Nuclear Reactor Physics

Diffusion equation

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Course info

Info about in-house (simulator) labs

In-house (simulator) labs

- In-house labs will run during end of October to end of November.
- Book a time slot In Canvas Calendar.
- A time slot can be booked by up to three students.
- Lab instructors will be Yi Meng Chan and Dmitry Grishchenko.
- The lab takes 3 hours.
- The meeting point is in front of **my office corridor B51 (5th floor) either at 9:00 or 13:00 (SHARP!)**.
- The “labs” folder in Canvas Files already contains:
  - **lab instructions**,
  - instructions on **how to write a technical report**
  - instructions on **how your report will be graded**,
  - a **list of acronyms for common stylistic errors**.
- Although labs are done in groups, lab reports are **individual**.
- You can revise the report **once**.

Deadlines for all labs

Deadlines for in-house simulator lab report:

- **December 12: Draft of the report** (if you upload the draft after the deadline then you will not receive any comments on it).
- **January 10: Final report** (if you upload the report after the deadline then the report will be graded, but the number of points will be divided by 2).

These reports will be graded by Yi Meng Chan <ymchan@kth.se> and Dmitry Grishchenko <dmitrygr@kth.se>.

Deadlines for VR-1 lab report:

- **December 19: Draft of the report** (if you upload the draft after the deadline then you will not receive any comments on it).
- **January 13: Final report** (if you upload the report after the deadline then the report will be graded, but the number of points will be divided by 2).

These reports will be graded by Vasily Arzhanov <arzhanov@kth.se>.

Diffusion approximation

What kind of calculations is the neutron diffusion approximation used in?

The **diffusion approximation** is the simplest deterministic method that allows to compute the neutron flux distribution in the system.

What are the simplifications made in the diffusion approximation?

- **Neutrons are mono-energetic** (all having the same speed). Hence, in the diffusion approximation, the neutron flux $\phi(E)$ and reaction rates $\Sigma(E)\phi(E)$ do not depend on the neutron energy E (speed v), and so, they are group constants. We will denote the group flux and macroscopic cross sections simply as ϕ and Σ, resp. **These variables still depend on the position.**
- **Neutrons scatter isotropically**. (It is assumed that neutron behavior is chaotic, similar to behavior of gas molecules.)

Fick's law

The neutron diffusion approximation is based on the Fick's law (originally used to account for chemical diffusion of a solute in solutions).

What are the basic ideas of the Fick's law?

- The idea is: neutrons diffuse **from the region of higher neutron concentration to the region of lower neutron concentration**.
- It was also found that the rate of flow is proportional to the **negative of the gradient** of the neutron concentration.

Fick's law

What is the physical meaning of the neutron current J_x in x-direction?

$J_x(\vec{x})$ equals the **net** number of neutrons that pass per unit time through a unit area perpendicular to the x-direction at $\vec{x}$ (J_x has the same unit as ϕ).

Calculate $J_x(\vec{x})$ for the case when 200 neutrons per second pass in the negative direction through a unit area (perpendicular to x-axis) at $\vec{x}$ and 100 neutrons per second pass in the positive direction through the same area at $\vec{x}$

In this case, $J_x(\vec{x})$ is negative and equals -100 neutrons per second.

Fick's law

Assume you know neutron currents in x, y and z directions at $\vec{x}$. How can you then calculate the current in an arbitrary direction $\vec{\omega}$? (Note that $\vec{\omega}$ is always a unit vector.)

Let's denote the neutron currents in x, y and z directions as J_x, J_y and J_z, and let $\vec{J} = (J_x, J_y, J_z)$ be the **neutron current density vector** or simply **the current**. If $\vec{\omega}$ is a unit vector pointing in any arbitrary direction then

$$\vec{J} \cdot \vec{\omega} = J_x\omega_x + J_y\omega_y + J_z\omega_z = J_\omega$$

equals the net flow of neutrons per second per unit area normal to the direction of $\vec{\omega}$.

Express the Fick's law for the neutron flux mathematically for 1-D problems (e.g. in x-direction).

Suppose that ϕ varies along the x-direction as shown on the figure then Fick's law is written as

$$J_x = -D\frac{d\phi}{dx}$$

The parameter D is called the diffusion coefficient (with unit of cm).

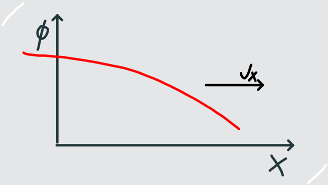

Figure 1: Diffusion of neutrons.

Fick's law

Express the Fick's law for the neutron flux mathematically for 3-D problems.

As the neutron flux $\phi(\vec{r})$ is a function of three spatial variables, the Fick's law can be written as

$$\vec{J} = -D \,\mathrm{grad}\, \phi = -D \nabla \phi$$

where $\vec{J}$ is the **neutron current density vector** or simply **the current**.

