Physical Principles in Biology
Biology 3550
Fall 2016

Lecture 17

Diffusion: Fick's Second Law

Friday, 30 September

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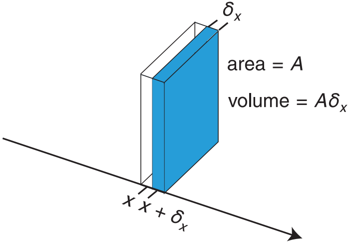
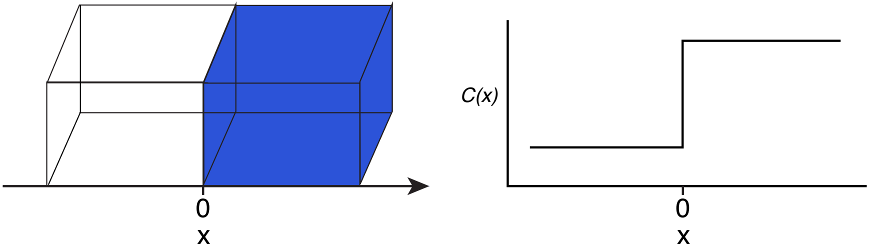
Fick's First Law of Diffusion

$$J = -\frac{\delta_x^2}{2\tau}\frac{dC}{dx} = -D\frac{dC}{dx}$$



- J = flux of molecules per unit area per unit time $(\text{moles}/(\text{s}\cdot\text{m}^2))$
- D = diffusion coefficient = $\frac{\delta_x^2}{2\tau}(\text{m}^2/\text{s})$
- δ_x = RMS step length along the x-direction (m)
- τ = average duration of random steps (s)
- $\frac{dC}{dx}$ = derivative of concentration with x $(\text{moles}/\text{m}^4)$

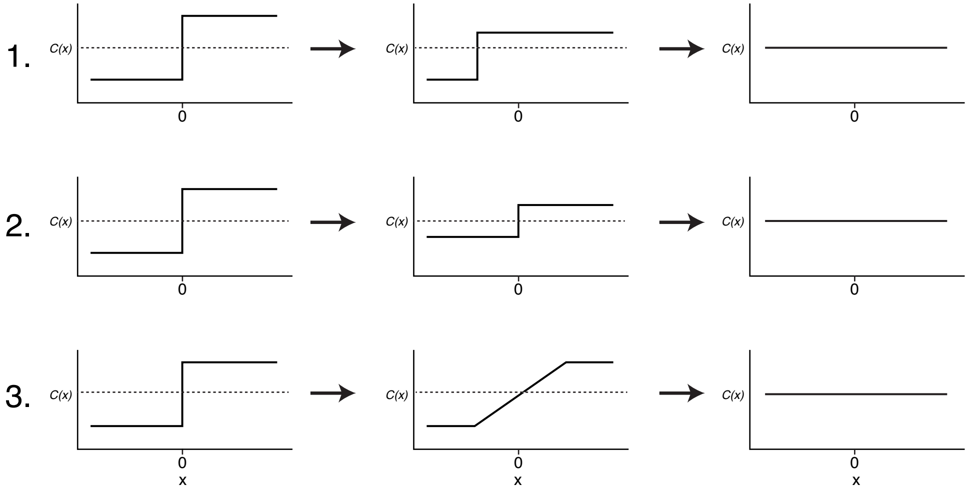
An Idealized Macroscopic Diffusion Experiment



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

Clicker Question #1

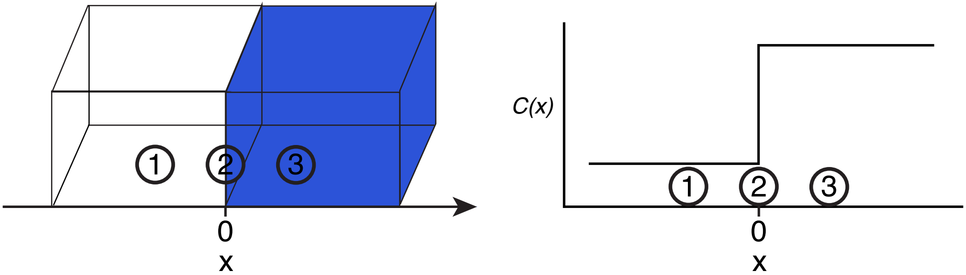
How will the concentration change with time?



All answers count for now!

