Aalto University
School of Science
and Technology

PHYS-E0562 Nuclear Engineering, advanced course
Lecture 4 – Diffusion theory

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Topics of this lecture

Derivation of diffusion theory:

- Transport theory revisited
- Neutron continuity equation
- Multi-group condensation
- Fick's law

Validity of diffusion approximation:

- Limitations of the method
- Physical interpretation of the diffusion coefficient

Solution In homogeneous medium:

- Separation of variables using one-group diffusion theory
- Time dependent amplitude function and Helmholtz equation for spatial dependence
- Point-kinetics approximation and k-eigenvalue equation
- Generalization to other geometries and multiple energy groups
- Boundary conditions

Transport theory: basic concepts revisited

As discussed in Lecture 2, deterministic transport theory describes the collective behavior of the neutron population using the concept of (angular) neutron flux, which is defined using the (angular) neutron density n and speed v:

$$\psi(\boldsymbol{r}, \hat{\boldsymbol{\Omega}}, E) = vn(\boldsymbol{r}, \hat{\boldsymbol{\Omega}}, E) \tag{1}$$

Both angular density and flux are density-like functions in the six-dimensional phase-space, depending on the position, direction of motion and energy of the neutrons.

The angular flux relates the collective motion of neutrons to physical reaction rates:

$$dR_x = \Sigma_x(\boldsymbol{r}, \hat{\boldsymbol{\Omega}}, E)\psi(\boldsymbol{r}, \hat{\boldsymbol{\Omega}}, E)dV\, d\hat{\boldsymbol{\Omega}} dE \tag{2}$$

The product of angular flux ψ and macroscopic cross section Σ gives the corresponding reaction rate density, which when integrated over the variables gives the corresponding reaction rate:[1]

$$R_x = \int_V \int_{\hat{\boldsymbol{\Omega}}} \int_E \Sigma_x(\boldsymbol{r}, \hat{\boldsymbol{\Omega}}, E)\psi(\boldsymbol{r}, \hat{\boldsymbol{\Omega}}, E)dV\, d\hat{\boldsymbol{\Omega}} dE \tag{3}$$

[1] From Lecture 2 it is recalled that the integration of neutron flux over space, direction, energy and time gives the total combined path length traveled by the neutrons, and that the macroscopic cross section is defined as the interaction probability per path length. This is also the physical principle behind the track-length estimate of neutron flux used in Monte Carlo simulation for calculating integral reaction rates, as discussed in Lecture 3.

Transport theory: basic concepts revisited

For scattering reactions the product of angular flux and the double-differential scattering cross section describes the differential reaction rate density, i.e. the rate at which neutrons are scattering from direction $\hat{\mathbf{\Omega}}$ to $\hat{\mathbf{\Omega}}'$ and energy E to E':

$$dR_{\mathrm{s}} = \Sigma_{\mathrm{s}}(\mathbf{r}, \hat{\mathbf{\Omega}} \rightarrow \hat{\mathbf{\Omega}}', E \rightarrow E')\psi(\boldsymbol{r}, \hat{\mathbf{\Omega}}, E)dV d\hat{\mathbf{\Omega}} dE d\hat{\mathbf{\Omega}}' dE' \tag{4}$$

The corresponding reaction rate is obtained by integration over volume and the direction and energy of the incident and emitted neutron. The change in direction is often written using the scattering cosine μ, in which case (4) becomes:

$$dR_{\mathrm{s}} = \Sigma_{\mathrm{s}}(\mathbf{r}, \mu, E \rightarrow E')\psi(\boldsymbol{r}, \hat{\mathbf{\Omega}}, E)dV d\hat{\mathbf{\Omega}} dE d\mu dE' \tag{5}$$

Replacing the absolute directions with scattering angle is a valid approximation in the case of isotropic medium.

In reactions where the incident neutron is lost or secondary neutrons are emitted isotropically,[2] angular flux can be replaced by the scalar flux, which is obtained by integration over full solid angle:

$$\phi(\boldsymbol{r}, E) = \int_{4\pi} \psi(\boldsymbol{r}, \hat{\mathbf{\Omega}}, E) d\hat{\mathbf{\Omega}} \tag{6}$$

Both angular and scalar flux are scalar quantities, and their practical significance is related to neutron-induced reaction rates.

[2] E.g. all capture and fission reactions.

Transport theory: basic concepts revisited

The vector equivalent of angular flux is the angular current density:

$$\boldsymbol{j}(\boldsymbol{r}, \hat{\boldsymbol{\Omega}}, E) = \hat{\boldsymbol{\Omega}}\psi(\boldsymbol{r}, \hat{\boldsymbol{\Omega}}, E) \tag{7}$$

which gives the rate at which neutrons traveling in direction $\hat{\boldsymbol{\Omega}}$ with energy E are passing through an infinitesimal surface element $d\mathbf{S}$ located at position $\mathbf{r}$:

$$dL = \boldsymbol{j}(\boldsymbol{r}, \hat{\boldsymbol{\Omega}}, E) \cdot d\mathbf{S} \tag{8}$$

When the angular current density is integrated over the full solid angle, the result is another vector quantity called neutron current density:[3]

$$\mathbf{J}(\boldsymbol{r}, E) = \int_{4\pi} \mathbf{j}(\boldsymbol{r}, \hat{\boldsymbol{\Omega}}, E) d\hat{\boldsymbol{\Omega}} \tag{9}$$

which gives the net rate of neutrons with energy E passing through an infinitesimal surface element $d\mathbf{S}$ located at position $\mathbf{r}$:

$$dL = \mathbf{J}(\boldsymbol{r}, E) \cdot d\mathbf{S} \tag{10}$$

The current densities are associated with the rates at which neutrons cross the boundaries of a specified volume. Most importantly, the total net current is given by:

$$J_{\text{net}} = \oint_S \mathbf{J}(\boldsymbol{r}, E) \cdot d\mathbf{S} \tag{11}$$

[3] It is important to note that even though $\boldsymbol{j} = \hat{\boldsymbol{\Omega}}\psi$, this is not the case for quantities integrated over the full solid angle, and $\mathbf{J} \neq \hat{\boldsymbol{\Omega}}\phi$.

Transport theory: transport equation revisited

The transport equation is a conservation equation, describing the neutron balance in the infinitesimal six-dimensional phase-space element:

$$\underbrace{\frac{1}{v}\frac{\partial}{\partial t}\psi(\boldsymbol{r},\hat{\boldsymbol{\Omega}},E,t)}_{\text{(A)}}+\underbrace{\hat{\boldsymbol{\Omega}}\cdot\nabla\psi(\boldsymbol{r},\hat{\boldsymbol{\Omega}},E,t)}_{\text{(B)}}+\underbrace{\Sigma(\boldsymbol{r},E)\psi(\boldsymbol{r},\hat{\boldsymbol{\Omega}},E,t)}_{\text{(C)}}=q(\boldsymbol{r},\hat{\boldsymbol{\Omega}},E,t) \tag{12}$$

where (A) is the time-rate of change in neutron density, (B) is the streaming term, (C) is the removal term, and q is the source term:

$$q(\boldsymbol{r},\hat{\boldsymbol{\Omega}},E,t)=Q(\boldsymbol{r},\hat{\boldsymbol{\Omega}},E,t)+S(\boldsymbol{r},\hat{\boldsymbol{\Omega}},E,t)+F(\boldsymbol{r},\hat{\boldsymbol{\Omega}},E,t) \tag{13}$$

composed of external source Q, and flux-dependent scattering:

$$S(\boldsymbol{r},\hat{\boldsymbol{\Omega}},E,t)=\int_{4\pi}\int_{0}^{\infty}\Sigma_{\mathrm{s}}(\mathbf{r},\hat{\boldsymbol{\Omega}}'\rightarrow\hat{\boldsymbol{\Omega}},E'\rightarrow E)\psi(\mathbf{r},\hat{\boldsymbol{\Omega}}',E',t)d\hat{\boldsymbol{\Omega}}'dE' \tag{14}$$

and fission source:

$$F(\boldsymbol{r},\hat{\boldsymbol{\Omega}},E,t)=\frac{\chi(E)}{4\pi}\int_{0}^{\infty}\nu\Sigma_{\mathrm{f}}(\mathbf{r},E')\phi(\mathbf{r},E',t)dE' \tag{15}$$

where $\nu\Sigma_{\mathrm{f}}$ is the fission neutron production cross section and $\chi(E)$ is the fission spectrum, i.e. the probability that the energy of the emitted neutron falls on interval dE about E. Factor $1/4\pi$ comes from the fact that fission neutrons are assumed to be emitted isotropically.

