Module 9: Mass Transfer

Lecture 37: Diffusive Mass Transfer

The Lecture Contains:

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Mass Diffusion Coefficient

Considerable attention has been given to predicting the mass diffusion coefficient D_{AB} for the binary mixture of two gases **A and B**. Assuming ideal gas behaviour, kinetic theory may be used to show that.

$$D_{AB} = p^{-1}T^{3/2}$$

This relation applies for restricted pressure and temperature ranges and is useful for estimating values of the diffusion coefficient at conditions other than those for which data are available.

Conservation of species for a control volume

The rate at which the mass of some species enters a control volume minus the rate at which this species mass leaves the control volume must equal the rate at which the species mass stored in the control volume.

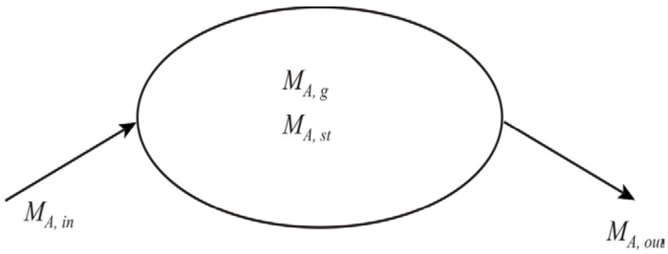

Figure 9.2 : Conservation of mass

$$\dot{M}_{A,in} + \dot{M}_{A,g} - \dot{M}_{A,out} = \frac{dM_A}{dt} = \dot{M}_{A,st} \quad \textbf{(9.22)}$$

Species generation exists when chemical reactions occur in the system.
There will be a net production of species **A** if a dissociation reaction of the form **AB** → **A + B** were occuring.

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Mass Diffusion Equation :-

We shall consider a homogeneous medium that is binary mixture of species A and B and that is stationary. The mass average or molar average velocity of the mixture is everywhere zero and mass transfer may occur only by diffusion. The resulting equation could be solved for the species concentration distribution, which could, in turn, be used with **Fick's** law to determine the species diffusion rate at any point in the medium.

We define a differential control volume **dx dy dz**, within the medium and then consider the processes that influence the distribution of species A. With the concentration gradients, diffusion must result in the transport of species A through the control surfaces. Moreover, relative to stationary coordinates, the species transport rates at opposite surfaces must be related by

