

A. Fick's Laws of Diffusion

For a species A in solution, its concentration becomes a function of both space and time:

$$C_A(x, t)$$

$$J_A = -D_A \frac{\partial C_A}{\partial x} \quad \text{Fick's First Law of Diffusion}$$

$$\frac{\partial C_A}{\partial t} = -\frac{\partial J_A}{\partial x} = D_A \frac{\partial^2 C_A}{\partial x^2} \quad \text{Fick's Second Law of Diffusion}$$

D_A is the diffusion constant for species A.

B. Instantaneous Plane Source Solution

Boundary Conditions:

$$C_A(x = 0, t = 0) =$$

$$C_A(x \neq 0, t = 0) = 0$$

Solution:

$$C_A = \frac{N_A}{2(\sqrt{D_A t})} \exp\left[-\frac{x^2}{4D_A t}\right]$$

where N_A is the total number of molecules:

$$N_A = \int_{-\infty}^{+\infty} C_A dx$$

C. Spreading Probability

What is the probability that a molecule has diffused a distance x in time t ?

We define $p(x)dx$ is the probability that a molecule has diffused to a region between x and $x + dx$:

$$p(x)dx = \frac{C_A}{N_A} dx = \frac{1}{2(\sqrt{D_A t})^{1/2}} \exp\left[-\frac{x^2}{4D_A t}\right] dx$$

The mean square distance diffused by a molecule in time t is:

$$\langle x^2 \rangle = \int_{-\infty}^{+\infty} x^2 p(x) dx = 2D_A t$$

$$\sqrt{\langle x^2 \rangle} = \sqrt{2D_A t}$$

