Physical Principles in Biology
Biology 3550
Fall 2018

Lecture 18:

Fick's Second Law: The Diffusion Equation

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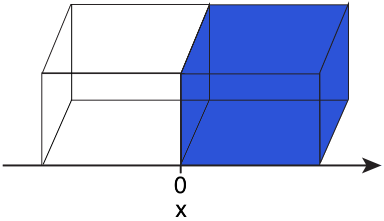
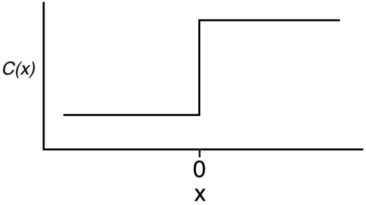
An Idealized Macroscopic Diffusion Experiment

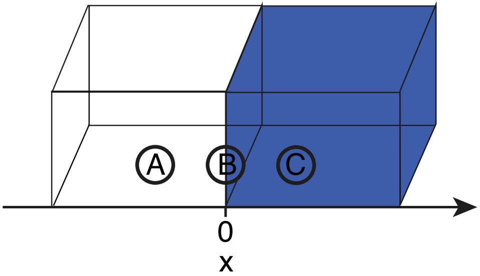


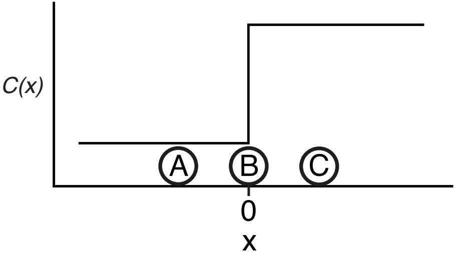


- How will plot of $C(x)$ versus x change with time?

Clicker Question #1

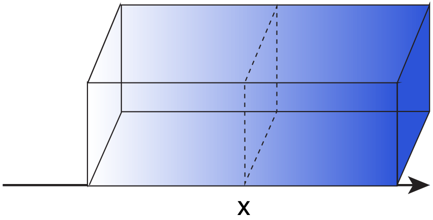
Where will the absolute value of the flux, $|J|$, be greatest?

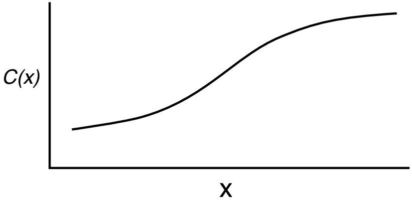




- At point B, where the concentration gradient is greatest.
- But, the molecules move at the same rate everywhere!

Fick's First and Second Laws of Diffusion





- First law:

$$J = -D\frac{dC}{dx}$$

- Flux, J, at position x is proportional to the concentration gradient at that position.

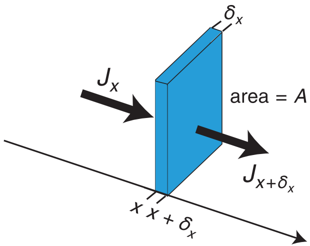
- Second law:

$$\frac{dC}{dt} = D\frac{d^2C}{dx^2}$$

- Rate of change in concentration at position x is proportional to the derivative of the concentration gradient.

Fick's Second Law of Diffusion

$$\frac{dC}{dt} = D\frac{d^2C}{dx^2}$$



- A "second-order differential equation".
- The solution to the equation is a function:

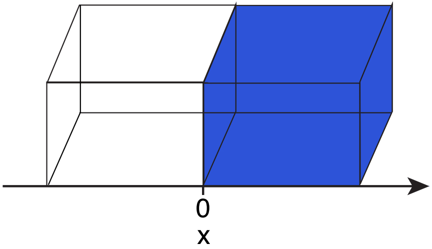
$$C = f(x, t)$$

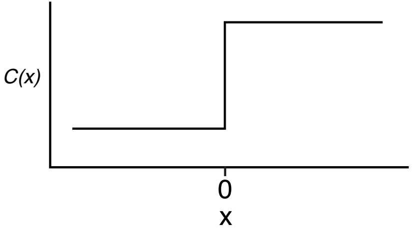
that satisfies the equation:

$$\frac{df(x,t)}{dt} = D\frac{d^2f(x,t)}{dx^2}$$

- The trick is to find the function, $C = f(x, t)$.
- The solution depends on the shape of the volume and the initial concentrations, the *boundary conditions*.

