# Introduction to Diffusion in Materials Science

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## Outline

- Brownian motion
- Fick's $1^{st}$ and $2^{nd}$ law of diffusion

## 1 Brownian Motion: The Origin of Diffusion

- **Observation**: Random zig-zag motion of pollen grains (Robert Brown, 1827)
- **Modern interpretation**: Thermal motion and collision of atoms/molecules
- **Key characteristics**
  - Uncorrelated: Each step of movement is independent and random
  - For Brownian 1D motion, the chance of find the particle at position $x$ after time $t$:

$$\rho(x,t) = \frac{1}{\sqrt{4\pi Dt}} \exp\left(-\frac{x^2}{4Dt}\right)$$

  - Mean squared displacement: $\langle x^2 \rangle = 2n \cdot Dt$, $n$ is the dimension

## 2 Fick's First Law

**Real-World Motivation: Food Packaging**

**Problem**: Potato chips become stale when oxygen diffuses through plastic packaging. How can we design bags that:

- Extend the shelf life of the product
- Use minimal plastic (reducing cost and environmental impact)

### Steady-State Diffusion

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

- $J$: Flux [mol/m²s]
- $D$: Diffusion coefficient
- $\partial c/\partial x$: Concentration gradient

**Solution for Food Packaging**

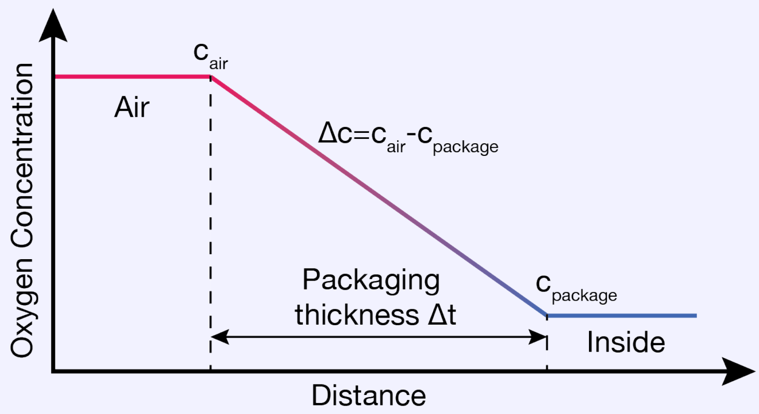
- Staleness: Chips become stale when oils oxidize with oxygen.
- Industrial standard: Oxygen concentration inside packaging $< 0.5\%$ (vs. 21% in air)

$$\boldsymbol{\Delta c = c_{\text{air}} - c_{\text{package}} \simeq 0.21}$$

- Flux requirement: For a standard package with 12-month shelf life,

$$\boldsymbol{J \leq 1 \times 10^{-10}\ \mathrm{mol/(m^2 s)}}, \text{ or, } \boldsymbol{J \leq 2.24 \times 10^{-11}\ m^3/(m^2\mathrm{s})}$$

- Diagram illustration:




- For biaxially oriented polypropylene (BOPP, $D \approx 5 \times 10^{-12}\ \mathrm{m^2/s}$ [1]):

$$\Delta x = \frac{D\Delta c}{J} = \frac{5 \times 10^{-12} m^2/s \times 0.21}{2.24 \times 10^{-11}\, m^3/(m^2\mathrm{s})} \approx 5\ \mathrm{cm}\ \text{(too thick!)}$$

- OPP-LDPE-OPP-PVdC copolymer ($D \approx 5 \times 10^{-14}\ \mathrm{m^2/s}$, 1/100 of BOPP [2] ):

$$\Delta x \approx 0.5\,\mathrm{mm}$$

### Diffusion Coeffient: Arrhenius Equation

$$D = D_0\, e^{-\frac{Q}{RT}}$$

- $D_0$: Pre-exponential factor ($\mathrm{m^2/s}$)
- $Q$: Activation energy [J/mol]
- $R$: Gas constant (8.314 J/mol·K)
- $T$: Absolute temperature [K]

## 3 Fick's Second Law

**Real-World Motivation: Case Hardening for Gears**

**Problem**: Hardened case by carbonization with a ductile core for the trade-off between hardness and toughness.

- What is carbon concentration profile: $c(x,t)$ as a function of distance and time

### Time-Dependent Diffusion

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

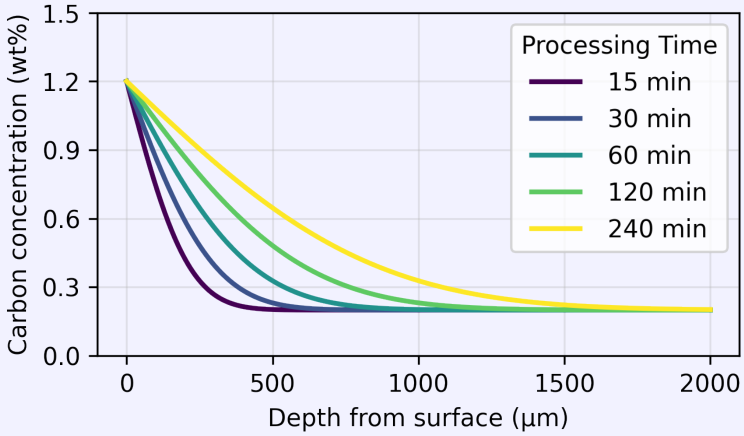
- $c(x,t)$: Concentration at depth $x$, time $t$
- $D$: Diffusivity
- $x$: Depth from surface
- $t$: Time

**Solution for Case Hardening**

With constant boundary concentration, the solution of Fick's second law is

$$c(x,t) = c_s - (c_s - c_0)\,\mathrm{erf}\left(\frac{x}{2\sqrt{Dt}}\right)$$

- $c_s$: Surface concentration (e.g., 1.2% C)
- $c_0$: Initial bulk concentration (e.g., 0.2% C)
- erf: Error function
- $D = 1.5 \times 10^{-11}\,\mathrm{m}^2/\mathrm{s}$ (at 900°C)
- Diagram illustration:




## Key Equations Summary

$$\begin{aligned}
\text{Brownian motion:} &\quad \langle x^2 \rangle = 2Dt \\
\text{Fick's first law:} &\quad J = -D\frac{\partial c}{\partial x} \\
\text{Fick's second Law:} &\quad \frac{\partial c}{\partial t} = D\frac{\partial^2 c}{\partial x^2} \\
\text{Arrhenius Equation:} &\quad D = D_0 e^{-Q/(RT)}
\end{aligned}$$

## Recommended Resources

- Callister, W. *Materials Science and Engineering: An Introduction* (Chapter. 5)
- Shewmon, P. *Diffusion in Solids*

## References

[1] M Trefry and B Patterson. An experimental determination of the effective oxygen diffusion coefficient for a high density polypropylene geomembrane. 2001.

[2] Gordon L Robertson. *Food packaging: Principles and practice, third edition.* CRC Press, 19 April 2016.