Clicker Question #2

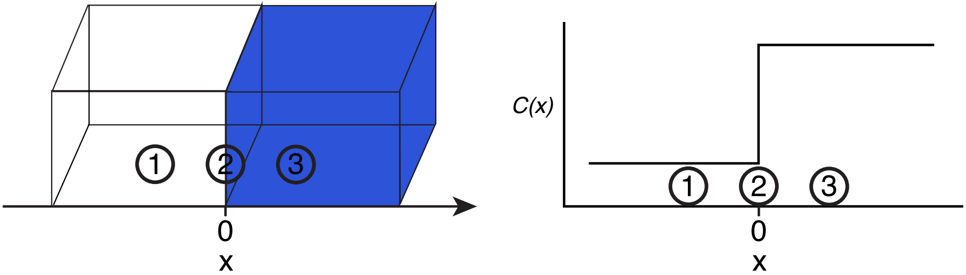
Where will the flux, *J*, be greatest?



At point 2, where the concentration gradient is greatest.

Clicker Question #3

Where will where will the concentration change most rapidly?



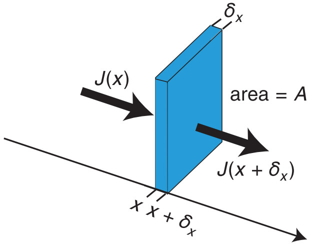
All answers count for now!

Fick's Second Law of Diffusion

- Net number of molecules moving to the right at two sides of a slice, during interval dt:

$$N(x) = J(x)Adt$$

$$N(x+\delta_x) = J(x+\delta_x)Adt$$



- Change in number of molecules in the slice:

$$dN = AJ(x)dt - AJ(x+\delta_x)dt$$

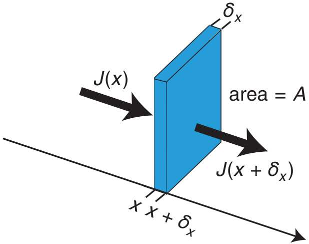
$$= Adt\big(J(x) - J(x+\delta_x)\big)$$

Fick's Second Law of Diffusion

- Change in concentration in the slice:

$$dC = \frac{dN}{A\delta_x} = \frac{Adt\left(J(x) - J(x+\delta_x)\right)}{A\delta_x}$$

$$= -dt\frac{J(x+\delta_x) - J(x)}{\delta_x}$$



- In the limit of small dt and small δ_x:

$$\frac{dC}{dt} = -\frac{J(x+\delta_x) - J(x)}{\delta_x} = -\frac{dJ}{dx}$$

- How does J change with x?

Fick's Second Law of Diffusion

- Fick's first law:

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

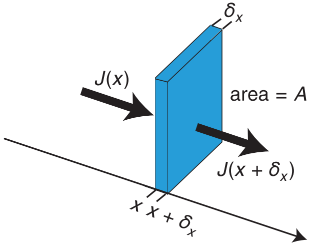
- Derivative of J with respect to x:

$$\frac{dJ}{dx} = -D\frac{d^2C}{dx^2}$$

- Fick's second law:

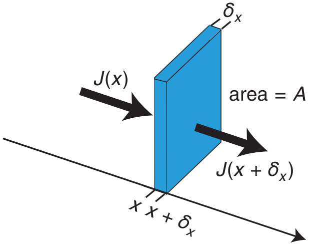
$$\frac{dC}{dt} = -\frac{dJ}{dx} = D\frac{d^2C}{dx^2}$$

Also called the diffusion equation.
What is it good for?



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:

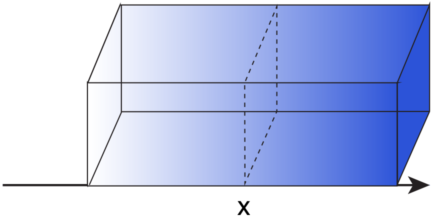
$$C = f(x, t)$$

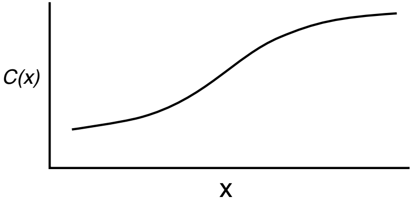
that satisfies the equation:

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

- The trick is to find $C = f(x, t)$.

Fick's First and Second Laws of Diffusion





- First law:

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

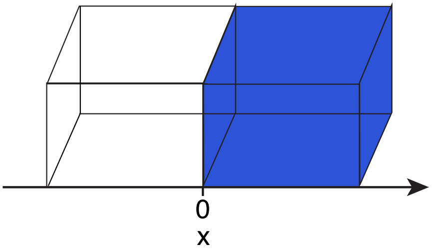
- Flux, J, at position x is proportional to the concentration gradient at that position.

