferrite	80	6.2×10^{-7}

b) What will be the case depth if carburizing time is doubled?

$C_o = 0.18$ wt %, $C_s = 0.8$ wt %, $T = 820°C = 1093 K$

$x = 800 \mu m$

$C_x = 0.4$ wt %

$$\left\{ \frac{C_x - C_o}{C_s - C_o} = 1 - \operatorname{erf}\left(\frac{x}{2\sqrt{Dt}}\right) \right\}$$

$$D = D_o \exp\left[\frac{-Q}{RT}\right]$$

$$= 1 \times 10^{-5} \times \exp\left[\frac{-136000}{8.314 \times 1093}\right]$$

$$D = 3.2 \times 10^{-12} m^2/s = 3.2 \mu m^2/s$$

Z	2nd Decimal of Z									
	0	1	2	3	4	5	6	7	8	9
0	0.00000	0.01128	0.02256	0.03384	0.04511	0.05637	0.06762	0.07886	0.09008	0.10128
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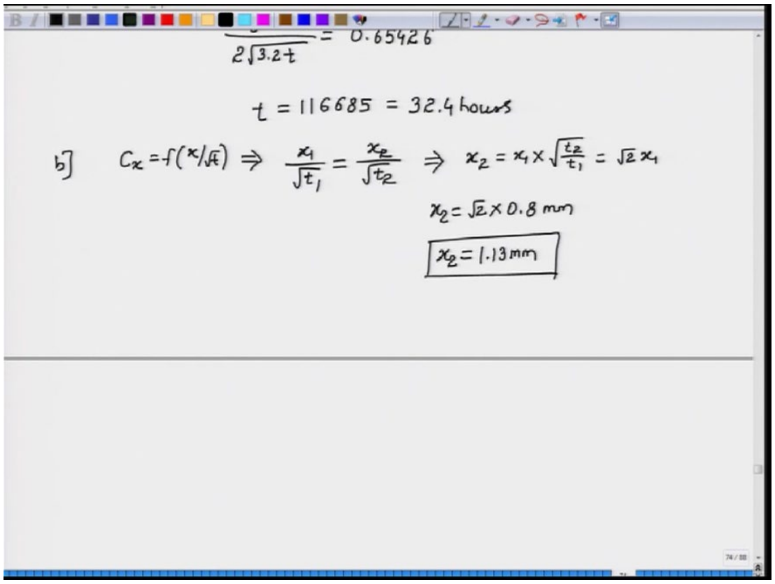
0.5	0.52050	0.52924	0.53790	0.54646	0.55494	0.56332	0.57162	0.57982	0.58792	0.59594



$$\frac{\quad}{2\sqrt{3.2t}} = 0.65426$$

$$t = 116685 = 32.4 \text{ hours}$$

b] $C_x = f(x/\sqrt{t}) \Rightarrow \frac{x_1}{\sqrt{t_1}} = \frac{x_2}{\sqrt{t_2}} \Rightarrow x_2 = x_1 \times \sqrt{\frac{t_2}{t_1}} = \sqrt{2} x_1$

$$x_2 = \sqrt{2} \times 0.8 \text{ mm}$$

$$\boxed{x_2 = 1.13 \text{mm}}$$

Now, the second part of the problem, what will be the case depth if carburizing time is doubled? This is simple as once we know when carburizing time for one case depth, we can straightaway use the Boltzmann parameter. As you see this equation here, C is a function of:

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

Everything else is constant included D, C_o and C_s.. It means, for part b:

$$\frac{x_1}{\sqrt{t_1}} = \frac{x_2}{\sqrt{t_2}} \quad , \quad x_2 = x_1 \times \frac{\sqrt{t_2}}{\sqrt{t_1}} = \sqrt{2}x_1 \quad , \quad x_2 = \sqrt{2} \times 0.8\,mm$$

We suggest that if we double the carburizing time, the case depth should become $\sqrt{2}$ times the original one. So:

$$x_2 = 1.13\,mm$$

This is how we can determine carburizing time for the given conditions or carburizing time for the given case depth or we can determine what should be the case depth in given carburizing time at a given temperature. Let us move on to the second problem today.

