# 10. The diffusion equation

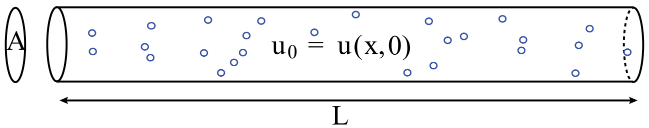
The equation

$$\frac{\partial u}{\partial t} = \alpha \frac{\partial^2 u}{\partial x^2}, \qquad 0 < x < L,\ t > 0 \tag{3.52}$$

was first introduced as a partial differential equation that describes the flow of heat in a rod. This equation can be used to model much more than heat flow, however, and appears across many fields in science and engineering. In the most general sense, equations of the above form are known as **Diffusion Equations.**

Diffusion Equations are used to model the “spreading out" of chemical species, biological cells, fluid vortices, and even people in a crowd. This all comes from the fact that the assumptions made when deriving the equation for heat are actual very simple assumptions based on the conservation of some quantity and the desire of that quantity to spread out in a simply way. We'll go through a problem that models the spreading of some chemical molecule along the length of a pipe. Such a model would be useful when designing a chemical reactor, an industrial device for synthesizing important chemicals from other more available inputs.

**The physics for modeling concentrations in mixtures.**



Imagine a pipe filled with carbonated water. In this fluid, the carbon dioxide, or $\mathrm{CO_2}$, has a concentration which varies along the length of the pipe. (Assume the length of the pipe is very large compared to its diameter; this lets us ignore the variations in concentration in the radial direction of the pipe.) The $\mathrm{CO_2}$ will "diffuse" through the pipe as it randomly moves about, tending to spread out from areas of high concentration to low concentration. We'll list some of the important quantities for the model below. Note the similarities to the model used for heat transfer in a rod:

| | |
|---|---|
| $L$ | length of the pipe |
| $A$ | cross sectional area of the inside of the pipe |
| $u_0$ | initial concentration of $\mathrm{CO_2}$ in the pipe |
| $t$ | time |
| $x$ | position along the length of the pipe |
| $u$ | the concentration of $\mathrm{CO_2}$ at a given point in the pipe at a given time, in terms of mass |
| $q$ | $\mathrm{CO_2}$ mass flux at a given point in the pipe at a given time |

Note that these variables are all directly analogous to those used in the heat formulation. In addition, we have 2 basic laws that guide us with the model.

1. **Conservation of Mass** The total amount of carbon dioxide in the pipe is fixed–none is leaving or being created. This means that if the mass is changing in any small segment of pipe, this must occur because $\mathrm{CO_2}$ is flowing into or out of the region.

2. **Fick's Law of Mass Transfer** The idea is that $\mathrm{CO_2}$ moves from regions of high concentration to regions of low concentration.

The equations that describe these two laws combine together (see below) to form the diffusion equation for concentration transfer:

$$\frac{\partial u}{\partial t} = \alpha \frac{\partial^2 u}{\partial x^2}. \tag{3.53}$$

**Putting it together to get the diffusion equation**

1. **Conservation of Mass:** The change in the total mass of chemical in any region equals the net mass flowing into or out of that region. (We assume that no $\mathrm{CO_2}$ being created through reactions—like active yeast cultures which produce $\mathrm{CO_2}$ in beer.)

   Concentration $u$ is a density, and therefore the units are $\mathrm{mass}/\mathrm{volume}$, which is equivalent to $\mathrm{mass}/\mathrm{length}^3$. Consider a small slice of pipe with cross sectional area $A$ and length $\Delta x$. The volume of this slice is $A\Delta x$, and the mass of $\mathrm{CO_2}$ inside is approximately $u\left(x\right)A\Delta x$.

   How does this mass change in a small amount of time $\Delta t$? The only way for the mass to change in our small volume is by diffusing in through either of the two ends. The diffusion through either end is called flux. Flux, in this case $\mathrm{CO_2}$ flux density, has units of $\mathrm{mass}/\left[\mathrm{time}\cdot\mathrm{length}^2\right]$. We can write the change in the $\mathrm{CO_2}$ mass in a small volume $A\Delta x$ that occurs in a short time $\Delta t$ as

   $$\left(u\left(x,t+\Delta t\right)-u\left(x,t\right)\right)A\Delta x = A\Delta t\left(q\left(x,t\right)-q\left(x+\Delta x,t\right)\right) \tag{3.54}$$

   The sign on the $q\left(x+\Delta x,t\right)$ term is negative because $Aq\left(x+\Delta x,t\right)\Delta t$ is the $\mathrm{CO_2}$ mass passing to the right, out of the small $\Delta x$ length over a small time interval $\Delta t$, while the flux on the left side is bringing new mass in. Note that Dividing by $\Delta t$ and $\Delta x$ we get

   $$A\frac{u\left(x,t+\Delta t\right)-u\left(x,t\right)}{\Delta t} = -A\frac{q\left(x+\Delta x,t\right)-q\left(x,t\right)}{\Delta x} \tag{3.55}$$

   We can take the limit as both $\Delta x$ and $\Delta t$ go to zero and divide through by $A$ to get a relationship between the change in concentration and the change in flux:

   $$\frac{\partial u}{\partial t} = -\frac{\partial q}{\partial x}. \tag{3.56}$$

2. **Fick's Law of Mass Transfer:** Analogous to Fourier's law of heat transfer, Fick's law of Mass transfer says that the flux between two points is proportional to the difference in concentration between the two points, with the appropriate sign so that the flow is from higher to lower concentration. We also note that it states that the flow between two points is inversely proportional to the distance between the

points. This makes intuitive sense, as a small difference in concentration is more likely to generate a greater flux when the difference is over a short distance compared to a longer one. If we imagine two points along our pipe, $x$ and $x + \Delta x$, then the $\mathrm{CO_2}$ concentration at these points will be $u\left(x, t\right)$ and $u\left(x + \Delta x, t\right)$, respectively. We can write Fick's Law of Mass Transfer as

$$q \propto -\frac{\partial u}{\partial x} \tag{3.57}$$

We can make this an equality by adding the "Diffusion Constant" $\alpha > 0$.

$$q = -\alpha \frac{\partial u}{\partial x} \tag{3.58}$$

Why is there a negative sign on the right of the expression above? We want $q$ to be positive whenever we have a flux to the right, which means that $u\left(x + \Delta x, t\right) < u\left(x, t\right)$ (and we assume $\Delta x > 0$).Thus we have a negative sign in the above relation.

With the above two laws each giving an equation in terms of $q$ and $u$, we can plug the second equation into the first to get a partial differential equation for just $u$ as

$$\frac{\partial u}{\partial t} = \frac{\partial}{\partial x}\left(\alpha \frac{\partial u}{\partial x}\right) \tag{3.59}$$

In the simplest cases, $\alpha$ will be a constant, which simplifies the above equation to the most familiar form of the Diffusion Equation:

$$\frac{\partial u}{\partial t} = \alpha \frac{\partial^2 u}{\partial x^2} \tag{3.60}$$

**Note:** In some cases, $\alpha$ may vary with $x$ (such as a non-homogenous material where it is easier for cells to move in one region vs. another) and this changes the form of the equation. We will just assume $\alpha$ is a constant, and thus get the familiar Diffusion Equation.

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