Diffusion from a Sharp Boundary

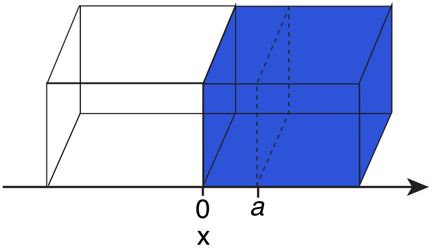


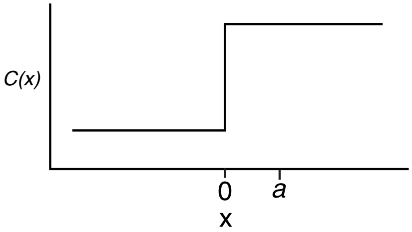


At $t = 0$

- For $x < 0$: $C(x) = 0$, $\quad \dfrac{dC}{dx} = 0$, $\quad \dfrac{d^2C}{dx^2} = 0$
- At $x = 0$, $\quad \dfrac{dC}{dx} \to \infty$
- For $x \geq 0$: $C(x) = 1$, $\quad \dfrac{dC}{dx} = 0$, $\quad \dfrac{d^2C}{dx^2} = 0$

Diffusion from a Sharp Boundary



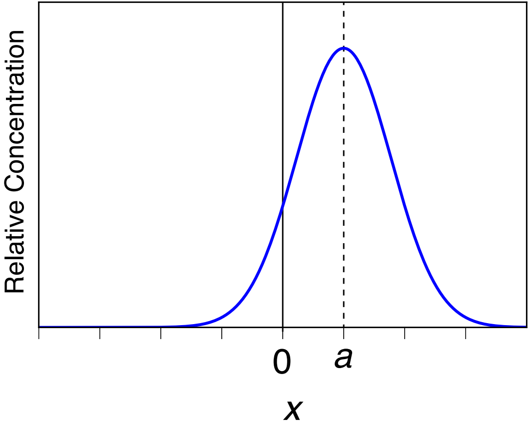


Consider molecules initially at a position $x = a > 0$:

- Molecules will begin to diffuse via a random walk.
- How will the molecules initially at position a be distributed after a time, t?
- A Gaussian distribution centered at $x = a$.

Diffusion from a Sharp Boundary

Distribution of molecules originally at position $x = a$

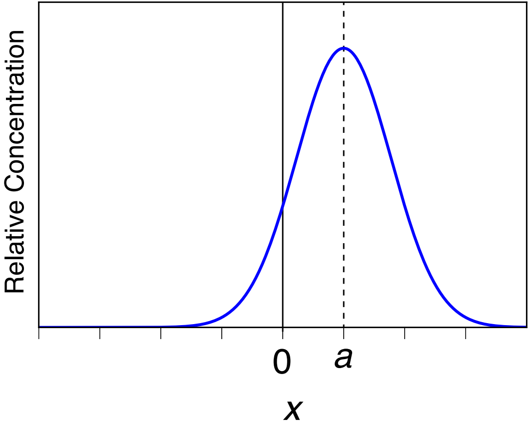


$$p(x) = \frac{1}{\sqrt{2\pi n\delta_x^2}} e^{-(x-a)^2/(2n\delta_x^2)}$$

- n = number of steps in random walk
- δ_x^2 = mean-square step displacement along x-axis
- $n\delta_x^2$ = mean-square end-to-end displacement after n steps

Diffusion from a Sharp Boundary

Distribution of molecules originally at position $x = a$



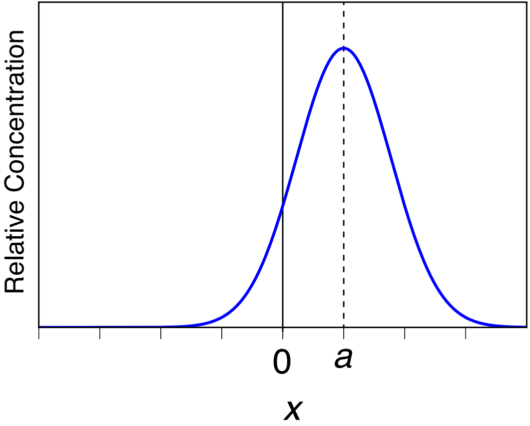
$$p(x) = \frac{1}{\sqrt{2\pi n \delta_x^2}} e^{-(x-a)^2/(2n\delta_x^2)}$$

