Diffusion in Multicomponent Solids
Professor Kaustubh Kulkarni
Department of Material Science and Engineering
Indian Institute of Technology, Kanpur
Lecture 23
Solution to Diffusion Equations for Multicomponent Diffusions Couple

Welcome back to this online class on Diffusion in Multicomponent Solids. Today we are going to solve diffusion equation for multicomponent system.

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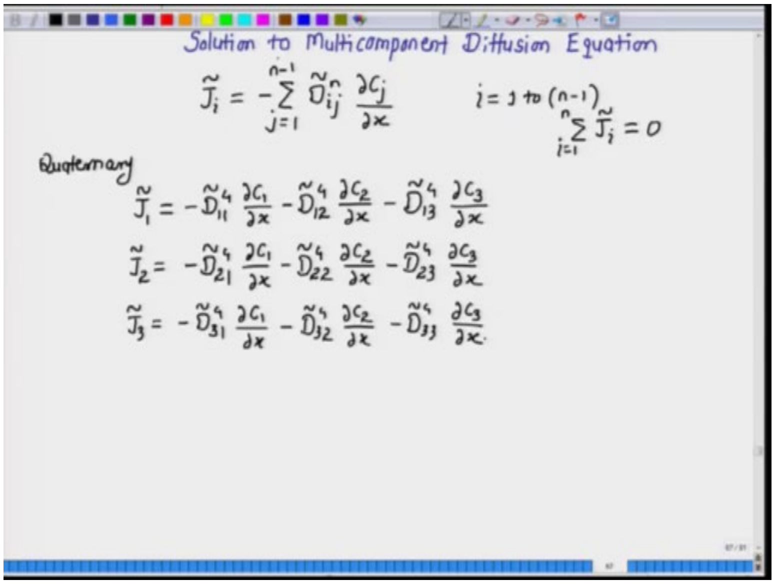


Solution to Multicomponent Diffusion Equation

$$\tilde{J}_i = -\sum_{j=1}^{n-1} \tilde{D}_{ij}^{n} \frac{\partial C_j}{\partial x} \qquad i = 1 \text{ to } (n-1)$$

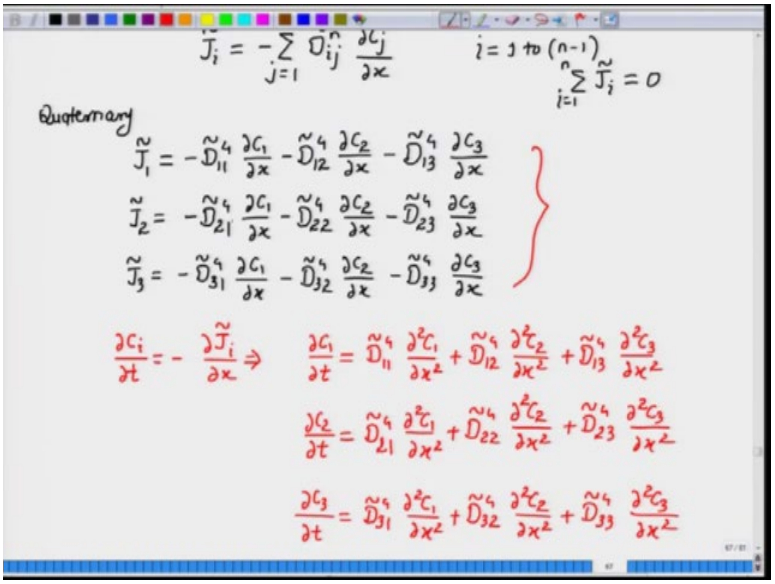
$$\sum_{i=1}^{n} \tilde{J}_i = 0$$

Quaternary

$$\tilde{J}_1 = -\tilde{D}_{11}^{4} \frac{\partial C_1}{\partial x} - \tilde{D}_{12}^{4} \frac{\partial C_2}{\partial x} - \tilde{D}_{13}^{4} \frac{\partial C_3}{\partial x}$$

$$\tilde{J}_2 = -\tilde{D}_{21}^{4} \frac{\partial C_1}{\partial x} - \tilde{D}_{22}^{4} \frac{\partial C_2}{\partial x} - \tilde{D}_{23}^{4} \frac{\partial C_3}{\partial x}$$

$$\tilde{J}_3 = -\tilde{D}_{31}^{4} \frac{\partial C_1}{\partial x} - \tilde{D}_{32}^{4} \frac{\partial C_2}{\partial x} - \tilde{D}_{33}^{4} \frac{\partial C_3}{\partial x}.$$



$$\tilde{J}_i = -\sum_{j=1}^{n} \tilde{D}^n_{ij} \frac{\partial C_j}{\partial x} \qquad i = 1 \text{ to } (n-1)$$