Transport theory: transport equation revisited

Transport theory is based on the following assumptions:

1) Neutrons can be treated as independent particles, traveling in straight lines between collisions
2) Neutron-neutron interactions can be ignored
3) Reaction cross sections are independent of flux and constant in time

With these assumptions the neutron transport equation describes a linear problem.[4] In the derivation of the neutron transport equation it is in addition assumed that:

4) All materials are isotropic, i.e. differential scattering cross sections depend only on scattering angles and not on neutron direction of motion
5) Fission neutrons are emitted isotropically
6) Fission spectrum is independent of incident neutron energy

Approximation 4 is valid in practically all applications, approximations 5 and 6 are valid at energies relevant for fission reactors.

[4] As pointed out in Lecture 2, assumption 3) does not hold in coupled problems describing an operating nuclear reactor subject to reactivity feedbacks and fuel burnup, in which case the transport problem actually becomes non-linear. The solution to the coupled problem is obtained by iteration between the different solvers, assuming that the transport problem can be linearized over sufficiently short time intervals.

Derivation of diffusion theory

The most obvious difficulty in the solution of the neutron transport problem is the complicated energy dependence of cross sections. In reality, however, this is relatively easily handled without major approximations by multi-group condensation, performed by preserving the reaction rate balance.

The difficult part is handling the angular dependence of the streaming and scattering source terms, and in general, the fact that angular neutron density, angular flux and angular current density can be strongly anisotropic in heterogeneous geometries.[5]

Treatment of angular dependence is one of the main factors that differentiate various deterministic solution methods from each other. In diffusion theory, the approximations made for the angular dependence are taken to the extreme.

The idea in neutron diffusion is that neutrons flow from regions of higher concentration towards lower concentrations by Brownian motion. For the transport equation this means a simple connection between the gradient of scalar flux and neutron current density, which makes the resulting diffusion equation easy to solve.

Diffusion theory is derived from the general transport theory in the following, and the limitations of the diffusion approximation are discussed.

[5] Even if the assumption of isotropic flux was a good approximation, scattering, in general, is not an isotropic process in the L-frame.

Derivation of diffusion theory

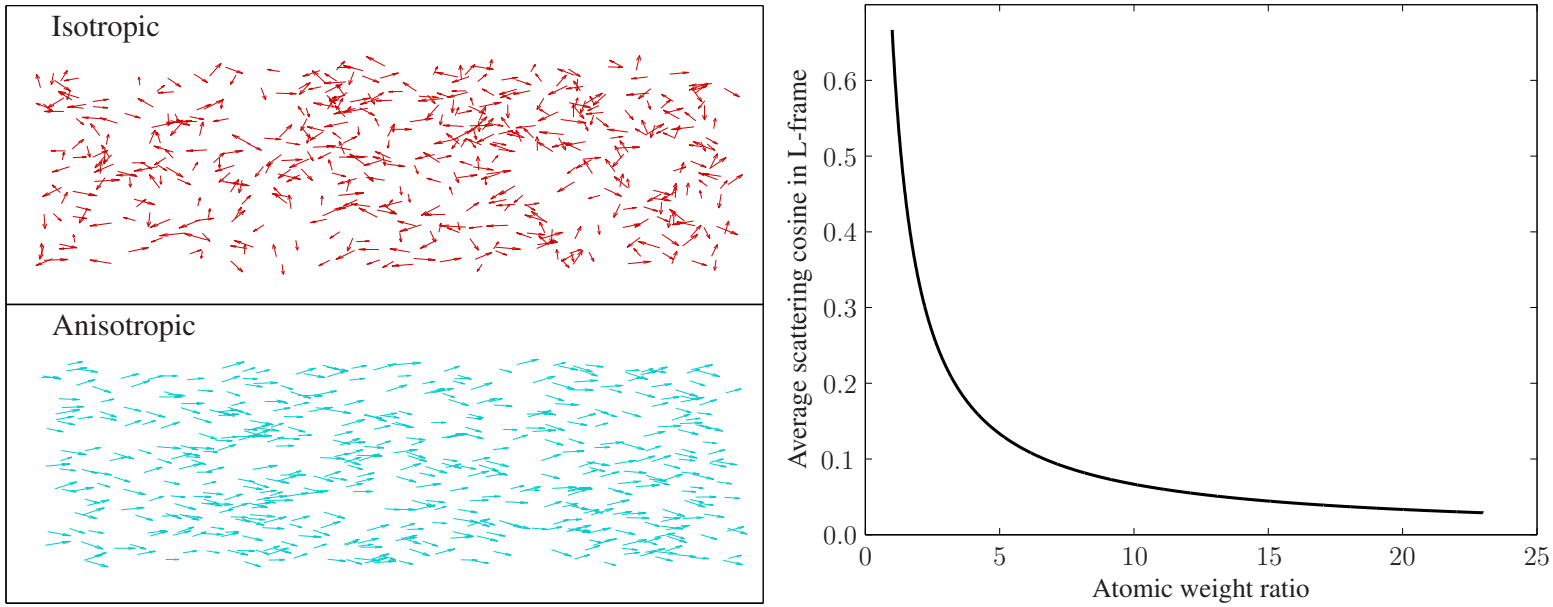


Figure 1 : Left: Illustration of an isotropic and anisotropic vector field, for example, neutron current density. In the isotropic case neutron directions are completely randomly distributed. In the anisotropic case there is a clear preferential direction. Right: Anisotropy of elastic potential scattering in the laboratory frame-of-reference (L-frame). Even though potential scattering is isotropic in the center-of-mass frame (C-frame), i.e. the average scattering cosine is zero, the anisotropy increases in the L-frame with decreasing nuclide mass. The curve shows that scattering from hydrogen, for example, has a clear forward bias.

Derivation of diffusion theory: directional dependence

The first task in the derivation of the neutron diffusion equation is to remove the directional dependence in such way that the transport equation can be written using the scalar flux. This can be done without introducing any additional approximations.

The downside of obtaining a simplified representation for flux is that the streaming term is written using the neutron current density, as seen in the final form in Eq. (24). This is not a problem for diffusion theory, as neutron current density is later related to flux gradient using an approximation called Fick's law (42).

The integration of the time-derivative term and the removal term over the full solid angle is straightforward:

$$\int_{4\pi} \frac{1}{v}\frac{\partial}{\partial t}\psi(\boldsymbol{r},\hat{\boldsymbol{\Omega}},E,t)d\hat{\boldsymbol{\Omega}} = \frac{1}{v}\frac{\partial}{\partial t}\int_{4\pi}\psi(\boldsymbol{r},\hat{\boldsymbol{\Omega}},E,t)d\hat{\boldsymbol{\Omega}} = \frac{1}{v}\frac{\partial}{\partial t}\phi(\boldsymbol{r},E,t) \tag{16}$$

and

$$\int_{4\pi}\Sigma(\boldsymbol{r},E)\psi(\boldsymbol{r},\hat{\boldsymbol{\Omega}},E,t)d\hat{\boldsymbol{\Omega}} = \Sigma(\boldsymbol{r},E)\int_{4\pi}\psi(\boldsymbol{r},\hat{\boldsymbol{\Omega}},E,t)d\hat{\boldsymbol{\Omega}} = \Sigma(\boldsymbol{r},E)\phi(\boldsymbol{r},E,t) \tag{17}$$

The fission source term (15) was already written without angular dependence.[6] The external source is independent of flux and its angular dependence depends on the source type. The integration of the two remaining terms is less straightforward.

[6] The integration over full solid angle only cancels the $1/4\pi$ factor in (15).

