Mathematics of Diffusion Problems

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Outline

1. Physical background;
2. General derivation of the diffusion equation;
3. One-dimensional problems;
4. Examples of applied problems;
5. Measurements of the diffusion coefficient.

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Particle density

Number of particles in a unit volume:

$$n(x, y, z, t)$$

Number of particles in an arbitrary volume Ω:

$$N(t) = \int_{\Omega} n \, d^3x$$

Change of $N(t)$ in an arbitrary volume:

$$\frac{dN}{dt} = (income) - (outcome)$$

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Income

It is convenient to let "incomes" be positive and negative so that we may write:

$$\frac{dN}{dt} = \sum(income)$$

There are two different reasons for changes in $N(t)$

- Volume income ("birth" (positive) and "death" (negative))
- Fluxes over the boundaries ("migration")

Volume sources

Number of particles that are created in a unit volume per unit time

$$q(x, y, z, t, n \ldots)$$

The corresponding change of $N(t)$ can be quantified

$$\frac{dN}{dt} = \int_{\Omega} q \; d^3x$$

Different source terms are possible

Predefined external source	$q(x, y, z, t)$
Chemical reaction	$q = \pm kn$
Nonlinear source, e.g.,	$q \sim n^2$

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Flux

Number of particles that flow through a unit surface per unit time

$$\mathbf{j}(x, y, z, t)$$

The corresponding change of $N(t)$ can be quantified

$$\frac{dN}{dt} = -\int_{\partial\Omega} \mathbf{j}\, d\mathbf{S}$$

Divergence theorem

$$\frac{dN}{dt} = -\int_{\Omega} (\nabla\mathbf{j})\, d^3x$$

Where

$$\nabla\mathbf{j} = \frac{\partial j_x}{\partial x} + \frac{\partial j_y}{\partial y} + \frac{\partial j_z}{\partial z}$$

Derivation

By the definition of $N(t)$

$$\frac{dN}{dt} = \frac{d}{dt}\int_\Omega n \; d^3x = \int_\Omega \frac{\partial n}{\partial t} \; d^3x$$

Fluxes and sources

$$\frac{dN}{dt} = \int_\Omega (-\nabla \mathbf{j} + q) \; d^3x$$

Therefore

$$\int_\Omega (\partial_t n + \nabla \mathbf{j} - q) \; d^3x = 0$$

that is valid for an arbitrary volume.

Continuity equation

We have just derived

One of the most important physical equations

$$\frac{\partial n}{\partial t} + \nabla \mathbf{j} = q$$

However we have only one equation for both n and $\mathbf{j}$.
The continuity equation can not be used as is, a physical model, e.g.,

$$\mathbf{j} = \mathbf{j}(n)$$

is required.

Flux models

Flux is caused by spatial changes in $n(x, y, z, t)$.

It is natural to assume that $\mathbf{j} \sim \nabla n$.

The proportionality coefficient is denoted $-D$.

- Fick's first law (for particles) $\mathbf{j} = -D\nabla n$.
- Nonuniform diffusion $\mathbf{j} = -D(x, y, z)\nabla n$.
- Non-isotropic diffusion $j_k = -\sum_{i=x,y,z} D_{ki}\partial_i n$.
- Non-linear diffusion $\mathbf{j} = -D(n)\nabla n$.
- Fourier's law (for energy) and many others.

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Diffusion equation

Having a physical model (**diffusion**) we can proceed with the derivation of a self-consistent mathematical equation:

$$\partial_t n + \nabla \mathbf{j} = q$$

$$\mathbf{j} = -D \nabla n$$

We have just obtained another fundamental equation

$$\partial_t n = \nabla (D \nabla n) + q$$

Let us consider only a uniform isotropic medium

$$\partial_t n = D \nabla (\nabla n) + q$$

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Laplacian

It is convenient to introduce the following notation

$$\triangle n = \nabla(\nabla n)$$

where

$$\triangle n = \frac{\partial^2 n}{\partial x^2} + \frac{\partial^2 n}{\partial y^2} + \frac{\partial^2 n}{\partial z^2}$$

E.g., stationary distributions of particles are given by the famous

Laplace (Poisson) equation

$$D \triangle n = -q$$

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Resume

Linear diffusion equation in 1D

$$\boxed{\frac{\partial n}{\partial t} = D\frac{\partial^2 n}{\partial x^2} + q(x,t)}$$

- $n = n(x,t)$ should be found;
- $D = \mathrm{const}$ and $q = q(x,t)$ are known;
- the solution should exist for all $t \geq 0$;
- the initial distribution $n_0(x) = n(x,0)$ is known;
- $a < x < b$ with the boundary conditions at $x = a$ and $x = b$;
- $x > 0$ and $-\infty < x < \infty$ are also possible.

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Boundary conditions

1. Dirichlet: edge concentrations are given, e.g.,

$$n(x = a, t) = 1$$

2. Neumann: edge fluxes are given, e.g.,

$$\partial_x n(x = b, t) = 0$$

3. More complicated: e.g., combined Dirichlet and Neumann

$$\Big[\alpha(t)n(x,t) + \beta(t)\partial_x n(x,t)\Big]_{x=a,b} = \gamma(t)$$

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Delta function

It was first introduced by Dirac to represent a unit point mass.

The physical definition of $\delta(x-a)$ (e.g., mass density) is

$$\begin{aligned} \delta(x-a) &= 0 && \text{if } x \neq a \\ \delta(x-a) &= \infty && \text{if } x = a \end{aligned}$$

and

$$\int_{-\infty}^{\infty} \delta(x-a)\, dx = 1$$

so that we have a unit mass at $x = a$.

