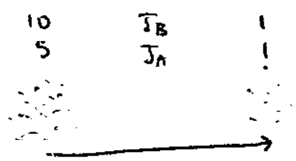
PRINT NEATLY *** **USE A BLACK PEN** *** **DO NOT STAPLE**

Course 565/665 Lecture Number ______ Date 4/21/03

Lecturer Dr. Silvia Cavagnero Note Taker Eric Fulmer

Concentration Gradients and Kinetics (Consider the Special Type)

(1) Molecules tend to flow from higher concentrations to lower concentrations.



Fick's First Law:

$$\boxed{J = -D \frac{dc}{dx}}$$

$D \equiv$ Diffusion coefficient ($cm^2\ sec^{-1}$)

Benzene $D = 1.02 \times 10^{-5}\ cm^2\ sec^{-1}$

Myosin $D = 1.16 \times 10^{-7}\ cm^2\ sec^{-1}$

In 3 dimensions,

$$\boxed{\vec{J} = -D\ \vec{\nabla} c}$$ where $\vec{\nabla} = \left(\frac{\partial}{\partial x}\right)\hat{i} + \left(\frac{\partial}{\partial y}\right)\hat{j} + \left(\frac{\partial}{\partial z}\right)\hat{k}$

Driving Force?

Driving force for flux across concentration gradients: tendency to equalize chemical potentials. $\mu_A > \mu_B \Rightarrow$ flux.

At Equilibrium:

$\mu_A = \mu_B \Rightarrow$ No Flux

PRINT NEATLY *** **USE A BLACK PEN** *** **DO NOT STAPLE**

Course 565/665 Lecture Number ______ Date 9/21/03

Lecturer Caragnero Note Taker Fulmer

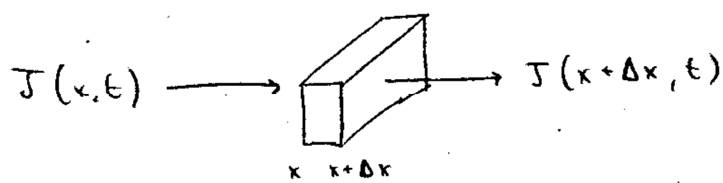
What about D?

$$J = L \cdot f = -D\frac{dc}{dx} = -\frac{L}{c}kT\frac{dc}{dx}$$

$$\boxed{D = \frac{L}{c}kT}$$ where $\frac{L}{c} \equiv u$ (mobility)

$$f_c = \frac{1}{u} = \frac{c}{L} \equiv \text{friction coefficient}$$

Concentration Gradients vs. Space and Time



$$\Delta J \cdot A \cdot \Delta t = A \cdot \Delta t \cdot [J(x,t) - J(x+\Delta x, t)]$$

- increase in the number of particles in vol. element A at time Δt (area?).

$= \text{Volume} \cdot (\text{midpoint concentration})$

$$= A \cdot \Delta x \left[c\left(x + \frac{\Delta x}{2}, t + \Delta t\right) - c(x + \Delta x, t)\right]$$

Course 565/665 Lecture Number ______ Date 4/21/03

Lecturer Caragnero Note Taker Fulmer

Combining the two: (and dividing by $\Delta x \cdot \Delta t$)

$$\frac{\cancel{A}\,\Delta t}{\Delta x\,\cancel{\Delta t}}\underbrace{\left[J(x,t) - J(x+\Delta x, t)\right]}_{-\Delta J} = \frac{\cancel{A}\,\cancel{\Delta x}}{\Delta t\,\cancel{\Delta x}}\underbrace{\left[c\left(x+\frac{\Delta x}{2}, t+\Delta t\right) - c(x+\Delta x, t)\right]}_{\Delta c}$$

$$\lim_{\Delta x \to dx} \frac{-\Delta J}{\Delta x} = -\left(\frac{\partial J}{\partial x}\right)_t \qquad \lim_{\Delta t \to dt} \frac{\Delta c}{\Delta t} = \left(\frac{dc}{dt}\right)_x$$

Thus,

$$-\left(\frac{\partial J}{\partial x}\right)_t = \left(\frac{dc}{dt}\right)_x$$

Also, $J = -D\left(\frac{dc}{dx}\right)_t$

Diffusion Equation: $$\boxed{D\left(\frac{\partial^2 c}{\partial x^2}\right)_t = \left(\frac{\partial c}{\partial t}\right)_x}$$ (1D)

3D Diffusion Equation: $$\boxed{\left(\frac{dc}{\partial t}\right)_x = D\nabla^2 c}$$

PRINT NEATLY *** **USE A BLACK PEN** *** **DO NOT STAPLE**

Course 565/665 Lecture Number ______ Date 4/21/03

Lecturer Cavagnero Note Taker Fulmer

The previous equation is a differential equation.

A partial differential equation. To solve, we need:

- 2 boundary conditions (c vs. spacial coordinates)
- 1 initial condition. (c vs time at $t=0$)

We will only consider steady-state conditions:

c is constant @ all times at each point in space.