$$\sum_{i=1}^{n} \tilde{J}_i = 0$$

Quaternary

$$\left.\begin{aligned} \tilde{J}_1 &= -\tilde{D}^4_{11}\frac{\partial C_1}{\partial x} - \tilde{D}^4_{12}\frac{\partial C_2}{\partial x} - \tilde{D}^4_{13}\frac{\partial C_3}{\partial x} \\ \tilde{J}_2 &= -\tilde{D}^4_{21}\frac{\partial C_1}{\partial x} - \tilde{D}^4_{22}\frac{\partial C_2}{\partial x} - \tilde{D}^4_{23}\frac{\partial C_3}{\partial x} \\ \tilde{J}_3 &= -\tilde{D}^4_{31}\frac{\partial C_1}{\partial x} - \tilde{D}^4_{32}\frac{\partial C_2}{\partial x} - \tilde{D}^4_{33}\frac{\partial C_3}{\partial x} \end{aligned}\right\}$$

$$\frac{\partial C_i}{\partial t} = -\frac{\partial \tilde{J}_i}{\partial x} \Rightarrow \begin{aligned} \frac{\partial C_1}{\partial t} &= \tilde{D}^4_{11}\frac{\partial^2 C_1}{\partial x^2} + \tilde{D}^4_{12}\frac{\partial^2 C_2}{\partial x^2} + \tilde{D}^4_{13}\frac{\partial^2 C_3}{\partial x^2} \\ \frac{\partial C_2}{\partial t} &= \tilde{D}^4_{21}\frac{\partial^2 C_1}{\partial x^2} + \tilde{D}^4_{22}\frac{\partial^2 C_2}{\partial x^2} + \tilde{D}^4_{23}\frac{\partial^2 C_3}{\partial x^2} \\ \frac{\partial C_3}{\partial t} &= \tilde{D}^4_{31}\frac{\partial^2 C_1}{\partial x^2} + \tilde{D}^4_{32}\frac{\partial^2 C_2}{\partial x^2} + \tilde{D}^4_{33}\frac{\partial^2 C_3}{\partial x^2} \end{aligned}$$

We will consider the infinite diffusion couple boundary conditions and we will consider a multicomponent system containing n components. When it comes to multicomponent systems, there are n-1 independent concentration variables. And when we define the flux of one component, we need to consider the concentration gradients of all the n-1 independent components. Based on Onsager's formalism of Fick's law, we can write the equation for flux of a component i in an n component system as:

$$\tilde{J}_i = -\sum_{j=1}^{n-1} \tilde{D}^n_{ij} \frac{\partial C_j}{\partial x} \qquad i = j \; to \; n-1$$

The flux of component i is related to the gradient of component j through the interdiffusion coefficient $\tilde{D}^n_{ij}$. The superscript n here denotes that component n is taken as the dependent component. Now, there are n-1 independent concentration gradients and that is why j varies from 1 to n-1. To define the flux of one component, we need n-1 interdiffusion coefficients. And we have n-1 independent fluxes. Because, if we assume the molar volume to be constant then the summation of all $\tilde{J}_i$, i going from 1 to n is equal to 0:

$$\sum_{i=1}^{n} \tilde{J}_i = 0$$

So, the nth flux is dependent. Therefore, we have $(n-1)^2$ interdiffusion coefficient that define the interdiffusion completely in an n component system at a particular composition.

Now we are going to assume that the set of interdiffusion coefficients is independent of composition for solving this equation. Let us see how do we solve the diffusion equation for an n component system. We consider here as an example quaternary system which means there are four components. So, three components are independent and we can write three interdiffusion fluxes:

$$\tilde{J}_1 = -\tilde{D}_{11}^4 \frac{\partial C_1}{\partial x} - \tilde{D}_{12}^4 \frac{\partial C_2}{\partial x} - \tilde{D}_{13}^4 \frac{\partial C_3}{\partial x}$$

$$\tilde{J}_2 = -\tilde{D}_{21}^4 \frac{\partial C_1}{\partial x} - \tilde{D}_{22}^4 \frac{\partial C_2}{\partial x} - \tilde{D}_{23}^4 \frac{\partial C_3}{\partial x}$$

$$\tilde{J}_3 = -\tilde{D}_{31}^4 \frac{\partial C_1}{\partial x} - \tilde{D}_{32}^4 \frac{\partial C_2}{\partial x} - \tilde{D}_{33}^4 \frac{\partial C_3}{\partial x}$$

To get to the diffusion equation we can apply the continuity equation for individual components, we can write:

$$\left(\frac{\partial C_i}{\partial t}\right)_x = -\left(\frac{\partial \tilde{J}_i}{\partial x}\right)_t$$

If we expand this continuity equation again for three components we can write:

$$\frac{\partial C_1}{\partial t} = \tilde{D}_{11}^4 \frac{\partial^2 C_1}{\partial x^2} + \tilde{D}_{12}^4 \frac{\partial^2 C_2}{\partial x^2} + \tilde{D}_{13}^4 \frac{\partial^2 C_3}{\partial x^2}$$

$$\frac{\partial C_2}{\partial t} = \tilde{D}_{21}^4 \frac{\partial^2 C_1}{\partial x^2} + \tilde{D}_{22}^4 \frac{\partial^2 C_2}{\partial x^2} + \tilde{D}_{23}^4 \frac{\partial^2 C_3}{\partial x^2}$$

$$\frac{\partial C_3}{\partial t} = \tilde{D}_{31}^4 \frac{\partial^2 C_1}{\partial x^2} + \tilde{D}_{32}^4 \frac{\partial^2 C_2}{\partial x^2} + \tilde{D}_{33}^4 \frac{\partial^2 C_3}{\partial x^2}$$

So, we can see in multicomponent system, the diffusion equation is coupled, which means if we consider the partial differential of any component's profile with respect to time, it is expressed in terms of second derivative or the second partial of each of the independent components with respect to x. And we have a problem here, how to solve this coupled equation.

