1 Diffusion

If a synapse releases a neurotransmitter, that neurotransmitter will diffuse across the synaptic cleft. In general, if you put a fluid in another fluid, the two fluids will mix through the process of diffusion. What causes this?

Various people originally thought that molecules of one kind feel a force from molecules of another kind. Einstein (good old Al) showed that diffusion is merely the result of a random walk. In other words, molecules with no preferred direction to go will follow the law of diffusion.

2 Diffusion as a Random Walk

Suppose you have a fluid at some temperature T. Using statistical mechanics, we can derive the velocity distribution (i.e. the percentages of molecules with velocity v). This is all fun and good, but it's a little more information than we really need. Suffice it to say that a more rigorous analysis will turn up the same results.

For simplicity, we'll only consider motion in one dimension.

Let the average time between collisions be τ. Let ϵ be the distance that the average particle moves in time τ.

Suppose a given particle p has a position $r_p(t)$ at time t. At time $t+\tau$, p will have a position

$$r_p(t+\tau) = \begin{cases} r_p(t)+\epsilon & \text{with probability } 1/2 \\ r_p(t)-\epsilon & \text{with probability } 1/2 \end{cases}$$

The expected value of the position $r_p(t+\tau)$ *squared*, is given by:

$$\begin{aligned} < r_p(t+\tau)^2 > &= < \tfrac{1}{2}(r_p(t)+\epsilon)^2 + \tfrac{1}{2}(r_p(t)-\epsilon)^2 > \\ &= < \tfrac{1}{2}(r_p(t)^2 + 2r_p(t)\epsilon + \epsilon^2) + \tfrac{1}{2}(r_p(t)^2 - 2r_p(t)\epsilon + \epsilon^2) > \\ &= < r_p(t)^2 + \epsilon^2 > \\ &= < r_p(t)^2 > + < \epsilon^2 > \\ &= < r_p(t)^2 > + \epsilon^2 \end{aligned}$$

Averaging over all particles p, we find that

$$< r(t+\tau)^2 > = < r(t)^2 > + \epsilon^2$$

If we set up our coordinates such that $r(0) = 0$, we have

$$\begin{aligned} < r(t)^2 > &= \tfrac{t}{\tau}\epsilon^2 \\ &= \tfrac{\epsilon^2}{\tau} t \end{aligned}$$

Usually (for reasons that'll be mentioned later), this is written as

$$< r(t)^2 > = 2Dt$$

This is the one dimensional version. In three dimensions, we have to look at the sum of the x, y and z displacements, which will give us a constant of 6 D.

Typical values of D (at room temperature) are on the order of 10^{-9} m^2/s. Typical diffusion distances are left as an exercise to the reader.

3 The Diffusion Equation

We've just looked at the question "how far do individual molecules diffuse?" Now let's turn it around. Suppose we stand at a given place. How many molecules pass by this point in a given time?

Again, we model it as a random walk.

Consider slabs of thickness ϵ and area A. Every time step τ, 1/2 of the molecules in each slab move to the left and 1/2 move to the right.

We want the molecular *flux*, i.e. the number of molecules per unit area per time step.

Let c(x) be the concentration of molecules at a point x. The number of molecules passing through x is

$$\begin{aligned} & \#\text{ of molecules in slab } x-\epsilon - \#\text{ of molecules in slab } x+\epsilon \\ = \; & K(c(x-\epsilon)V - c(x+\epsilon)V) \\ = \; & K(c(x-\epsilon) - c(x+\epsilon))A\epsilon \end{aligned}$$

Where K is a constant factor meaning that some fixed fraction of the molecules in each slab have enough velocity to get to the next slab in time τ. (The actual geometry is a little sticky.)

So the flux M, which is molecules per area per time, is given by

$$\begin{aligned} M &= \frac{\#of molecules}{A\tau} \\ &= \frac{K(c(x-\epsilon)-c(x+\epsilon))A\epsilon}{A\tau} \\ &= \frac{K(c(x-\epsilon)-c(x+\epsilon))\epsilon}{\tau} \\ &= \frac{2K\epsilon^2}{\tau}\frac{c(x-\epsilon)-c(x+\epsilon)}{2\epsilon} \\ &= -\frac{2K\epsilon^2}{\tau}\frac{c(x+\epsilon)-c(x-\epsilon)}{2\epsilon} \\ &= -\frac{2K\epsilon^2}{\tau}\frac{\partial c}{\partial x} \\ &= -\frac{2K\epsilon^2}{\tau}\frac{\partial c}{\partial x} \\ &= -D\frac{\partial c}{\partial x} \end{aligned}$$

(So K=1/4. We shall not comment further on K.)

This explains the value of $2D$ in the other equation.