Exercise 1.2.5

Derive an equation for the concentration $u(x,t)$ of a chemical pollutant if the chemical is produced due to chemical reaction at the rate of $\alpha u(\beta - u)$ per unit volume.

Solution

The Differential Formulation

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.

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

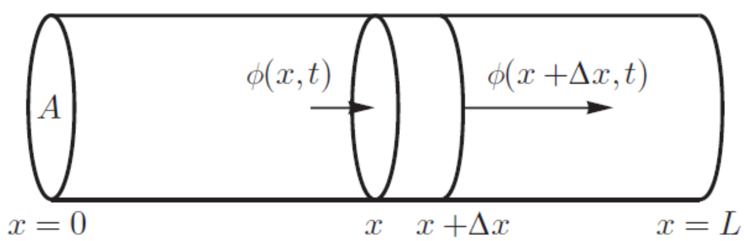

Figure 1: This is a schematic of the shell that the pollutant flows through (differential formulation).

The production of pollutant due to chemical reaction will be included on the left side as one of the terms for "rate of pollutant in." Since $\alpha u(\beta - u)$ is the rate per unit volume, it will be multiplied by the volume $V = A\Delta x$ of the shell. 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

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

Factor $-A$ from the terms containing ϕ on the left side.

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

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

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

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

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

Divide both sides by $A\Delta x$.

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

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

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

The second term on the left is how the first derivative of ϕ with respect to x is defined.

$$\alpha u(\beta - u) - \frac{\partial \phi}{\partial x} = \frac{\partial u}{\partial t}$$

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.

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

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

$$\frac{\partial u}{\partial t} = k\frac{\partial^2 u}{\partial x^2} + \alpha u(\beta - u)$$

The Integral Formulation

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.

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

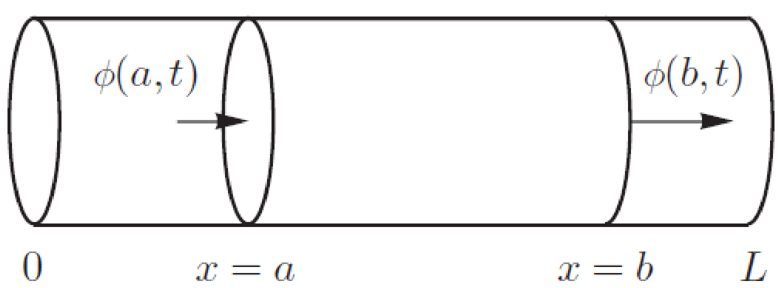

Figure 2: This is a schematic of the pipe that the pollutant flows through (integral formulation).

The production of pollutant due to chemical reaction will be included on the left side as one of the terms for "rate of pollutant in." Since $\alpha u(\beta - u)$ is the rate per unit volume, it will be integrated over the volume of the pipe. 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 pipe, then the mass balance over it is

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

Factor $-A$ from the two terms containing ϕ.

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

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

$$\int_{\text{pipe}} \alpha u(\beta - u)\,dV - A\int_a^b \frac{\partial \phi}{\partial x}\,dx = \left.\frac{dm}{dt}\right|_{\text{pipe}}$$

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

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

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

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

Divide both sides by A, combine the two integrals on the left into one, and bring the derivative inside the integral on the right side.

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

The integrands must be equal to one another.

$$\alpha u(\beta - u) - \frac{\partial \phi}{\partial x} = \frac{\partial u}{\partial t}$$

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.

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

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

$$\frac{\partial u}{\partial t} = k\frac{\partial^2 u}{\partial x^2} + \alpha u(\beta - u)$$