Derivation of diffusion theory: directional dependence

The integration of the scattering source (14) is written as:

$$\int_{4\pi}\left[\int_{4\pi}\int_{0}^{\infty}\Sigma_{\mathrm{s}}(\mathbf{r},\hat{\mathbf{\Omega}}'\rightarrow\hat{\mathbf{\Omega}},E'\rightarrow E)\psi(\mathbf{r},\hat{\mathbf{\Omega}}',E',t)d\hat{\mathbf{\Omega}}'dE'\right]d\hat{\mathbf{\Omega}} \tag{18}$$

Since the integration is carried over the full solid angle, and because the double-differential scattering cross section depends only on the angle between directions $\hat{\mathbf{\Omega}}'$ and $\hat{\mathbf{\Omega}}$, the integral over the double-differential scattering cross section can be written using the scattering cosine:

$$\int_{4\pi}\int_{0}^{\infty}\left[\int_{-1}^{1}\Sigma_{\mathrm{s}}(\mathbf{r},\mu,E'\rightarrow E)d\mu\right]\psi(\mathbf{r},\hat{\mathbf{\Omega}}',E',t)d\hat{\mathbf{\Omega}}'dE' \tag{19}$$

The term in brackets describes the total scattering probability from energy E' to E, and can be written as:

$$\begin{aligned}&\int_{4\pi}\int_{0}^{\infty}\Sigma_{\mathrm{s}}(\mathbf{r},E'\rightarrow E)\psi(\mathbf{r},\hat{\mathbf{\Omega}}',E',t)d\hat{\mathbf{\Omega}}'dE'\\&=\int_{0}^{\infty}\Sigma_{\mathrm{s}}(\mathbf{r},E'\rightarrow E)\left[\int_{4\pi}\psi(\mathbf{r},\hat{\mathbf{\Omega}}',E',t)d\hat{\mathbf{\Omega}}'\right]dE'\end{aligned} \tag{20}$$

The term in brackets is the scalar flux, and the final form can be written as:

$$\int_{0}^{\infty}\Sigma_{\mathrm{s}}(\mathbf{r},E'\rightarrow E)\phi(\mathbf{r},E',t)dE' \tag{21}$$

Derivation of diffusion theory: directional dependence

The final term in (12) left to be integrated is the streaming term, which can also be written using the angular current density (7):

$$\hat{\boldsymbol{\Omega}} \cdot \nabla \psi(\boldsymbol{r}, \hat{\boldsymbol{\Omega}}, E, t) = \nabla \cdot \hat{\boldsymbol{\Omega}} \psi(\boldsymbol{r}, \hat{\boldsymbol{\Omega}}, E, t) = \nabla \cdot \mathbf{j}(\boldsymbol{r}, \hat{\boldsymbol{\Omega}}, E, t) \tag{22}$$

Integration over the full solid angle yields

$$\int_{4\pi} \nabla \cdot \mathbf{j}(\boldsymbol{r}, \hat{\boldsymbol{\Omega}}, E, t) d\hat{\boldsymbol{\Omega}} = \nabla \cdot \int_{4\pi} \mathbf{j}(\boldsymbol{r}, \hat{\boldsymbol{\Omega}}, E, t) d\hat{\boldsymbol{\Omega}} = \nabla \cdot \mathbf{J}(\boldsymbol{r}, E, t) \tag{23}$$

where $\mathbf{J}(\boldsymbol{r}, E)$ is the neutron current density (9).

When the results (16)-(23) are collected, the transport equation can be written as:

$$\frac{1}{v} \frac{\partial}{\partial t} \phi(\boldsymbol{r}, E, t) + \nabla \cdot \mathbf{J}(\boldsymbol{r}, E, t) + \Sigma(\boldsymbol{r}, E) \phi(\boldsymbol{r}, E, t) = q(\boldsymbol{r}, E, t) \tag{24}$$

where q is again the source term composed of external source Q and the flux-dependent scattering and fission source:

$$S(\boldsymbol{r}, E, t) = \int_0^\infty \Sigma_{\mathrm{s}}(\mathbf{r}, E' \rightarrow E) \phi(\mathbf{r}, E', t) dE' \tag{25}$$

$$F(\boldsymbol{r}, E, t) = \chi(E) \int_0^\infty \nu \Sigma_{\mathrm{f}}(\mathbf{r}, E') \phi(\mathbf{r}, E', t) dE' \tag{26}$$

This form of transport equation is also known as the neutron continuity equation, and as pointed out earlier, no approximations were made in the derivation of (24) from the original transport equation (12) written for the angular flux.

The same derivation of the neutron continuity equation was presented in Lecture 2.

Derivation of diffusion theory: energy dependence

Energy group condensation is an approximation that is common to practically all deterministic transport methods. This means that the continuous energy-dependence is discretized into G energy groups with boundaries E_{g-1} and E_g, indexed in such way that:

$$E_0 > E_1 > E_2 > \cdots > E_G \tag{27}$$

Indexing the groups in the order of decreasing energy results from the fact that neutrons are born at high energy and scatter towards lower energies during their random walk.

The group-wise flux and current density can then be written as:

$$\phi_g(\boldsymbol{r}, t) = \int_{E_g}^{E_{g-1}} \phi(\boldsymbol{r}, E, t) dE \tag{28}$$

and

$$\mathbf{J}_g(\boldsymbol{r}, t) = \int_{E_g}^{E_{g-1}} \mathbf{J}(\boldsymbol{r}, E, t) dE \tag{29}$$

When energy group condensation is applied to the neutron continuity equation (24), the integration of time derivative and streaming terms over energy can be written simply as:

$$\int_{E_g}^{E_{g-1}} \frac{1}{v} \frac{\partial}{\partial t} \phi(\boldsymbol{r}, E, t) dE = \frac{1}{v_g} \frac{\partial}{\partial t} \phi_g(\boldsymbol{r}, t) \tag{30}$$

and:

$$\int_{E_g}^{E_{g-1}} \nabla \cdot \mathbf{J}(\boldsymbol{r}, E) dE = \nabla \cdot \mathbf{J}_g(\boldsymbol{r}, t) \tag{31}$$

Derivation of diffusion theory: energy dependence

Integration of the removal term can be written as:

$$\int_{E_g}^{E_{g-1}} \Sigma(\boldsymbol{r}, E)\phi(\boldsymbol{r}, E, t)dE = \Sigma_g \phi_g(\boldsymbol{r}, t) \tag{32}$$

where Σ_g is the group-wise macroscopic total cross section, defined in such way that the total reaction rate is preserved in the energy group condensation:

$$\int_V \Sigma_g \phi_g(\boldsymbol{r})dV = \int_V \int_{E_g}^{E_{g-1}} \Sigma(\boldsymbol{r}, E)\phi(\boldsymbol{r}, E)dVdE \tag{33}$$

Which combined with Eq. (28) gives:

$$\Sigma_g = \frac{\int_V \int_{E_g}^{E_{g-1}} \Sigma(\boldsymbol{r}, E)\phi(\boldsymbol{r}, E)dVdE}{\int_V \int_{E_g}^{E_{g-1}} \phi(\boldsymbol{r}, E)dVdE} \tag{34}$$

In other words, Σ_g is calculated as the flux-volume weighted average of the corresponding space- and energy-dependent cross section.[7] Similar energy group condensation is applied for the inverse neutron speed in Eq. (30).

[7] Removing the spatial dependence at this point implies that the flux solutions will be obtained in homogeneous material regions and combined together by boundary conditions (interface conditions).

Derivation of diffusion theory: energy dependence

The calculation of flux-volume weighted cross sections in (34) reveals a fundamental paradox in multi-group transport calculation:

- Solution to the transport problem (neutron flux) is needed for the calculation of flux-volume weighted cross sections
- Flux-volume weighted cross sections are needed for the solution of the transport problem

Calculation of multi-group cross sections forms the first part of the reactor physics calculation chain, introduced in Lecture 2. In practice, the procedure starts with a simplified geometry description and high energy resolution, and the number of energy groups is gradually reduced, while moving towards larger spatial scale.

This procedure is revisited in Lecture 7. From here on it is assumed that integrals similar to those in Eq. (34) can be evaluated, i.e. that the accurate space- energy-dependent flux solution is known.[8]

[8] In practice, integration over energy group g is replaced by summation over the micro-group structure $h \in g$, in which the flux solution is obtained by some higher-order deterministic transport method. Continuous-energy Monte Carlo codes are capable of producing stochastic estimates for the integrals without intermediate micro-group condensation, which is one of the advantages of using the method in group constant generation.

