Flux Notes

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There are two common usages of the word "flux" in science: (1) the flow vector field for the transport of some substance across a surface measuring the amount of stuff flowing across a small piece of surface in a small time including the direction of the flow and (2) the amount per time of the transport of some substance across a surface. The units for the flux in usage (1) are the amount of stuff per area per time and the units for flux in usage (2) are amount per time.

Typical type-1 fluxes are

$$\text{diffusion flux } \frac{\text{mol}}{\text{m}^2\text{s}}, \quad \text{volume flux } \frac{\text{m}^3}{\text{m}^2\text{s}}, \quad \text{and mass flux } \frac{\text{kg}}{\text{m}^2\text{s}};$$

they correspond to the type-2 fluxes

$$\frac{\text{mol}}{\text{s}}, \quad \frac{\text{m}^3}{\text{s}}, \quad \frac{kg}{s}.$$

What are typical type-1 fluxes? Fluxes are ubiquitous in science. While an exact description of the movement of substances across surfaces is not known, useful approximations (which yield excellent results in many cases) are obtained from the simple principle that stuff usually flows from regions of high concentration toward regions of low concentration. This is the content of Fick's law (Adolf Fick 1855) for molecular diffusion, Fourier's law (Joseph Fourier 1822) of heat diffusion, and Darcy's law (Henry Darcy 1856) for flow through porous media. The stuff for Fick is molecules, for Fourier heat, and for Darcy fluid. Mathematically, the flow from higher to lower concentration

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is given by the gradient. For example, imagine a substance distributed in one direction with coordinate x. You might imagine that the substance has the same concentration in the plane perpendicular to the given direction. Let the concentration of the substance at position x and time t be $C(x,t)$. Fick's law says the flux vector is proportional to the spatial derivative of C; or, more precisely,

$$X = -\lambda\frac{\partial C}{\partial x},$$

where the positive number λ (called the diffusivity) is measured in square meters per second. The negative sign is there to ensure that X points in the direction of lower concentration. If the concentration increases with x, the derivative is positive and X is negative; if the concentration decreases X is positive.

Suppose the concentration of some substance is distributed in a round pipe with radius a and length L whose central axis is our line with coordinate x on the interval $(0, L)$. For example, suppose the concentration in the cross section at x is $C(x,t) = c(x/L)^2/2$ moles per cubic meter in a medium whose diffusivity is λ square meters per second. The corresponding flux field is

$$X(x,t) = -\frac{\lambda c}{L}\Big(\frac{x}{L}\Big),$$

measured in moles per square meter per second. Note that c has units moles per cubic meter.

How much of the substance is crossing the cross section of the pipe at position x? Answer:

$$\frac{\pi a^2 \lambda c x}{L}$$

moles per second in the negative direction of the coordinate axes. A typical diffusivity is $\lambda = 10^{-10}$ square meters per second.

In many instances we don't know the concentration in the pipe. Perhaps we know the concentrations at the ends of the pipe, and we wish to know the concentration profile inside the pipe.

What is a good candidate for a law that tells us the concentration changes in space and time. The units for the change in concentration per time $\partial C/\partial t$ are amount per volume per time. This should be related to the flux, which is given in amount per area per time. To match these units, we must either multiply the rate of change of concentration by a length or divide the flux by a length. We might imagine many different ways to do this. The correct

way is to differentiate the flux with respect to length and change the sign to get

$$\frac{\partial C}{\partial t} = \lambda \frac{\partial^2 C}{\partial x^2}.$$

At least the units are correct. Why should this equation be the correct model for the diffusion of our substance?

Let's consider an subinterval $[\beta, \gamma]$ on our line. Imagine the distribution of our substance in the pipe along this interval. The total amount of stuff in the pipe over the interval is obtained by adding up the stuff in each slice. How do we do this? We break up the interval into small subintervals and pick a point in each subinterval where the concentration at the chosen point is representative of the concentration along the entire subinterval. Over this subinterval, the amount of stuff in the pipe is πa^2 times the length of the subinterval multiplied by the concentration at the representative point. We add all these products together to approximate the amount of stuff over the entire interval.

Does this prescription remind you of a mathematical concept? It should! Indeed, the mathematical representation of this process is the definite integral of the amount of stuff over the interval; that is,

$$\int_{\beta}^{\gamma} \pi a^2 C(x, t) \, dx.$$

How does the total amount of stuff in the interval change with time; or equivalently, what is

$$\frac{d}{dt} \int_{\beta}^{\gamma} \pi a^2 C(x, t) \, dx \, ?$$

The rate of change in the amount of stuff (assuming that none of the stuff is created or destroyed in the portion of the pipe over the interval $[\beta, \gamma]$) is the rate of stuff going in minus the rate going out of the cylinder over the interval. The only place for stuff to go in or out is through the cross sections at the ends of the interval. Under our assumption that the concentration does not change on a cross section, the amount of stuff per time crossing the section at β should be the flux times the area $-\lambda \pi a^2 C(\beta, t)$. We have to be careful about the sign. Which way does the stuff cross this boundary? Suppose the concentration is higher outside the the cylinder under consideration than inside. At both boundaries (at β and γ) stuff is flowing into the cylinder over $[\beta, \gamma]$. The rate of change of the concentration with respect to position

