Module 4:

Multicomponent Transport

Lecture 36:

Solving the Multi-component Flux Equations

Given the "continuity equation"

$$\frac{\partial C_i}{\partial t} + \nabla.(\underline{v}C_i) = -\nabla.\underline{F}_i \qquad (3.7.35)$$

Where the multicomponent flux $\underline{F}_i = -\sum_{j=1}^{n} D_{ij} \ \nabla C_j \qquad (3.7.36)$

Reformulate this problem in a form resembling a binary diffusion problem.

Eqs. (3.7.35), (3.7.36) can be written in matrix form

$$\frac{\partial \mathbf{C}}{\partial t} + \nabla.(\mathbf{vC}) = -\nabla.\mathbf{F} \qquad (3.7.37)$$

$$\mathbf{F} = -\mathbf{D} \cdot \nabla \mathbf{C} \qquad (3.7.38)$$

Where **C** is the vector of species "concentrations" and **D** <u>is the "multicomponent diffusion" matrix</u>

These are subject to

$$Initial\ Conditions: \qquad \Delta \underline{C}(x, y, z, t=0) = \Delta \underline{C}_0 \qquad (3.7.39)$$

$$\Delta \underline{C}(B, t) = 0 \qquad (3.7.40)$$

$$Boundary\ Conditions:$$

$$\frac{\partial \underline{C}}{\partial Z}(b, t) = 0 \qquad (3.7.41)$$

Where B and b represent boundaries of the system, ΔC is a concentration difference that generally varies with position and time.

Note: The boundary condition on all concentrations must have the same functional form for this analysis to be applicable. This may be a serious restriction where chemical reactions on boundaries take place.

Assume there exists a non-singular matrix $\underline{\underline{t}}$ which can diagonalize $\underline{\underline{D}}$, i.e

$$\underline{\underline{t}}^{-1}.\underline{\underline{D}}.\underline{\underline{t}} = \underline{\underline{\sigma}} = \begin{bmatrix} \sigma_1 & 0 & 0 & .... \\ 0 & \sigma_2 & 0 & .... \\ 0 & 0 & \sigma_3 & .... \\ .... & .... & .... & .... \end{bmatrix} \qquad (3.7.42)$$

Here $\underline{\underline{t}}^{-1}$ is the inverse of $\underline{\underline{t}}$, and $\underline{\underline{\sigma}}$ is the diagonal matrix of the eigenvalues of matrix $\underline{\underline{D}}$.

For a ternary mixture

$$\underline{\underline{t}} = \begin{bmatrix} t_{11} & t_{12} \\ t_{21} & t_{22} \end{bmatrix} = \frac{\begin{bmatrix} 1 & \dfrac{D_{12}}{D_{22}-\sigma_1} \\ \dfrac{D_{22}-\sigma_2}{D_{12}} & 1 \end{bmatrix}}{\det(\underline{\underline{t}})}$$

Note: find the components of $\underline{\underline{\sigma}}$ for a ternary mixture

Now, use matrix $\underline{\underline{t}}$ to define a new concentration $(\underline{\psi})$ variable, such that

$$\underline{C} = \underline{\underline{t}}.\underline{\psi} \qquad (3.7.43)$$

Combining (3.7.37), (3.7.38) and (3.7.43)

$$\frac{\partial \psi}{\partial t} + \nabla.\underline{v}\underline{\psi} = \underline{\underline{\sigma}}\nabla^2\underline{\underline{\psi}} \qquad (3.7.44)$$

Which represents a set of scalar equations

$$\frac{\partial \psi_i}{\partial t} + \nabla.\underline{v}\underline{\psi}_i = \sigma_i\nabla^2\underline{\underline{\psi}}_i \qquad (3.7.45)$$

Note: We have assumed that $\underline{\underline{D}}$ (hence both $\underline{\underline{t}}$ and $\underline{\underline{\sigma}}$) are not functions of composition.

Eqs. (3.7.39) – (3.7.41) can also be written in terms of $\underline{\psi}$.

$$\Delta\underline{\psi}(x,y,z,t=0)=\Delta\underline{\psi}_0=\underline{\underline{t}}^{-1}.\ \Delta\underline{C}_0 \qquad (3.7.46)$$

$$\Delta\underline{\psi}(B,t)=0 \qquad (3.7.47)$$

$$\frac{\partial\underline{\psi}}{\partial Z}(b,t)=0 \qquad (3.7.48)$$

This way, a set of <u>coupled</u> PDEs has been reduced to a set of <u>uncoupled</u> PDEs in terms of $\underline{\psi}$.

Eqs. (3.7.45) – (3.7.48) are of the same form as the associated <u>binary</u> diffusion problem.

$$\frac{\partial C_1}{\partial t}+\nabla.\underline{v}\,C_1=D\nabla^2 C_1$$

If this binary problem has the solution

$$\Delta C_1=G(D)\,\Delta C_{10}$$

Then eqs. (3.7.45) – (3.7.48) have the solution

$$\Delta\psi_i=G(\sigma_i)\Delta\psi_{i0}$$

Where the eigenvalue σ_i is substituted everywhere that the diffusivity occurring in the binary solution. In terms of the actual concentration,

$$\Delta \underline{C} = \underline{\underline{t}}.\underline{\underline{G}}(\underline{\underline{\sigma}}).\underline{\underline{t}}^{-1}.\,\Delta C_0 \qquad (3.7.49)$$