Derivation of diffusion theory: energy dependence

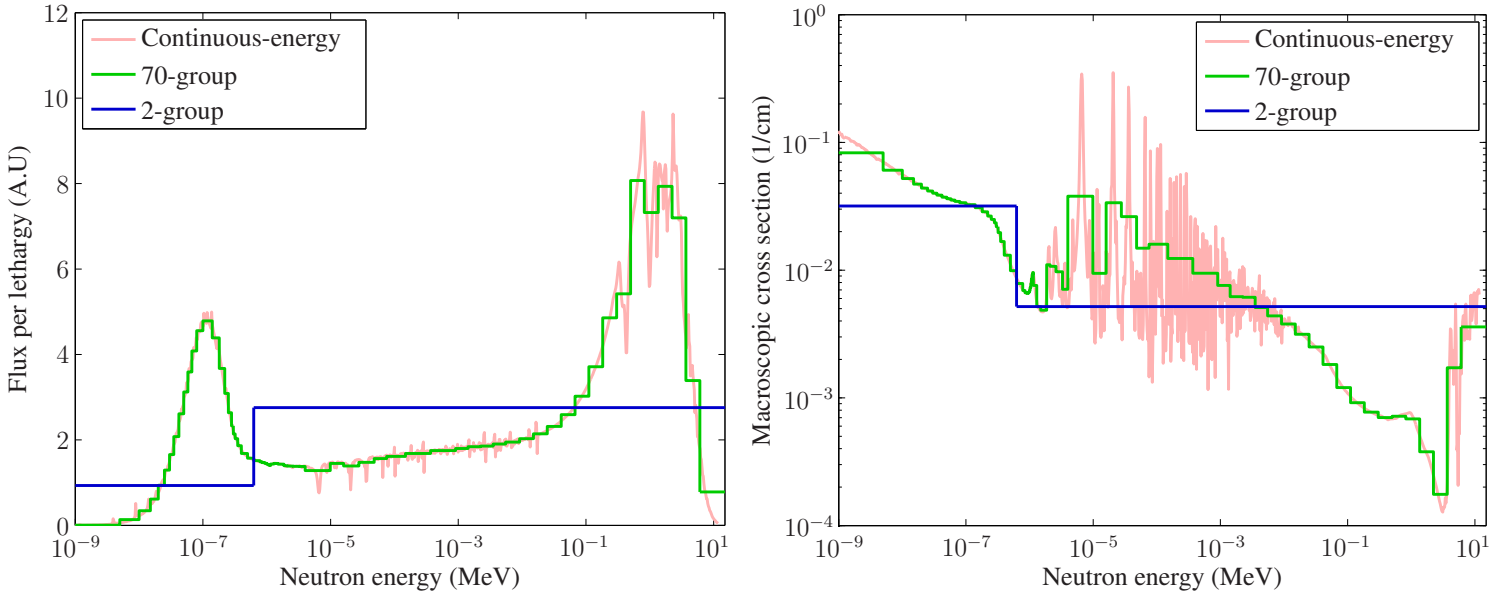


Figure 2 : Illustration of energy group condensation for flux (left) and total absorption cross section (right). Condensation of flux is performed by integration over energy groups as in Eq. (28). Condensation of cross sections is carried out by calculating flux-volume-weighted averages that preserve the reaction rate balance as in Eq. (34). This topic is revisited in Lecture 7.

Derivation of diffusion theory: energy dependence

Similar group condensation gives for the scattering source:

$$S_g(\boldsymbol{r},t) = \sum_{g'} \Sigma_{\mathrm{s},g'g}\phi_{g'}(\boldsymbol{r},t) \tag{35}$$

where

$$\Sigma_{\mathrm{s},g'g} = \frac{\int_V \int_{E_{g'}}^{E_{g'-1}} \int_{E_g}^{E_{g-1}} \Sigma_{\mathrm{s}}(\mathbf{r},E' \rightarrow E)\phi(\mathbf{r},E')dVdE'dE}{\int_V \int_{E_{g'}}^{E_{g'-1}} \phi(\mathbf{r},E')dVdE'} \tag{36}$$

is the group-transfer cross section, and for the fission source:

$$F_g(\boldsymbol{r},t) = \chi_g \sum_{g'} \nu\Sigma_{\mathrm{f},g'}\phi_{g'}(\boldsymbol{r},t) \tag{37}$$

where χ_g is the group-wise fission spectrum, i.e. the probability that the fission neutron is emitted in group g and the group-wise fission production cross section is calculated similar to (34):

$$\nu\Sigma_{\mathrm{f},g} = \frac{\int_V \int_{E_g}^{E_{g-1}} \nu\Sigma_{\mathrm{f}}(\boldsymbol{r},E)\phi(\boldsymbol{r},E)dVdE}{\int_V \int_{E_g}^{E_{g-1}} \phi(\boldsymbol{r},E)dVdE} \tag{38}$$

Derivation of diffusion theory: energy dependence

When the results of (30)-(38) are collected, the multi-group transport equation can be written as:

$$\frac{1}{v_g}\frac{\partial}{\partial t}\phi_g(\boldsymbol{r},t)+\nabla\cdot\mathbf{J}_g(\boldsymbol{r},t)+\Sigma_g\phi_g(\boldsymbol{r},t)=Q_g(\boldsymbol{r},t)+\sum_{g'}\Sigma_{\mathrm{s},g'g}\phi_{g'}(\boldsymbol{r},t)+\chi_g\sum_{g'}\nu\Sigma_{\mathrm{f},g'}\phi_{g'}(\boldsymbol{r},t) \tag{39}$$

where Q_g is the group-wise external source. By separating the contribution of intra-group scattering ($g\rightarrow g$) from the scattering source term, the equation can be written as:

$$\frac{1}{v_g}\frac{\partial}{\partial t}\phi_g(\boldsymbol{r},t)+\nabla\cdot\mathbf{J}_g(\boldsymbol{r},t)+\Sigma_{\mathrm{r},g}\phi_g(\boldsymbol{r},t)=Q_g(\boldsymbol{r},t)+\sum_{g'\neq g}\Sigma_{\mathrm{s},g'g}\phi_{g'}(\boldsymbol{r},t)+\chi_g\sum_{g'}\nu\Sigma_{\mathrm{f},g'}\phi_{g'}(\boldsymbol{r},t) \tag{40}$$

where the group-removal cross section:

$$\Sigma_{\mathrm{r},g}=\Sigma_g-\Sigma_{\mathrm{s},gg} \tag{41}$$

includes all reactions that remove neutrons from group g.

The result of removing the energy dependence from the continuity equation is a set of G equations, coupled together by the scattering and fission source terms.

Derivation of diffusion theory: Fick's law

The final step in the derivation of diffusion equation is to assume a simple connection between neutron current density and flux gradient:

$$\mathbf{J}_g(\boldsymbol{r}, t) = -D_g \nabla \phi_g(\boldsymbol{r}, t) \tag{42}$$

This relation is known as the diffusion approximation or Fick's law, and it was originally developed to account for the movement of molecules in chemical diffusion from higher to lower concentration.

Fick's law (42) can also be derived from transport theory. This is not a trivial task, but without going into the details it can be accomplished by assuming linear anisotropy for the angular flux:

$$\psi(\boldsymbol{r}, \hat{\boldsymbol{\Omega}}, E, t) \approx \frac{1}{4\pi}\left[\phi(\boldsymbol{r}, E, t) + 3\hat{\boldsymbol{\Omega}} \cdot \mathbf{J}(\boldsymbol{r}, E, t)\right] \tag{43}$$

and integrating the so-called first-moment equation[9] over full solid angle.

Additional approximations include:

1) The medium is infinite and homogeneous
2) Neutron source is isotropic
3) The time-rate of change of neutron current density is small compared to flux gradient
4) The anisotropic contribution to scattering energy transfer can be neglected

[9] The first-moment equation is obtained by multiplying all terms of the transport equation by direction vector $\hat{\boldsymbol{\Omega}}$.

Derivation of diffusion theory: Fick's law

With the previous approximations it can be shown that the relation between flux gradient and neutron current density is reduced into:[10]

$$\frac{1}{3}\nabla\phi_g(\boldsymbol{r}) + \Sigma_g \mathbf{J}_g(\boldsymbol{r}) = \sum_{g'} \overline{\mu}\,\Sigma_{\mathrm{s},g'g}\mathbf{J}_{g'}(\boldsymbol{r})\,. \tag{44}$$

For one dimension this can be written as:

$$J_g(x) = -\frac{1}{3}\left[\Sigma_g - \frac{\sum_{g'} \overline{\mu}\,\Sigma_{\mathrm{s},g'g} J_{g'}(x)}{J_g(x)}\right]^{-1} \frac{d}{dx}\phi_g(x)\,, \tag{45}$$

which is of the same form as (42) when the diffusion coefficient is written as:

$$D_g = \frac{1}{3}\left[\Sigma_g - \frac{\sum_{g'} \overline{\mu}\,\Sigma_{\mathrm{s},g'g} J_{g'}(x)}{J_g(x)}\right]^{-1} = \frac{1}{3\Sigma_{\mathrm{tr},g}}\,, \tag{46}$$

where $\Sigma_{\mathrm{tr},g}$ is the transport-corrected total cross section (or simply transport cross section).

