Radiation Heat Transfer

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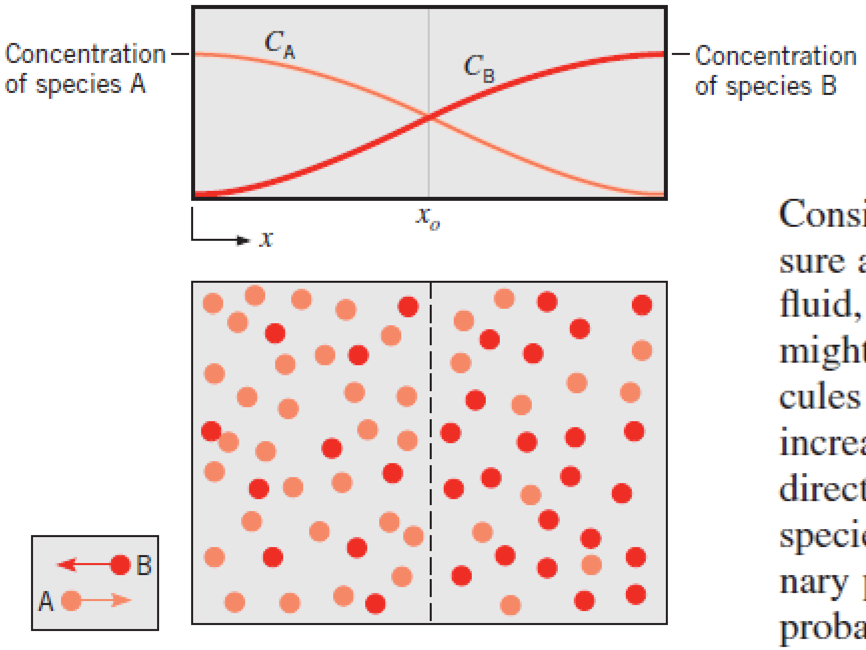
Lecture 7 Mass Transfer: Basic Concepts

Mass transfer is mass in transit as the result of a species concentration difference in a mixture.



Mass transfer by diffusion in a binary gas mixture.

Consider a chamber in which two different gas species at the same temperature and pressure are initially separated by a partition. If the partition is removed without disturbing the fluid, both species will be transported by diffusion. Figure shows the situation as it might exist shortly after removal of the partition. A higher concentration means more molecules per unit volume, and the concentration of species A (light dots) decreases with increasing x, while the concentration of B increases with x. Since mass diffusion is in the direction of decreasing concentration, there is net transport of species A to the right and of species B to the left. The physical mechanism may be explained by considering the imaginary plane shown as a dashed line at x_o. Since molecular motion is random, there is equal probability of any molecule moving to the left or the right. Accordingly, more molecules of species A cross the plane from the left (since this is the side of higher A concentration) than from the right. Similarly, the concentration of B molecules is higher to the right of the plane than to the left, and random motion provides for *net* transfer of species B to the left. Of course, after a sufficient time, uniform concentrations of A and B are achieved, and there is no *net* transport of species A or B across the imaginary plane.

Important parameters

A mixture consists of two or more chemical constituents (*species*), and the amount of any species i may be quantified in terms of its *mass density* ρ_i (kg/m^3) or its *molar concentration* C_i (kmol/m^3). The mass density and molar concentration are related through the species molecular weight, $\mathcal{M}_i$ (kg/kmol), such that

$$\rho_i = \mathcal{M}_i C_i \tag{1}$$

With ρ_i representing the mass of species i per unit volume of the mixture, the mixture mass density is

$$\rho = \sum_i \rho_i \tag{2}$$

Similarly, the total number of moles per unit volume of the mixture is

$$C = \sum_i C_i \tag{3}$$

The amount of species i in a mixture may also be quantified in terms of its *mass fraction*

$$m_i = \frac{\rho_i}{\rho} \tag{4}$$

or its *mole fraction*

$$x_i = \frac{C_i}{C} \tag{5}$$

From Equations 2 and 3, it follows that

$$\sum_i m_i = 1 \tag{6}$$

and

$$\sum_i x_i = 1 \tag{7}$$

For a mixture of ideal gases, the mass density and molar concentration of any constituent are related to the partial pressure of the constituent through the ideal gas law. That is,

$$\rho_i = \frac{p_i}{R_i T} \tag{8}$$

and

$$C_i = \frac{p_i}{\mathfrak{R} T} \tag{9}$$

where R_i is the gas constant for species i and $\mathfrak{R}$ is the universal gas constant. Using Equations 5 and 9 with *Dalton's law* of partial pressures,

$$p = \sum_i p_i \tag{10}$$

it follows that

$$x_i = \frac{C_i}{C} = \frac{p_i}{p} \tag{11}$$

Fick's Law of Diffusion

equation for mass diffusion is known as *Fick's law,* and for the transfer of species A in a *binary mixture* of A and B, it may be expressed in vector form as

$$\mathbf{j}_A = -\rho D_{AB} \nabla m_A \qquad (12)$$

or

$$\mathbf{J}_A^* = -C D_{AB} \nabla x_A \qquad (13)$$

The form of these expressions is similar to that of Fourier's law, as Fourier's law serves to define one important transport property, the thermal conductivity, Fick's law defines a second important transport property, namely, the *binary diffusion coeffi cient* or *mass diffusivity,* D_{AB}.

