

Physical Principles in Biology  
Biology 3550  
Fall 2017

## Lecture 16

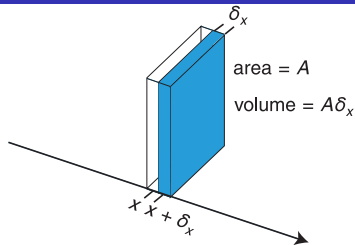
### Diffusion: Fick's Second Law

Wednesday, 27 September

©David P. Goldenberg  
University of Utah  
goldenberg@biology.utah.edu

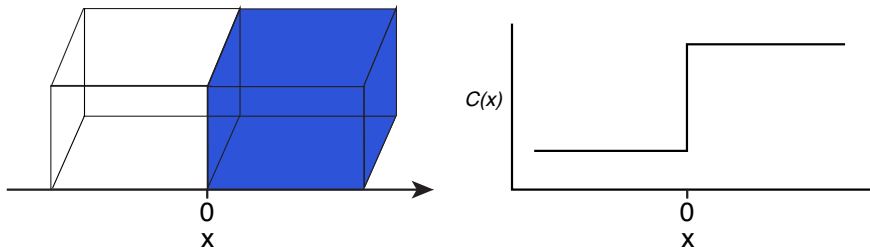
# Fick's First Law of Diffusion

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



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

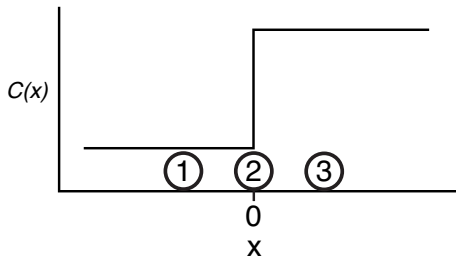
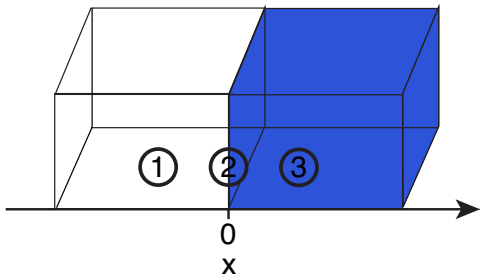
# An Idealized Macroscopic Diffusion Experiment



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

# Clicker Question #1

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



At point 2, where the concentration gradient is greatest.

# Fick's Second Law of Diffusion

- How does the concentration at a given point change with time?
- Net number of molecules moving to the right at two sides of a slice, during interval  $dt$ :

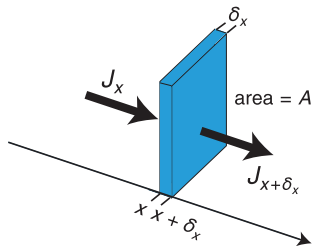
$$N_x = J_x A dt$$

$$N_{x+\delta_x} = J_{x+\delta_x} A dt$$

- Change in number of molecules in the slice:

$$dN = AJ_x dt - AJ_{x+\delta_x} dt$$

$$= A dt (J_x - J_{x+\delta_x})$$



# Fick's Second Law of Diffusion

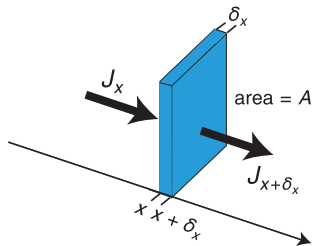
- Change in concentration in the slice:

$$\begin{aligned}dC &= \frac{dN}{A\delta_x} = \frac{A dt (J_x - J_{x+\delta_x})}{A\delta_x} \\ &= -dt \frac{J_{x+\delta_x} - J_x}{\delta_x}\end{aligned}$$

- In the limit of small  $dt$  and small  $\delta_x$ :

$$\frac{dC}{dt} = -\frac{J_{x+\delta_x} - J_x}{\delta_x} = -\frac{dJ}{dx}$$

- 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  $x$ :

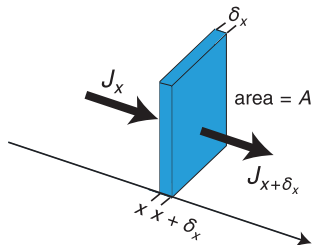
$$\frac{dJ}{dx} = -D \frac{d^2C}{dx^2}$$

- Fick's second law:

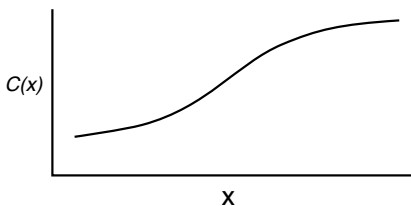
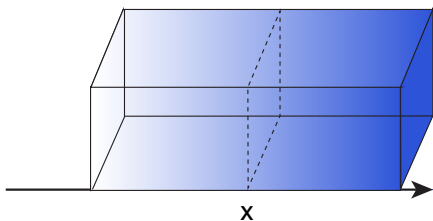
$$\frac{dC}{dt} = -\frac{dJ}{dx} = D \frac{d^2C}{dx^2}$$

Also called the diffusion equation.