We first need to decouple the equation. And we can do that easily if we use matrix algebra. If we carefully look at the equation for the fluxes, for example here it is easy to see that we can express this in the form of a matrix equation. If we define a column matrix of fluxes on the left side, column matrix of gradients on the right side and square matrix of interdiffusion coefficients.

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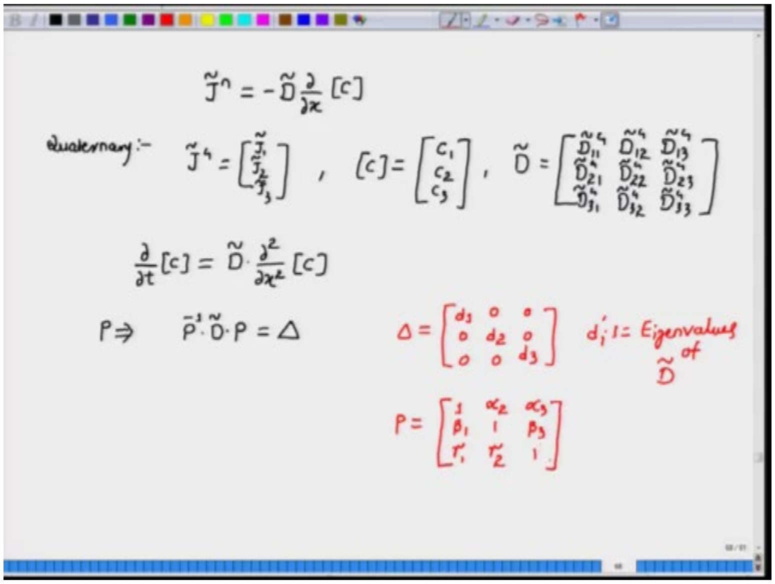


$$\tilde{J}^n = -\tilde{D}\frac{\partial}{\partial x}[c]$$

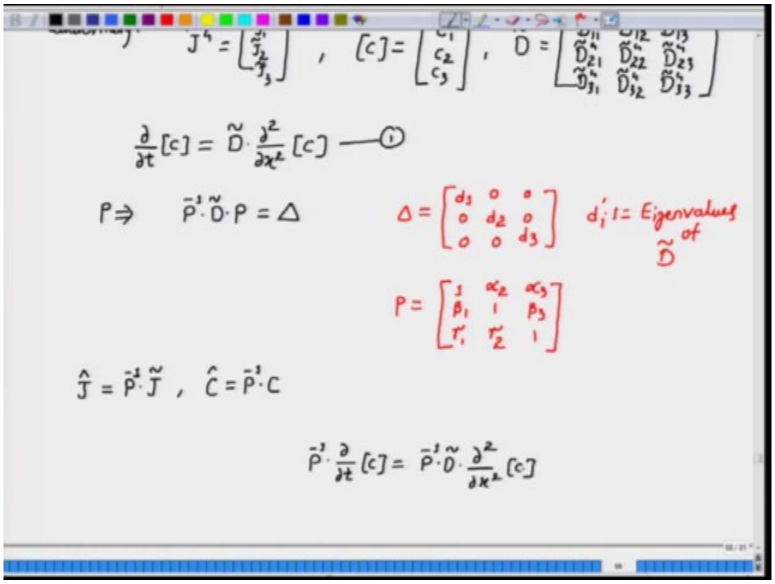
Quaternary:- $\tilde{J}^4 = \begin{bmatrix}\tilde{J}_1\\ \tilde{J}_2\\ \tilde{J}_3\end{bmatrix}$, $[c] = \begin{bmatrix}c_1\\ c_2\\ c_3\end{bmatrix}$, $\tilde{D} = \begin{bmatrix}\tilde{D}^4_{11} & \tilde{D}^4_{12} & \tilde{D}^4_{13}\\ \tilde{D}^4_{21} & \tilde{D}^4_{22} & \tilde{D}^4_{23}\\ \tilde{D}^4_{31} & \tilde{D}^4_{32} & \tilde{D}^4_{33}\end{bmatrix}$

$$\frac{\partial}{\partial t}[c] = \tilde{D}\cdot\frac{\partial^2}{\partial x^2}[c]$$

$P \Rightarrow \quad P^{-1}\cdot\tilde{D}\cdot P = \Delta$

$\Delta = \begin{bmatrix}d_1 & 0 & 0\\ 0 & d_2 & 0\\ 0 & 0 & d_3\end{bmatrix}$ d_i' := Eigenvalues of $\tilde{D}$

$P = \begin{bmatrix}1 & \alpha_2 & \alpha_3\\ \beta_1 & 1 & \beta_3\\ \gamma_1 & \gamma_2 & 1\end{bmatrix}$



