

Recitation #2

Fick's first law $\phi(x,t) = -D \frac{\partial c(x,t)}{\partial x}$

Continuity equation $-\frac{\partial \phi(x,t)}{\partial x} = \frac{\partial c(x,t)}{\partial t}$

Diffusion equation $\frac{\partial c(x,t)}{\partial t} = D \frac{\partial^2 c(x,t)}{\partial x^2}$

Steady state solution: Time-invariant
($\frac{\partial c}{\partial t} = 0, \frac{\partial \phi}{\partial t} = 0$)

$\phi(x,t) = \phi_0$ (constant flux)

$c(x,t) = -\frac{\phi_0}{D} x + \alpha$

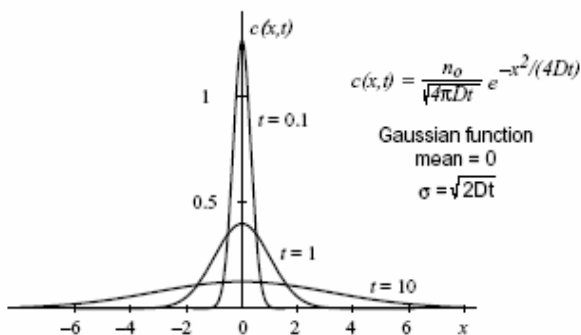
Equilibrium: Zero flux + ~~time~~ time invariant

$\therefore \phi_0 = 0$ $c(x,t) = \text{constant}$
 \Rightarrow uniform distribution.

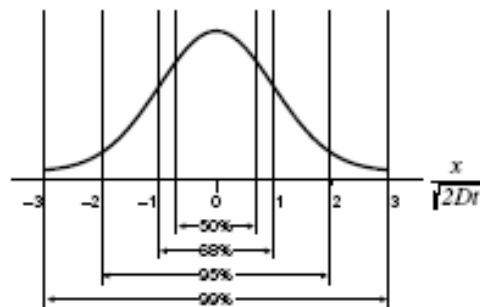
Impulse Response

Given $c(x,t) = n_0 \delta(x)$ at $t=0$

Solve $\frac{\partial c(x,t)}{\partial t} = D \frac{\partial^2 c(x,t)}{\partial x^2}$ for $t > 0$



How long till half the solute diffuses to $|x| > x_{1/2}$



$c(x,t) = \frac{n_0}{\sqrt{4\pi Dt}} e^{-x^2/(4Dt)}$

$\frac{x_{1/2}}{\sqrt{2Dt}} \approx \frac{2}{3}$
 $\frac{2}{3} \sqrt{2Dt} \approx x_{1/2}$
 $\frac{4}{9} 2Dt \approx x_{1/2}^2$
 $t \approx \frac{x_{1/2}^2}{D} = t_{1/2}$

Problem 1. Consider a cell composed of a cell body to which is attached a long thin tubular “process” (e.g., the axon of a neuron or the flagellum of a sperm cell) of length l cm (Figure 1). Suppose some substance n (e.g., a metabolite) is generated in the cell body and diffuses along the

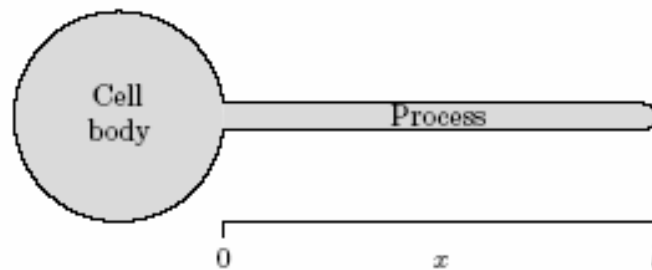


Figure 1: Cell body with a process.

process, all along which the substance is consumed at a constant uniform rate, α_n mol/s per unit length. The continuity equation for the substance thus becomes

$$\frac{\partial c_n}{\partial t} = -\frac{\partial \phi_n}{\partial x} - \frac{\alpha_n}{A}$$

where A is the (assumed constant) cross-sectional area of the process.

