

Physical Principles in Biology
Biology 3550
Fall 2016

Lecture 19
Diffusion and Molecular Motion

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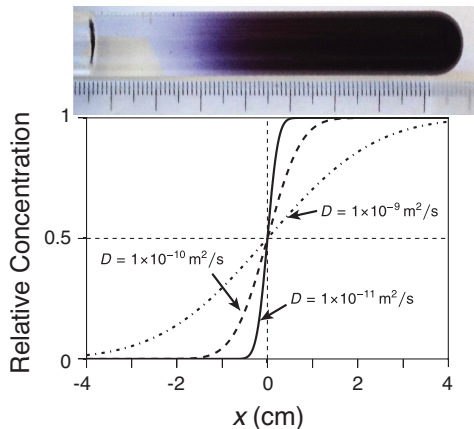
Estimating D from Diffusion from a Sharp Boundary

$$C(x, t) = \frac{1}{2} + \int_0^x \frac{1}{\sqrt{4\pi Dt}} e^{-x^2/(4Dt)} dx$$

$$t = 48 \text{ hr} = 1.7 \times 10^5 \text{ s}$$

$$D \approx 2 \times 10^{-10} \text{ m}^2/\text{s}$$

$$D = \frac{\delta_x^2}{2\tau}$$



What are the average length (δ_x) and duration (τ) of the random walk steps?

Energy and Work

- Energy: the capacity to do work
- Work: The application of force over distance

$$w = \int_a^b F dx$$

- The units of work and energy.
 - Force: Units defined by Newton's second law: $F = \text{mass} \times \text{acceleration}$
SI unit of mass: Kg
Acceleration: change in velocity (m/s) with time. SI units: m/s^2
SI units of Force: $\text{Kg} \cdot \text{m/s}^2$ $1 \text{ N} = 1 \text{ Kg} \cdot \text{m/s}^2$
 - Work or energy: $\text{Kg} \cdot \text{m}^2/\text{s}^2$ $1 \text{ J} = 1 \text{ N} \cdot \text{m} = 1 \text{ Kg} \cdot \text{m}^2/\text{s}^2$

Kinetic Energy

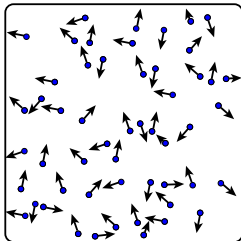
- An object of mass, m , moving with velocity, v_x , in the x -direction has kinetic energy in that direction of:

$$E_{k,x} = mv_x^2/2$$

- The energy required to accelerate the mass, m , from rest to velocity, v_x .
- Also the energy released during the deceleration of the mass from velocity, v_x , to rest.
- Kinetic energy does not depend on the rate of acceleration, only the final velocity.

Kinetic Energy of Molecules

- Temperature is the measure of kinetic energy of molecules.
- How do we measure temperature?
- Pressure of a gas is due to the collision of molecules against container walls.



$$PV = nRT$$

P = pressure, V = volume, n = number of moles, T = temperature,
 R = gas constant.

Clicker Question #1

What are the units of the gas constant?

$$R = \frac{PV}{nT}$$

- 1 pascal · L · K⁻¹ mol⁻¹
- 2 Kg · m² s⁻² K⁻¹ mol⁻¹
- 3 m³ bar · K⁻¹ mol⁻¹
- 4 JK⁻¹ mol⁻¹
- 5 L · atm · K⁻¹ mol⁻¹
- 6 N · m · K⁻¹ mol⁻¹

All of the above!

Units of the Gas Constant

- From the ideal gas law: $R = \frac{PV}{nT}$

- In SI basic units:

Pressure, force per unit area: $\text{Kg} \cdot \text{m} \cdot \text{s}^{-2} \div \text{m}^2 = \text{Kg} \cdot \text{m}^{-1}\text{s}^{-2} = \text{Pa}$

Volume: m^3

Gas constant: $\text{Kg} \cdot \text{m}^2\text{s}^{-2}\text{K}^{-1}\text{mol}^{-1}$

- Joule (unit of energy) = $\text{Nm} = \text{Kg} \cdot \text{m}^2\text{s}^{-2}$
- The gas constant expressed in energy units:

$$R \approx 8.314 \text{ JK}^{-1}\text{mol}^{-1} \approx 1.987 \text{ cal/K}^{-1}\text{mol}^{-1}$$

- RT is proportional to the kinetic energy of one mole of molecules at a temperature T .