$\tilde{J}^4 = \begin{bmatrix}\tilde{J}_1\\ \tilde{J}_2\\ \tilde{J}_3\end{bmatrix}$, $[c] = \begin{bmatrix}c_1\\ c_2\\ c_3\end{bmatrix}$, $\tilde{D} = \begin{bmatrix}\tilde{D}^4_{11} & \tilde{D}^4_{12} & \tilde{D}^4_{13}\\ \tilde{D}^4_{21} & \tilde{D}^4_{22} & \tilde{D}^4_{23}\\ \tilde{D}^4_{31} & \tilde{D}^4_{32} & \tilde{D}^4_{33}\end{bmatrix}$

$$\frac{\partial}{\partial t}[c] = \tilde{D}\cdot\frac{\partial^2}{\partial x^2}[c] \quad \text{—①}$$

$P \Rightarrow \quad P^{-1}\cdot\tilde{D}\cdot P = \Delta$

$\Delta = \begin{bmatrix}d_1 & 0 & 0\\ 0 & d_2 & 0\\ 0 & 0 & d_3\end{bmatrix}$ d_i' := Eigenvalues of $\tilde{D}$

$P = \begin{bmatrix}1 & \alpha_2 & \alpha_3\\ \beta_1 & 1 & \beta_3\\ \gamma_1 & \gamma_2 & 1\end{bmatrix}$

$\hat{J} = P^{-1}\cdot\tilde{J}$, $\hat{C} = P^{-1}\cdot C$

$$P^{-1}\cdot\frac{\partial}{\partial t}[c] = P^{-1}\cdot\tilde{D}\cdot\frac{\partial^2}{\partial x^2}[c]$$

we can write the Fick's law equation as:

$$\tilde{J}^n = -\tilde{D}\frac{\partial}{\partial x}[C]$$

In this case if we write this for quaternary system, you can define these matrices as:

$$\tilde{J}^4 = \begin{bmatrix}\tilde{J}_1\\ \tilde{J}_2\\ \tilde{J}_3\end{bmatrix}$$

$\tilde{J}^4$ is a column matrix of 3 independent fluxes. C is a column matrix of 3 independent concentrations and $\widetilde{D}$ is a square matrix:

$$[C] = \begin{bmatrix} C_1 \\ C_2 \\ C_3 \end{bmatrix}, \qquad \widetilde{D} = \begin{bmatrix} \widetilde{D}^4_{11} & \widetilde{D}^4_{12} & \widetilde{D}^4_{13} \\ \widetilde{D}^4_{21} & \widetilde{D}^4_{22} & \widetilde{D}^4_{23} \\ \widetilde{D}^4_{31} & \widetilde{D}^4_{32} & \widetilde{D}^4_{33} \end{bmatrix}$$

In case of quaternary, $\widetilde{D}$ is a 3x3 matrix containing 9 interdiffusion coefficients which are given above. We can also write the three diffusion equations in the form of a matrix equation as:

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

Now to make it even simpler, let us try to transform the original matrices into a new form. Let us call this new form as cap basis. So, we have to first define what we call as similarity transformation matrix for $\widetilde{D}$. This similarity transformation matrix P is defined such that if we pre multiply $\widetilde{D}$ by inverse of P, and post multiply $\widetilde{D}$ by P, we get a diagonal matrix Δ:

$$P^{-1}.\widetilde{D}.P = \Delta$$

and it is obtained by arranging the eigen values of this $\widetilde{D}$ matrix along the diagonal. Δ is:

$$\Delta = \begin{bmatrix} d_1 & 0 & 0 \\ 0 & d_2 & 0 \\ 0 & 0 & d_3 \end{bmatrix}$$

These $d_i's$ are eigen values of $\widetilde{D}$ and matrix P is obtained by arranging the eigen vectors of $\widetilde{D}$ column by column. For convenience, we write eigen vectors such that the corresponding diagonal elements are normalized to 1:

$$P = \begin{bmatrix} 1 & \alpha_2 & \alpha_3 \\ \beta_1 & 1 & \beta_3 \\ \gamma_1 & \gamma_2 & 1 \end{bmatrix}$$

Now to proceed further, we define fluxes and compositions in a new basis which we call as cap basis. We obtained the matrix $\hat{J}$ by pre-multiplying the original matrix with P^{-1}. :

$$\hat{J} = P^{-1}.\tilde{J}$$

and $\hat{C}$ is obtained by pre-multiplying the original matrix C with P^{-1}:

$$\hat{C} = P^{-1}.C$$

So, how this transformation helps us, just try to look at it. If we now pre-multiply the diffusion equation in the matrix form with P^{-1}, we get:

$$P^{-1}.\frac{\partial}{\partial t}[C] = P^{-1}.\widetilde{D}.\frac{\partial^2}{\partial x^2}[C]$$

