~~Applications~~ Diffusion in a Potential

$$\frac{\partial}{\partial t} p(x,t) = -\frac{\partial}{\partial x} j(x,t)$$

$$j(x,t) = -\mu \frac{\partial U(x)}{\partial x} P(x,t) - D \frac{\partial P(x,t)}{\partial t}$$

where $U(x)$ is the potential energy.

Using $D = \mu k_B T$

$$\frac{\partial}{\partial t} p(x,t) = D \frac{\partial}{\partial x}\left[\frac{\partial}{\partial x} + \beta \frac{\partial U(x)}{\partial x}\right] p(x,t)$$

One dimensional Fokker Planck equation

Note that $D = \mu k_B T$ is necessary so that

$P(x,t) \propto e^{-\beta U(x)}$, $\beta = 1/(k_B T)$

is a stationary solution

For isotropic medium, in 3D

$$\frac{\partial}{\partial t} p(\vec{x},t) = D \vec{\nabla}\left(\vec{\nabla} + \beta(\vec{\nabla} U)\right) P(\vec{x},t)$$

When $U = 0$ we get the Diffusion Equation

$$\frac{\partial}{\partial t} P(\vec{x},t) = D\nabla^2 P(\vec{x},t)$$

For many non-interacting particles concentration follows the same equation.

$$\frac{\partial}{\partial t} C(\vec{x},t) = D\vec{\nabla}\left(\vec{\nabla} + \beta\vec{\nabla}U(\vec{x})\right)C(\vec{x},t)$$

No potential: Fick's law

$$J = -D\frac{\partial c}{\partial x}$$

Boundary conditions:

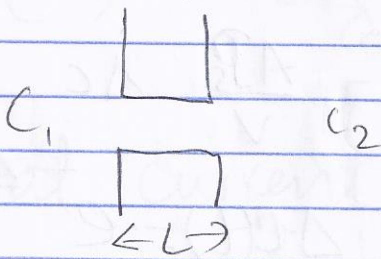
Reflecting Boundary: $\vec{J}(x) = 0$ at bdry

No potential $\nabla_n C(x) = 0$

Absorbing Boundary: $C(x) = 0$ at boundary.

Biological Applications

Permeability



$C(0) = C_1$

$C(L) = C(2)$

$$\frac{\partial c}{\partial t} = 0 \qquad \boxed{J(x) = \frac{\partial c}{\partial x}}$$

$$\Rightarrow \frac{\partial}{\partial x} J(x) = 0$$

$$C(x) = C(0) - \frac{Jx}{D}$$

$$C(L) = C(0) - \frac{JL}{D}$$

$$J = -D\,\frac{\Delta C}{L} \qquad \Delta C = C_2 - C_1$$

With a permeable surface

$$J_s = -P_s\,\Delta C$$

If Concentrations inside a volume is not forced to be fixed

$$\frac{d}{dt} V(\Delta c) = j_s A = -AP_s \Delta c$$

or $$\frac{d\Delta c}{dt} = -\frac{AP_s}{V} \Delta c$$

Leading to $$\Delta c(t) = e^{-\frac{AP_s}{V}t} \Delta c(0)$$
$$= e^{-t/\tau} \Delta c(0)$$

$$\frac{V}{AP_s} = \tau$$

Diffusion limited absorption/reaction

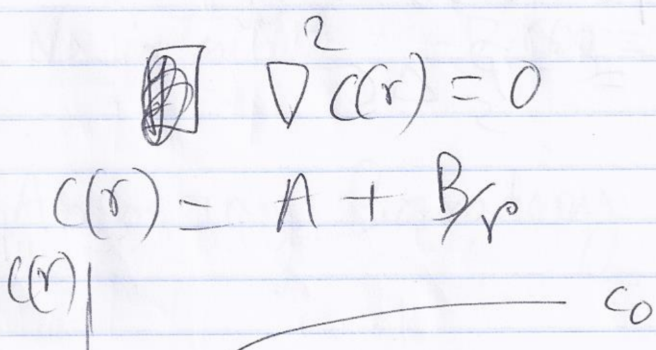
$c(r)$

$$j(r) = -D \frac{\partial c(r)}{\partial r}$$

$$\nabla^2 c(r) = 0$$

$$c(r) = A + B/r$$

$c(R) = 0$
Absorbing bdry cond.



