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Course 565/665 Lecture Number ______ Date 4/22/03

Lecturer Dr. Silvia Cavagnero Note Taker Eric Fulmer

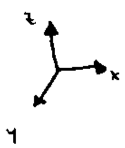
Last Time: The Differential Equation

1 D Diffusion

$\longrightarrow x$

$$\left(\frac{\partial c}{\partial t}\right)_x = D\left(\frac{\partial^2 c}{\partial x^2}\right)$$

3D Diffusion



$$\left(\frac{\partial c}{\partial t}\right)_{x,y,z} = D\nabla^2 c$$

In order to solve the differential equation, you need

1. Initial Conditions (ie. $t=0$ behavior)
2. 2 Boundary Conditions (ie. behavior at certain spacial positions)

Exam Information:

- Exam II
  - Chapter 10 - 16
  - Protein Stability

- Final Exam
  - Chapter 1 – 18
  - Protein Stability
  - Energy Landscapes

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Stokes - Einstein Equation

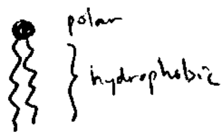
$$D = \frac{kT}{6\pi\eta a}$$

η - viscosity of medium

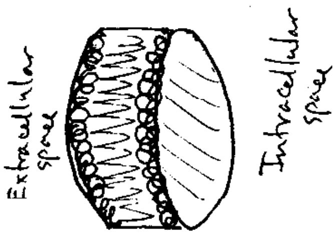
a - radius of sphere

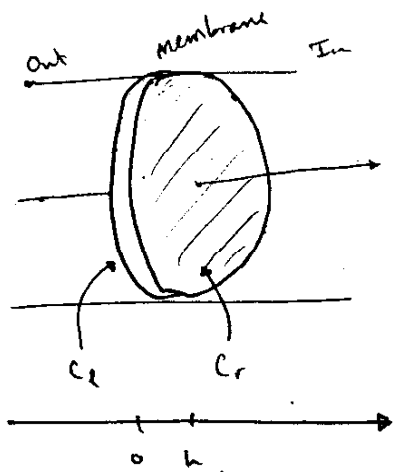
k - Boltzmann Constant

$\boxed{\text{Example}}$ Consider a lipid membrane. Lipits are composite molecules, having a polar head and a hydrophobic tail.



Can we describe the diffusion of a drug across a biological membrane?





$\Delta c = c_r - c_l$

$\left(\frac{\partial c}{\partial t}\right)_x = 0$ (Steady State Approximation)

Not equilibrium - material and energy flow.

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$$\left(\frac{\partial^2 c}{\partial x^2}\right)_t = 0$$

<u>Integration Once</u>

$$\int d\, f(x) = f(x) + c$$

$$\int \left(\frac{\partial^2 c}{\partial x^2}\right)_t dx = \frac{\partial c}{\partial x} + A_1'$$

$$\int \left[\left(\frac{\partial c}{\partial x}\right)_t + A_1'\right] dx = c + A_1' x + A_2'$$

$$\left(\frac{\partial c}{\partial t}\right)_x = 0 = D\,\frac{\partial^2 c}{\partial x^2}$$

$$0 = c + A_1' x + A_2'$$

$$-A_1' = A_1$$

$$-A_2' = A_2$$

$$c = A_1 x + A_2$$

<u>Boundary Conditions</u>

$x = 0$ $\qquad c(0) = K c_x$

$x = h$ $\qquad c(h) = K c_r$

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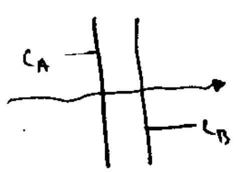
$x = 0$ $\quad c = A_1 \cancel{x}^{0} + A_2 = kc_\ell \qquad A_2 = kc_\ell$

$x = h$ $\quad c = A_1 h + A_2 = A_1 h + kc_\ell = kc_r$

$$A_1 = \frac{k}{h}(c_r - c_\ell)$$

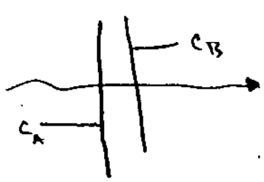
$c_r < c_\ell$ typically for media that oppose some resistance to the flow

$$\boxed{c = \frac{k}{h}(c_r - c_\ell)x + kc_\ell}$$



passive transport

spontaneous.



active transport

requires energy