$D$ is a function of molecule size, fluid phase, and temperature.

Size: Larger molecules have smaller $D$ ($k$ smaller).

Phase: Freer systems (gases) have larger $D$ ($\delta x$ bigger).

Temp: Hotter systems have larger $D$ ($\delta x$ bigger).

\[ D = k (\delta x)^2 \]

Refer Table 1.1 (Handout)

Typical value of $D$

For water \( \approx O (10^{-9}) \) \( \frac{m^2}{s} \)

For air \( \approx O (10^{-5}) \) \( \frac{m^2}{s} \)

\( \sim O (10^4) \) difference
Example: Diffusion in a lake

Lake contaminated by arsenic

* Show figs 1.5 and 1.6 in Handout *

**Thermocline** at \( z = -3 \text{ m} \), area \( A = 2 \times 10^4 \text{ m}^2 \)

Region of highest density gradient

**Diffusion coefficient (molecular):** \( D_m = 10^{-10} \text{ m}^2/\text{s} \)

**Find:** Magnitude and direction of diffusive flux of arsenic through the thermocline.

Fick's law

\[
\frac{\partial C}{\partial z} = -D_m \frac{\partial^2 C}{\partial z^2} \approx -D_m \frac{C_2 - C_1}{z_2 - z_1}
\]

\[
= -\left(10^{-10}\right) \frac{10 - 6}{-2 - (-4)} \frac{1000 \text{ L}}{1 \text{ m}^3}
\]

\[
= -2.0 \times 10^{-7} \frac{\mu g}{\text{m}^2 \cdot \text{s}} \quad \text{(negative = going downward)}
\]

**Total flux**

\[
\dot{m} = A \frac{\partial C}{\partial z} = (2 \times 10^4) \left(2.0 \times 10^{-7}\right) = 4.0 \times 10^{-3} \frac{\mu g}{\text{s}}
\]

**Note:** In reality, the diffusion coefficient (due to turbulence) at a lake thermocline would be \(10^4\) times larger.
Diffusion Equation

Consider a small control volume

\[ \frac{\partial M}{\partial t} = \sum \dot{m}_{in} - \sum \dot{m}_{out} \]

Conservation of mass:

Consider only the x-direction

\[ \delta \dot{m}_x = \delta_1 \delta y \delta z - \delta_2 \delta y \delta z \]

\[ = (\delta_1 - \delta_2) \delta y \delta z \]

Apply Fick's law

\[ \frac{\partial}{\partial x} \left|_1 \right. \]

\[ = -D \left. \frac{\partial c}{\partial x} \right|_1 \]

\[ \frac{\partial}{\partial x} \left|_2 \right. \]

\[ = -D \left. \frac{\partial c}{\partial x} \right|_2 \]

\[ \delta \dot{m}_x = -D \delta y \delta z \left( \left. \frac{\partial c}{\partial x} \right|_1 - \left. \frac{\partial c}{\partial x} \right|_2 \right) \]
Taylor Series expansion

\[
    f(x_2) = f(x_1 + \delta x) \\
    = f(x_1) + \frac{\partial f}{\partial x} \bigg|_1 \delta x + \frac{1}{2} \frac{\partial^2 f}{\partial x^2} \bigg|_1 (\delta x)^2 + \cdots \underbrace{O(\delta x^3)}_{H.O.T.}, \text{ higher order terms}
\]

Substituting \( \frac{\partial C}{\partial x} \) for \( f \)

\[
    \frac{\partial C}{\partial x} \bigg|_2 = \frac{\partial C}{\partial x} \bigg|_1 + \frac{2}{\partial x} \left( \frac{\partial C}{\partial x} \right) \bigg|_1 \delta x + O(\delta x^2)
\]

Substitute back to \( \delta m_x \)

\[
    \delta m_x = -D \delta y \delta z \left[ \frac{\partial C}{\partial x} \bigg|_1 - \left( \frac{\partial C}{\partial x} \bigg|_1 + \frac{2}{\partial x} \left( \frac{\partial C}{\partial x} \right) \bigg|_1 \right) \delta x + O(\delta x^2) \right]
\]

\[
    \approx + D \frac{\partial^2 C}{\partial x^2} \delta x \delta y \delta z \quad \text{(neglect the H.O.T.)}
\]

Similarly for \( y \) \& \( z \) directions

\[
    \delta m_y = + D \frac{\partial^2 C}{\partial y^2} \delta x \delta y \delta z
\]

\[
    \delta m_z = + D \frac{\partial^2 C}{\partial z^2} \delta x \delta y \delta z
\]

Since \( \delta M = C \delta x \delta y \delta z \) and \( \delta m = \frac{\partial m}{\partial t} \)

\[
    = \frac{\partial C}{\partial t} \delta x \delta y \delta z
\]

Substitute back to conservation of mass, \( \sum \delta m_{in} - \sum \delta m_{out} = \delta m_x + \delta m_y + \delta m_z \)
\[ \frac{\partial C}{\partial t} \delta x \delta y \delta z = \left( D \frac{\partial^2 C}{\partial x^2} + D \frac{\partial^2 C}{\partial y^2} + D \frac{\partial^2 C}{\partial z^2} \right) \delta x \delta y \delta z \]

\[ \frac{\partial C}{\partial t} = D \left( \frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2} + \frac{\partial^2 C}{\partial z^2} \right) \]

or

\[ \frac{\partial C}{\partial t} = D \nabla^2 C \]

(or \( \frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x_i^2} \) in tensor form)

This is the diffusion equation.

Note: The diffusion equation is the same as the heat equation. It is a parabolic PDE requiring initial & boundary conditions to solve.

Example: Steady concentration profile in a narrow channel with zero velocity

\[ C_1 \quad \quad \quad C_2 \]

\[ x = 0 \quad L \quad x = L \]

\( C_1, C_2 \) : fixed concentrations

narrow: \( 1D \), \( \frac{\partial}{\partial y} \) & \( \frac{\partial}{\partial z} = 0 \)

steady: \( \frac{\partial}{\partial t} = 0 \)
Diffusion eqn: \[
\frac{\partial^2 C}{\partial x^2} = 0
\]

Integrate twice: \[
C = C_1 x + C_2^* \quad C_1, C_2 = \text{constant}
\]

BCs: \[
C(x=0) = C_1 \quad \Rightarrow C_2^* = C_1
\]
\[
C(x=L) = C_2 \quad \Rightarrow C_1^* = \frac{C_2 - C_1}{L}
\]

\[
C = \frac{C_2 - C_1}{L} x + C_1 \quad (\text{concentration profile is linear})
\]

Next,

Using perfume example \(\Rightarrow\) solve for point source problem.