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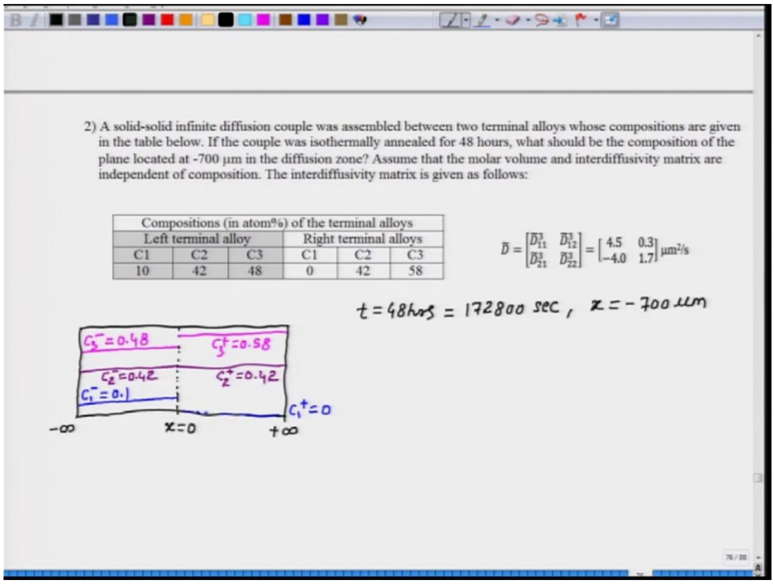
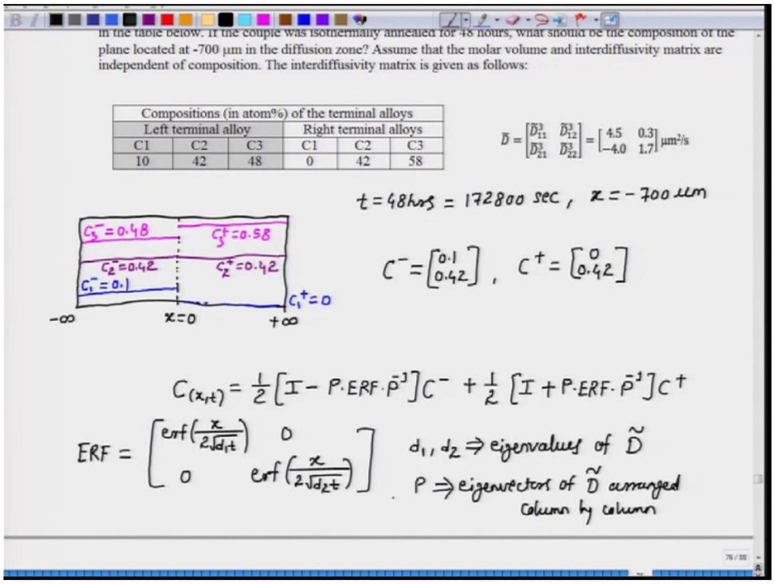


2) A solid-solid infinite diffusion couple was assembled between two terminal alloys whose compositions are given in the table below. If the couple was isothermally annealed for 48 hours, what should be the composition of the plane located at -700 μm in the diffusion zone? Assume that the molar volume and interdiffusivity matrix are independent of composition. The interdiffusivity matrix is given as follows:

Compositions (in atom%) of the terminal alloys					
Left terminal alloy			Right terminal alloys		
C1	C2	C3	C1	C2	C3
10	42	48	0	42	58

$$\tilde{D} = \begin{bmatrix} \tilde{D}^3_{11} & \tilde{D}^3_{12} \\ \tilde{D}^3_{21} & \tilde{D}^3_{22} \end{bmatrix} = \begin{bmatrix} 4.5 & 0.3 \\ -4.0 & 1.7 \end{bmatrix} \mu m^2/s$$

$t = 48\,hrs = 172800\,sec$, $x = -700\,\mu m$



in the table below. If the couple was isothermally annealed for 48 hours, what should be the composition of the plane located at -700 μm in the diffusion zone? Assume that the molar volume and interdiffusivity matrix are independent of composition. The interdiffusivity matrix is given as follows:

Compositions (in atom%) of the terminal alloys					
Left terminal alloy			Right terminal alloys		
C1	C2	C3	C1	C2	C3
10	42	48	0	42	58

$$\tilde{D} = \begin{bmatrix} \tilde{D}^3_{11} & \tilde{D}^3_{12} \\ \tilde{D}^3_{21} & \tilde{D}^3_{22} \end{bmatrix} = \begin{bmatrix} 4.5 & 0.3 \\ -4.0 & 1.7 \end{bmatrix} \mu m^2/s$$

$t = 48 hrs = 172800$ sec, $x = -700 \mu m$

$$C^- = \begin{bmatrix} 0.1 \\ 0.42 \end{bmatrix}, \quad C^+ = \begin{bmatrix} 0 \\ 0.42 \end{bmatrix}$$

$$C_{(x,t)} = \frac{1}{2}\left[I - P \cdot ERF \cdot P^{-1}\right] C^- + \frac{1}{2}\left[I + P \cdot ERF \cdot P^{-1}\right] C^+$$

$$ERF = \begin{bmatrix} \mathrm{erf}\left(\frac{x}{2\sqrt{d_1 t}}\right) & 0 \\ 0 & \mathrm{erf}\left(\frac{x}{2\sqrt{d_2 t}}\right) \end{bmatrix}$$

$d_1, d_2 \Rightarrow$ eigenvalues of $\tilde{D}$

$P \Rightarrow$ eigenvectors of $\tilde{D}$ arranged column by column

This problem is calculating the concentration at given x and t in a multi component diffusion couple. Again, we will assume constant interdiffusivity matrix and we will consider a ternary diffusion couple example. This will give you an idea about how to use the multi component diffusion equation to actually calculate the concentrations at various x and t in an infinite diffusion couple. We will solve this for ternary but it will be equally applicable for quaternary or higher order system and we will be using the analytical solutions for constant interdiffusivity matrix. The problem says a solid-solid infinite diffusion couple was assembled between 2 terminal alloys whose compositions are given in the table below.