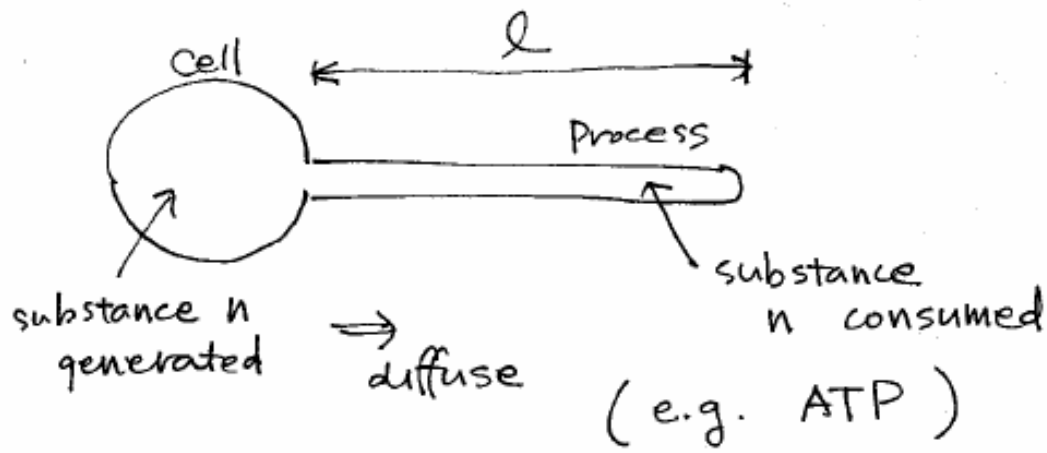
- Combine the modified continuity equation given above with Fick's Law to obtain a modified form of the diffusion equation that must be satisfied by c_n .
- Show that a solution of this equation in the steady-state ($\partial c_n / \partial t = \partial \phi_n / \partial t = 0$) is

$$c_n(x) = \frac{\alpha_n}{2DA}x^2 + a_0x + b_0$$

and find values of the constants a_0 and b_0 corresponding to the boundary conditions $c_n(0) = C_0$ and $\phi_n(l) = 0$.

- Show that the requirement that α_n mol/(s·cm) be consumed uniformly along the process sets an upper limit (if C_0 , D , A , and α_n are fixed) on the possible length l of the process, and find a formula for this upper bound.

1.



α_n : consumption rate (mol/s per unit length)

[Continuity equation]

$$\underbrace{\frac{\partial C_n}{\partial t}}_{\text{increase rate of local concentration}} = - \underbrace{\frac{\partial \phi_n}{\partial x}}_{\text{spatial gradient in flux}} - \underbrace{\frac{\alpha_n}{A}}_{\text{reaction loss}}$$

a) Fick's law $\phi_n = -D_n \frac{\partial C_n}{\partial x}$

$$\therefore \underline{\underline{\frac{\partial C_n}{\partial t} = + D_n \frac{\partial^2 C_n}{\partial x^2} - \frac{\alpha_n}{A}}}$$

b) In the steady state ($\frac{\partial}{\partial t} \rightarrow 0$)

$$D_n \frac{d^2 C_n(x)}{dx^2} - \frac{\alpha_n}{A} = 0$$

$$\frac{d^2 C_n(x)}{dx^2} = \frac{\alpha_n}{D_n A}$$

general solution $\Rightarrow C_n(x) = \frac{\alpha_n}{2D_n A} x^2 + a_0 x + b_0$
 (a_0, b_0 : constants)

Boundary conditions $\left\{ \begin{array}{l} C_n(0) = C_0 : \text{meaning?} \\ \text{(Intracellular concentration is maintained.)} \\ \phi_n(l) = 0 \\ \text{(At the end of process,} \\ \text{molecules cannot go further)} \end{array} \right.$

$\therefore C_n(0) = C_0 \Rightarrow b_0 = C_0$

$\phi_n(l) = -D_n \frac{\partial C_n}{\partial x} \Big|_{x=l} = -D_n \left(\frac{\alpha_n}{D_n A} x + a_0 \right) \Big|_{x=l} = 0$

$\therefore a_0 = -\frac{\alpha_n l}{D_n A}$

$\therefore C_n(x) = \frac{\alpha_n}{2D_n A} x^2 - \frac{\alpha_n l}{D_n A} x + C_0$

c) what is the minimum concentration?
 Where does it happen? $\Rightarrow x=l$.