To better understand the meaning of the diffusion coefficient D we need to use a new variable "transport mean free path" λ_{tr}. What is the physical meaning of λ_{tr}?

The transport mean free path λ_{tr} is an average distance a neutron will move in its original direction after an infinite number of scattering collisions.

Note that $\Sigma_{tr} = 1/\lambda_{tr}$ is called the macroscopic transport cross section.

Fick's law

Calculation of the transport mean free path λ_{tr}

- The value of λ_{tr} closely relates to the average value $\bar{\mu}$ of the cosine of the angle in the lab system at which neutrons are scattered in the medium. For most neutron energies it holds that

$$\bar{\mu} = \frac{2}{3A}$$

- After each collision, the neutron's direction may be shifted from its original direction, and, the projection of the path between the collisions into the original direction get smaller and smaller, by the factor $\bar{\mu}$ after each collision.
- We can then calculate λ_{tr} as

$$\lambda_{tr} = \lambda_s + \lambda_s\bar{\mu} + \lambda_s\bar{\mu}^2 + \ldots = \frac{\lambda_s}{1 - \bar{\mu}}$$

Fick's law

What is the relation between the diffusion coefficient D and the transport mean free path λ_{tr}?

It can be shown that D is given approximately by

$$D = \frac{\lambda_{\mathrm{tr}}}{3}$$

What are the limitations of the Fick's law? At which situation the Fick's law is not accurate?

Fick's law is not accurate:

- about 3 mfp **around (and inside) strong sources or absorbers**,
- around interfaces between various environments,
- when scattering is strongly anisotropic.

The equation of continuity

The neutron transport can be mathematically expressed via the so-called equation of continuity

The equation of continuity states that the **time rate of change of the number of neutrons**, a, in a volume V is given by a combination of several terms:

$$a = b - c - d$$

Suggest the physical meaning of the above terms

- the **rate of production**, b, of neutrons in V
- minus the **rate of absorption**, c, of neutrons in V
- minus the **rate of leakage**, d, of neutrons from V.

The equation of continuity

a - the time rate of change of the number of neutrons in a volume V.

- The number of neutrons in V is

$$\int_V n dV$$

where n is the neutron density at any point and time in V.

- The rate of change in the number of neutrons is then

$$\frac{d}{dt}\int_V n dV$$

which equals

$$a = \int_V \frac{\partial n}{\partial t} dV = \int_V \frac{1}{v}\frac{\partial \phi}{\partial t} dV$$

The equation of continuity

The rate of production, b, of neutrons in a volume V.

Let s be the rate at which neutrons are emitted from sources per cm^3 in V. (Neutron emission from fission and other nuclear reactions are included here.) The rate at which neutrons are produced in V is then

$$b = \int_V s dV$$

The rate of absorption, c, of neutrons in a volume V.

The rate at which neutrons get lost by absorption per cm^3 is equal to $\Sigma_a \phi$, where Σ_a is the macroscopic absorption cross section. The total loss rate of neutrons due to absorption in V is then

$$c = \int_V \Sigma_a \phi dV$$

The equation of continuity

The rate of leakage, d, of neutrons from V.

- If $\vec{J}$ is the current density vector on the surface of V and $\vec{n}$ is a unit normal vector pointing outward from the surface, then

$$\vec{J} \cdot \vec{n}$$

  is the **net** number of neutrons passing outward through the surface per cm^2/sec (may be positive or negative).

- The rate of leakage of neutrons through the surface A of volume V is then

$$\int_A \vec{J} \cdot \vec{n} \, dA$$

The equation of continuity

The leakage term, $\int_A \vec{J} \cdot \vec{n}\, dA$, is a surface integral over the surface A of the volume V. Is it possible to convert it into an integral over the volume V?

- The surface integral

$$d = \int_A \vec{J} \cdot \vec{n}\, dA$$

can be transformed into a volume integral by using the divergence theorem:

$$\int_A \vec{J} \cdot \vec{n}\, dA = \int_V \mathrm{div}\vec{J}\, dV$$

where

$$\mathrm{div}\vec{J} = \nabla \cdot \vec{J}$$

- Therefore,

$$d = \int_V \mathrm{div}\vec{J}\, dV$$

The equation of continuity

The equation of continuity now has the following form:

$$\int_V \frac{1}{v}\frac{\partial \phi}{\partial t} dV = \int_V s dV - \int_V \Sigma_a \phi dV - \int_V \mathrm{div}\vec{J}\, dV$$

Can we simplify the above equation somehow?

- Since the equation of continuity must hold for any volume V the integrands on the right when summed must equal the integrand on the left.
- Therefore it holds that:

$$\frac{1}{v}\frac{\partial \phi}{\partial t} = s - \Sigma_a \phi - \mathrm{div}\vec{J}$$

State the steady-state equation of continuity.