- Diffusion coefficient, $D = \dfrac{\delta_x^2}{2\tau}$
- τ = average time of each RW step
- After time, t, $n = t/\tau$

$$n\delta_x^2 = \frac{t\delta_x^2}{\tau} = 2Dt$$

Diffusion from a Sharp Boundary

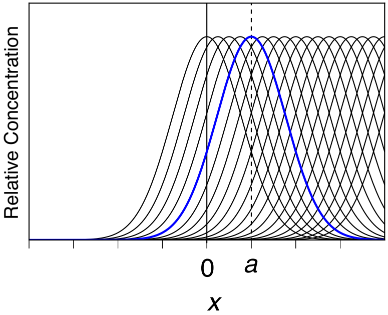
Distribution of molecules originally at position $x = a$



$$p(x) = \frac{1}{\sqrt{4\pi D t}} e^{-(x-a)^2/(Dt)}$$

Diffusion from a Sharp Boundary

- Distribution of molecules from all starting points, $a \geq 0$.



- At position x, concentration is the sum of molecules that have diffused from $a \geq 0$

$$C(x,t) = \int_0^\infty \frac{1}{\sqrt{4\pi Dt}} e^{-(x-a)^2/(4Dt)} da$$

Does the "Solution" Satisfy Fick's Second Law?

- Putative solution:

$$C(x,t) = \int_0^\infty \frac{1}{\sqrt{4\pi Dt}} e^{-(x-a)^2/(4Dt)} da$$

- Fick's second law:

$$\frac{dC}{dt} = D\frac{d^2C}{dx^2}$$

- Need to evaluate $\frac{dC}{dt}$ and $\frac{d^2C}{dx^2}$ and see if they satisfy the equation.
- They do!

Different Ways of Writing the Solution

- My way:

$$C(x,t) = \int_0^{\infty} \frac{1}{\sqrt{4\pi D t}} e^{-(x-a)^2/(4Dt)} da$$

- The textbook way:

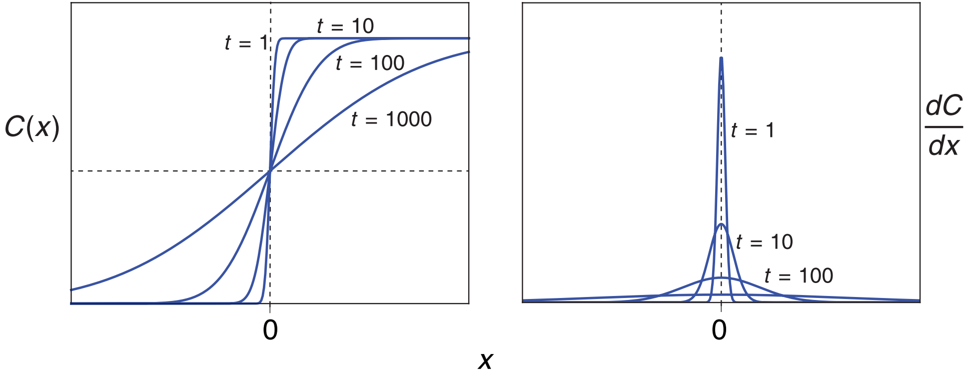
$$C(x,t) = \frac{1}{2}\left[1 + \text{erf}\left(\frac{x}{\sqrt{4Dt}}\right)\right]$$

$$= \frac{1}{2} + \int_0^{x} \frac{1}{\sqrt{4\pi D t}} e^{-x^2/(4Dt)} dx$$

erf(x) is the "error function",
the integral of the Gaussian function from 0 to x.

- Two ways of writing the solution are equivalent.
- Cannot be analytically evaluated. Can be numerically evaluated.