Now we are assuming that, $\widetilde{D}$ matrix is constant. And this P and P^{-1} matrices are also constant, so we can take them inside the derivatives. Further, we know:

$$\hat{C} = P^{-1}.C$$

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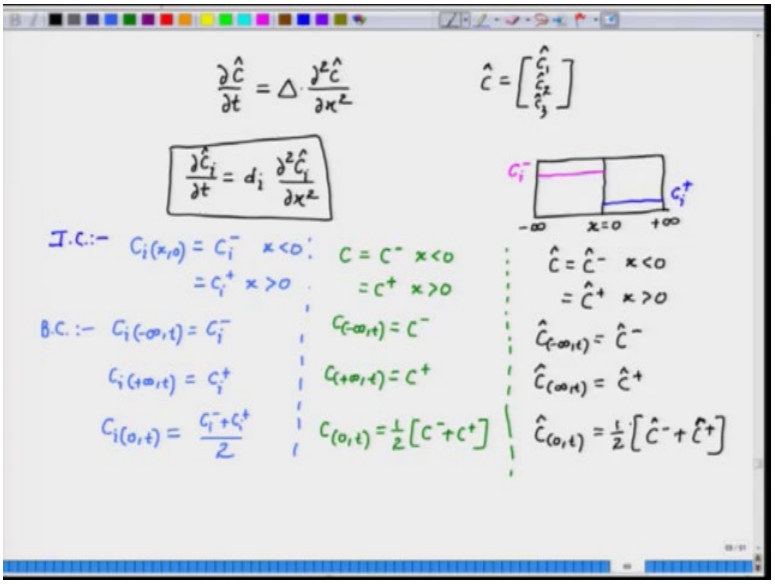

$$\frac{\partial \hat{C}}{\partial t} = \Delta \cdot \frac{\partial^2 \hat{C}}{\partial x^2} \qquad \hat{C} = \begin{bmatrix} \hat{C}_1 \\ \hat{C}_2 \\ \hat{C}_3 \end{bmatrix}$$

$$\boxed{\frac{\partial \hat{C}_i}{\partial t} = d_i \frac{\partial^2 \hat{C}_i}{\partial x^2}}$$

I.C.:- $C_i(x,0) = C_i^- \quad x<0$ $\quad C = C^- \quad x<0$ $\quad \hat{C} = \hat{C}^- \quad x<0$

$= C_i^+ \quad x>0$ $\quad = C^+ \quad x>0$ $\quad = \hat{C}^+ \quad x>0$

B.C. :- $C_i(-\infty,t) = C_i^-$ $\quad C(-\infty,t) = C^-$ $\quad \hat{C}(-\infty,t) = \hat{C}^-$

$C_i(+\infty,t) = C_i^+$ $\quad C(+\infty,t) = C^+$ $\quad \hat{C}(\infty,t) = \hat{C}^+$

$C_i(0,t) = \frac{C_i^- + C_i^+}{2}$ $\quad C(0,t) = \frac{1}{2}[C^- + C^+]$ $\quad \hat{C}(0,t) = \frac{1}{2}[\hat{C}^- + \hat{C}^+]$

So, we can write:

$$\frac{\partial \hat{C}}{\partial t} = P^{-1}.\widetilde{D}.\frac{\partial^2}{\partial x^2}[C]$$

We insert a matrix defined by the product of P and P^{-1} which is an identity matrix on the right hand side between $\widetilde{D}$ and $\frac{\partial^2}{\partial x^2}[C]$ we get:

$$\frac{\partial \hat{C}}{\partial t} = P^{-1}.\widetilde{D}.(P.P^{-1})\frac{\partial^2}{\partial x^2}[C] = \left(P^{-1}.\widetilde{D}.P\right).P^{-1}\frac{\partial^2}{\partial x^2}[C]$$

Now on substituting the following we get:

$$P^{-1}.\widetilde{D}.P = \Delta$$

$$\frac{\partial \hat{C}}{\partial t} = \Delta\,.P^{-1}\frac{\partial^2}{\partial x^2}[C]$$

We can take P^{-1} inside and $P^{-1}.C$ is again matrix of concentration in cap basis. So:

$$\frac{\partial \hat{C}}{\partial t} = \Delta.\frac{\partial^2 \hat{C}}{\partial x^2}$$

We now by the transformation got the diffusion equation in a simpler form. In terms of individual components of this, you know $\hat{C}$ would be a column vector of $\hat{C}_1$, $\hat{C}_2$ and $\hat{C}_3$. And Δ is a diagonal matrix. Individually we can write:

$$\frac{\partial \hat{C}_i}{\partial t} = d_i\frac{\partial^2 \hat{C}_i}{\partial x^2}$$

We have now obtained a decoupled partial differential equation which looks now easier to solve. But we also need to look at the initial and boundary conditions now. Initial conditions for a diffusion couple is a step function. If we consider any single component, on the left terminal alloy composition was C_i^- and on the right terminal alloy the composition was C_i^+ to start with.

And it is a step function or at $x = 0$ there is a discontinuity. The thicknesses of the two blocks are such that the diffusion species does not penetrate all the way to the other end. These ends are $\pm\infty$. The concentration of the alloy blocks remain as the original concentration in these two ends.

