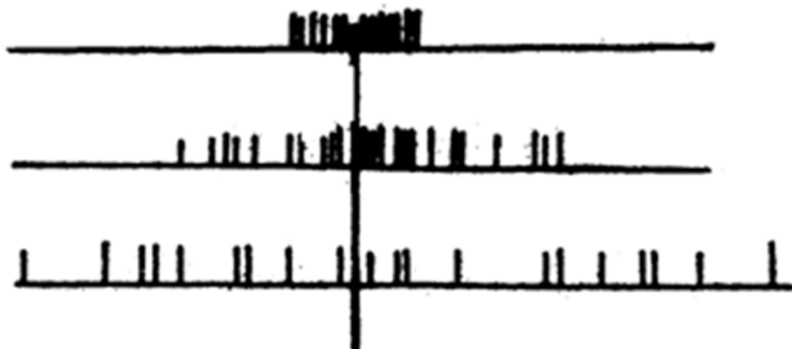
TRANSPORT PHENOMENON
FICK'S LAW OF DIFFUSION
ATP-POWERED PUMPS
-II-

Yalçın İŞLER, PhD
Izmir Katip Celebi University
Department of Biomedical Engineering
isleryа@yahoo.com

DIFFUSION

- Diffusion describes the spread of particles through random motion from the regions of higher concentration to the regions of lower concentration.
- After a period of time the particles are distributed randomly.
- At the end of a certain period, the average travelled distances by the particles will be zero.
  - Because the number of particles moving in one direction is almost equal to the number of particles moving in the reverse direction



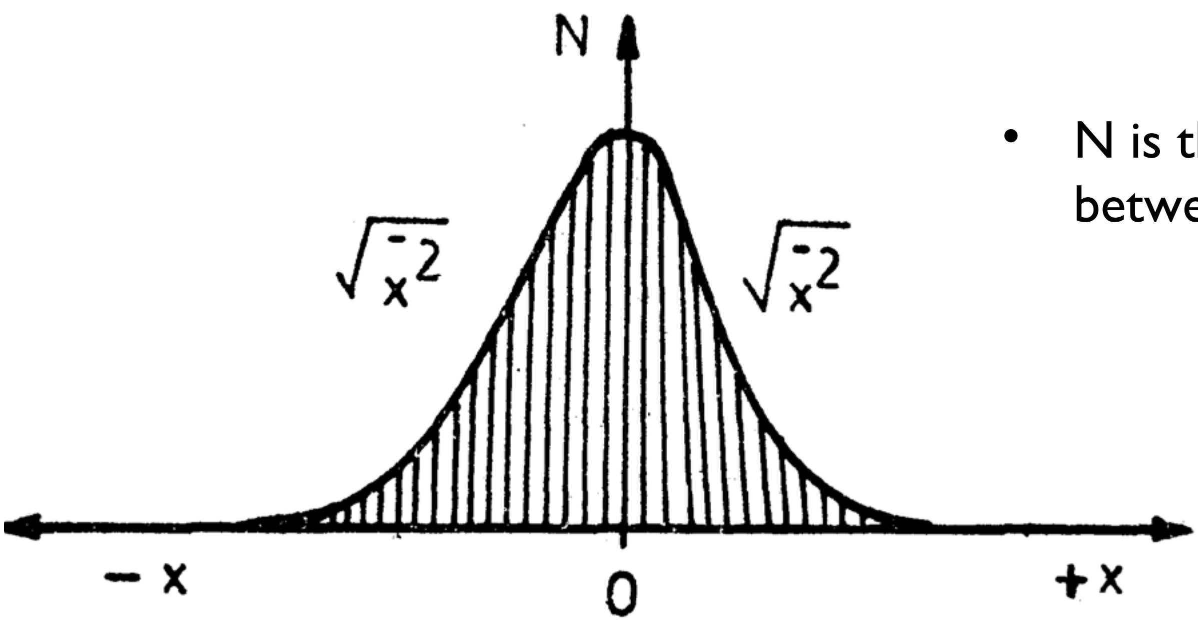
Diffusion

- The root mean square of the distances travelled by particles is always a positive.

$$x_{rms} = \sqrt{\bar{x}} = \sqrt{\frac{\sum x^2}{n}}$$

Diffusion

- After a period of time, particles reach such locations along the motion axis that
  - the graph of the number of particles and their distances from the starting point gives a "GAUSS" curve.



