Exercise 5

Derive the equation of one-dimensional diffusion in a medium that is moving along the x axis to the right at constant speed V.

Solution

There are two ways (among others) to go about this problem. One is the integral formulation, where we consider the mass flowing into and out of a fixed finite volume known as a control volume. The other is the differential formulation, where we consider the mass flowing into and out of a fixed infinitesimal volume element. In both cases we come to the same governing PDE, so use whichever you prefer.

There are two fluxes to consider in this exercise: the one due to diffusion (the random motion of fluid molecules) and the one due to advection (the bulk fluid motion). To find the governing PDE for the concentration we have to invoke the law of conservation of mass, which says that mass can neither be created nor destroyed. If there's a certain amount of mass entering a control volume and there's less mass coming out of it, then there must be mass accumulating within it. Mathematically this is expressed as

$$\frac{dm}{dt} = \text{rate of mass in} - \text{rate of mass out}, \tag{1}$$

where m denotes the amount of mass and dm/dt represents how fast mass is accumulating. The mass flux is defined as the amount of mass flowing axially per unit time per unit area. Therefore, if we multiply the mass flux by the area of the control volume's cross section, we get the rate of mass that is flowing through it.

The mass flux due to diffusion ϕ is given by Fick's first law, which states it is proportional to the concentration gradient. The concentration is defined as mass per unit volume. Let $u(x,t)$ represent it.

$$\phi \propto \frac{\partial u}{\partial x}$$

To change this to an equation we can use, we introduce a constant of proportionality k, which is known as the chemical diffusivity.

$$\phi = -k\frac{\partial u}{\partial x} \tag{2}$$

The minus sign is present to account for the fact that mass flows down a concentration gradient; that is, it diffuses from areas of high concentration to ones of low concentration.

The mass flux due to advection ψ is obtained simply by multiplying the concentration u by the speed V that the mass travels per unit time. This is apparent if we look at the units.

$$[V][u] = \left[\frac{\text{meter}}{\text{second}}\right]\left[\frac{\text{kilogram}}{\text{meter}^3}\right] = \left[\frac{\text{kilogram}}{\text{second} \cdot \text{meter}^2}\right]$$

We end up with units of mass per unit time per unit area, which are the units of mass flux. Thus,

$$\psi = Vu. \tag{3}$$

The Integral Formulation

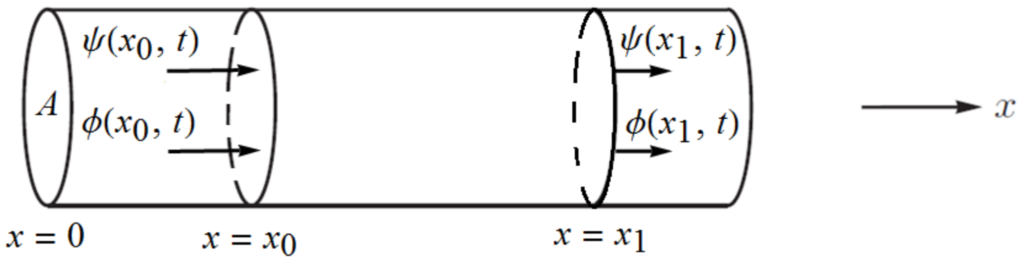

Figure 1: Schematic of the control volume (integral formulation).

If we consider the control volume between $x = x_0$ and $x = x_1$ as shown in Figure 1, mass is flowing by diffusion into it at $x = x_0$ and out of it at $x = x_1$, as indicated by the arrows.

$$\begin{aligned} \text{Rate of mass flow in:} &\quad \phi(x_0, t)A \\ \text{Rate of mass flow out:} &\quad \phi(x_1, t)A \end{aligned}$$

These are the rates due to diffusion. The bulk fluid motion is causing the particles to move from left to right with speed V, so mass flows by advection into the control volume at $x = x_0$ and out of it at $x = x_1$, as indicated by the arrows.

$$\begin{aligned} \text{Rate of mass flow in:} &\quad \psi(x_0, t)A \\ \text{Rate of mass flow out:} &\quad \psi(x_1, t)A \end{aligned}$$

These are the rates due to advection. Substituting these results into the law of conservation of mass (1), we get

$$\frac{dm}{dt} = \phi(x_0, t)A + \psi(x_0, t)A - \phi(x_1, t)A - \psi(x_1, t)A.$$

Divide both sides by A and group similar terms together on the right side.

$$\frac{d}{dt}\left(\frac{m}{A}\right) = -[\phi(x_1, t) - \phi(x_0, t)] - [\psi(x_1, t) - \psi(x_0, t)]$$

Volume can be used on the bottom as long as we integrate over the length of the control volume.

$$\frac{d}{dt}\int_{x_0}^{x_1}\left(\frac{m}{V}\right) dx = -[\phi(x_1, t) - \phi(x_0, t)] - [\psi(x_1, t) - \psi(x_0, t)]$$

According to the fundamental theorem of calculus,

$$\int_a^b f(x)\, dx = F(b) - F(a),$$

so we can write the two expressions in square brackets as

$$\begin{aligned} \phi(x_1, t) - \phi(x_0, t) &= \int_{x_0}^{x_1} \frac{\partial}{\partial x}[\phi(x, t)]\, dx \\ \psi(x_1, t) - \psi(x_0, t) &= \int_{x_0}^{x_1} \frac{\partial}{\partial x}[\psi(x, t)]\, dx. \end{aligned}$$