In steady-state, the time derivative is zero, and the equation becomes

$$0 = s - \Sigma_a \phi - \mathrm{div}\vec{J}$$

The diffusion equation

The equation of continuity contains two unknowns: the neutron flux and the neutron current. How can we solve this problem?

We can apply the Fick's law here, and convert the neutron current in the eq. of continuity into the neutron flux. The resulting equation is called the **diffusion equation**.

- The Fick's law states
$$\vec{J} = -D\nabla\phi$$
- Applying the law on the term $\mathrm{div}\vec{J}$ gives
$$\mathrm{div}\vec{J} = -\mathrm{div}D\nabla\phi = -\nabla \cdot D\nabla\phi$$
- This can be written for systems where D is not dependent on the position (homogeneous systems) as
$$-D\nabla^2\phi$$
where $\nabla^2 = \mathrm{div}\,\mathrm{grad}$ is called the Laplacian (sometimes denoted as Δ).

The diffusion equation

- The diffusion equation has the resulting form

$$\frac{1}{v}\frac{\partial \phi}{\partial t} = s - \Sigma_a \phi + \nabla \cdot D \nabla \phi$$

- and for homogeneous systems:

$$\frac{1}{v}\frac{\partial \phi}{\partial t} = s - \Sigma_a \phi + D \nabla^2 \phi$$

- For time-independent problems the **steady-state diffusion equation** (for homogeneous systems) becomes

$$D \nabla^2 \phi - \Sigma_a \phi + s = 0$$

which is often divided by D and written as

$$\nabla^2 \phi - \frac{1}{L^2}\phi + \frac{s}{D} = 0$$

where

$$L^2 = \frac{D}{\Sigma_a}$$

is called the diffusion area.

What is the physical meaning of the diffusion area?

The diffusion area L^2 equals one-sixth the average square of the straight distance a neutron travels from its origin to its absorption

$$L^2 = \frac{1}{6}\overline{r^2}$$

Boundary equation

Can you give examples of common boundary conditions for the diffusion equation?

The diffusion equation is a partial differential equation, so we need to specify boundary conditions to obtain a solution. Examples:

- **Reflective boundary condition**: the gradient of the flux on the boundary is zero.
- **Void boundary condition** (also known as black boundary condition) for systems that neutrons can leave but cannot re-enter. Higher order methods suggest that the diffusion approximation may give acceptable solution for systems with the void boundary condition when the flux function is assumed to hit zero at a small **extrapolation distance** d beyond the surface. (Beware however, that the flux computed this way has no relevance outside the system.)

How can we calculate the extrapolation distance d?

For most cases, the extrapolation distance may be taken as

$$d = 0.71\lambda_{\mathrm{tr}}$$

Solutions of the diffusion equation - infinite planar source

Let's assume the case of an infinite planar source (perpendicular to x-axis) emitting S neutrons per cm^2/sec in an infinite diffusing medium.

Can we simplify the diffusion equation for this case?

- As the source is fixed in time we may assume only steady-state solution.
- No variation in the y or z direction $\Rightarrow \phi$ is a function of x only.
- Solution must by symmetrical about $x = 0 \Rightarrow$ solution can be obtained for $x > 0$ only and mirrored for $x < 0$.
- As there is no source for $x > 0$ the diffusion equation

$$\nabla^2\phi - \frac{1}{L^2}\phi + \frac{s}{D} = 0$$

becomes for $x > 0$

$$\nabla^2\phi - \frac{1}{L^2}\phi = 0$$

Solutions of the diffusion equation - infinite planar source

The general solution is

$$\phi = Ae^{-x/L} + Ce^{x/L}$$

What is the value of the C constant?

Since the second term in

$$\phi = Ae^{-x/L} + Ce^{x/L}$$

increases to infinity for $x \to \infty$, it follows that $C = 0$
(The system cannot have an infinite neutron flux at infinite distance from the source.)

Therefore,

$$\phi = Ae^{-x/L}$$

Solutions of the diffusion equation - infinite planar source

How can we calculate the value of A in equation $\phi = Ae^{-x/L}$?

- For $x \to 0^+$, half of the source neutrons is emitted to the negative and other half to the positive x direction. Therefore,

$$\lim_{x \to 0^+} J(x) = \frac{S}{2}$$

- From Fick's law,

$$J_x = -D\frac{d\phi}{dx} = \frac{DA}{L}e^{-x/L}$$

- Hence,

$$\lim_{x \to 0^+} \frac{DA}{L}e^{-x/L} = \frac{DA}{L} = \frac{S}{2}$$

$$\Rightarrow A = \frac{SL}{2D}$$

- The solution for $x > 0$ is thus $\phi = \frac{SL}{2D}e^{-x/L}$, and the solution for all x must be

$$\phi = \frac{SL}{2D}e^{-|x|/L}$$

In the same way, we could also derive the solution of the diffusion equation for the infinite homogeneous system with a point source of neutrons.

The solution is

$$\phi = \frac{S}{4\pi D}\frac{e^{-r/L}}{r}$$