The quantity $\mathbf{j}_A$ (kg/s·m^2) is defined as the diffusive mass flux of species A. It is the amount of A that is transferred by diffusion per unit time and per unit area perpendicular to the direction of transfer, and it is proportional to the mixture mass density, $\rho = \rho_A + \rho_B$ (kg/m^3), and to the gradient in the species mass fraction, $m_A = \rho_A/\rho$. The species flux may also be evaluated on a molar basis, where $\mathbf{J}_A^*$ (kmol/s·m^2) is the diffusive molar flux of species A. It is proportional to the total molar concentration of the mixture, $C = C_A + C_B$ (kmol/m^3), and to the gradient in the species mole fraction, $x_A = C_A/C$. The foregoing forms of Fick's law may be simplified when the total mass density ρ or the total molar concentration C is a constant.

Absolute and Diffusive Species Fluxes

The absolute mass (or molar) flux of a species is defined as the total flux relative to a fixed coordinate system. To obtain an expression for the absolute mass flux, consider species A in a binary mixture of A and B. The absolute mass flux $\mathbf{n}''_A$ is related to the species absolute velocity $\mathbf{v}_A$ by

$$\mathbf{n}''_A \equiv \rho_A \mathbf{v}_A \tag{14}$$

$$\mathbf{n}''_B \equiv \rho_B \mathbf{v}_B \tag{15}$$

A *mass-average velocity for the mixture*

$$\left.\begin{aligned} &\rho \mathbf{v} = \mathbf{n}'' = \mathbf{n}''_A + \mathbf{n}''_B = \rho_A \mathbf{v}_A + \rho_B \mathbf{v}_B \\ &\text{giving} \\ &\mathbf{v} = m_A \mathbf{v}_A + m_B \mathbf{v}_B \end{aligned}\right\} \tag{16}$$

Note

It is important to note that we have defined the velocities ($\mathbf{v}_A$, $\mathbf{v}_B$, $\mathbf{v}$) and the fluxes ($\mathbf{n}''_A$, $\mathbf{n}''_B$, $\mathbf{n}''$) as *absolute* quantities. That is, they are referred to axes that are fixed in space. The mass-average velocity $\mathbf{v}$ is a useful parameter of the binary mixture, for two reasons. First, it need only be multiplied by the total mass density to obtain the total mass flux with respect to fixed axes. Second, it is the mass-average velocity which is required in the equations expressing conservation of mass, momentum, and energy

the *mass* flux *of species* A *relative to the mixture mass-average velocity* as $\mathbf{j}_A \equiv \rho_A(\mathbf{v}_A - \mathbf{v})$ (17)

Whereas $\mathbf{n}''_A$ is the *absolute* flux of species A, $\mathbf{j}_A$ is the *relative* or *diffusive* flux of the species and is the quantity previously given by Fick's law, Equation 12. It represents the motion of the species relative to the average motion of the mixture. It follows from Equations 14 and 17 that $\mathbf{n}''_A = \mathbf{j}_A + \rho_A \mathbf{v}$ (18)

Significance of equation 18

This expression delineates the two contributions to the absolute flux of species A: a contribution due to *diffusion* (i.e., due to the motion of A *relative* to the mass-average motion of the mixture) and a contribution due to *advection* (i.e., due to motion of A *with* the mass-average motion of the mixture).

Substituting we obtain $\mathbf{n}''_A = -\rho D_{AB}\nabla m_A + m_A(\mathbf{n}''_A + \mathbf{n}''_B)$ (19)

Question: Prove that $\mathbf{n}''_B = -\rho D_{AB}\nabla m_B + m_B(\mathbf{n}''_A + \mathbf{n}''_B)$

$\mathbf{j}_B \equiv \rho_B(\mathbf{v}_B - \mathbf{v})$ (20)

where $\mathbf{j}_B = -\rho D_{BA}\nabla m_B$

From eqs. (16), (17) and (20) $\Rightarrow$ $\mathbf{j}_A + \mathbf{j}_B = 0$

$\nabla m_A = -\nabla m_B$, since $m_A + m_B = 1$ for a binary mixture, it follows that $D_{BA} = D_{AB}$

Hence, $\mathbf{n}''_B = -\rho D_{AB}\nabla m_B + m_B(\mathbf{n}''_A + \mathbf{n}''_B)$

Assignment 1 Prove that $\mathbf{N}''_A = -CD_{AB}\nabla x_A + x_A(\mathbf{N}''_A + \mathbf{N}''_B)$ **and** $\boxed{\mathbf{J}^*_A + \mathbf{J}^*_B = 0}$

use

$\mathbf{N}''_A \equiv C_A\mathbf{v}_A$ and $\mathbf{N}''_B \equiv C_B\mathbf{v}_B$