$c(\infty) = c(0)$

$$c(r) = c_0\left(1 - \frac{R}{r}\right)$$

$$j(r) = -D\frac{\partial}{\partial r}c(r) = -D\frac{c_0 R}{r^2}$$

Total current $4\pi r^2 j(r) = -4\pi D R c_0$

This is the rate of "absorption"

Two applications;

a) Prokaryotic cells

$R = ?$ Conc. of O_2 $c_0 = 0.2\ \text{moles}/m^3$

$D = 2\times10^{-9}\ m^2/s$

$$4\pi D R c_0 = 4\pi \times 2\times10^{-9}\ \frac{m^2}{s} \times 0.2\ \frac{\text{moles}}{m^3} \times R$$

If metabolic activity requires $10^{-3}\ \frac{\text{mole}}{kg\ s}$ O_2

then for radius R

$$\frac{4\pi}{3}R^3 \times 10^3\ \frac{kg}{m^3} \times 10^{-3}\ \frac{\text{mole}}{kg\ s} \leq 4\pi \times 2 \times 10^{-9}\ \frac{m^2}{s} \times 0.2\ \frac{\text{moles}}{m^3} \times R$$

$$R^2 \leq 12\times10^{-10}\ m^2 \Rightarrow R \leq 3.4\times10^{-5}\ m$$
$$= 34\ \mu m$$

b) For two molecules to interact

Rate of of hitting a region of size R is

$$4\pi D R c_0$$

For a molecule of size a

$$D = \frac{k_B T}{6\pi \eta a}$$

So $\frac{4\pi k_B T R}{6\pi \eta a} c_0$ is the diffusion limited rate.

For $R \simeq a$

$\frac{k_B T}{\eta}$ decides maximum kinetic constant

$$\frac{4 \times 10^{-21}\ \mathrm{Nm}}{8.9 \times 10^{-4}\ \mathrm{Pa\,s}} \simeq 0.5 \times 10^{-17}\ \frac{m^3}{s}$$

This is when c_0 is in $\frac{1}{m^3}$

If c_0 is in $\frac{moles}{m^3}$

$$\frac{0.5 \times 10^{-17}}{6 \times 10^{-23}}\ \frac{m^3}{moles\ s} \simeq 10^3\ s^{-1} \left(\frac{moles}{m^3}\right)^{-1}$$

Chemical ~~Reactions~~ Concentrations often are described in Molar

$M = \frac{\text{mole}}{\text{Liter}}$ ~~mole~~

$k_{max} \sim 10^6\, s^{-1} M^{-1} \sim 10^9\, s^{-1} mM^{-1}$

1 nM is one molecule in a bacterial cell
1 mM is 10^3 molecules " " " "

Nernst Relation

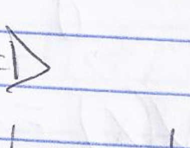
Charged particles in a potential.

$U(x) = q\, V(x)$

$J(x) = 0$, say through a channel

$$J(x) = -\mu \frac{\partial U(x)}{\partial x} c(x) - D \frac{\partial c(x)}{\partial x}$$
$$= -D \left(\frac{\partial c(x)}{\partial x} + \frac{1}{k_B T} \frac{\partial U(x)}{\partial x} \right)$$

$J(x) = 0 \implies c(x) \propto e^{-\frac{U(x)}{k_B T}} = e^{-\frac{qV(x)}{k_B T}}$

c_1, V_1  $c_2 V_2$

$$\frac{c_2}{c_1} = e^{-\frac{q(V_2 - V_1)}{k_B T}}$$

$$\Delta \ln C = -q\Delta V / k_B T$$

When conc. ratios are of the order e, $\Delta V \sim \frac{k_B T}{q}$

$$\frac{k_B T}{\text{electron charge}} = \frac{4.1 \times 10^{-21} J}{1.6 \times 10^{-19} C} \simeq \frac{1}{40} \text{ Volt}$$

$$= 25 mV$$

Neurons fire by letting ions in and out and altering channels conductivities. If a particular ion channel is very conducting, charges flow and voltages alter so that Nernst relation is approximately satisfied.

During neurons firing the voltage drop across the membrane is of the order of

10–100 mV.

Conductance / Resistance

One more a $j \neq 0$ stationary solution.

$$U(x) = q V(x) = -q E x$$

$c(x)$ constant

Charge current $qJ = -\frac{Dq}{k_BT}\frac{\partial U(x)}{\partial x}\, c = \frac{Dq^2 cE}{k_BT} = \sigma E$

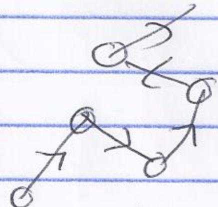
Conductance $\sigma = \frac{Dq^2 c}{k_BT}$

Resistance $= \frac{\Delta V}{I} = \frac{EL}{(qJ)A} = \cancel{k_B T}\,\frac{EL}{\sigma E A}$

$$= \frac{L}{\sigma A} = \frac{k_BTL}{Dq^2 cA}$$

Detour: Random walk and Polymers

Polymer



Long molecule made of N monomers

Freely jointed model: End to end separation

$\vec{X}_N = \sum_{i=1}^{N} \vec{l}_i$ Each $\vec{l}_i$ is random vector of length b.

'Same' as random walk of N steps

$\langle \vec{X}_N \rangle = 0$ $\quad \langle \vec{X}_N^2 \rangle = \sum_{ij} \langle \vec{l}_i \cdot \vec{l}_j \rangle = \sum_{i=1}^{N} \langle \vec{l}_i^2 \rangle$
$= Nb^2$

Asymptotic distr^n for large N

$P(\vec{X}_N) \propto e^{-3\vec{X}_N^2/2Nb^2}$. Size of polymer $\sim \sqrt{N}\, b$.