- N is the number of particles between **x** and **x+Δx**

Diffusion

- In addition to diffusion particles there may be other dissolved particles in the solution.
- In this case, the distribution rate of the particles, (travelled distance per unit of time) will be changed.
- High energy particles will lead to scattering of the low energy particles

Diffusion

The Boltzmann Equation describes the relationship between the particles in gases and solutions.

- the number of particles (N_y) which have E_y energy and
- the number of particles (N_d) which have E_d energy

$$\ln \frac{N_y}{N_d} = -\frac{(E_y - E_d)}{kT}$$

k= Boltzmann constant = 1,38 x10^{-23} J/°K

T= absolute temperature (°K)

Diffusion

- The kinetic energy of a particle is: $E_{kin} = \frac{1}{2}mv^2$
- If this formula is written in Boltzmann Equation;

$$\ln \frac{N_y}{N_d} = -\frac{(mv_y^2 - mv_d^2)}{2kT}$$

will be obtained.

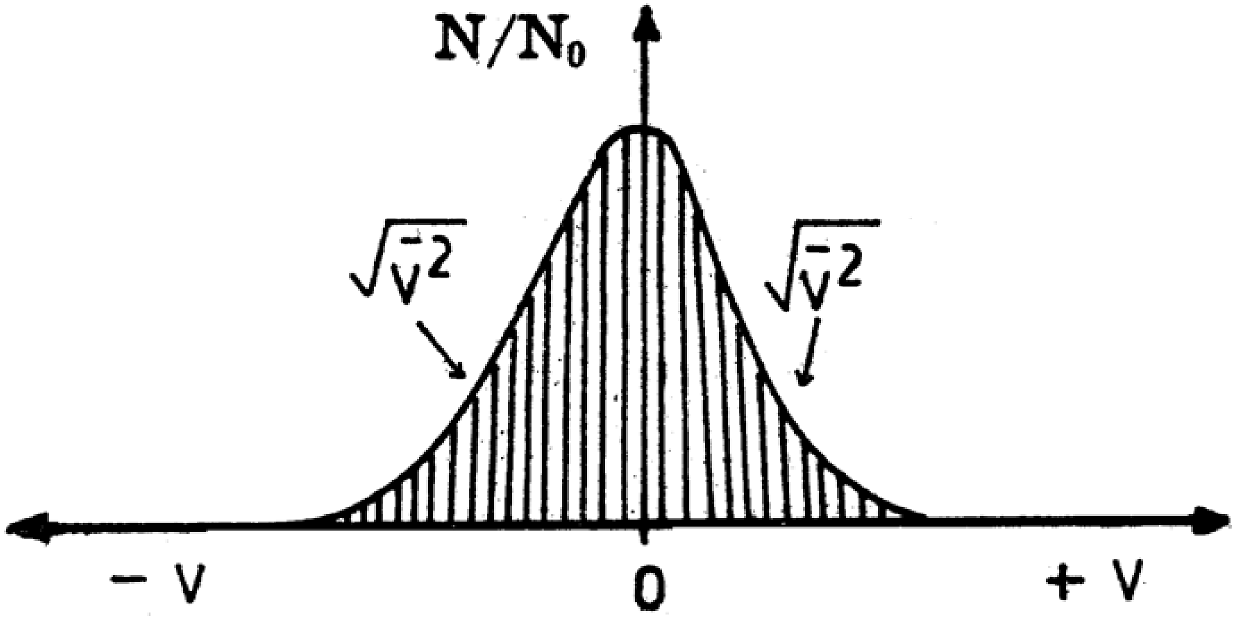
- If the low energy level E_d=0, then V_d=0.

Therefore, instead of N_d, N_0 could be used and equation will be as follows;

$$\ln \frac{N_y}{N_0} = -\frac{mv_y^2}{2kT}$$

Diffusion

- This new equation is also a Gaussion function.
- Each vertical line in the graph, represents the ratio of the number of the particles whose velocities are between v and v+Δv and the number of stable particles.