What is it good for? How do we use it?



# 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:

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

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



# Fick's Second Law of Diffusion

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

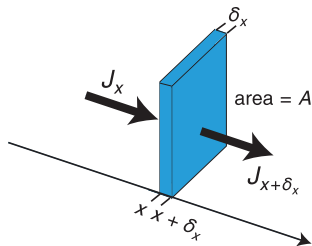
- A “second-order differential equation”.
- The solution to the equation is a function:

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

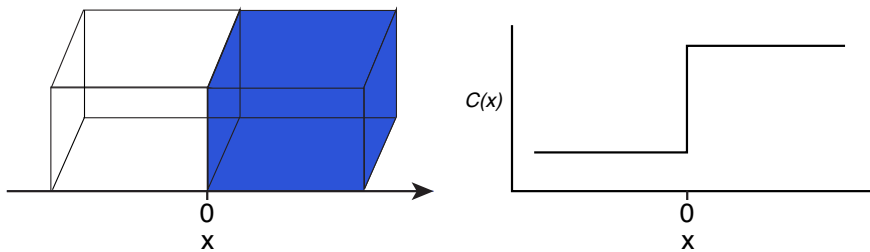
that satisfies the equation:

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

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



# Diffusion from a Sharp Boundary



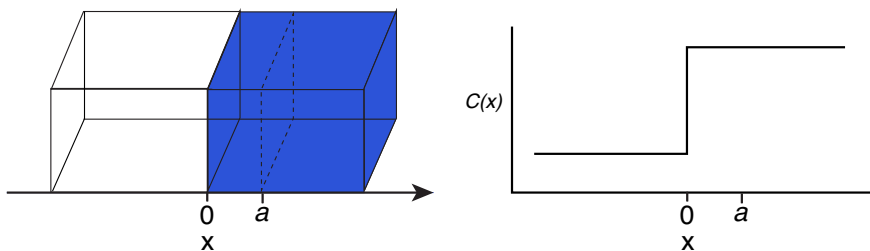
At  $t = 0$

■ For  $x < 0$ :  $C(x) = 0$ ,  $\frac{dC}{dx} = 0$ ,  $\frac{d^2C}{dx^2} = 0$

■ At  $x = 0$ ,  $\frac{dC}{dx} \rightarrow \infty$

■ For  $x \geq 0$ :  $C(x) = 1$ ,  $\frac{dC}{dx} = 0$ ,  $\frac{d^2C}{dx^2} = 0$

# Diffusion from a Sharp Boundary

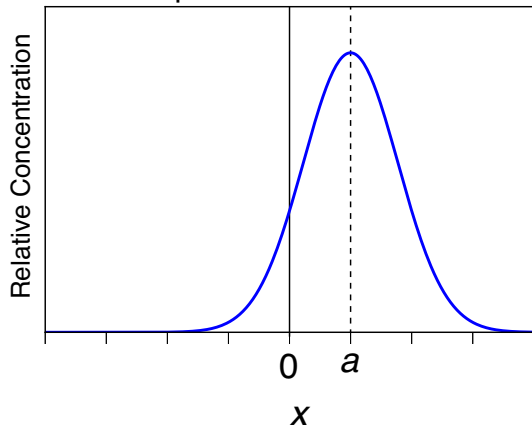


Consider molecules at a position  $x = a > 0$ :

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

# Diffusion from a Sharp Boundary

Distribution of molecules originally at position  $x = a$



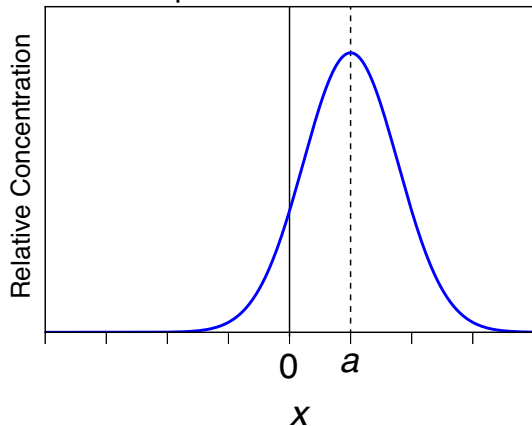
$$p(x) = \frac{1}{\sqrt{2\pi n \langle \delta_x^2 \rangle}} e^{-(x-a)^2 / (2n \langle \delta_x^2 \rangle)}$$