Kinetic Energy of Molecules

- The Boltzmann constant, k , the “gas constant per molecule”:

$$\begin{aligned}k &= R/N_A = 8.314 \text{ JK}^{-1}\text{mol}^{-1} \div 6.02 \times 10^{23} \text{ molecule/mol} \\ &= 1.38 \times 10^{-23} \text{ JK}^{-1}\end{aligned}$$

- Molecules at a given temperature do not have unique velocities or kinetic energies.
- Molecules have a broad distribution of energies, with RMS average kinetic energy in each direction (x , y or z):

$$\text{RMS}(E_{k,x}) = kT/2$$

- In context of molecular motion, “ $E_{k,x}$ ” will imply RMS value.

Velocities of Molecules

- Kinetic energy of a molecule, in x -direction: $\text{RMS}(E_{k,x}) = kT/2$
- Kinetic energy of any object: $E_{k,x} = mv_x^2/2$
- Solving for v :

$$mv_x^2/2 = kT/2$$

$$v_x^2 = kT/m$$

$$v_x = \sqrt{kT/m}$$

(also an RMS value)

- Velocity increases with \sqrt{T} and decreases with \sqrt{m} .

Velocity of an N₂ Molecule at Room Temperature

- Mass

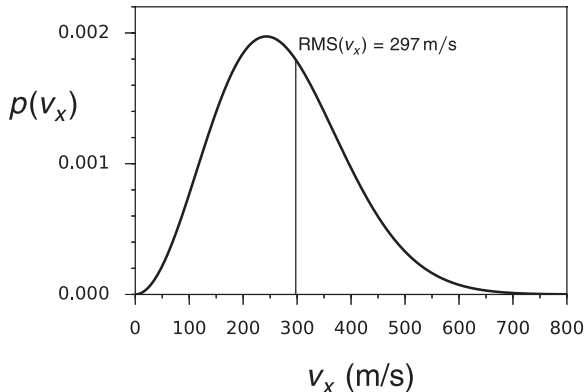
$$\begin{aligned}m &= 28 \text{ g/mol} \div 6.02 \times 10^{23} \text{ molecules/mol} \\ &= 4.65 \times 10^{-23} \text{ g} = 4.65 \times 10^{-26} \text{ Kg}\end{aligned}$$

- Temperature = 25°C = 298 K

- Velocity:

$$\begin{aligned}\text{RMS}(v_x) &= \sqrt{kT/m} \\ &= \sqrt{1.38 \times 10^{-23} \text{ Kg} \cdot \text{m}^2\text{s}^{-2}\text{K}^{-1} \times 298 \text{ K} / 4.65 \times 10^{-26} \text{ Kg}} \\ &\approx 300 \text{ ms} \quad (100 \text{ km/hr})\end{aligned}$$

Distribution of N_2 Velocities in a Gas at 298 K



- The Maxwell-Boltzmann distribution

$$p(v_x) = \left(\frac{m}{2\pi kT} \right)^{3/2} 12\pi v_x^2 e^{-3mv_x^2/(2kt)}$$

(assumes ideal gas behavior)

Diffusion of Bromophenol Blue Revisited

■ From diffusion experiment: $D = 2 \times 10^{-10} \text{ m}^2/\text{s}$

■ Definition of the diffusion coefficient: $D = \frac{\delta_x^2}{2\tau}$.

■ $\delta_x/\tau = \text{velocity}$, which we can calculate now!

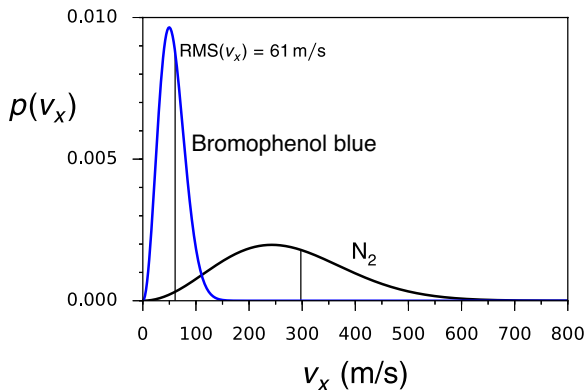
- $v = \sqrt{kT/m}$

- Molar mass = 670 gm/mol

- Molecular mass = $1.11 \times 10^{-24} \text{ Kg}$

$$v = \sqrt{1.38 \times 10^{-23} \text{ Kg} \cdot \text{m}^2\text{s}^{-2}\text{K}^{-1} \times 298 \text{ K} / 1.1 \times 10^{-24} \text{ Kg}}$$
$$= 61 \text{ m/s}$$

Distribution of Velocities at 298 K



- Average (RMS) kinetic energies of molecules are the same.
- Based on ideal gas behavior.
- Distribution is similar in liquids.