In the diffusion couple, this is the initial interface between 2 terminal alloy, let us call it x=0 and this is an infinite diffusion couple. The left most terminal is at $-\infty$, right most terminal is $+\infty$. Again this means that the diffusing species do not penetrate by diffusion all the way to the terminal ends, that the infinite boundary conditions are maintained.

Now in the left terminal alloy, the initial concentrations which we typically denote by C^- in mole fractions are: $C_1^- = 0.1$, $C_2^- = 0.42$, $C_3^- = 0.48$. $C_1^+ = 0$, $C_2^+ = 0.42$, $C_3^+ = 0.58$. Composition of component 2 is same in both the terminal alloy to start with. So this is the initial concentration profile, you can see it is a step function or it has a discontinuity at x=0, except for C_2 because in this case C_2 is constant on both sides.

$$C^- = \begin{bmatrix} 0.1 \\ 0.42 \end{bmatrix}, \qquad C^+ = \begin{bmatrix} 0 \\ 0.42 \end{bmatrix}$$

The couple was isothermally annealed for 48 hours. The diffusion annealing time t is equal to 48 hours, we can convert it into seconds, because we use diffusivities in $\frac{m^2}{s}$ or $\frac{\mu m^2}{s}$. So, it will be 172800 second. Then, what should be the composition of the plane located at -700 μm in the diffusion zone? -700 means it would be on the left side of the couple as x = -700 μm. Assume that the molar volume and interdiffusivity matrix are independent of composition and the interdiffusivity matrix is given here:

$$\left\{\widetilde{D}_{11}^{3} = 4.5, \quad \widetilde{D}_{12}^{3} = 0.3, \quad \widetilde{D}_{21}^{3} = -4.0, \quad \widetilde{D}_{22}^{3} = 1.7\right\} \frac{\mu m^2}{s}$$

These are the ternary interdiffusion coefficients. We need 4 interdiffusion coefficients since there are 2 independent components. Now, we can use the multi component diffusion solution in order to obtain the concentrations at the given x and t in the matrix form. We can write $C_{(x,t)}$, where C is a column matrix since there are 2 independent concentrations, so it is a 2x1 column matrix. It will contain the term C_1 and C_2 since we have interdiffusivities with component 3 as dependent, the superscript denotes the dependent component. This should be:

$$C = \frac{1}{2}[I - P.ERF.P^{-1}]C^{-} + \frac{1}{2}[I + P.ERF.P^{-1}]C^{+}$$

C^{-} and C^{+} is the column matrix of independent concentrations in the left and right terminal alloys respectively. Now, we know what are these matrices P, ERF and P^{-1}. ERF is essentially a diagonal matrix containing error function terms. This error function terms are in terms of the Eigen values of the diffusivity matrix. So, it looks like:

$$ERF = \begin{bmatrix} \frac{x}{2\sqrt{d_1 t}} & 0 \\ 0 & \frac{x}{2\sqrt{d_2 t}} \end{bmatrix}$$

The non-diagonal elements are 0 and $1D443$ is a matrix formed by Eigen vectors of $\widetilde{D}$. Eigen vectors are arranged column by column, since $\widetilde{D}$ is a 2 by 2 matrix, there are 2 Eigen vectors. P is again a 2 by 2 matrix.

Now we first need to find out the Eigen values and Eigen vectors of $\widetilde{D}$. This is a little bit of revision of part of mathematical concepts, we already gone over some of those like Laplace transforms. You will get an opportunity to revise your matrix algebra concepts, that is why *I* am going over these problems.

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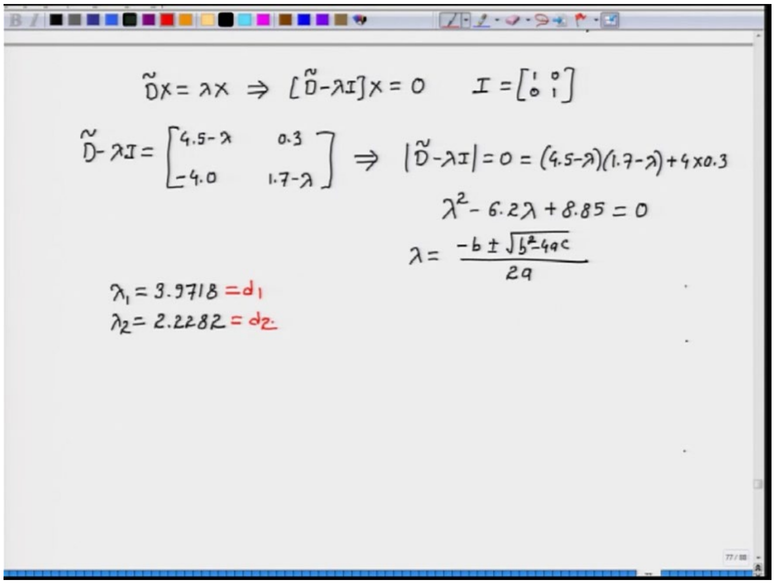