$n$  = number of steps in random walk

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

# Diffusion from a Sharp Boundary

Distribution of molecules originally at position  $x = a$



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

■ Diffusion coefficient,  $D = \frac{\delta_x^2}{2\tau}$

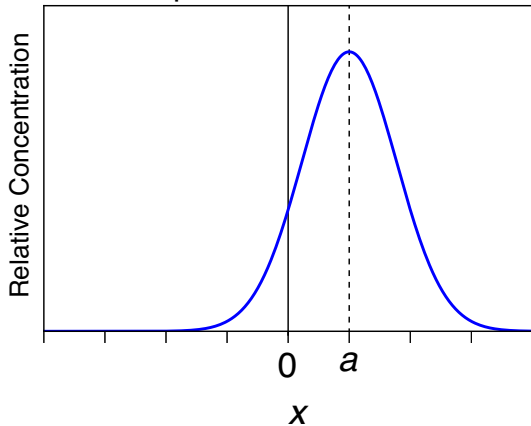
$\tau$  = average time of each RW step

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

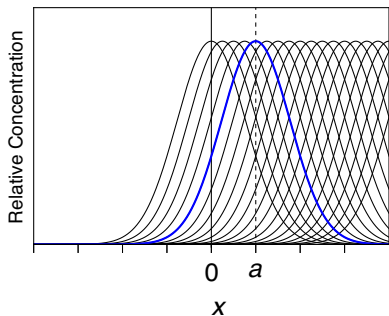
Distribution of molecules originally at position  $x = a$



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

# 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:

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

- Fick’s second law:

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

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

They do!



# Different Ways of Writing the Solution

- My way:

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

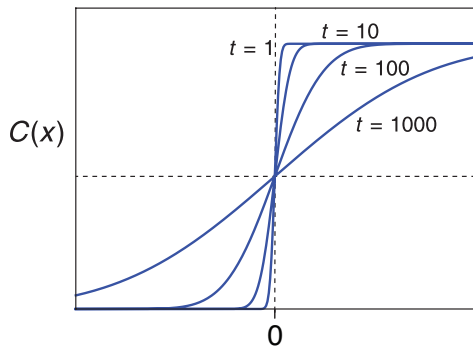
- The textbook way:

$$\begin{aligned} C(x, t) &= \frac{1}{2} \left[ 1 + \operatorname{erf} \left( \frac{x}{\sqrt{4Dt}} \right) \right] \\ &= \frac{1}{2} + \int_0^x \frac{1}{\sqrt{4\pi Dt}} e^{-x^2/(4Dt)} dx \end{aligned}$$

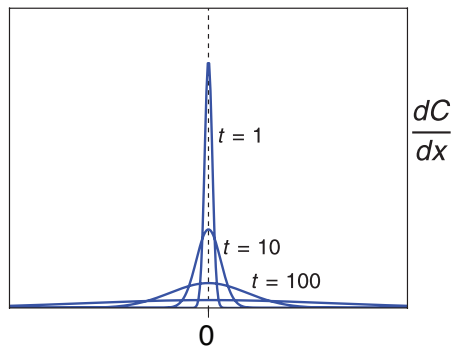
$\operatorname{erf}(x)$  is the “error function”,  
the integral of the Gaussian function from 0 to  $x$ .

- Cannot be analytically evaluated. Can be numerically evaluated.

# Diffusion from a Sharp Boundary



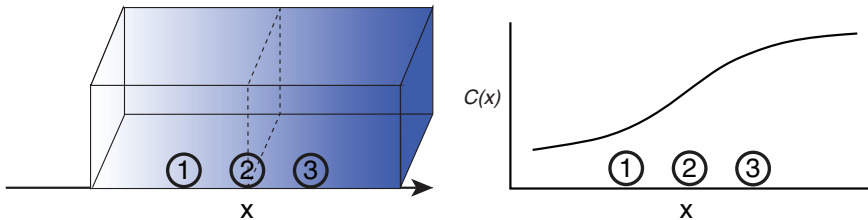
$x$



$\frac{dC}{dx}$

## Clicker Question #2

Where will the concentration increase most rapidly?



At point 1, where the concentration gradient increases most rapidly with respect to  $x$ .

# Diffusion from a Sharp Boundary