[10] In the literature this is referred to as one of the two P_1 equations.

Derivation of diffusion theory: Fick's law

The definition of transport-cross section in Eq. (46):

$$\Sigma_{\mathrm{tr},g} = \Sigma_g - \frac{\sum_{g'} \overline{\mu}\, \Sigma_{\mathrm{s},g'g} J_{g'}(x)}{J_g(x)} \tag{47}$$

is known as the in-scattering approximation. This is often difficult to calculate, and transport cross section is obtained by applying the out-scattering approximation:

$$\sum_{g'} \overline{\mu}\, \Sigma_{\mathrm{s},g'g} J_{g'}(x) \approx \sum_{g'} \overline{\mu}\, \Sigma_{\mathrm{s},gg'} J_g(x)\,, \tag{48}$$

which essentially implies that the contribution of scattering from all other groups to group g (in-scattering) is assumed to be equal to the contribution of scattering from group g to all other groups (out-scattering). Transport cross section is then reduced to:

$$\Sigma_{\mathrm{tr},g} = \Sigma_g - \sum_{g'} \overline{\mu}\, \Sigma_{\mathrm{s},gg'} \tag{49}$$

or:

$$\Sigma_{\mathrm{tr},g} = \Sigma_g - \overline{\mu}\, \Sigma_{\mathrm{s},g} \tag{50}$$

where Σ_{s} is the total scattering cross section.

Derivation of diffusion theory: Fick's law

Constant $\overline{\mu}$ in Eqs. (44)-(50) is the average scattering angle:

$$\overline{\mu} = \frac{\int_{-1}^{1}\int_{E_g}^{E_{g-1}} \mu\Sigma_{\mathrm{s}}(\mu, \boldsymbol{r}, E)d\mu}{\int_{-1}^{1}\int_{E_g}^{E_{g-1}} \Sigma_{\mathrm{s}}(\mu, \boldsymbol{r}, E)d\mu} . \tag{51}$$

Calculation of transport-cross section and diffusion coefficient is a non-trivial topic, and there are additional approximations related to the energy group condensation of these constants. These topics are related to spatial homogenization and revisited in Lecture 7.

For the reminder of this lecture it is sufficient to assume that diffusion coefficient is a given constant that relates neutron current density to flux gradient according to Fick's law (42).

Derivation of diffusion theory

The final form of the multi-group diffusion equation is then written as:

$$\frac{1}{v_g}\frac{\partial}{\partial t}\Phi_g(\boldsymbol{r},t) - D_g\nabla^2\Phi_g(\boldsymbol{r},t) + \Sigma_{\mathrm{r},g}\Phi_g(\boldsymbol{r},t) = Q_g(\boldsymbol{r},t) + \sum_{g'\neq g}\Sigma_{\mathrm{s},g'g}\Phi_{g'}(\boldsymbol{r},t) + \chi_g\sum_{g'}\nu\Sigma_{\mathrm{f},g'}\Phi_{g'}(\boldsymbol{r},t) \tag{52}$$

The behavior of the neutron population is now described using a single density-like function, Φ, and a balance equation (52) that is possible to solve.[11]

As stated earlier, the derivation of diffusion theory is based on a number of crude approximations, which do not hold particularly well in heterogeneous reactor geometries. Even so, neutron transport codes based on diffusion methods are routinely used in reactor analysis, with considerable accuracy.

The reason why diffusion theory works in reactor applications is that the heterogeneity of the geometry is reduced by spatial homogenization, and a major part of the transport physics is actually included in the homogenized group constants. This topic is revisited in Lectures 7 and 8. The validity of the various approximations is considered in the following.

[11] Solution to the neutron diffusion equation is from here on denoted with a capital phi, Φ. For clarity, Φ is referred to as the diffusion flux in contexts where it is easily confused with the scalar flux, ϕ, obtained from the solution of the transport equation.

Validity of the diffusion approximation

In the derivation of Fick's law it was assumed that the flux is linearly anisotropic, which is a poor approximation in or near:

1) Localized sources
2) Strong absorbers
3) Vacuum boundaries and low-density material regions
4) Large moderator regions

For strong absorbers and vacuum boundaries the anisotropy is caused by the lack of back-flow through the boundary surface. For large moderator regions there is a large inward component of fast neutrons and an outward component of thermal neutrons, which disrupts the flux isotropy.

In addition to linear flux anisotropy, diffusion theory assumes that:

- Flux is a relatively smooth function of spatial coordinates, without steep gradients
- Absorption is much less likely than scattering

In reality, local heterogeneities also inflict steep gradients in the neutron flux. Scattering is the dominant reaction mode in moderator and structural materials, but not in fuel and certainly not in strong absorbers.

Most of these problems are resolved when the heterogeneous reactor geometry is homogenized at the fuel assembly level. The spatial detail is reduced to homogeneous nodes with dimensions considerably larger than the neutron mean-free-path.

Validity of the diffusion approximation

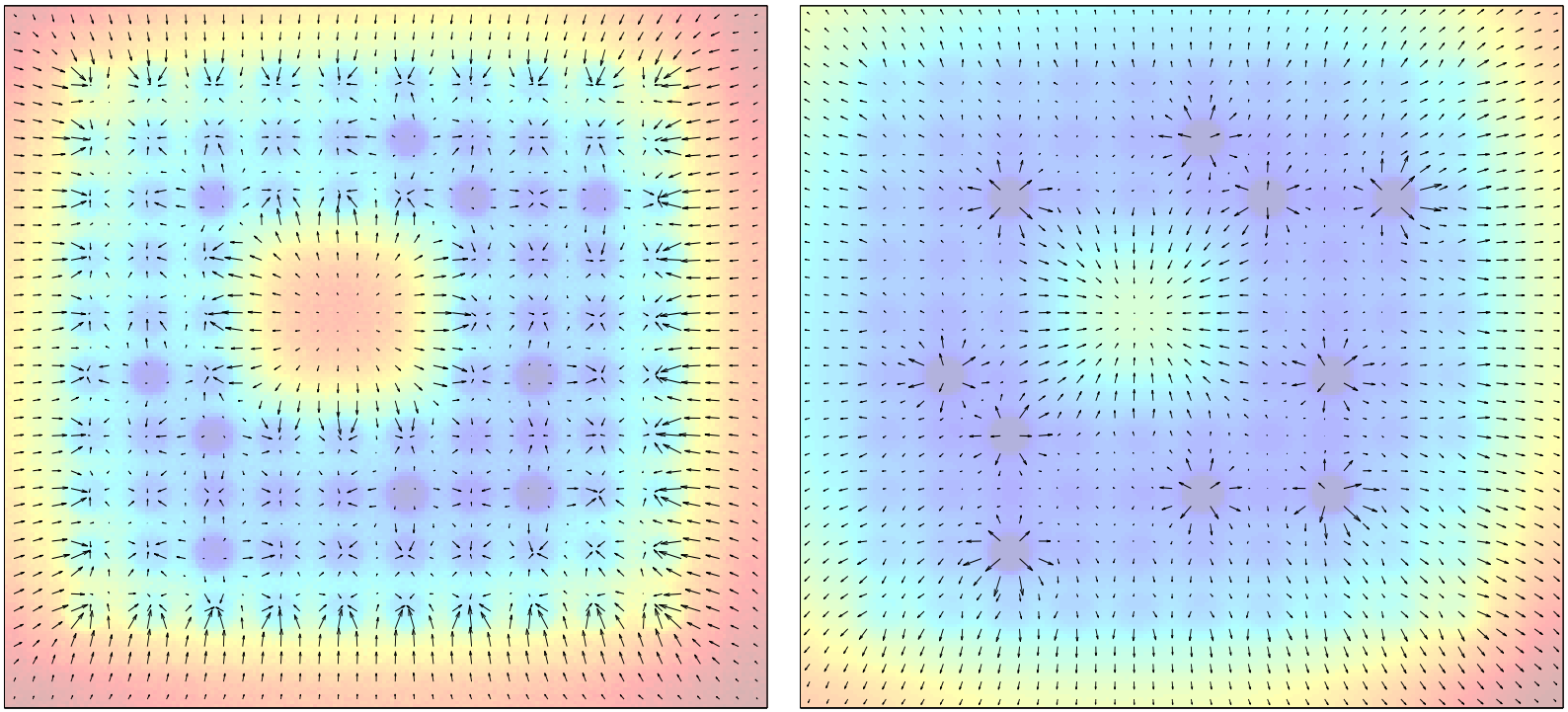


Figure 3 : Flux gradient field in fast (left) and thermal (right) energy group in a BWR fuel assembly, demonstrating the heterogeneity of the flux solution. Neutron density distribution is plotted in the background. Energy group boundary is set to 0.625 eV. Calculations carried out using Monte Carlo simulation.