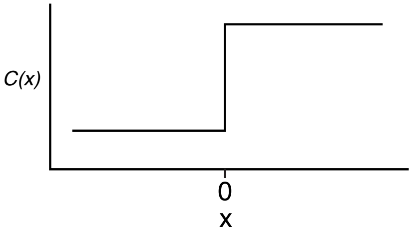
- Second law:

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

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

Diffusion from a Sharp Boundary

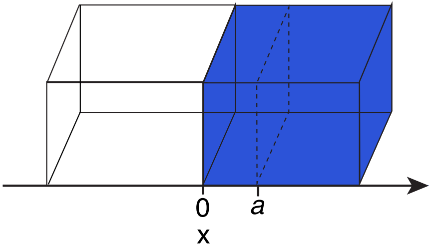


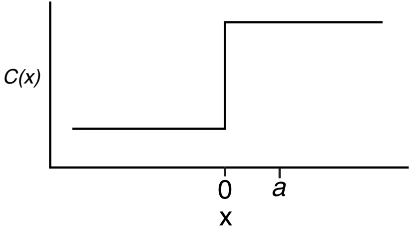


At $t = 0$

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

Diffusion from a Sharp Boundary





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

- Molecules will begin to diffuse via a random walk.
- After a time, t, molecules from this position will be distributed along the x-axis, according to a Gaussian distribution:

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

Diffusion from a Sharp Boundary

- Distribution of molecules originally at position $x = a$

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

n = number of steps in random walk

$\langle\delta_x^2\rangle$ = mean-square step distance along x-axis

- Diffusion coefficient, $D = \dfrac{\delta_x^2}{2\tau}$

$\tau =$ average time of each RW step

After time, t, $n = t/\tau$

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

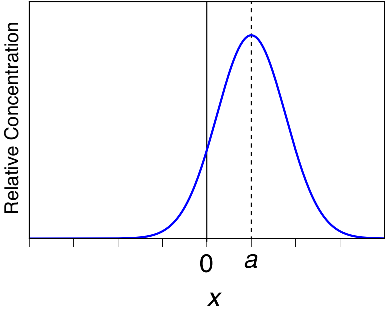
Diffusion from a Sharp Boundary

- Distribution of molecules originally at position $x = a$

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

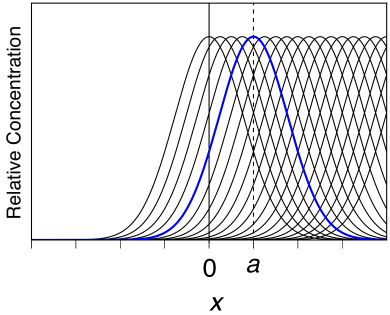
D = diffusion coefficient

t=time



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 $a \geq 0$

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

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:

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

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

  $\text{erf}(x)$ is the "error function",
  the integral of the Gaussian function from 0 to x.

- Cannot be analytically evaluated. Can be numerically evaluated.

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

- Putative solution:

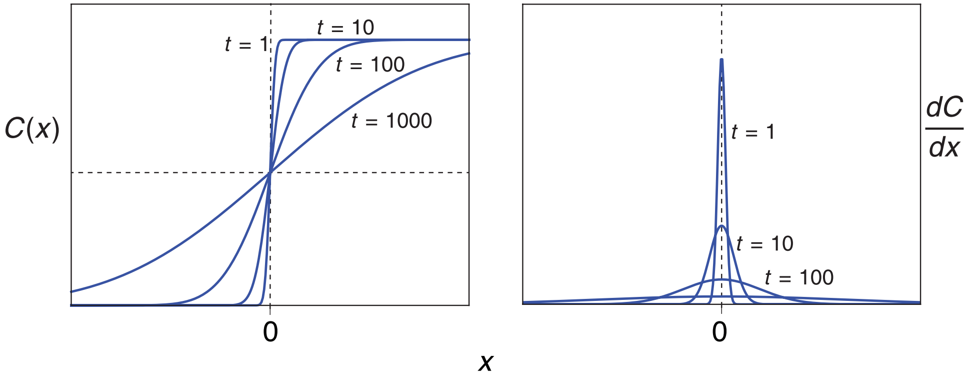
$$C(x,t) = \frac{1}{2} + \int_0^x \frac{1}{\sqrt{4\pi Dt}} e^{-x^2/(4Dt)} dx$$

- 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!

Diffusion from a Sharp Boundary



Diffusion from a Sharp Boundary