$$\tilde{D}X = \lambda X \Rightarrow [\tilde{D} - \lambda I]X = 0 \qquad I = \begin{bmatrix}1 & 0\\ 0 & 1\end{bmatrix}$$

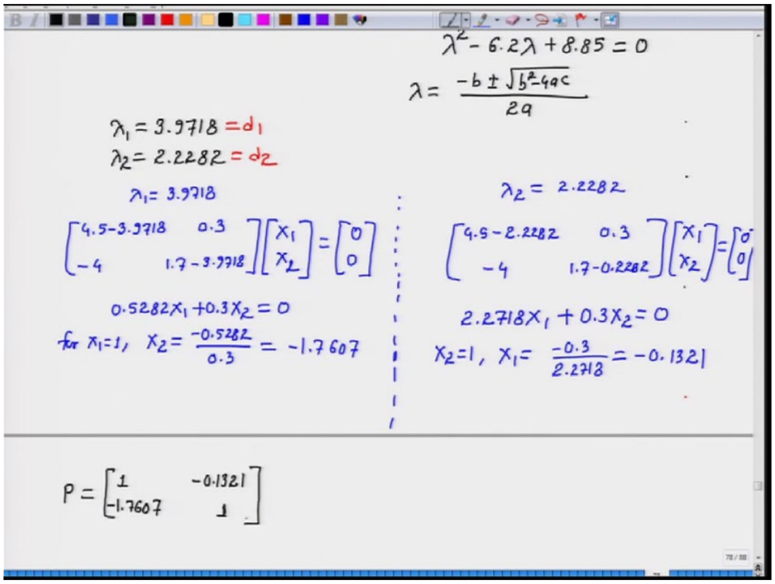
$$\tilde{D} - \lambda I = \begin{bmatrix}4.5-\lambda & 0.3\\ -4.0 & 1.7-\lambda\end{bmatrix} \Rightarrow |\tilde{D}-\lambda I| = 0 = (4.5-\lambda)(1.7-\lambda) + 4\times 0.3$$

$$\lambda^2 - 6.2\lambda + 8.85 = 0$$

$$\lambda = \frac{-b \pm \sqrt{b^2-4ac}}{2a}$$

$$\lambda_1 = 3.9718 = d_1$$

$$\lambda_2 = 2.2282 = d_2$$



$$\lambda^2 - 6.2\lambda + 8.85 = 0$$

$$\lambda = \frac{-b \pm \sqrt{b^2-4ac}}{2a}$$

$$\lambda_1 = 3.9718 = d_1$$

$$\lambda_2 = 2.2282 = d_2$$

$$\lambda_1 = 3.9718$$

$$\begin{bmatrix}4.5-3.9718 & 0.3\\ -4 & 1.7-3.9718\end{bmatrix}\begin{bmatrix}x_1\\ x_2\end{bmatrix} = \begin{bmatrix}0\\ 0\end{bmatrix}$$

$$0.5282x_1 + 0.3x_2 = 0$$

$$\text{for } x_1 = 1,\ x_2 = \frac{-0.5282}{0.3} = -1.7607$$

$$\lambda_2 = 2.2282$$

$$\begin{bmatrix}4.5-2.2282 & 0.3\\ -4 & 1.7-0.2282\end{bmatrix}\begin{bmatrix}x_1\\ x_2\end{bmatrix} = \begin{bmatrix}0\\ 0\end{bmatrix}$$

$$2.2718x_1 + 0.3x_2 = 0$$

$$x_2 = 1,\ x_1 = \frac{-0.3}{2.2718} = -0.1321$$

$$P = \begin{bmatrix}1 & -0.1321\\ -1.7607 & 1\end{bmatrix}$$

To evaluate the eigenvalues and eigenvectors of $\widetilde{D}$, we write the typical equation:

$$\widetilde{D}X = \lambda X,$$

This will give me:

$$\left[\widetilde{D} - \lambda I\right]X = 0, \qquad I = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

where I is a 2x2 identity matrix. Obviously $X = 0$ is a trivial solution. If we evaluate the D tilde minus λ I matrix. Since I is an identity matrix λI would be, again a diagonal matrix with both the diagonal terms being λ and the non-diagonal terms being 0. So we get:

$$\widetilde{D} - \lambda I = \begin{bmatrix} 4.5 - \lambda & 0.3 \\ -4.0 & 1.7 - \lambda \end{bmatrix}$$