Validity of the diffusion approximation

Spatial homogenization does not change the fact that scattering is an anisotropic reaction in the L-frame,[12] in particular for light elements (See Fig. 9). Since more than 90% of all neutron interactions in LWR's consist of elastic scattering from hydrogen in water, the requirement of isotropic scattering is clearly not met.

To be precise, the assumption of isotropic source was made in order to evaluate some of the integrals in the derivation of diffusion theory, and the introduction of transport cross section (47) actually attempts to correct this flaw. As most clearly seen in the out-scattering definition:

$$\Sigma_{\mathrm{tr}}(\boldsymbol{r}, E) = \Sigma(\boldsymbol{r}, E) - \overline{\mu}\,\Sigma_{\mathrm{s}}(\boldsymbol{r}, E) \tag{53}$$

the value of transport cross section is smaller when scattering is forward-biased ($\overline{\mu} > 0$). It is later shown that the diffusion coefficient:

$$D \sim \frac{1}{\Sigma_{\mathrm{tr}}} \tag{54}$$

can be associated to the distance migrated by the neutrons in the medium, which is increased by scattering anisotropy.

In a way, the directional component of the double-differential scattering rate (5) is contained within the transport cross section, while the group-transfer cross section (36) contains the energy-transfer component. The use of a coarse energy group structure reduces the error introduced by this approximation.

[12] Scattering isotropy in the L-frame must not be confused with isotropy in the C-frame, which is generally a good approximation.

Multi-group diffusion equation

What complicates the solution of the neutron diffusion equation is that (52) consists of a set of G coupled differential equations with space- and time-dependence. There exists solution methods that are capable of handling an arbitrary number of energy groups in a systematic manner, but the basic principles are easily demonstrated using one- and two-group diffusion theory.

Diffusion calculation in general is an extensive topic, and the following examples involving non-multiplying and multiplying medium are presented as an introduction to the nodal diffusion method, covered in Lecture 8. More examples are found in various text books.[13]

Even though one-group diffusion theory has very little practical use in reactor analysis, it does conveniently lead to some of the same results introduced for the transport equation in Lecture 2. Some of these results are easily generalized for the two-group diffusion theory, which is the workhorse in deterministic LWR core analysis.

[13] See, for example, W. M. Stacey, *Nuclear Reactor Physics*, Wiley, 2001.

Multi-group diffusion equation

With only one energy group covering the flux spectrum the multi-group diffusion equation (52) is reduced into:

$$\frac{1}{v}\frac{\partial}{\partial t}\Phi(\boldsymbol{r},t) - D\nabla^2\Phi(\boldsymbol{r},t) + \Sigma_{\mathrm{a}}\Phi(\boldsymbol{r},t) = Q(\boldsymbol{r},t) + \nu\Sigma_{\mathrm{f}}\Phi(\boldsymbol{r},t) \tag{55}$$

The two-group diffusion equations can be written by setting χ_1 = 1 and χ_2 = 0 and re-grouping some of the terms in (52):[14]

$$\begin{aligned}\frac{1}{v_1}\frac{\partial}{\partial t}\Phi_1(\boldsymbol{r},t) - D_1\nabla^2\Phi_1(\boldsymbol{r},t) + \left(\Sigma_{\mathrm{a},1} + \Sigma_{\mathrm{rem}}\right)\Phi_1(\boldsymbol{r},t) &= Q_1(\boldsymbol{r},t) + F_1(\boldsymbol{r},t)\\ \frac{1}{v_2}\frac{\partial}{\partial t}\Phi_2(\boldsymbol{r},t) - D_2\nabla^2\Phi_2(\boldsymbol{r},t) + \Sigma_{\mathrm{a},2}\Phi_2(\boldsymbol{r},t) &= Q_2(\boldsymbol{r},t) + S_2(\boldsymbol{r},t)\end{aligned} \tag{56}$$

where the contribution from up-scattering is included in the removal cross section:

$$\Sigma_{\mathrm{rem}} = \Sigma_{\mathrm{s},12} - \frac{\Phi_2}{\Phi_1}\Sigma_{\mathrm{s},21} \tag{57}$$

and the fission and scattering source terms are written as:

$$\begin{aligned}F_1(\boldsymbol{r},t) &= \nu\Sigma_{\mathrm{f},1}\Phi_1(\boldsymbol{r},t) + \nu\Sigma_{\mathrm{f},2}\Phi_2(\boldsymbol{r},t)\\ S_2(\boldsymbol{r},t) &= \Sigma_{\mathrm{rem}}\Phi_1(\boldsymbol{r},t)\end{aligned} \tag{58}$$

[14] The energy boundary between fast and thermal group is typically set to 0.625 eV.

Physical interpretation of diffusion coefficient

Even though the diffusion coefficient cannot be directly related to any physical continuous-energy reaction rate, it is possible to obtain a physical interpretation for this parameter by considering neutron diffusion from a constant point source through an infinite source-free medium.

The problem is solved in the following using one-group diffusion theory in spherical coordinate system centered at the point source. In the absence of neutron multiplication, the source term is written as:

$$Q = \begin{cases} S & \text{when } r = 0 \\ 0 & \text{when } r > 0 \end{cases} \tag{59}$$

Because S is constant in time, also the time-dependence in Eq. (55) can be dropped, and the one-group diffusion equation outside the point source is written as:

$$-D\nabla^2\Phi(\boldsymbol{r}) + \Sigma_{\mathrm{a}}\Phi(\boldsymbol{r}) = 0 \tag{60}$$

or by writing the Laplacian in spherical coordinates and re-arranging the terms:

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{d}{dr}\Phi(r)\right) - \frac{1}{M^2}\Phi(r) = 0 \tag{61}$$

where

$$M^2 = \frac{D}{\Sigma_{\mathrm{a}}} \tag{62}$$

Physical interpretation of diffusion coefficient

Eq. (61) is a standard second-order homogeneous differential equation, which is easily solved using conventional techniques. The general solution can be written in form:

$$\Phi(r) = C_1 \frac{1}{r} e^{r/M} + C_2 \frac{1}{r} e^{-r/M} \tag{63}$$

The first exponential term can be dropped by requiring that:

$$\lim_{r \to \infty} \Phi(r) = 0 \Rightarrow C_1 = 0 \tag{64}$$

Constant C_2 can be fixed by setting the current over a sphere enclosing the source equal to source rate as the radius approaches zero. The current density is given by Fick's law:

$$\mathbf{J}(r) = -D\nabla\Phi(r) = -D\frac{d}{dr}\Phi(r) = DC_1 \left(\frac{1}{rM} + \frac{1}{r^2} \right) e^{-r/M} \tag{65}$$

The current over a sphere with radius r is obtained by surface integral:

$$J(r) = \oint_{4\pi} \mathbf{J}(r) \cdot d\mathbf{S} = 4\pi r^2 DC_1 \left(\frac{1}{rM} + \frac{1}{r^2} \right) e^{-r/M} = 4\pi DC_1 \left(\frac{r}{M} + 1 \right) e^{-r/M} \tag{66}$$

Current over an infinitesimal sphere is then set equal to source rate:

$$\lim_{r \to 0} J(r) = 4\pi DC_1 = S \Rightarrow C_1 = \frac{S}{4\pi D} \tag{67}$$

Physical interpretation of diffusion coefficient

The final form of the flux solution outside the point source is then written as:

$$\Phi(r) = \frac{S}{4\pi D}\frac{1}{r}e^{-r/M} \tag{68}$$

It is noted that the function has a singularity at $r = 0$. This is not considered a problem, because diffusion theory is not valid near sources anyway.