$C_n(l) = \frac{\alpha_n}{2D_n A} l^2 - \frac{\alpha_n l^2}{D_n A} + C_0$
 $= C_0 - \frac{\alpha_n l^2}{2D_n A}$

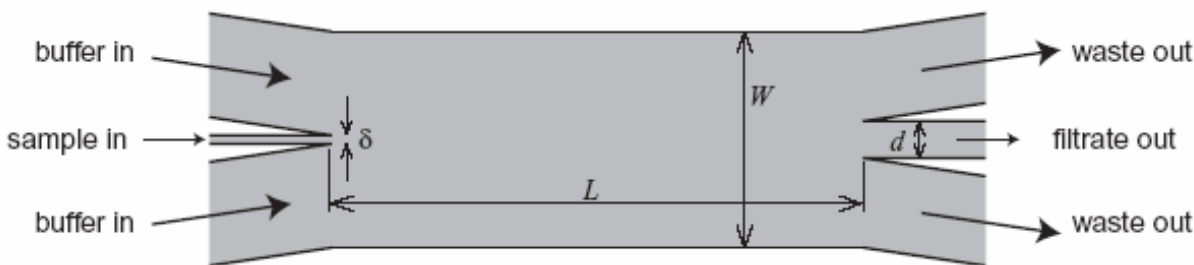
Since negative concentration does not make sense,

$C_0 \geq \frac{\alpha_n l^2}{2D_n A} \quad l^2 \leq \frac{2D_n A C_0}{\alpha_n}$

If this is violated (If the process becomes longer)

\Rightarrow End of the process cannot get the molecule at all.

Problem 2. As your first assignment at Tinyfluidics Inc., you are asked to design a microfluidic device that will remove small molecules from a sample of fluid that contains both large molecules and small molecules. After some thinking, you design the laminar flow device shown below.



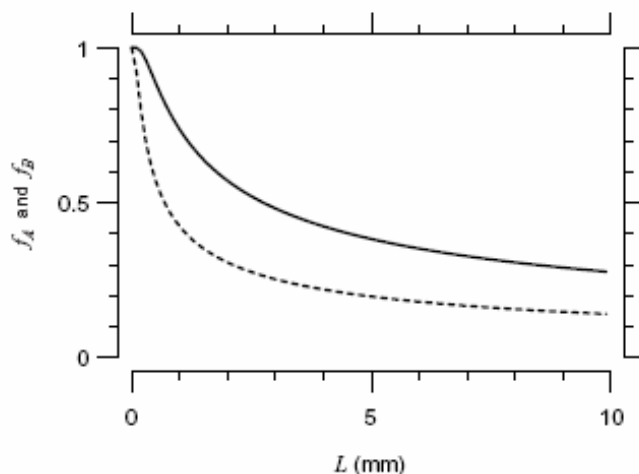
The sample is injected in a port with width δ . The sample flow is surrounded by buffers injected on both sides of the sample. The combined flow then passes through a channel that has width W and length L after which the fluids are separated into a desired filtrate output (in a channel of width d) and two waste outputs. Assume that the fluid moves with the same speed v in all parts of the microfluidic device (although this is not generally true, it is a convenient starting point). Assume that $\delta \ll d$, and that W is sufficiently large that it can be taken to be infinity.

To test the device, you mix a solution that contains equal concentrations of 2 proteins, A and B. The diffusivity of solute B is four times that of solute A.

Part a. Briefly explain how this device takes advantage of differences in diffusivities to achieve separation.