Plugging in these results and u for m/V, the equation becomes

$$\frac{d}{dt}\int_{x_0}^{x_1} u\,dx = -\int_{x_0}^{x_1} \frac{\partial}{\partial x}[\phi(x,t)]\,dx - \int_{x_0}^{x_1} \frac{\partial}{\partial x}[\psi(x,t)]\,dx.$$

Bring the t-derivative inside the integral on the left side and combine the two integrals on the right side.

$$\int_{x_0}^{x_1} \frac{\partial u}{\partial t}\,dx = \int_{x_0}^{x_1} \left(-\frac{\partial \phi}{\partial x} - \frac{\partial \psi}{\partial x}\right) dx$$

Hence, the integrands must be equal.

$$\frac{\partial u}{\partial t} = -\frac{\partial \phi}{\partial x} - \frac{\partial \psi}{\partial x}$$

Plugging in (2) for ϕ and (3) for ψ gives us

$$\frac{\partial u}{\partial t} = -\frac{\partial}{\partial x}\left(-k\frac{\partial u}{\partial x}\right) - \frac{\partial}{\partial x}(Vu).$$

Therefore,

$$\frac{\partial u}{\partial t} = k\frac{\partial^2 u}{\partial x^2} - V\frac{\partial u}{\partial x}.$$

The Differential Formulation

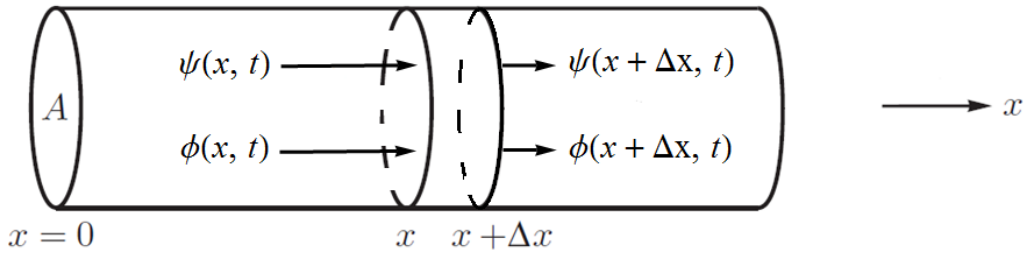

Figure 2: Schematic of the control volume (differential formulation).

If we consider the control volume between x and $x + \Delta x$ as shown in Figure 1, mass is flowing by diffusion into the portion at x and out of it at $x + \Delta x$, as indicated by the arrows.

$$\begin{aligned} \text{Rate of mass flow in:} &\quad \phi(x,t)A \\ \text{Rate of mass flow out:} &\quad \phi(x+\Delta x,t)A \end{aligned}$$

These are the rates due to diffusion. The bulk fluid motion is causing the particles to move from left to right with speed V, so mass flows by advection into the control volume at x and out of it at $x + \Delta x$, as indicated by the arrows.

$$\begin{aligned} \text{Rate of mass flow in:} &\quad \psi(x,t)A \\ \text{Rate of mass flow out:} &\quad \psi(x+\Delta x,t)A \end{aligned}$$

These are the rates due to advection. Substituting these results into the law of conservation of mass (1), we get

$$\frac{dm}{dt} = \phi(x,t)A + \psi(x,t)A - \phi(x+\Delta x,t)A - \psi(x+\Delta x,t)A.$$

Divide both sides by A and group similar terms together on the right side.

$$\frac{d}{dt}\left(\frac{m}{A}\right) = -[\phi(x+\Delta x,t) - \phi(x,t)] - [\psi(x+\Delta x,t) - \psi(x,t)]$$

The volume of the control volume is $V = A\,\Delta x$, so we have

$$\frac{d}{dt}\left(\frac{m}{V}\right)\Delta x = -[\phi(x+\Delta x,t) - \phi(x,t)] - [\psi(x+\Delta x,t) - \psi(x,t)]$$

Divide both sides by Δx and recall that m/V is the concentration u.

$$\frac{\partial u}{\partial t} = -\frac{\phi(x+\Delta x,t) - \phi(x,t)}{\Delta x} - \frac{\psi(x+\Delta x,t) - \psi(x,t)}{\Delta x}$$

Now let $\Delta x \to 0$.

$$\frac{\partial u}{\partial t} = -\lim_{\Delta x\to 0}\frac{\phi(x+\Delta x,t) - \phi(x,t)}{\Delta x} - \lim_{\Delta x\to 0}\frac{\psi(x+\Delta x,t) - \psi(x,t)}{\Delta x}$$

The first derivative is defined as

$$\frac{df}{dx} = \lim_{h\to 0} \frac{f(x+h) - f(x)}{h},$$

so we can write the two limits as

$$\lim_{\Delta x\to 0} \frac{\phi(x+\Delta x, t) - \phi(x,t)}{\Delta x} = \frac{\partial}{\partial x}[\phi(x,t)]$$
$$\lim_{\Delta x\to 0} \frac{\psi(x+\Delta x, t) - \psi(x,t)}{\Delta x} = \frac{\partial}{\partial x}[\psi(x,t)].$$

The equation becomes

$$\frac{\partial u}{\partial t} = -\frac{\partial \phi}{\partial x} - \frac{\partial \psi}{\partial x}.$$

Plugging in (2) for ϕ and (3) for ψ gives us

$$\frac{\partial u}{\partial t} = -\frac{\partial}{\partial x}\left(-k\frac{\partial u}{\partial x}\right) - \frac{\partial}{\partial x}(Vu).$$

Therefore,

$$\frac{\partial u}{\partial t} = k\frac{\partial^2 u}{\partial x^2} - V\frac{\partial u}{\partial x}.$$