The attention is next turned to the physical interpretation of parameter M. The absorption rate in a small spherical shell located between r and $r + dr$ is given by:

$$dR = \Sigma_{\mathrm{a}}\Phi(r)dV = \Sigma_{\mathrm{a}}\Phi(r)4\pi r^2 dr = \Sigma_{\mathrm{a}}\frac{S}{D}re^{-r/M}dr = \frac{S}{M^2}re^{-r/M}dr \tag{69}$$

The probability that a source neutron is absorbed between r and $r + dr$ is simply the absorption rate divided by source strength:

$$p(r)dr = \frac{dR}{S} = \frac{r}{M^2}e^{-r/M}dr \tag{70}$$

This probability can be used for calculating the mean square-distance from the point source at which the neutrons are absorbed:

$$\overline{r^2} = \int_0^\infty r^2 p(r)dr = \int_0^\infty \frac{r^3}{M^2}e^{-r/M}dr = \cdots = 6M^2 = 6\frac{D}{\Sigma_{\mathrm{a}}} \tag{71}$$

Physical interpretation of diffusion coefficient

The diffusion coefficient can now be related to a physical property, namely the mean square-distance the neutrons travel in a homogeneous medium before being removed from the flux by absorption. Constant:

$$M^2 = \frac{D}{\Sigma_{\mathrm{a}}} \tag{72}$$

is known as the migration area and the square value M the migration length.

Since the mean square distance of neutron diffusion, $\overline{r^2}$, is easily evaluated using Monte Carlo simulation, Eq. (71) can be used for providing a stochastic estimate for the diffusion coefficient.

Similar result can be derived from the multi-group diffusion equation, by looking at the contribution of neutrons emitted from the point source only, i.e. by ignoring the contribution of scattering source.

In two-group diffusion theory the migration area is replaced by two similar parameters:

- Fast diffusion area L_1^2 and the corresponding fast diffusion length L_1, also called the slowing-down length.[15]
- Thermal diffusion area L_2^2 and the corresponding thermal diffusion length L_2.

[15] Because of historical reasons, L_1^2 is also known as the neutron age or Fermi-age, since it essentially depends on how long it takes a fission neutron to slow down to the thermal energy region.

One-group diffusion equation in multiplying medium

Non-multiplying media are encountered in reflectors and some control rod constructions.[16] The solution of neutron diffusion equation in the multiplying part of the active core is simplified by the fact that the heterogeneity of the geometry is reduced by spatial homogenization.

The flux solution is typically obtained in regularly-shaped homogeneous nodes, which means that the flux shape can even be described using analytical functions. This reduces the computational task to coupling the intra-nodal solutions together by boundary conditions.

Nodal diffusion methods are left for Lecture 8, and the remainder of this lecture is focused on solving the diffusion equation in homogeneous medium. An important part of the solution is the separation of the remaining variables, which also leads to some of the same conclusions introduced in Lecture 2.

As in the previous example with non-multiplying medium, the essential results are first derived from the one-group diffusion equation, and then generalized to multi- and two-group theory.

[16] For example, fast reactors and VVER-440 control elements.

One-group diffusion equation in multiplying medium

In one-group diffusion theory the only remaining variables are space and time, for which the separation can be written as:

$$\Phi(\boldsymbol{r},t) = \Phi(\boldsymbol{r})\mathcal{T}(t) \tag{73}$$

Also, the external source is dropped at this point for convenience.[17]

The substitution of (73) into (55) yields:

$$\frac{1}{v}\frac{\partial}{\partial t}\Phi(\boldsymbol{r})\mathcal{T}(t) - D\nabla^2\Phi(\boldsymbol{r})\mathcal{T}(t) + \Sigma_{\mathrm{a}}\Phi(\boldsymbol{r})\mathcal{T}(t) = \nu\Sigma_{\mathrm{f}}\Phi(\boldsymbol{r})\mathcal{T}(t) \tag{74}$$

or by re-grouping the terms:

$$\Phi(\boldsymbol{r})\frac{1}{v}\frac{\partial}{\partial t}\mathcal{T}(t) = \mathcal{T}(t)\left[D\nabla^2\Phi(\boldsymbol{r}) - \Sigma_{\mathrm{a}}\Phi(\boldsymbol{r}) + \nu\Sigma_{\mathrm{f}}\Phi(\boldsymbol{r})\right] \tag{75}$$

Division of (75) by $\Phi(\boldsymbol{r})\mathcal{T}(t)$ yields:

$$\frac{1}{\mathcal{T}(t)}\frac{\partial}{\partial t}\mathcal{T}(t) = \frac{v}{\Phi(\boldsymbol{r})}\left[D\nabla^2\Phi(\boldsymbol{r}) - \Sigma_{\mathrm{a}}\Phi(\boldsymbol{r}) + \nu\Sigma_{\mathrm{f}}\Phi(\boldsymbol{r})\right] \tag{76}$$

This is an equation where time-dependence is confined to the left-hand side (LHS) and spatial dependence to the right-hand side (RHS).

[17] Including the external source in the following calculations would require similar separation of variables for the source term $Q(\boldsymbol{r},t)$.

One-group diffusion equation in multiplying medium

The only way for the equality to hold is that both LHS and RHS of (76) are equal to a constant, independent of all variables.

When this constant is written as ω, the LHS becomes:

$$\frac{1}{\mathcal{T}(t)}\frac{\partial}{\partial t}\mathcal{T}(t) = \omega \tag{77}$$

or:

$$\frac{\partial}{\partial t}\mathcal{T}(t) - \omega\mathcal{T}(t) = 0 \tag{78}$$

with solution:

$$\mathcal{T}(t) = \mathcal{T}(0)e^{\omega t} \tag{79}$$

From Lecture 2 it is recalled that the exponential coefficient ω is the inverse period, related to the reactor period T:

$$T = \frac{1}{\omega} \tag{80}$$

which is the time taken for the neutron population to grow by factor 2.7 (when $\omega > 0$) or decrease by factor 0.37 (when $\omega < 0$).

One-group diffusion equation in multiplying medium

The RHS of (76) is written:

$$\frac{v}{\Phi(\boldsymbol{r})}\left[D\nabla^2\Phi(\boldsymbol{r}) - \Sigma_\mathrm{a}\Phi(\boldsymbol{r}) + \nu\Sigma_\mathrm{f}\Phi(\boldsymbol{r})\right] = \omega \tag{81}$$

or:

$$\frac{\omega}{v}\Phi(\boldsymbol{r}) - D\nabla^2\Phi(\boldsymbol{r}) + \Sigma_\mathrm{a}\Phi(\boldsymbol{r}) - \nu\Sigma_\mathrm{f}\Phi(\boldsymbol{r}) = 0 \tag{82}$$

By re-grouping the terms, Eq. (82) can be written as:

$$D\nabla^2\Phi(\boldsymbol{r}) + \left[\nu\Sigma_\mathrm{f} - \Sigma_\mathrm{a} - \frac{\omega}{v}\right]\Phi(\boldsymbol{r}) = 0 \tag{83}$$

or:

$$\nabla^2\Phi(\boldsymbol{r}) + B^2\Phi(\boldsymbol{r}) = 0 \tag{84}$$

where:

$$B^2 = \frac{\nu\Sigma_\mathrm{f} - \Sigma_\mathrm{a} - \dfrac{\omega}{v}}{D} \tag{85}$$

Equation (84) is identified as the Helmholtz equation, encountered in many fields of physics and engineering.

One-group diffusion equation in multiplying medium

The significance of the previous result is that the spatial solution is now written using a simple equation, and the formulation of the solution depends only on:

1) The coordinate system, which determines the form of the Laplacian operator ∇^2
2) The boundary conditions, which fix the values of any undefined constants

In addition, constant B^2, fixed by the geometry configuration, is related to the material properties by (85) and therefore to the inverse period in the time-dependent solution (79) by:

$$\omega = v\left(\nu\Sigma_{\mathrm{f}} - DB^2 - \Sigma_{\mathrm{a}}\right) \tag{86}$$

It is also seen from Eq. (84) that

$$B^2 = -\frac{\nabla^2\Phi(\boldsymbol{r})}{\Phi(\boldsymbol{r})} \tag{87}$$

is a measure of flux curvature. Because of this interpretation, parameter B^2 is called the buckling, or more precisely, the geometry buckling.[18]

The solution to the Helmholtz equation is next studied in the simplest one-dimensional geometry: bare infinite slab reactor, but the main results can be generalized to other geometries as well.