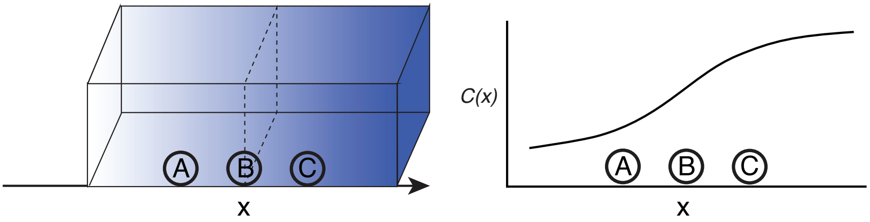
Diffusion from a Sharp Boundary



- The derivative, dC/dx is a Gaussian function because the function $C(x)$ is the integral of a Gaussian function!

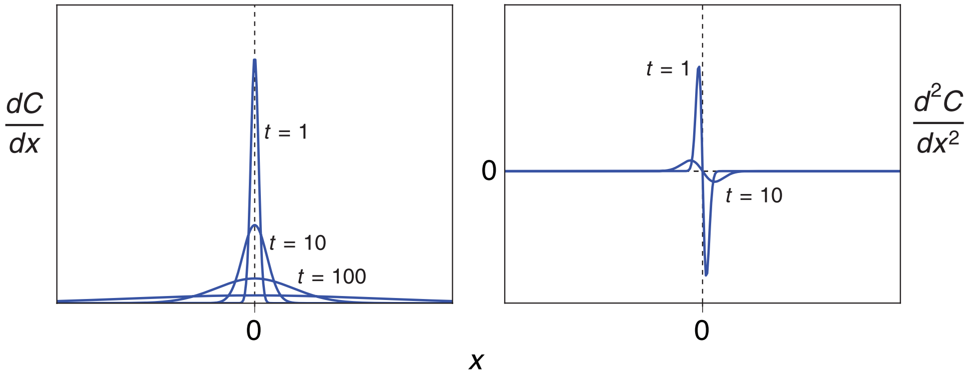
Clicker Question #2

Where will the concentration increase most rapidly?

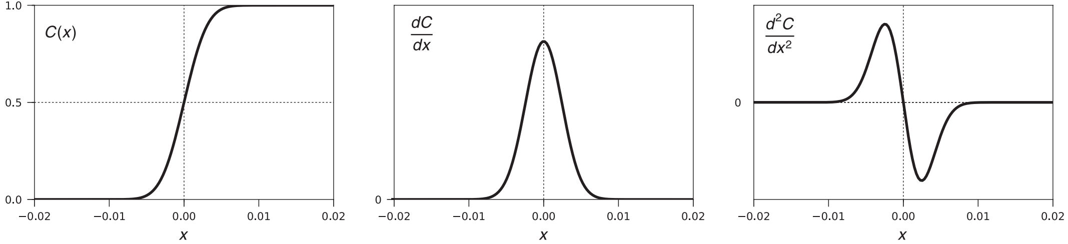


At point A, where the concentration gradient increases most rapidly with respect to x.

Diffusion from a Sharp Boundary



$C(x)$ and its Derivatives, for Diffusion from a Sharp Boundary



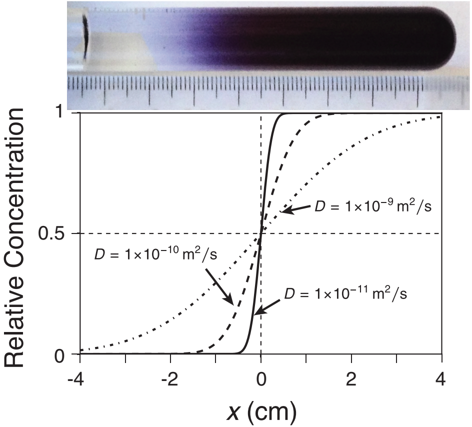
Estimating D from Diffusion from a Sharp Boundary

$$C(x,t) = \int_0^\infty \frac{1}{\sqrt{4\pi D t}} e^{-(x-a)^2/(4Dt)}\, da$$

$$t = 48\,\text{hr} = 1.7\times10^5\,\text{s}$$

$$D \approx 2\times10^{-10}\,\text{m}^2/\text{s}$$

$$D = \frac{\delta_x^2}{2\tau}$$



- What are the average length (δ_x) and duration (τ) of the random walk steps?