Diffusion

1 Molecular Diffusion

Molecular diffusion, often simply called diffusion, is the process by which molecules move from an area of high concentration to an area of low concentration. It's a fundamental phenomenon in physics and chemistry, driven by the random thermal motion of molecules.

The rate at which diffusion occurs depends on several factors, including the concentration gradient (the difference in concentrations between two areas), the temperature (with higher temperatures leading to faster diffusion), the mass of the particles (with lighter particles diffusing more quickly), and the medium in which diffusion is taking place.

2 Heat Diffusion

Temperature represents the molecules' kinetic energy. During the molecular diffusion, molecules will exchange kinetic energy, which will cause different types of heat transfer.

1. **Heat Conduction:** If the thermally vibrating molecules pass their kinetic energy to adjacent molecules, we call the process "conduction".
2. **Heat Diffusion:** If the heat conduction is time dependent, we call the process "diffusion".
3. **Heat Advection:** If heat is physically transported by larger-sale motion of a solid or fluid, we call the process "advection".
4. **Heat Convention:** If the motion resulting in advection is driven by the distribution of heat, we call it "convection".

To quantify the heat transfer in molecular view, we use **Fouriers's Law**:

$$\rho\epsilon \underline{\boldsymbol{C}} = \underline{\boldsymbol{q}} = -k\nabla T \tag{1}$$

If assume 1D:

$$\rho\epsilon\bar{C}_k = q_k = -k\frac{dT}{dx} = \frac{k}{c_v}\frac{de}{dx} \tag{2}$$

Here:

1. $\rho\epsilon\bar{C}_k$ can be regarded as a moving mass $\rho\bar{C}_k$ carrying energy ϵ. Here $\bar{C}_k$ is mean velocity, with unit as m/s, and ϵ is specific energy, with unit as J/kg and ρ is the density, with unit as kg/m^3
2. q_k is defined as the heat flux, with the unit as $\frac{J}{m^2 \cdot s}$, interpreted as energy per area per second, which is the meaning of flux.
3. k is the **heat conductivity**, with the unit as $W/(m \cdot K)$.
4. e is the internal energy.

This equation can be approximated by mean free path λ:

$$\rho\epsilon\bar{C} \approx \frac{k}{c_v}\frac{\epsilon}{\lambda} \tag{3}$$

$$\frac{k}{\rho c_v} \propto \lambda\bar{C} \tag{4}$$

Normally we define **thermal diffusivity:**

$$\alpha = \frac{k}{\rho c_p} = \frac{k}{\rho\gamma c_v} \propto \lambda\bar{C} \tag{5}$$

Notice that the unit of α is m^2/s.

3 Mass Diffusion

Mass diffusion is a process that describes how particles move from regions of high concentration to regions of low concentration. This is due to the random motion of particles, also known as Brownian motion. Over time, this leads to a net flow of particles from high- to low-concentration areas until a state of equilibrium is reached where the concentration is uniform.

This process normally is quantified by **Fick's Law:**

$$\underline{\boldsymbol{J}} = -D\nabla\phi \tag{6}$$

If assume 1D:

$$J = -D\frac{d\phi}{dx} \tag{7}$$

Here:

1. $\underline{\boldsymbol{J}}$ is the diffusion flux, with the unit as $\frac{molec}{m^2 \cdot s}$, or simply is $\frac{1}{m^2 \cdot s}$
2. ϕ is the concentration, with the unit as $\frac{molec}{m^3}$, or simply as $\frac{1}{m^3}$
3. D is the diffusivity, with the unit as m^2/s

With some minor change, this can express the mass diffusion:

$$\rho \bar{C}_k = j_k = -D\frac{d\rho}{dx} \tag{8}$$

Here j_k is the mass flux, with unit as $\frac{kg}{m^2 \cdot s}$.
We can also approximate the distance by mean free path, then we get:

$$D \propto \lambda \bar{C} \tag{9}$$

4 Momentum Diffusion

Details could be found in **Viscous Flow Viscosity** chapter, for the Newtonian flow:

$$\rho \bar{C}_i \bar{C}_k = \tau_{ik} = \mu\frac{du_i}{dx_i} \tag{10}$$

Here:

1. τ_{ik} is the stress, with the unit as $\frac{N}{m^2}$ (**Same as pressure**). Notice that due to $F = ma$:

   $$N = kg \cdot \frac{m}{s^2} \tag{11}$$

   Recall that momentum can be expressed as:

   $$p = mv \tag{12}$$

   Therefore, the unit of momentum is $kg \cdot \frac{m}{s}$. Based on this, we can interpret stress as the **momentum flux**:

   $$\frac{N}{m^2} = (kg \cdot m/s) \cdot \frac{1}{m^2 \cdot s} \tag{13}$$

2. μ is the dynamic viscosity, with the unit as $\frac{kg}{m \cdot s}$

3. u_i is the velocity, with the unit as m/s

Rearrange the equation and approximate the distance by mean free path:

$$\frac{\mu}{\rho} = \nu \propto \lambda \bar{C} \tag{14}$$

Here ν is the kinematic viscosity, or we can call it momentum diffusivity, with the unit as m^2/s.

5 Diffusion Scaling

Recall the last three sections, summarize:

1. **Mass Diffusivity:** D, gradient in mass of species i
2. **Thermal Diffusivity:** α, gradient in temperature
3. **Momentum Diffusivity:** ν, gradient in velocity

All of them are proportional to $\lambda\bar{C}$. Based on kinetic theory:

$$\lambda = \frac{1}{\sqrt{2}n\sigma} \tag{15}$$

$$\bar{C} = \sqrt{8k_BT/\pi m} \tag{16}$$

Therefore:

$$\lambda\bar{C} \propto \frac{\sqrt{T}}{\rho} \tag{17}$$

6 Dimensionless Ratio

1. **Prandtl Number:**
$$Pr = \frac{\nu}{\alpha} \tag{18}$$
2. **Schmidt Number:**
$$Sc = \frac{\nu}{D} \tag{19}$$
3. **Lewis Number:**
$$Le = \frac{\alpha}{D} \tag{20}$$

7 Other Driving Forces

1. **Soret Effect:** Large gradients in temperature can result in mass diffusion since light molecules diffuse from low to high-temperature regions, and heavy molecules diffuse from high to low-temperature.
2. **Dufour Effect:** Based on **Onsagers Reciprocal Relations**, if Soret effect occurs, concentration gradients must produce a heat flux.