So, initial condition is:

$$\begin{aligned} I.C. \quad : \quad & C_i(x,0) = C_i^- \qquad x < 0 \\ & C_i(x,0) = C_i^+ \qquad x > 0 \end{aligned}$$

Boundary condition is:

$$B.C. \quad : \quad C_i(-\infty,t) = C_i^-$$

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

When we solve the diffusion equation for the binary diffusion couple, we also used the condition:

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

Since the diffusivity are constant, $C_i(0, t)$ should be average of the two end concentrations. Now if you define this in terms of matrices, we can write:

$$\begin{aligned} I.C. \quad : \quad & C(x, 0) = C^- \qquad x < 0 \\ & C(x, 0) = C^+ \qquad x > 0 \\ B.C. \quad : \quad & C(-\infty, t) = C^- \\ & C(\infty, t) = C^+ \\ & C(0, t) = \frac{C^- + C^+}{2} \end{aligned}$$

where C is the matrix of concentrations, C^- is the matrix of three independent concentrations in the left terminal alloy and C^+ is the column matrix of three independent concentrations for right terminal alloy. We can apply the similar transformation to the initial and boundary conditions. If we pre-multiply on both sides by P inverse, we get the concentrations in cap basis.

If we pre-multiply both side by P^{-1}, we can write:

$$\begin{aligned} I.C. \quad : \quad & \hat{C}(x, 0) = \hat{C}^- \qquad x < 0 \\ & \qquad\quad\;\; = \hat{C}^+ \qquad x > 0 \\ B.C. \quad : \quad & \hat{C}(-\infty, t) = \hat{C}^- \\ & \hat{C}(\infty, t) = \hat{C}^+ \\ & \hat{C}(0, t) = \frac{\hat{C}^- + \hat{C}^+}{2} \end{aligned}$$

We have to solve, now this diffusion equations and the initial and boundary conditions are defined by these matrix equations. If you write in terms of individual components $\hat{C}_i$, then we will see that now we have obtained a decoupled partial differential equation with the initial and boundary conditions which we have solved before for binary diffusion.

Except that here, the concentration variable is now defined in the new basis, the cap basis. And instead of the single diffusivity term that appeared earlier for binary diffusion, here we see is d_i which is the eigen value of $\widetilde{D}$. Now we know the solution for this as we have derived the solution for this.

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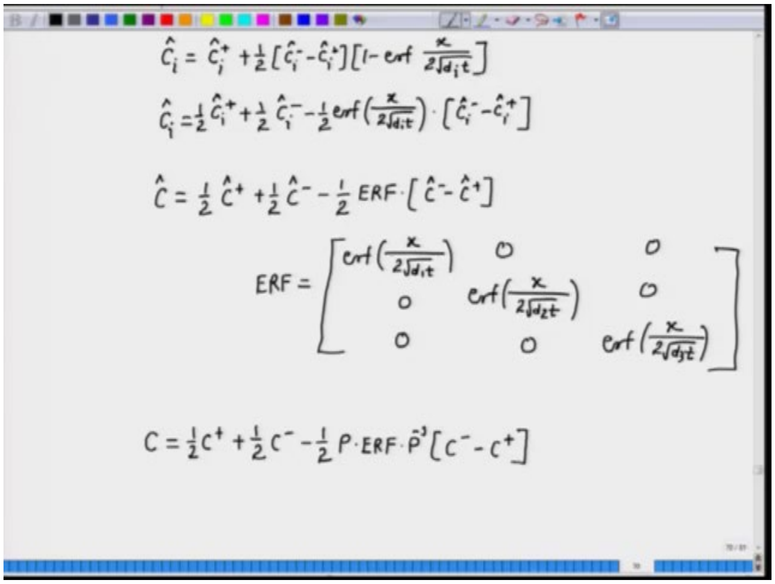


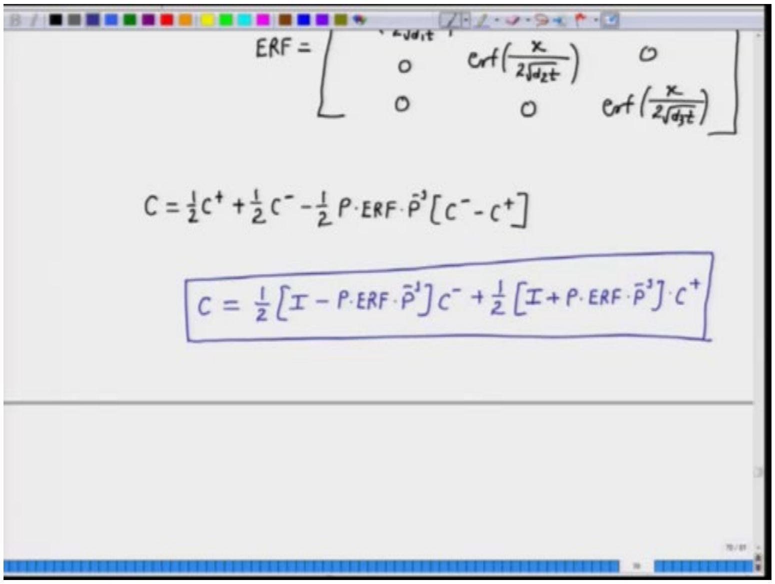
$$\hat{C}_i = \hat{C}_i^+ + \frac{1}{2}[\hat{C}_i^- - \hat{C}_i^+][1 - erf \frac{x}{2\sqrt{d_i t}}]$$

$$\hat{C}_i = \frac{1}{2}\hat{C}_i^+ + \frac{1}{2}\hat{C}_i^- - \frac{1}{2} erf\left(\frac{x}{2\sqrt{d_i t}}\right) \cdot [\hat{C}_i^- - \hat{C}_i^+]$$

$$\hat{C} = \frac{1}{2}\hat{C}^+ + \frac{1}{2}\hat{C}^- - \frac{1}{2} ERF \cdot [\hat{C}^- - \hat{C}^+]$$

$$ERF = \begin{bmatrix} erf\left(\frac{x}{2\sqrt{d_1 t}}\right) & 0 & 0 \\ 0 & erf\left(\frac{x}{2\sqrt{d_2 t}}\right) & 0 \\ 0 & 0 & erf\left(\frac{x}{2\sqrt{d_3 t}}\right) \end{bmatrix}$$