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is negative at β and positive at γ. We want a positive contribution to the rate of change of the amount of stuff at both ends. Thus, the sign of the flux over the boundary has to be positive at both ends. This means the rate in minus the rate out is

$$-\lambda \pi a^2 \frac{\partial C}{\partial x}(\beta, t) + \lambda \pi a^2 \frac{\partial C}{\partial x}(\gamma, t).$$

Thus, we have

$$\int_\beta^\gamma \pi a^2 C(x, t)\, dx = \lambda \pi a^2 \frac{\partial C}{\partial x}(\gamma, t) - \lambda \pi a^2 \frac{\partial C}{\partial x}(\beta, t),$$

where the right-hand side is a type-2 flux. Does this right-hand side remind you of something from calculus? It should! The right-hand side is in the form $f(\gamma) - f(\beta)$. Using the Fundamental Theorem of Calculus, we may recast the equality in the form

$$\pi a^2 \frac{d}{dt} \int_\beta^\gamma C(x, t)\, dx = \pi a^2 \lambda \int_\beta^\gamma \frac{\partial^2 C}{\partial x^2}(x, t)\, dx.$$

Or, equivalently, we have

$$\int_\beta^\gamma \frac{\partial C}{\partial t}(x, t)\, dx = \lambda \int_\beta^\gamma \frac{\partial^2 C}{\partial x^2}(x, t)\, dx.$$

Our interval $[\beta, \gamma]$ is arbitrary along the axis of the pipe. So, how could it be that the same integral relation is true for every interval? There is only one way:

$$\frac{\partial C}{\partial t} = \frac{\partial^2 C}{\partial x^2}.$$

This gives a partial differential equation for the change in concentration over time. This equation is called the diffusion equation (and sometimes Fick's second law).

We have just seen how our substance diffuses in its medium. What happens when it meets a permeable membrane? In this case, there are two concentrations to consider: the concentrations on the two sides of the membrane. Let's suppose the concentration to the left of our membrane, which is a cross section of our pipe, is C^L and the concentration on the right is C^R. For definiteness, suppose the membrane is at the position $x = \beta$. The

constitutive law for the flux across the membrane that respects Fick's law is that the flux is proportional to the difference in concentration across the membrane. From the point of view of the left side of the membrane, the flux is given by

$$-\lambda \pi a^2 \frac{\partial C^L}{\partial x}(\beta, t) = \alpha(C^L(\beta, t) - C^R(\beta, t).$$

From the point of view of the right side,

$$-\lambda \pi a^2 \frac{\partial C^R}{\partial x}(\beta, t) = \alpha(C^L(\beta, t) - C^R(\beta, t)).$$

Of course, this is for an ideal membrane that has zero thickness. The values of the concentrations at the membrane are limits from the left and right-hand sides.

We are building up to a complete model of the diffusion in the pipe containing the membrane. We simply put together the diffusion equations for the right and left sides, the boundary conditions at the membrane and the boundary conditions at the ends of the pipe.

For our pipe with fixed concentration at its left end and with a cap at the right end, a reasonable model would be

$$\begin{aligned}
\frac{\partial C^L}{\partial t} &= \lambda \frac{\partial^2 C^L}{\partial t^2}, \\
\frac{\partial C^R}{\partial t} &= \lambda \frac{\partial^2 C^R}{\partial t^2}, \\
C^L(0, t) &= c, \\
-\lambda \pi a^2 \frac{\partial C^L}{\partial x}(\beta, t) &= \alpha(C^L(\beta, t) - C^R(\beta, t)), \\
-\lambda \pi a^2 \frac{\partial C^R}{\partial x}(\beta, t) &= \alpha(C^L(\beta, t) - C^R(\beta, t)), \\
\frac{\partial C^R}{\partial x}(L, t) &= 0.
\end{aligned}$$

Given initial concentration profiles for C^L and C^R (that is, $C^L(x, 0) = f(x)$ for x in the interval $(0, \beta)$ and $C^R(x, 0) = g(x)$ for x in the interval (β, L)), we can find the concentrations predicted by the model at each position x and every time $t > 0$.

How would we solve the equations making our model? This is a very good question and a long story that you will soon learn how to read if you continue to study mathematics.

How do we get the second type of flux from the first in general? Obvious answer: multiply by area! But, life is not quite this simple.

Imagine a surface that is in the domain of a flow. Surfaces usually have two sides. (Can you think of a one-sided surface?) For a two sided surface, it is possible that it is being crossed in both direction by the same flow with flux X. We may cover the surface with small non-overlapping patches where X crosses the surface in the same direction on each patch. On each such patch, the vector X is the sum of a normal and a tangential component with the tangential component given a plus or negative sign according to a preliminary choice of direction across the two-sided surface. Clearly, only the tangential components count in determining the transport. We pick one representative point on each patch, consider the signed normal component of X at this point, multiply its length by the area of the patch, and add together all of the resulting numbers. This is the type-2 flux over the surface corresponding to the type-1 flux X. If you have taken calculus, you should recognize the sum just mentioned as an integral.