$\mathbf{N}'' = \mathbf{N}''_A + \mathbf{N}''_B = C\mathbf{v}^* = C_A\mathbf{v}_A + C_B\mathbf{v}_B$

$\mathbf{v}^* = x_A\mathbf{v}_A + x_B\mathbf{v}_B$

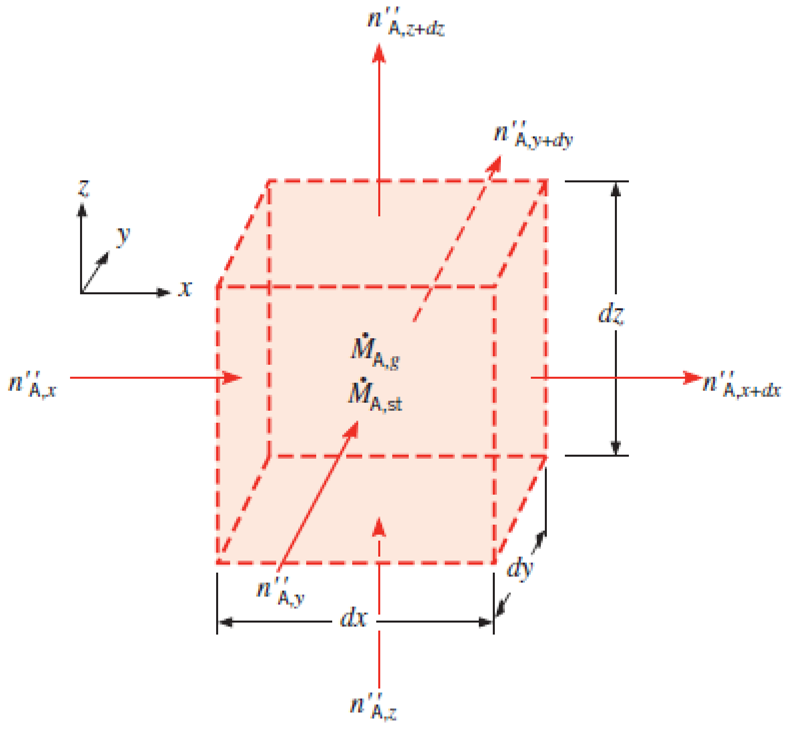
Conservation of Species for a Control Volume *for a Stationary Medium*

The rate at which the mass of some species enters a control volume, plus the rate at which the species mass is generated within the control volume, minus the rate at which this species mass leaves the control volume must equal the rate of increase of the species mass stored within the control volume.

For example, any species A may enter and leave the control volume due to both fluid motion and diffusion across the control surface; these processes are *surface* phenomena represented by $\dot{M}_{A,in}$ and $\dot{M}_{A,out}$. The same species A may also be generated, $\dot{M}_{A,g}$, and accumulated or stored, $\dot{M}_{A,st}$, *within* the control volume. The conservation equation may then be expressed on a rate basis as

$$\dot{M}_{A,in} + \dot{M}_{A,g} - \dot{M}_{A,out} = \frac{dM_A}{dt} \equiv \dot{M}_{A,st}$$

Species generation exists when chemical reactions occur in the system. For example, for a dissociation reaction of the form $AB \rightarrow A + B$, there would be net production of species A and B, as well as net reduction of the species AB.



Differential control volume, $dx\,dy\,dz$, for species diffusion analysis in Cartesian coordinates.

$$n''_{A,x+dx}\,dy\,dz = n''_{A,x}\,dy\,dz + \frac{\partial[n''_{A,x}\,dy\,dz]}{\partial x}dx$$

$$n''_{A,y+dy}\,dx\,dz = n''_{A,y}\,dx\,dz + \frac{\partial[n''_{A,y}\,dx\,dz]}{\partial y}dy$$

$$n''_{A,z+dz}\,dx\,dy = n''_{A,z}\,dx\,dy + \frac{\partial[n''_{A,z}\,dx\,dy]}{\partial z}dz$$

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

$$\dot{M}_{A,g} = \dot{n}_A \, dx \, dy \, dz$$

where $\dot{n}_A$ is the rate of increase of the mass of species A per unit volume of the mixture (kg/s·m^3). Finally, these processes may change the mass of species A stored within the control volume, and the rate of change is

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

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

we obtain

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

In terms of the molar concentration, a similar derivation yields

$$\frac{\partial}{\partial x}\left(C D_{AB} \frac{\partial x_A}{\partial x}\right) + \frac{\partial}{\partial y}\left(C D_{AB} \frac{\partial x_A}{\partial y}\right) + \frac{\partial}{\partial z}\left(C D_{AB} \frac{\partial x_A}{\partial z}\right) + \dot{N}_A = \frac{\partial C_A}{\partial t}$$

Assignment 2

Gaseous hydrogen is stored at elevated pressure in a rectangular container having steel walls 10 mm thick. The molar concentration of hydrogen in the steel at the inner surface is 1 $kmol/m^3$, while the concentration of hydrogen in the steel at the outer surface is negligible. The binary diffusion coefficient for hydrogen in steel is 0.26×10^{-12} m^2/s. What is the molar diffusive flux for hydrogen through the steel?

Thank you