Now we need to evaluate λ by putting determinant of $\widetilde{D} - \lambda I$ equal to 0. If we evaluate the determinant of this matrix, it will be:

$$\left|\widetilde{D} - \lambda I\right| = 0 = (4.5 - \lambda)(1.7 - \lambda) + 4 \times 0.3$$

We will get a quadratic equation in the form:

$$\lambda^2 - 6.2\lambda + 8.85 = 0$$

and the roots of this equation would be:

$$\lambda = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}$$

Substituting the values of $a = 1,\ b = -6.2,\ c = 8.85$ we will get:

$$\lambda_1 = 3.9718 = d_1 \quad , \quad \lambda_2 = 2.2282 = d_2$$

These are the 2 Eigen values in our terminology, d_1 and d_2. Now, we need to find the Eigen vectors. To find the Eigen vectors, we substitute each value of λ one by one back into the solution. For $\lambda_1 = 3.9718$:

$$\begin{bmatrix} 4.5 - 3.9718 & 0.3 \\ -4.0 & 1.7 - 3.9718 \end{bmatrix} \begin{bmatrix} X_1 \\ X_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

We will get 2 equations, we can solve any one of them. So, we get:

$$0.5282X_1 + 0.3X_2 = 0$$

The second one basically we will get the same equation.

We have two unknowns, but only 1 equation. So, we can fix one value and get the other one. This indicates why we take the matrix P with the diagonal elements being one. Tt is easier to do the calculations. here if we assume the first element $X_1 = 1$, as we can find X_2:

$$For \quad X_1 = 1 \quad , \quad X_2 = -\frac{0.5282}{0.3} = -1.7607$$

Similarly, we can do for $\lambda_2 = 2.2282$:

$$\begin{bmatrix} 4.5 - 2.2282 & 0.3 \\ -4.0 & 1.7 - 2.2282 \end{bmatrix} \begin{bmatrix} X_1 \\ X_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

We get an equation of the form:

$$2.2718X_1 + 0.3X_2 = 0$$

For the second Eigen vector, we take $X_2 = 1$:

$$For \quad X_2 = 1 \quad , \quad X_1 = -\frac{0.3}{2.2718} = -0.1321$$

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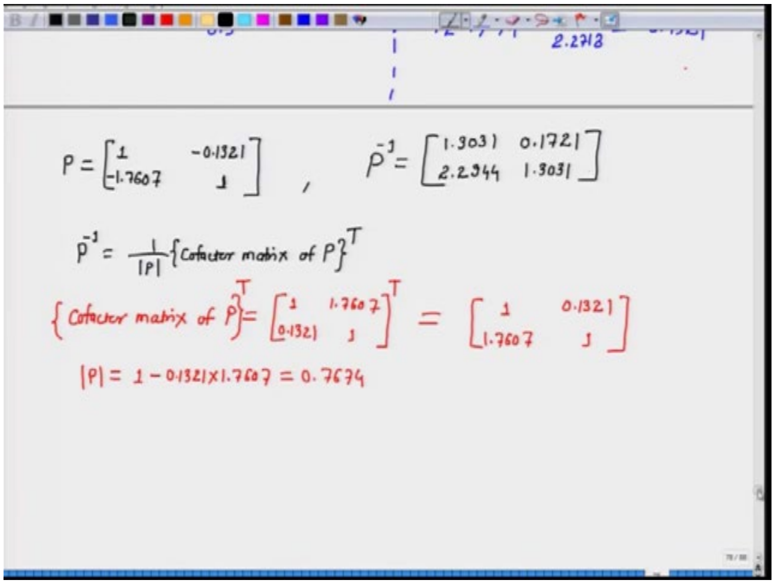
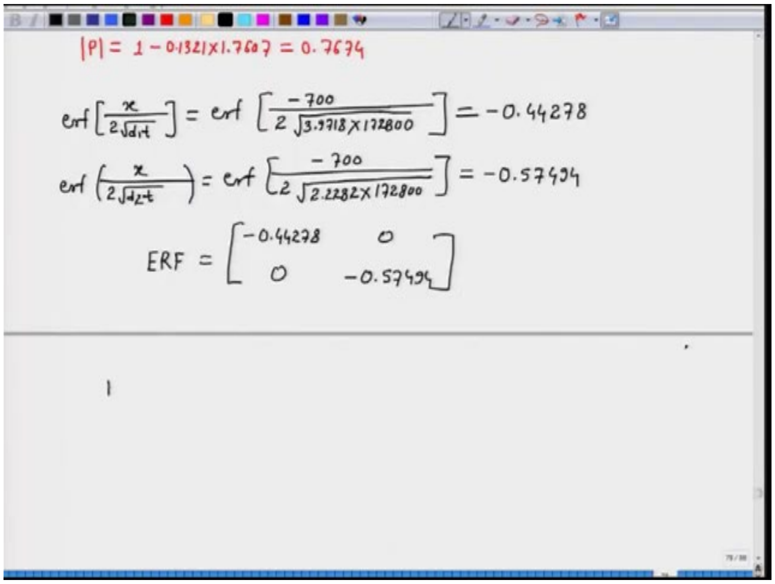