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



$$ERF = \begin{bmatrix} 0 & erf\left(\frac{x}{2\sqrt{d_2 t}}\right) & 0 \\ 0 & 0 & erf\left(\frac{x}{2\sqrt{d_3 t}}\right) \end{bmatrix}$$

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

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

If you write the solution for Ci cap:

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

Remember we are using the eigen value of $\widetilde{D}$ instead of single diffusivity term. For binary there was a single diffusivity term. We can rearrange the term and write the last solution as:

$$\hat{C}_i = \frac{1}{2}\hat{C}_i{}^{+} + \frac{1}{2}\hat{C}_i{}^{-} - \frac{1}{2} erf\left(\frac{x}{2\sqrt{d_i t}}\right).\left(\hat{C}_i{}^{-} - \hat{C}_i{}^{+}\right)$$

Now if we want to get back to the original basis because we want the solution for composition in the original basis we first need to convert this into matrix form:

If we write this in the matrix form you get:

$$\hat{C} = \frac{1}{2}\hat{C}^{+} + \frac{1}{2}\hat{C}^{-} - \frac{1}{2}ERF.\left(\hat{C}^{-} - \hat{C}^{+}\right)$$

And this ERF is nothing but the diagonal matrix defined by arranging the error function terms. These error function term for different components are arranged along the diagonal of this matrix as:

$$ERF = \begin{bmatrix} \frac{x}{2\sqrt{d_1 t}} & 0 & 0 \\ 0 & \frac{x}{2\sqrt{d_2 t}} & 0 \\ 0 & 0 & \frac{x}{2\sqrt{d_3 t}} \end{bmatrix}$$

Now we have to get back to the original basis what. So, we defined the cap basis as:

$$\hat{C} = P^{-1}.C$$

If we pre-multiply now by P on both sides of the equation:

$$P.\hat{C} = C$$

$$C = \frac{1}{2}C^{+} + \frac{1}{2}C^{-} - \frac{1}{2}P.ERF\left(\hat{C}^{-} - \hat{C}^{+}\right)$$

and introducing $I = P^{-1}.P$ after ERF we get back the original matrix:

$$C = \frac{1}{2}C^{+} + \frac{1}{2}C^{-} - \frac{1}{2}P.ERF.P^{-1}(C^{-} - C^{+})$$

C^+ and C^- are the matrices of independent concentrations in right and left terminal alloy respectively.

This is the solution for all the concentrations in a multi-component diffusion couple. We can arrange this in a better more good looking form as:

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

This is a very simple looking solution in the matrix form. And remember I illustrated this for quaternary while deriving the solution but this is applicable for an n component system. Just to verify if I apply this for binary system.

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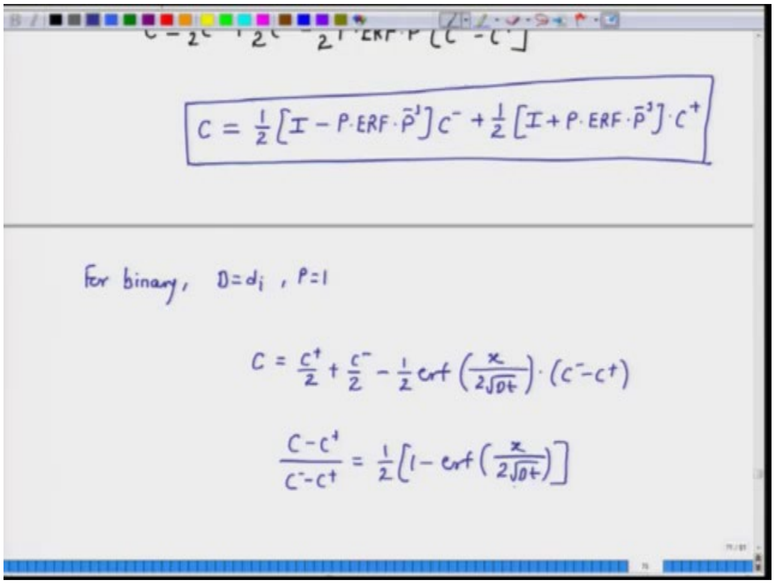

$$\boxed{C = \frac{1}{2}[I - P\cdot ERF\cdot P^{-1}]C^- + \frac{1}{2}[I + P\cdot ERF\cdot P^{-1}]\cdot C^+}$$

For binary, $D = d_i$, $P = 1$

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

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

For binary we have a single diffusivity term. $D = d_i$, $P = 1$ and we get back the solution that we have derived:

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

And if you rearrange the term we get the more popular form:

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

Remember this matrix ERF here for binary will have only one term that is $erf\left(\frac{x}{2\sqrt{Dt}}\right)$ where D is the binary diffusivity there. So, this can be verified for binary.