Diffusion

- According to the kinetic theory of gases, there is a relationship between the kinetic energy of a particle and the absolute temperature of the system.

$$\overline{E} = \frac{1}{2} m \overline{v}^2 = \frac{3}{2} kT$$

k= Boltzmann constant

- Because the movement has 3 dimension, velocity has 3 dimension (V_x, V_y, V_z).
- Therefore, the kinetic energy in one dimension is the 1/3 of the total kinetic energy of the system

$$\overline{E}_x = \frac{1}{2} m \overline{v}_x^2 = \frac{1}{3}\left(\frac{3}{2} kT\right) = \frac{1}{2} kT$$

Diffusion

- The movement of particles (molecules or ions) in aqueous solutions is more complex- than the movements of molecules in gases. Because in these systems, particles are under the effect of friction forces.
- Friction force is proportional to the particle velocity and has opposite direction.
- For example, a particle which has V_x velocity in x-axis is under the effect of the following friction force:

$$F_x = -fV_x$$

f= Friction coefficient

Diffusion

- Friction coefficient for the spherical molecules is:

$$f = 6\pi\eta r$$

$\eta =$ viscosity coefficient of the system

$r =$ radius of the molecule

Diffusion

- By the help of velocity, distance and energy equations, the following formula will be obtained:

$$\bar{x}^2 = \frac{2kT}{f} t_1$$

- This is the 'random walk' of particles in one dimension.
- In 3 dimension the equation will be:

$$\bar{r}^2 = \bar{x}^2 + \bar{y}^2 + \bar{z}^2 = \frac{2kT}{f} t_1 + \frac{2kT}{f} t_1 + \frac{2kT}{f} t_1 = \frac{6kT}{f} t_1$$

Diffusion

- Diffusion coefficient (D)

$$D = \frac{kT}{f} = \frac{kT}{6\pi\eta r}$$

- Diffusion coefficient (D) will vary depending on
  - the absolute temperature,
  - the viscosity of the medium
  - size and shape of the particle
- 'Random walk' equations in 3 dimensions could be written in terms of diffusion coefficient as follows:

$$\bar{x}^2 = 2Dt$$

$$\bar{s}^2 = 4Dt$$

$$\bar{r}^2 = 6Dt$$

Diffusion - Example

- **Question:**

How long will it take for a water molecule to diffuse 0.01 m in three dimensions?

- Diffusion coefficient of a water molecule in room temperature is: $D=2x10^{-9}$ m^2/s

Diffusion - Example

- Solution:

$$\bar{r}^2 = 6Dt$$

$$(0.01)^2 = 6 \times 2 \times 10^{-9} \times t$$

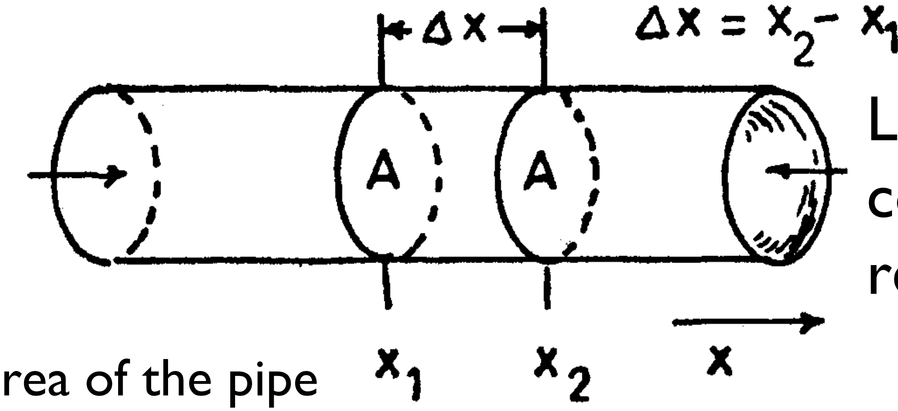
$$t = \frac{10^{-4}}{1.2 \times 10^{-8}} = 8333\,\text{second}\,(2.31\,\text{hour})$$

Fick's Law of Diffusion

- Because the particles in a solution move randomly, the probability of movement in all directions is equal.
- If the molecules are highly concentrated in a region, the number of molecules leaving the area will be more than the number of the molecules arriving this region.
- Thus, there will be a net flow of molecules from highly concentrated region to the low concentrated region. This phenomenon is called "diffusion".

Flow of molecules in one dimension

Highly concentrated region



Low concentrated region

A = Cross-section area of the pipe

Fick's Law of Diffusion

c_1 is the concentration in x_1 and

c_2 is the concentration in x_2

A is the cross-section area of the pipe

Net amount of particle (**Δm**) which flow from x_1 to x_2 in **Δt** time is:

$$\frac{\Delta m}{\Delta t} \alpha (Ac_1 - Ac_2) \quad \text{or} \quad \frac{\Delta m}{\Delta t} \alpha A(c_1 - c_2)$$

With a proportionality constant the equation will be:

$$\frac{\Delta m}{\Delta t} = kA(c_1 - c_2) = -kA\Delta c$$

Fick's Law of Diffusion

- If the x_1 and x_2 planes are too far apart from each other, then the amount of flowing particles between these planes will be very low.
- On the other hand, if these two planes are very close to each other, then the amount of flowing particles will be very high.
- Therefore, **k** constant in Fick's Diffusion equation is inversely proportional with $(x_2 - x_1) = \Delta x$.

$$k = \frac{D}{\Delta x}$$

k is referred to **Fick's diffusion constant**.
D is the **diffusion coefficient**.