Diffusion of Bromophenol Blue Revisited

- $D = \delta_x^2 / (2\tau) = 2 \times 10^{-10} \text{ m}^2/\text{s}$
- Express D in terms of velocity:

$$D = v\delta_x/2$$

- $v = \delta_x/\tau = 61 \text{ m/s}$
- Solve for δ_x

$$\begin{aligned}\delta_x &= 2D/v = 2 \times 2 \times 10^{-10} \text{ m}^2/\text{s} \div 61 \text{ m/s} \\ &= 6.5 \times 10^{-12} \text{ m}\end{aligned}$$

Diffusion of Bromophenol Blue Revisited

- From the previous slide

$$\delta_x = v \cdot \tau = 6.5 \times 10^{-12} \text{ m}$$

- Solve for τ

$$v = \delta_x / \tau$$

$$\begin{aligned}\tau &= \delta_x / v = 6.5 \times 10^{-12} \text{ m} \div 61 \text{ m/s} \\ &= 10^{-13} \text{ s} = 0.1 \text{ ps}\end{aligned}$$

- VERY short distances and times!

RMS Distance of Diffusion

- Random walk along one direction: $\langle x^2 \rangle = n\delta_x^2$

- For diffusion: $D = \frac{\delta_x^2}{2\tau}$

$$\delta_x^2 = 2D\tau$$

$$n = t/\tau$$

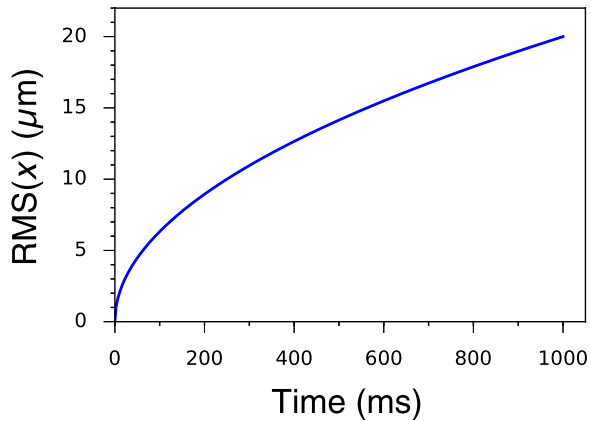
$$\langle x^2 \rangle = n\delta_x^2 = \frac{t}{\tau} \frac{2D\tau}{\tau} = 2Dt$$

$$\text{RMS}(x) = \sqrt{2Dt}$$

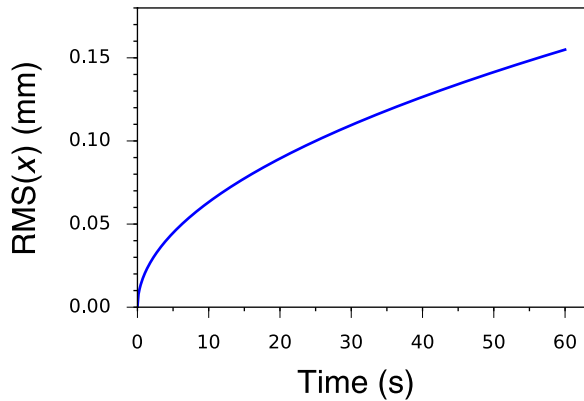
- For bromophenol blue (and molecules of similar size):

$$\text{RMS}(x) = \sqrt{t/s} \times 2 \times 10^{-5} \text{ m}$$

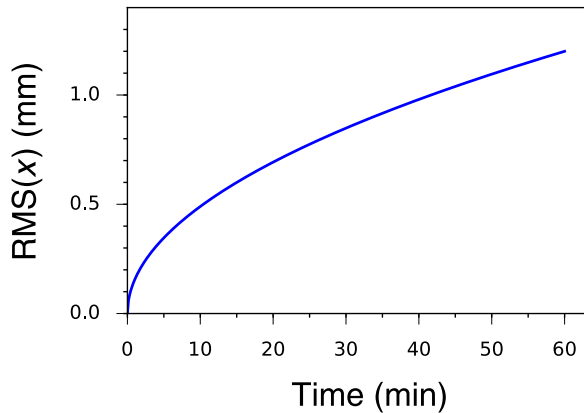
RMS Distance of Diffusion



RMS Distance of Diffusion



RMS Distance of Diffusion



“Velocity” of Diffusion

- RMS(x) as a function of time:

$$\text{RMS}(x) = \sqrt{2Dt} = \sqrt{2D} \cdot t^{1/2}$$

- Derivative of RMS(x) with respect to time:

$$\frac{d\text{RMS}(x)}{dt} = \frac{\sqrt{2D} \cdot t^{-1/2}}{2} = \frac{\sqrt{2D/t}}{2}$$

- Units: $\sqrt{\text{m}^2/\text{s} \div \text{s}} = \sqrt{\text{m}^2/\text{s}^2} = \text{m}/\text{s}$

It's a velocity!

“Velocity” of Diffusion