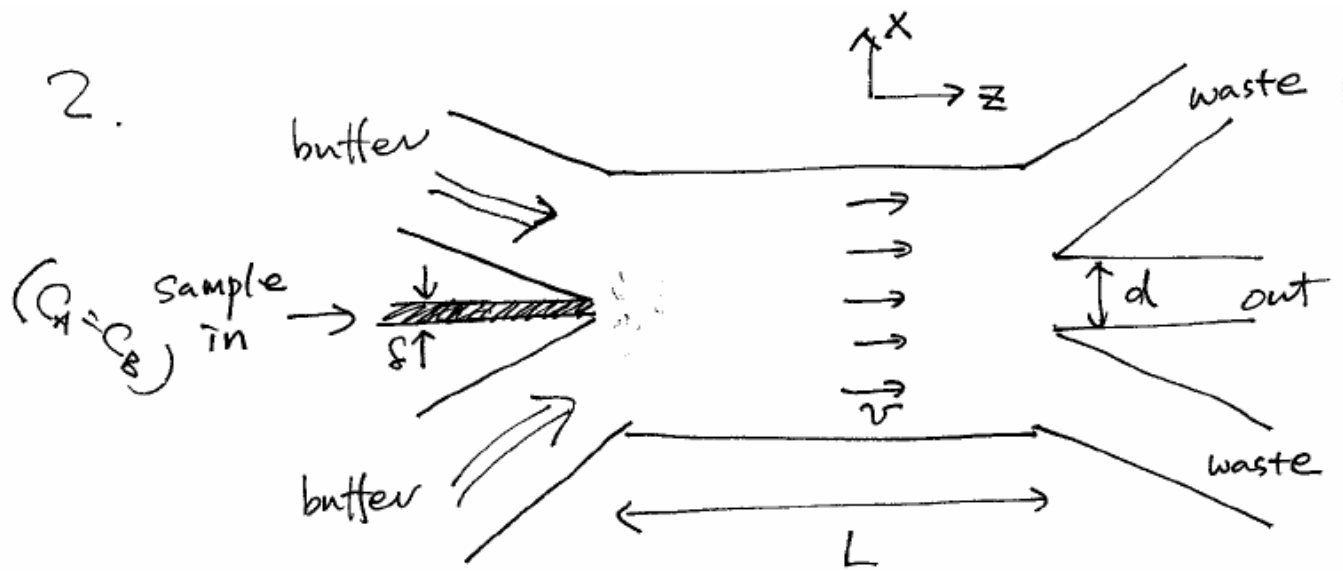
Part b. Let f_A represent the ratio of the amount of solute A found in the filtrate divided by the amount of solute A in the sample. Determine an expression for f_A . Determine an expression for the analogous ratio f_B for solute B.

The following figure shows a plot of the dependence of f_A and f_B on L , when $\delta = 1\mu\text{m}$, $d = 20\mu\text{m}$, $v = 1\text{ mm/s}$, and $D_A = 10^{-7}\text{ cm}^2/\text{s}$.



Part c. Which curve (dashed or solid) represents f_A ? Explain.

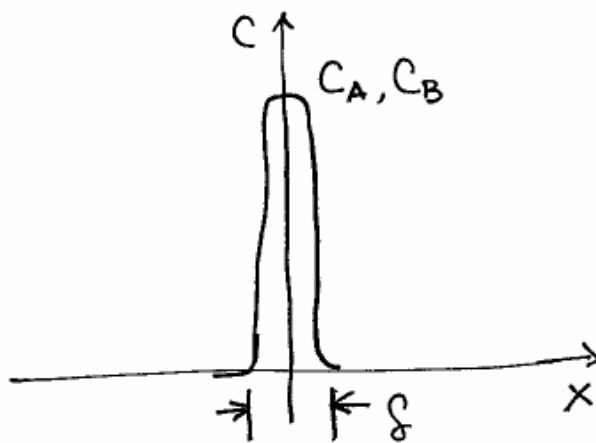
Part d. Determine L_0 , the value of L that maximizes the difference between f_A and f_B . Briefly explain why this difference is smaller when $L \ll L_0$ and when $L \gg L_0$.