Fick's Law of Diffusion

Put **k** equation in the place of the Fick's Diffusion equation and:

$$\frac{\Delta m}{\Delta t} = -kA\Delta c = -\frac{D}{\Delta x}A\Delta c = -DA\frac{\Delta c}{\Delta x} = \frac{\Delta m}{\Delta t}\frac{1}{A} = -D\frac{\Delta c}{\Delta x}$$

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

J: Diffusion flux: the amount of substance per unit area per unit time

Fick's first law postulates that the flux goes from regions of high concentration to regions of low concentration, with a magnitude that is proportional to the concentration gradient (spatial derivative).

Fick's Law of Diffusion

$$\frac{\partial c}{\partial t} = D\frac{\partial^2 c}{\partial^2 x}$$

Fick's second law predicts how diffusion causes the concentration to change with time

If the inial conditions are considered as;

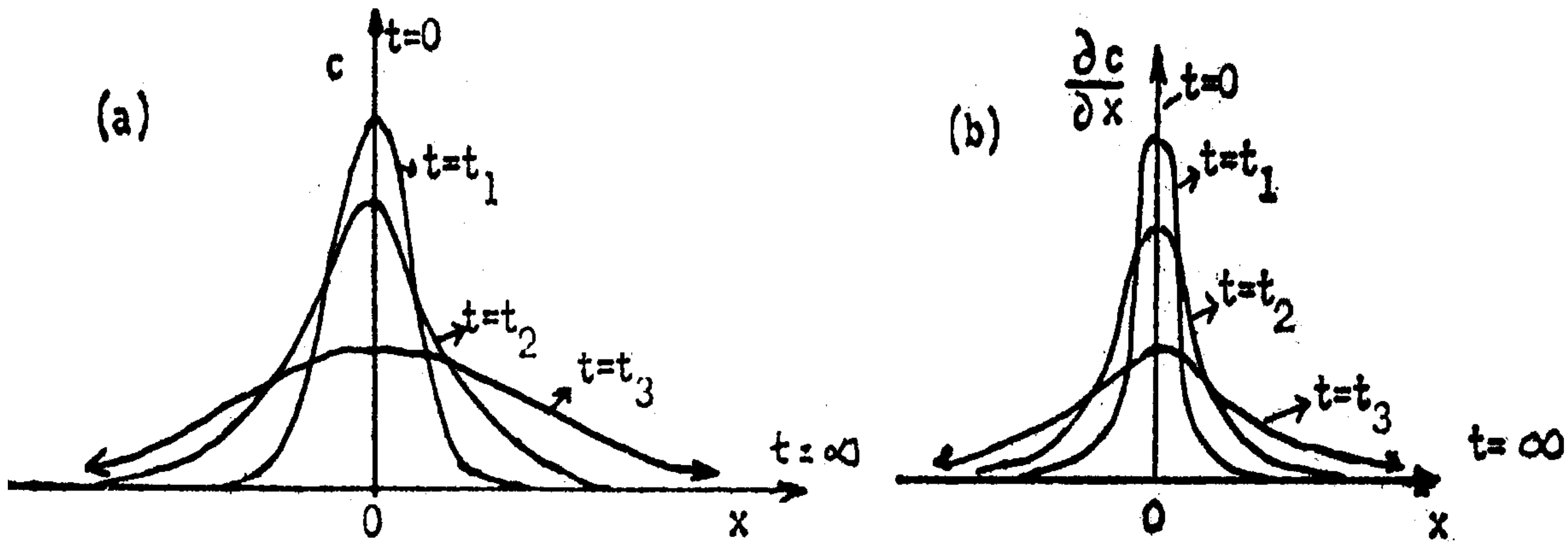
all the particles being in position $x = 0$ at time $t=0$

and in time particles walk away in both directions

then the solution of the equation will be as follows;

$$c = \frac{1}{(4\pi Dt)^{0,5}} e^{-x^2/4Dt}$$

Fick's Law of Diffusion



(a) **The Concentration** and change in time and with distance (b) **The concentration gradient**

References

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