Exercise 1.2.4

Derive the diffusion equation for a chemical pollutant.

(a) Consider the total amount of the chemical in a thin region between x and $x + \Delta x$.

(b) Consider the total amount of the chemical between $x = a$ and $x = b$.

Solution

Part (a)

The law of conservation of mass states that matter is neither created nor destroyed. If some amount of pollutant enters the left side of a shell at x, then that same amount must exit the right side of it at $x + \Delta x$, assuming it all flows through. If the pollutant enters at x faster (slower) than it leaves at $x + \Delta x$, then it will accumulate (diminish) within the shell. The mathematical expression for this idea, a mass balance, is as follows.

$$\text{rate of pollutant in} - \text{rate of pollutant out} = \text{rate of pollutant accumulation}$$

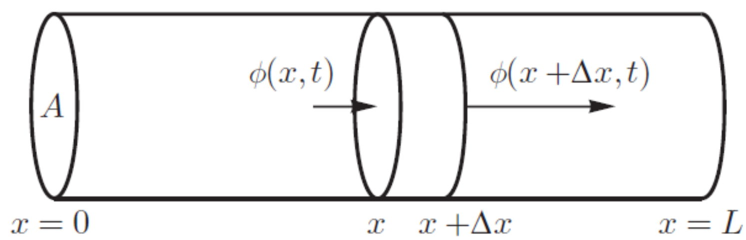

Figure 1: This is a schematic of the shell that the pollutant flows through (differential formulation).

The flux is defined to be the rate that the pollutant flows through the shell per unit area, and we denote it by $\phi = \phi(x, t)$. If we let m represent the mass of pollutant in the shell, then the mass balance over it is

$$A\phi(x,t) - A\phi(x + \Delta x, t) = \left.\frac{dm}{dt}\right|_{\text{shell}}.$$

Factor $-A$ from the left side.

$$-A[\phi(x + \Delta x, t) - \phi(x,t)] = \left.\frac{dm}{dt}\right|_{\text{shell}}$$

The mass of pollutant is equal to the concentration $u(x,t)$ times the volume ΔV of the shell.

$$-A[\phi(x + \Delta x, t) - \phi(x,t)] = \frac{\partial(u\Delta V)}{\partial t}$$

The volume of the shell is $\Delta V = A\Delta x$, a constant.

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

Divide both sides by $A\Delta x$.

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

Now take the limit as $\Delta x \to 0$.

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

The left side is how the negative of the first derivative of ϕ with respect to x is defined.

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

According to Fick's law of diffusion, the mass flux is proportional to the concentration gradient.

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

where k is a proportionality constant known as the chemical diffusivity. As a result, the mass balance becomes an equation solely for the concentration.

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

Therefore, the equation for the concentration of pollutant is the one-dimensional diffusion equation.

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

Part (b)

The law of conservation of mass states that matter is neither created nor destroyed. If some amount of pollutant enters the left side of a pipe at $x=a$, then that same amount must exit the right side of it at $x=b$, assuming it all flows through. If the pollutant enters at $x=a$ faster (slower) than it leaves at $x=b$, then it will accumulate (diminish) within the pipe. The mathematical expression for this idea, a mass balance, is as follows.

$$\text{rate of pollutant in} - \text{rate of pollutant out} = \text{rate of pollutant accumulation}$$

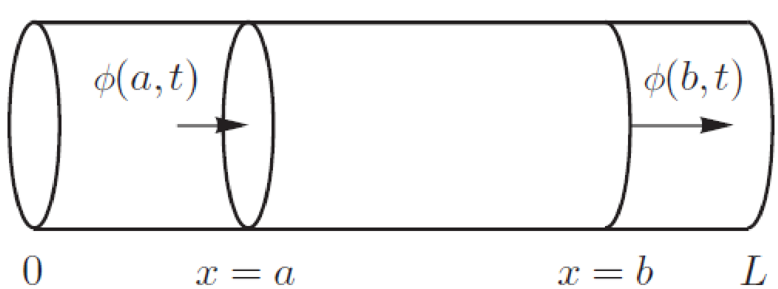

Figure 2: This is a schematic of the pipe that the pollutant flows through (integral formulation).

The flux is defined to be the rate that the pollutant flows through the pipe per unit area, and we denote it by $\phi = \phi(x,t)$. If we let m represent the mass of pollutant in the pipe, then the mass balance over it becomes

$$A\phi(a,t) - A\phi(b,t) = \left.\frac{dm}{dt}\right|_{\text{pipe}}.$$

Factor $-A$ from the left side.

$$-A[\phi(b,t) - \phi(a,t)] = \left.\frac{dm}{dt}\right|_{\text{pipe}}$$

By the fundamental theorem of calculus, the term in square brackets is an integral.

$$-A\int_a^b \frac{\partial \phi}{\partial x}\,dx = \left.\frac{dm}{dt}\right|_{\text{pipe}}$$

The mass of pollutant is obtained by integrating the concentration $u(x,t)$ over the volume of the pipe.

$$-A\int_a^b \frac{\partial \phi}{\partial x}\,dx = \frac{d}{dt}\int_{\text{pipe}} u(x,t)\,dV$$

The volume differential is $dV = A\,dx$.

$$-A\int_a^b \frac{\partial \phi}{\partial x}\,dx = \frac{d}{dt}\int_a^b u(x,t)A\,dx$$

Divide both sides by A and bring the minus sign and derivative inside the integrals.

$$\int_a^b \left(-\frac{\partial \phi}{\partial x}\right)dx = \int_a^b \frac{\partial u}{\partial t}\,dx$$

The integrands must be equal to one another.

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

According to Fick's law of diffusion, the mass flux is proportional to the concentration gradient.

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

where k is a proportionality constant known as the chemical diffusivity. As a result, the mass balance becomes an equation solely for the concentration.

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

Therefore, the equation for the concentration of pollutant is the one-dimensional diffusion equation.

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