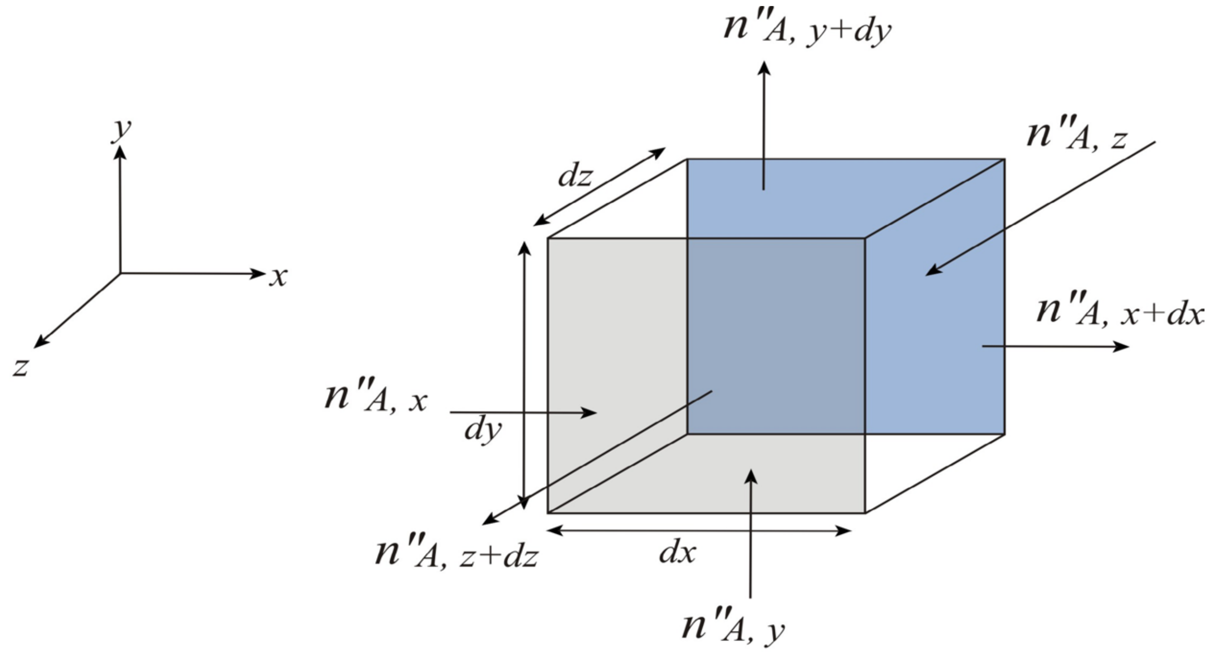

Figure 9.3 : Differential control volume dx; dy; dz for species diffusion analysis in cortisone coordinates

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$$n''_{A,x+dx} dz\ dy = n''_{A,x} dy\ dz + \frac{\partial [n''_{A,x} dy\ dz]}{\partial x} dx \quad \textbf{(9.23a)}$$

$$n''_{A,y+dy} dx\ dz = n''_{A,y} dx\ dz + \frac{\partial [n''_{A,y} dx\ dz]}{\partial y} dy \quad \textbf{(9.23b)}$$

$$n''_{A,z+dz} dx\ dy = n''_{A,z} dx\ dy + \frac{\partial [n''_{A,z} dx\ dy]}{\partial z} dz \quad \textbf{(9.23c)}$$

In addition, there may also be volumetric **(homogeneous)** chemical reactions throughout the medium. The rate at which species A is generated within the control volume due to such reactions may be expressed as

$$\dot{M}_{A,g} = \dot{n}_A\, dx\, dy\, dz \quad \textbf{(9.24)}$$

Where n''_A is the rate of increase of the mass of species A per unit volume of the mixture **(kg/sm3)**. Finally, these processes may change the mass of species A stored within the control volume **.**

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The rate of change is

$$\dot{M}_{A,st} = \frac{\partial \rho_A}{\partial t}\, dx\, dy\, dz \qquad (9.25)$$

With mass inflow rates determined by $n''_{A,x}$, $n''_{A,y}$ and $n''_{A,z}$ and the out flow rates determined by **(9.23), equations (9.23) to (9.25)** may be substituted in **(9.22)** to obtain.

$$-\frac{\partial n''_A}{\partial x} - \frac{\partial n''_A}{\partial y} - \frac{\partial n''_A}{\partial z} + \dot{n}_A = \frac{\partial \rho_A}{\partial t}$$

For a stationary medium, the mass average velocity **v** is zero, and from **equation (9.8)** it follows

that $n''_A = j_A$. Hence substituting the **x, y and z** components in the above equation, we get

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$$\frac{\partial}{\partial x}\left(\rho D_{AB}\frac{\partial m_A}{\partial x}\right)+\frac{\partial}{\partial y}\left(\rho D_{AB}\frac{\partial m_A}{\partial y}\right)+\frac{\partial}{\partial z}\left(\rho D_{AB}\frac{\partial m_A}{\partial z}\right)+\dot{n}_A=\frac{\partial \rho_A}{\partial t} \quad \textbf{(9.26)}$$

In terms of the molar concentration, a similar derivation yields **.**

$$\frac{\partial}{\partial x}\left(CD_{AB}\frac{\partial x_A}{\partial x}\right)+\frac{\partial}{\partial y}\left(CD_{AB}\frac{\partial x_A}{\partial y}\right)+\frac{\partial}{\partial z}\left(CD_{AB}\frac{\partial x_A}{\partial z}\right)+\dot{N}_A=\frac{\partial C_A}{\partial t} \quad \textbf{(9.27)}$$

If D_{AB} and ρ are constants:

$$\frac{\partial^2 \rho_A}{\partial x^2}+\frac{\partial^2 \rho_A}{\partial y^2}+\frac{\partial^2 \rho_A}{\partial z^2}+\frac{\dot{n}_A}{D_{AB}}=\frac{1}{D_{AB}}\frac{\partial \rho_A}{\partial t} \quad \textbf{(9.28)}$$

$$\frac{\partial^2 C_A}{\partial x^2}+\frac{\partial^2 C_A}{\partial y^2}+\frac{\partial^2 C_A}{\partial z^2}+\frac{\dot{N}_A}{D_{AB}}=\frac{1}{D_{AB}}\frac{\partial C_A}{\partial t} \quad \textbf{(9.29)}$$

The foregoing species diffusion equations may be expressed in **cylindrical and spherical coordinates**.

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