$$P = \begin{bmatrix} 1 & -0.1321 \\ -1.7607 & 1 \end{bmatrix} \quad , \quad P^{-1} = \begin{bmatrix} 1.3031 & 0.1721 \\ 2.2944 & 1.3031 \end{bmatrix}$$

$$P^{-1} = \frac{1}{|P|} \{\text{Cofactor matrix of } P\}^T$$

$$\{\text{Cofactor matrix of } P\}^T = \begin{bmatrix} 1 & 1.7607 \\ 0.1321 & 1 \end{bmatrix}^T = \begin{bmatrix} 1 & 0.1321 \\ 1.7607 & 1 \end{bmatrix}$$

$$|P| = 1 - 0.1321 \times 1.7607 = 0.7674$$

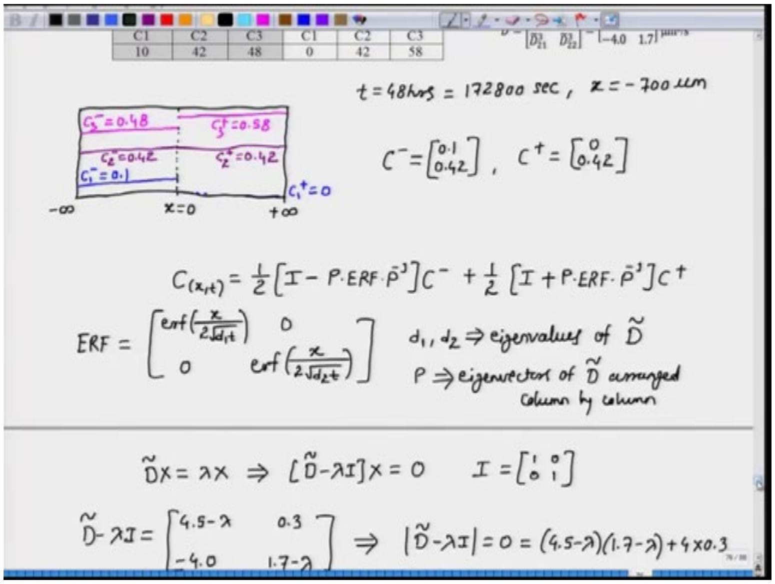


$|P| = 1 - 0.1321 \times 1.7607 = 0.7674$

$$\text{erf}\left[\frac{x}{2\sqrt{d_1 t}}\right] = \text{erf}\left[\frac{-700}{2\sqrt{3.9718 \times 172800}}\right] = -0.44278$$

$$\text{erf}\left(\frac{x}{2\sqrt{d_2 t}}\right) = \text{erf}\left[\frac{-700}{2\sqrt{2.2282 \times 172800}}\right] = -0.57494$$

$$ERF = \begin{bmatrix} -0.44278 & 0 \\ 0 & -0.57494 \end{bmatrix}$$



C1	C2	C3	C1	C2	C3
10	42	48	0	42	58

$\begin{bmatrix} \tilde{D}_{21} & \tilde{D}_{22} \end{bmatrix}$ $\begin{bmatrix} -4.0 & 1.7 \end{bmatrix}$

$t = 48\,\text{hrs} = 172800\ \text{sec}, \quad x = -700\ \mu m$

$$C^- = \begin{bmatrix} 0.1 \\ 0.42 \end{bmatrix}, \quad C^+ = \begin{bmatrix} 0 \\ 0.42 \end{bmatrix}$$

$$C_{(x,t)} = \frac{1}{2}\left[I - P \cdot ERF \cdot P^{-1}\right]C^- + \frac{1}{2}\left[I + P \cdot ERF \cdot P^{-1}\right]C^+$$

$$ERF = \begin{bmatrix} \text{erf}\left(\frac{x}{2\sqrt{d_1 t}}\right) & 0 \\ 0 & \text{erf}\left(\frac{x}{2\sqrt{d_2 t}}\right) \end{bmatrix}$$

$d_1, d_2 \Rightarrow$ eigenvalues of $\tilde{D}$

$P \Rightarrow$ eigenvectors of $\tilde{D}$ arranged column by column

$$\tilde{D}X = \lambda X \Rightarrow [\tilde{D} - \lambda I]X = 0 \qquad I = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

$$\tilde{D} - \lambda I = \begin{bmatrix} 4.5-\lambda & 0.3 \\ -4.0 & 1.7-\lambda \end{bmatrix} \Rightarrow |\tilde{D} - \lambda I| = 0 = (4.5-\lambda)(1.7-\lambda) + 4 \times 0.3$$