Two proteins A and B
 $4D_A = D_B$

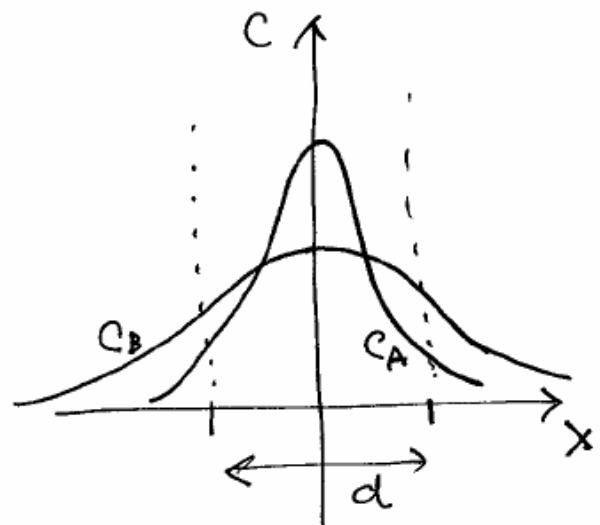
a) As the narrow sample stream enters the device, the proteins will get diffused in the lateral (x) dimension. The larger the diffusivity, the farther it will diffuse.

At the entrance

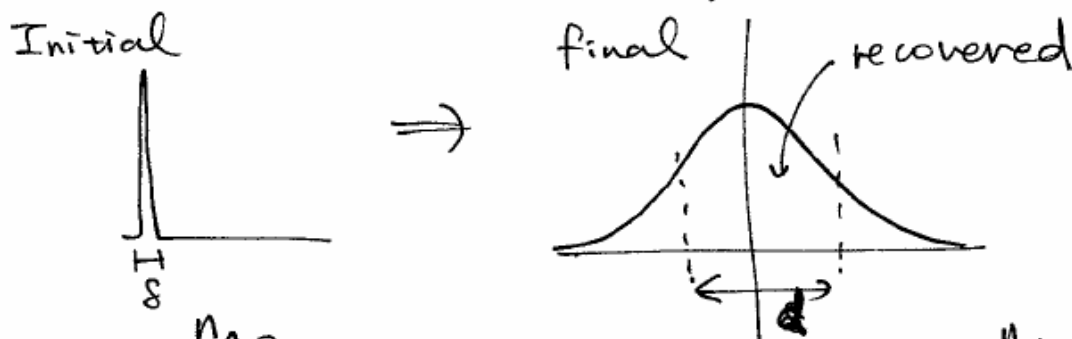


\Rightarrow

At the outlet



$$(b) f_A = \frac{\text{Amount of A recovered}}{\text{Amount of A injected}}$$



$$C_A(x) = n_A \delta(x) \quad \Rightarrow \quad C_A(x, t_0) = \frac{n_A}{\sqrt{4\pi D_A t_0}} e^{-x^2/4D_A t_0}$$

at $t=0$ (at injection) (at $t=t_0$)

What is t_0 ? $\Rightarrow v t_0 = L \quad t_0 = L/v$

$$f_A = \frac{\int_{-d/2}^{d/2} \left(\frac{n_A}{\sqrt{4\pi D_A t_0}} e^{-x^2/4D_A t_0} \right) dx}{\int_{-\infty}^{\infty} n_A \delta(x) dx} = \int_{-d/2}^{d/2} \frac{e^{-x^2/4D_A t_0}}{\sqrt{4\pi D_A t_0}} dx$$

$$\text{If } \frac{d}{2} = \sqrt{4D_A t_0} \Rightarrow f_A = 0.68$$

$$= 2\sqrt{4D_A t_0} \Rightarrow f_A = 0.95$$

(c) Since B diffuses faster, dotted line represents B.

(d) One can estimate (from the graph) that L_0 should be about ~ 1.5 mm.