Point source

Let N particles be initially placed at $x = a$. Their concentration $n(x, t)$ is subject to the diffusion equation

$$\partial_t n(x, t) = D\partial_x^2 n(x, t)$$

with

- $-\infty < x < \infty$,

where one usually assumes that

$$n(x, t) \to 0 \quad \text{at} \quad x \to \pm\infty;$$

and the following initial condition

- $n(x, 0) = N\delta(x - a)$.

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Kernel solution

The "point source" problem can be solved explicitly

$$n(x,t) = NK(x,a,t),$$

where the kernel solution

$$K(x,a,t) = \frac{1}{\sqrt{4\pi Dt}} \exp\left[-\frac{(x-a)^2}{4Dt}\right].$$

Here

- $\partial_t K = D\partial_x^2 K$;
- $K(x,a,t) = K(a,x,t)$;
- $\lim_{x\to\pm\infty} K(x,a,t) = 0$;
- $\lim_{t\to+\infty} K(x,a,t) = 0$;
- $\lim_{t\to 0} K(x,a,t) = \delta(x-a)$.

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Initial value problem

We can now give a formal solution of the initial value problem

$$\partial_t n(x,t) = D\partial_x^2 n(x,t),$$

where

- $-\infty < x < \infty$;
- $\lim_{|x|\to\infty} n(x,t)$ is finite;
- $n(x,0) = n_0(x)$.

One replaces N with $n_0(a)da$ for each $x = a$ and uses linearity

$$n(x,t) = \int_{-\infty}^{\infty} K(x,a,t) n_0(a) da.$$

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Diffusion problem with a source term

Problem with the trivial initial distribution $n_0(x) = 0$ and a source term

$$\partial_t n(x,t) = D\partial_x^2 n(x,t) + q(x,t)$$

where

- $-\infty < x < \infty$;
- $\lim_{|x|\to\infty} n(x,t)$ is finite;
- $n(x,0) = 0$.

The idea of solution is similar. The results reads

$$n(x,t) = \int_{-\infty}^{\infty}\int_0^t K(x,a,t-\tau)q(a,\tau)d\tau da.$$

General diffusion problem

It is also easy to solve the general problem

$$\partial_t n(x,t) = D\partial_x^2 n(x,t) + q(x,t),$$

where

- $-\infty < x < \infty, \quad n(x,0) = n_0(x);$
- $\lim_{|x|\to\infty} n(x,t)$ is finite.

The solution is a simple combination of the two previous results:

$$n(x,t) = \int_{-\infty}^{\infty} K(x,a,t) n_0(a) da + \\ + \int_{-\infty}^{\infty}\int_0^t K(x,a,t-\tau) q(a,\tau) d\tau da.$$

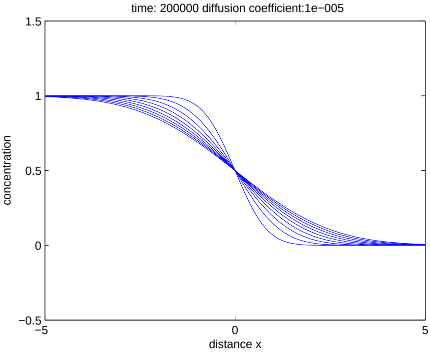
Application

This is an important standard situation for many applications:

$$\partial_t n(x,t) = D\partial_x^2 n(x,t),$$

where

$$n_0(x) = \begin{cases} 1 & \text{for} \quad x < 0, \\ 0 & \text{for} \quad x > 0. \end{cases}$$



The solution reads

$$n(x,t) = \frac{1}{2}\,\mathrm{Erf}\left(\frac{x}{2\sqrt{Dt}}\right),$$

$$\mathrm{Erf}(x) = \frac{2}{\sqrt{\pi}}\int_0^x e^{-s^2}\,ds.$$

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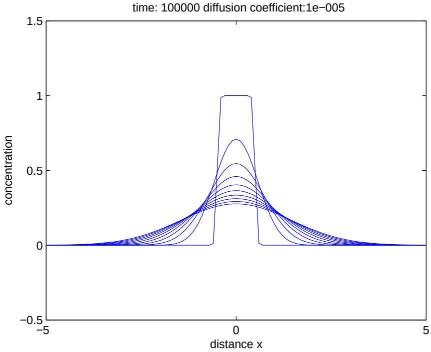
Another application

Another important standard solution of

$$\partial_t n(x,t) = D\partial_x^2 n(x,t),$$

where

$$n_0(x) = \begin{cases} 1 & \text{if } a < x < b, \\ 0 & \text{otherwise.} \end{cases}$$



The solution is found by a direct integration

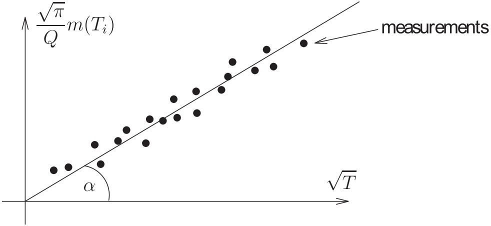
$$n(x,t) = \frac{1}{2}\left[\mathrm{Erf}\left(\frac{x-b}{2\sqrt{Dt}}\right) - \mathrm{Erf}\left(\frac{x-a}{2\sqrt{Dt}}\right)\right].$$

How D can be measured

We start from the standard solution $n(x,t) = \frac{1}{2}\,\mathrm{Erf}\left(\frac{x}{2\sqrt{Dt}}\right)$,

and measure amount of particles $m(T)$ that have passed through $x = 0$ into the region $x > 0$ as a function of time T

$$m(T) = \text{Area} \int_0^T (-D\partial_x n)_{x=0}\, dt = Q\sqrt{\frac{DT}{\pi}}$$



The dependence m vs $\sqrt{T}$ is linear and therefore

$$D = \frac{\pi \tan^2 \alpha}{Q^2}.$$