The advantage of using the matrix approach for solving the diffusion equation with the transformations that we did is very clear here. Because, we could solve very simplistically and got a very simple form of solution. Now people have derived before the solutions for ternary and you can see it can take a very complicated form. The advantage of matrix approaches is that we get the solution in a very simple form.

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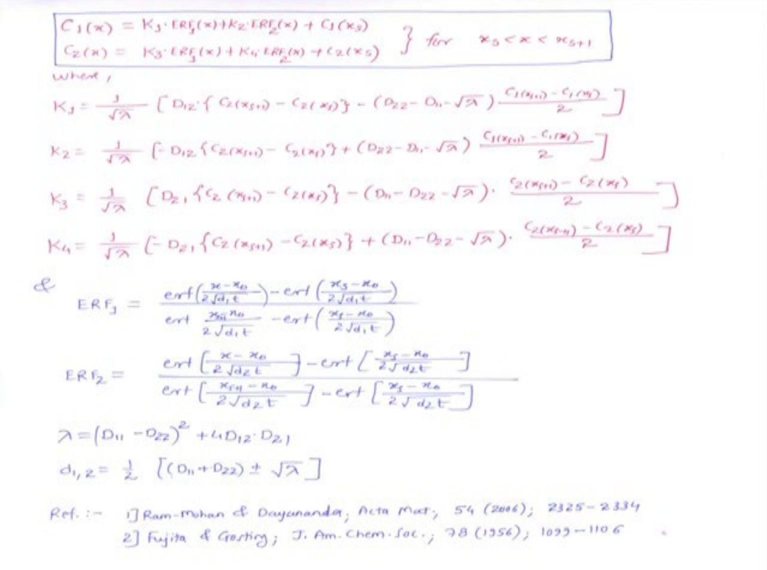

$$\boxed{\left.\begin{array}{l} C_1(x) = K_1\cdot ERF_1(x) + K_2\cdot ERF_2(x) + C_1(x_s) \\ C_2(x) = K_3\cdot ERF_1(x) + K_4\cdot ERF_2(x) + C_2(x_s) \end{array}\right\} \text{for} \quad x_s < x < x_{s+1}}$$

where,

$$K_1 = \frac{1}{\sqrt{\lambda}}\left[D_{12}\cdot\{C_2(x_{s+1}) - C_2(x_s)\} - (D_{22} - D_{11} - \sqrt{\lambda})\frac{C_1(x_{s+1}) - C_1(x_s)}{2}\right]$$

$$K_2 = \frac{1}{\sqrt{\lambda}}\left[-D_{12}\{C_2(x_{s+1}) - C_2(x_s)\} + (D_{22} - D_{11} - \sqrt{\lambda})\frac{C_1(x_{s+1}) - C_1(x_s)}{2}\right]$$

$$K_3 = \frac{1}{\sqrt{\lambda}}\left[D_{21}\{C_2(x_{s+1}) - C_2(x_s)\} - (D_{11} - D_{22} - \sqrt{\lambda})\cdot\frac{C_2(x_{s+1}) - C_2(x_s)}{2}\right]$$

$$K_4 = \frac{1}{\sqrt{\lambda}}\left[-D_{21}\{C_2(x_{s+1}) - C_2(x_s)\} + (D_{11} - D_{22} - \sqrt{\lambda})\cdot\frac{C_2(x_{s+1}) - C_2(x_s)}{2}\right]$$

&

$$ERF_1 = \frac{erf\left(\frac{x - x_0}{2\sqrt{d_1 t}}\right) - erf\left(\frac{x_s - x_0}{2\sqrt{d_1 t}}\right)}{erf\,\frac{x_{s+1} - x_0}{2\sqrt{d_1 t}} - erf\left(\frac{x_s - x_0}{2\sqrt{d_1 t}}\right)}$$

$$ERF_2 = \frac{erf\left[\frac{x - x_0}{2\sqrt{d_2 t}}\right] - erf\left[\frac{x_s - x_0}{2\sqrt{d_2 t}}\right]}{erf\left[\frac{x_{s+1} - x_0}{2\sqrt{d_2 t}}\right] - erf\left[\frac{x_s - x_0}{2\sqrt{d_2 t}}\right]}$$

$$\lambda = (D_{11} - D_{22})^2 + 4D_{12}\cdot D_{21}$$

$$d_{1,2} = \frac{1}{2}\left[(D_{11} + D_{22}) \pm \sqrt{\lambda}\right]$$

Ref. :- 1] Ram-Mohan & Dayananda; Acta Mat; 54 (2006); 2325-2334
2] Fujita & Gosting; J. Am. Chem. Soc.; 78 (1956); 1099-1106

For example if you want to see the solution for a ternary system which was derived earlier by Fujita and Gosting. This is the solution for ternary concentrations. We have two independent concentrations C_1 and C_2 and you can see it is a very complicated form. But using the matrix approach we obtained the solution in a very simple form. We will stop here for today, thank you.