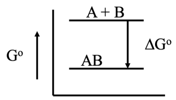
1 Molecular interactions

$A + B \underset{\mathrm{k_1}}{\overset{\mathrm{k_{-1}}}{\rightleftharpoons}} \mathrm{AB}$, $K = \frac{[\mathrm{AB}]}{[A][B]} = \frac{k_1}{k_{-1}}$

$\Delta G^\circ = -\mathrm{RT} \ln K$

The AB complex is stable relative to $A + B$. k_1, the on-rate constant: $A + B \xrightarrow{k_1} \mathrm{AB}$ (on-rate: k_1)



The rate of complex formation (or any bimolecular reaction) is limited by the diffusional limit of the rate of collisions

1.1 Translation diffusion

- Fick's first law: concentration gradient across the reference plane $J = -D\left(\frac{\mathrm{dn}}{\mathrm{dx}}\right) = \frac{\mathrm{moles\ (net)}}{\mathrm{area} * \mathrm{time}}$, D: diffusion coefficient, $\left(\frac{\mathrm{cm}^2}{\mathrm{sec}}\right)$, n = concentration, J: flux, mol · m^{-2} · s^{-1}

(PS: Use J at boundary conditions to solve for 2nd law)

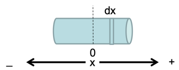
- Fick's second law: $\left(\frac{\mathrm{dn}}{\mathrm{dt}}\right) = -\frac{dJ}{dx} = D\left(\frac{\mathrm{d}^2\mathrm{n}}{\mathrm{dx}^2}\right)$

change in # particles per unit volume per unit time

- Constant gradient: same amount leaves as enters the box – concentration is constant
- Gradient higher on left: more enters the box than leaves – concentration changes

Example: one-dimensional diffusion in an infinite pipe (initial cond. $n_0 = \frac{N}{A}$)

$$\frac{dn(x,t)}{dt} = D\left(\frac{d^2 n(x,t)}{dx^2}\right)$$



Diffusion only in the x direction: $n(x,t)$ = number of particles per unit area between x and $x + dx$ at time t

SOLUTION: $n(x,t) = \frac{n_0}{\sqrt{4\pi Dt}} e^{-x^2/4Dt}$ Particles per unit area, where $n_0 = \frac{N}{A}$

Probability of finding molecules between $(x, x + dx)$ = $p(x,t)dx$

$$\frac{n(x,t)}{n_0} = \left[\frac{1}{\sqrt{4\pi Dt}} e^{-x^2/4Dt}\right] = p(x,t)$$

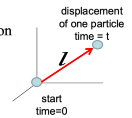
Units: fraction of molecules per unit distance, cm⁻¹

$$\langle x^2 \rangle = \int_{-\infty}^{+\infty} x^2 \boxed{p(x,t)dx} = \int_{-\infty}^{+\infty} x^2 \left[\frac{1}{\sqrt{4\pi Dt}} e^{-x^2/4Dt}\right] dx = 2Dt$$

3D diffusion: l is proportional to $\sqrt{t}$

$D_x = D_y = D_z$ isotropic diffusion

3-dimensional diffusion
$$\langle x^2 \rangle = 2D_x t$$
$$\langle y^2 \rangle = 2D_y t$$
$$\langle z^2 \rangle = 2D_z t$$



$$\langle x^2 \rangle + \langle y^2 \rangle + \langle z^2 \rangle = \langle l^2 \rangle$$
$$\langle l^2 \rangle = 6Dt$$
$$\sqrt{\langle l^2 \rangle} = \langle |l| \rangle = \sqrt{6Dt}$$
$$\langle |l| \rangle = \sqrt{6D}\sqrt{t}$$

$$D = \frac{\langle l^2 \rangle}{6t}$$

Units of the diffusion coefficient

cm^2/s

2 Diffusion

1. 1 dimension: protein along DNA or RNA
2. 2 dimensions: lipid or protein in a membrane bilayer
3. 3 dimensions: molecules in the cytoplasm