Now, we have obtained our matrix *P* here:

$$P = \begin{bmatrix} 1 & -0.1321 \\ -1.7607 & 1 \end{bmatrix}$$

So, we arranged the Eigen vectors column by column. The first Eigen vector is 1,-1.7607, second one is -0.1321, 1. Now next we need to find the inverse of *P*. To find the inverse of *P*, we can use the formula:

$$P^{-1} = \frac{1}{|P|}\{cofactor\ of\ P\}^T$$

So, we have to first find co-factor matrix of P and take its transpose and divided by the determinant of P. Let us see the cofactor matrix of P. For a 2 x2 matrix, it is easy. We just switch the positions of diagonal elements among themselves and the non-diagonal elements among themselves and multiply the non-diagonals by -1. This becomes:

$$cofactor\ of\ P = \begin{bmatrix} 1 & 1.7607 \\ 0.1321 & 1 \end{bmatrix}$$

And we take its transpose, which means we arrange rows as columns or columns as rows. This comes out to be:

$$\{cofactor\ of\ P\}^T = \begin{bmatrix} 1 & 1.7607 \\ 0.1321 & 1 \end{bmatrix}^T = \begin{bmatrix} 1 & 0.1321 \\ 1.7607 & 1 \end{bmatrix}$$

and we need determinant of P. This should be equal to:

$$|P| = 1 - 0.1321 \times 1.7607 = 0.7674$$

To find P inverse, we divide the transpose of co-factor of P by the determinant of P:

$$P^{-1} = \begin{bmatrix} 1.3031 & 0.1721 \\ 2.2944 & 1.3031 \end{bmatrix}$$

We need to find the error function terms. The first error function term is:

$$erf\left(\frac{x}{2\sqrt{d_1 t}}\right) = erf\left(\frac{-700}{2\sqrt{3.9718 \times 172800}}\right)$$

using the first Eigen value. Now, we can refer back to the same error function tables and we can evaluate the error function of this term. Now the most error function tables will give you error function for only the positive values of z. But we know:

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

It is easy to refer to those tables and get the values of error functions of negative values. This comes out to be:

$$erf\left(\frac{x}{2\sqrt{d_1 t}}\right) = erf\left(\frac{-700}{2\sqrt{3.9718 \times 172800}}\right) = -0.44278$$

Similarly, for the second error function term, referring back to the error function table, we will find the error function of this to be:

$$erf\left(\frac{x}{2\sqrt{d_2 t}}\right) = erf\left(\frac{-700}{2\sqrt{2.2282 \times 172800}}\right) = -0.57494$$

So:

$$ERF = \begin{bmatrix} -0.44278 & 0 \\ 0 & -0.57494 \end{bmatrix}$$

Referring back to the solution, we need this product $P.ERF.P^{-1}$.

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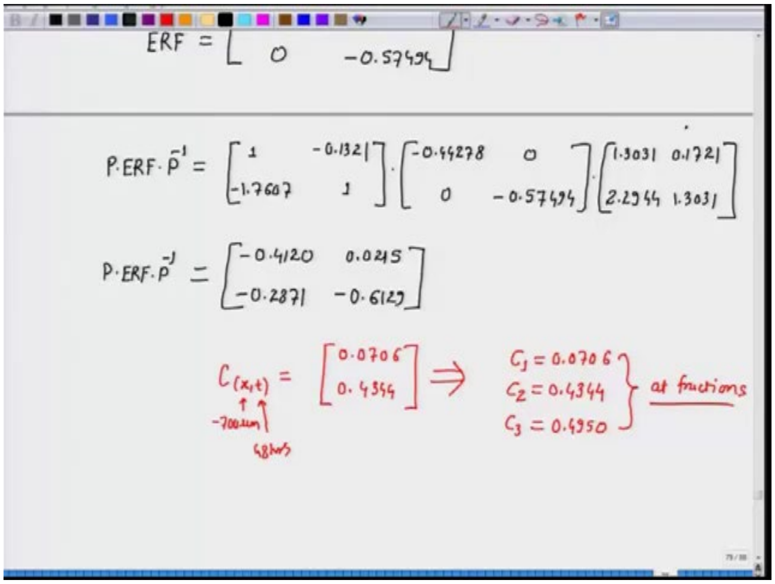
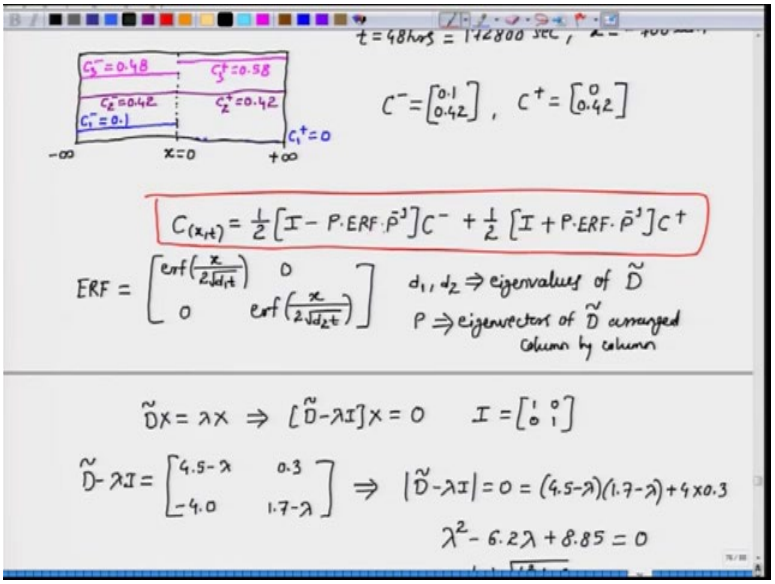


$$ERF = \begin{bmatrix} 0 & -0.57494 \end{bmatrix}$$

$$P \cdot ERF \cdot P^{-1} = \begin{bmatrix} 1 & -0.1321 \\ -1.7607 & 1 \end{bmatrix} \cdot \begin{bmatrix} -0.44278 & 0 \\ 0 & -0.57494 \end{bmatrix} \cdot \begin{bmatrix} 1.3031 & 0.1721 \\ 2.2944 & 1.3031 \end{bmatrix}$$

$$P \cdot ERF \cdot P^{-1} = \begin{bmatrix} -0.4120 & 0.0245 \\ -0.2871 & -0.6129 \end{bmatrix}$$

$$\underset{\substack{\uparrow\ \ \uparrow \\ -700\,\mu m\ \ 48\,hrs}}{C_{(x,t)}} = \begin{bmatrix} 0.0706 \\ 0.4344 \end{bmatrix} \Rightarrow \left.\begin{matrix} C_1 = 0.0706 \\ C_2 = 0.4344 \\ C_3 = 0.4950 \end{matrix}\right\} \underline{\text{at fractions}}$$



$t = 48\,hrs = 172800$ sec,

$$C^- = \begin{bmatrix} 0.1 \\ 0.42 \end{bmatrix}, \quad C^+ = \begin{bmatrix} 0 \\ 0.42 \end{bmatrix}$$

$$\boxed{C_{(x,t)} = \frac{1}{2}\left[I - P \cdot ERF \cdot P^{-1}\right]C^- + \frac{1}{2}\left[I + P \cdot ERF \cdot P^{-1}\right]C^+}$$

$$ERF = \begin{bmatrix} \mathrm{erf}\left(\frac{x}{2\sqrt{d_1 t}}\right) & 0 \\ 0 & \mathrm{erf}\left(\frac{x}{2\sqrt{d_2 t}}\right) \end{bmatrix}$$

$d_1, d_2 \Rightarrow$ eigenvalues of $\tilde{D}$

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$$\lambda^2 - 6.2\lambda + 8.85 = 0$$

We can obtain this product $P.ERF.P^{-1}$ as:

$$P.ERF.P^{-1} = \begin{bmatrix} 1 & -0.1321 \\ -1.7607 & 1 \end{bmatrix} \begin{bmatrix} -0.44278 & 0 \\ 0 & -0.57494 \end{bmatrix} \begin{bmatrix} 1.3031 & 0.1721 \\ 2.2944 & 1.3031 \end{bmatrix}$$

$$P.ERF.P^{-1} = \begin{bmatrix} -0.4120 & -0.0215 \\ -0.2871 & -0.6129 \end{bmatrix}$$

Now, we have to substitute back in the solution right:

$$C = \frac{1}{2}[I - P.ERF.P^{-1}]C^- + \frac{1}{2}[I + P.ERF.P^{-1}]C^+$$

We know I is the identity matrix 2 x2 here, we know this $P.ERF.P^{-1}$ and we know C^- and C^+. So, we substitute in them and find C at x and t. It will come out to be again a column matrix:

$$C_{(x,t)} = \begin{bmatrix} 0.0706 \\ 0.4344 \end{bmatrix} \quad , C_1 = 0.0706 \quad , \quad C_2 = 0.4344$$

What it tells me at x= -700 μm after 48 hours of diffusion annealing, the composition plane that will be developed is $C_1 = 0.0706$, $C_2 = 0.4344$ and because $C_3 = 1 - C_1 - C_2$:

$$C_3 = 0.4950$$

This will be in atom fraction. So, this is how we can use the multi-component diffusion solution to get the concentration as a function of x and t in any multi-component diffusion couple. Again we illustrated this with a ternary diffusion couple, but similar procedure you can apply to quaternary, quinary or higher order diffusion couples, okay. We assumed the interdiffusivity matrix is constant throughout the diffusion zone and also molar volume was assumed constant.

Instead of moles per centimeter cube, we can also use the atom fraction or even weight fraction because molar volume is constant, it is independent of composition. Okay, with that we will stop here for today. Thank you.