[18] Another buckling term, material buckling, is introduced with the criticality equation.

Spatial dependence in one dimension

In the bare slab geometry confined between $-a/2 \leq x \leq a/2$ the Helmholtz equation (84) is written in Cartesian coordinates as:

$$\frac{d^2\Phi(x)}{dx^2} + B^2\Phi(x) = 0 \tag{88}$$

The equation has a periodic solution, written as:

$$\Phi(x) = \sum_{n=0}^{\infty} \left[C_{1,n} \sin(B_n x) + C_{2,n} \cos(B_n x) \right] \tag{89}$$

where

$$B_n = \frac{(n+1)\pi}{a} \tag{90}$$

and $C_{1,n}$ and $C_{2,n}$ are constants fixed by the boundary conditions. In the case of bare slab, the symmetry of the geometry configuration requires that:[19]

$$\Phi(-x) = \Phi(x) \tag{91}$$

which means that the antisymmetric solution (sin-function) must disappear and $C_{1,n} = 0$. The solution is then written as:

$$\Phi(x) = \sum_{n=0}^{\infty} C_{2,n} \cos(B_n x) \tag{92}$$

[19] The exact formulation of the boundary conditions is considered later.

Spatial dependence in one dimension

This example demonstrates what was noted in Lecture 2, that the flux solution consists of a linear combination of different flux modes:

$$\Phi(\boldsymbol{r}) = \Phi_0(\boldsymbol{r}) + \Phi_1(\boldsymbol{r}) + \Phi_2(\boldsymbol{r}) + \dots \tag{93}$$

where Φ_0 is called the fundamental mode and the remaining modes the transient modes.

It is also seen in Eq. (90) that:

$$B_0^2 < B_1^2 < B_2^2 < \dots \tag{94}$$

Since Eq. (86) relates each B_n^2 to inverse period ω_n by:

$$\omega_n = v\left(\nu\Sigma_\mathrm{f} - DB_n^2 - \Sigma_\mathrm{a}\right) \tag{95}$$

it easy to see that:

$$\omega_0 > \omega_1 > \omega_2 > \dots \tag{96}$$

Which leads to the conclusion presented in Lecture 2 that the fundamental mode flux solution persists as $t \to \infty$, and the transient modes fade away. This is best understood by considering the three possible cases:

1) $\omega_0 > 0$: the fundamental mode grows faster than the transient modes, which are left behind
2) $\omega_0 = 0$: the fundamental mode represents the steady-state solution and all transient modes are characterized by exponentially decaying time dependence
3) $\omega_0 < 0$: all flux modes are exponentially decaying, but the transient modes decay faster than the fundamental mode

Spatial dependence in one dimension

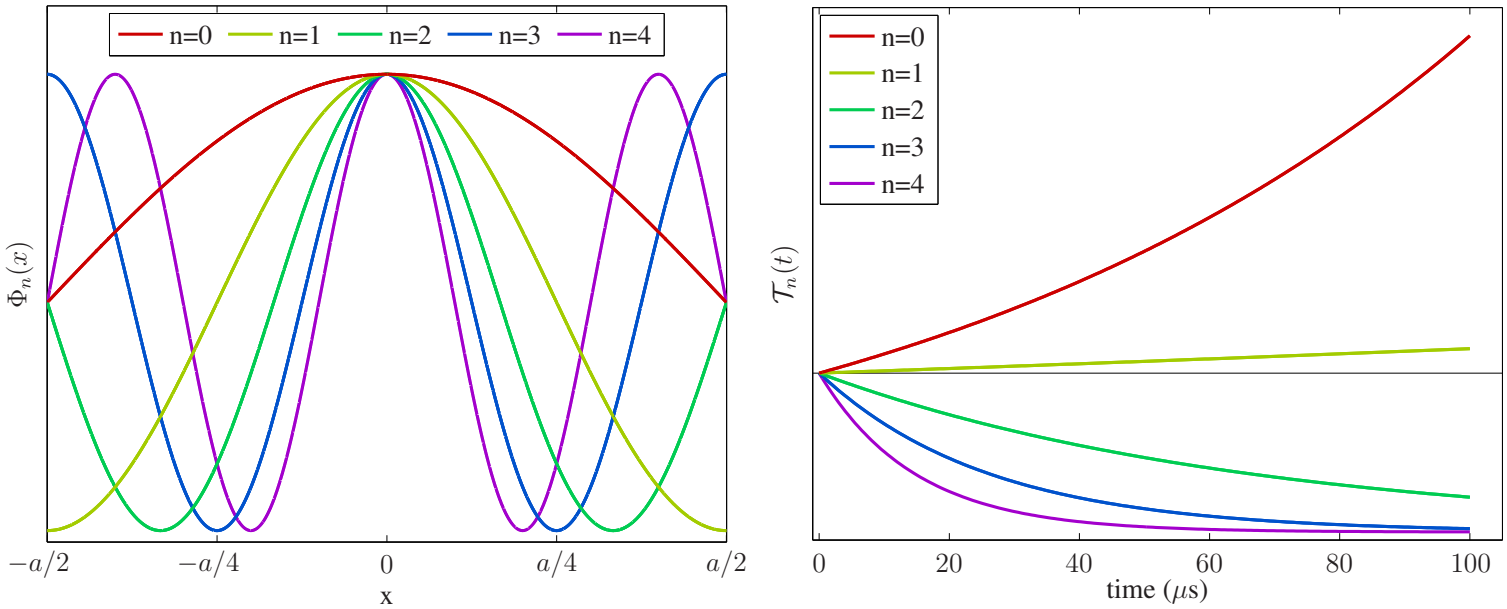


Figure 4 : Illustration of spatial flux modes (left) and time-dependent amplitude functions (right) for a bare infinite slab reactor. The first flux mode $n = 0$ is the fundamental mode and the remaining modes $n = 1, 2, 3, 4$ the first four transient modes. The first two modes are exponentially growing and the last three decaying. The fundamental mode determines the asymptotic flux shape and period of the reactor as $t \to \infty$, and the transient modes are left behind. For simplicity, $C_{2,0} = C_{2,1} = C_{2,2} = C_{2,3} = C_{2,4}$.

Spatial dependence in one dimension

As discussed in Lecture 2, the reactor period depends on neutron multiplication, i.e. the length and branching of fission chains, and the speed at which the chains proceed. This relation can be written as:[20]

$$\omega_n = \frac{k_n - 1}{\tau_{\mathrm{r},n}} \tag{97}$$

where the multiplication factor is written as:

$$k_n = \frac{\nu\Sigma_\mathrm{f}}{\Sigma_\mathrm{a} + DB_n^2} \tag{98}$$

and the prompt removal lifetime as:

$$\tau_{\mathrm{r},n} = \frac{1}{v(\Sigma_\mathrm{a} + DB_n^2)} \tag{99}$$

From (94) it results that:

$$k_0 > k_1 > k_2 > \dots \tag{100}$$

as stated in Lecture 2, but also that:[21]

$$\tau_{\mathrm{r},0} > \tau_{\mathrm{r},1} > \tau_{\mathrm{r},2} > \dots \tag{101}$$

[20] In lecture 2 the relation was written as $\omega = \rho/\Lambda$, where $\rho = (k_\mathrm{eff} - 1)/k_\mathrm{eff}$ is the reactivity and $\Lambda = \tau_\mathrm{r}/k_\mathrm{eff}$ is the generation time.

[21] The interpretation of (100) and (101) is not straightforward. The sum of all flux modes can be related to physical fission chains, but the same does not apply to individual modes (fundamental or transient).

Point-kinetics and eigenvalue equation

In Lecture 2, the fundamental mode flux was related to two solution methods for the transport equation:

1) The point-kinetics approximation of the time-dependent transport equation
2) The k-eigenvalue solution of the steady-state transport equation

The point-kinetics approximation was attained by separation of variables, which is exactly what was done for the one-group diffusion equation, and (97) with $n = 0$ represents the same relation between neutron multiplication, prompt neutron time constant and inverse reactor period.

$$\omega_0 = \frac{k_0 - 1}{\tau_{\mathrm{r},0}} \tag{102}$$

The k-eigenvalue form of the transport equation was obtained by dropping the time-dependence and scaling the fission source by effective multiplication factor k_{eff}. The same approach can be applied to the diffusion equation:

$$-D\nabla^2\Phi(\boldsymbol{r}) + \Sigma_{\mathrm{a}}\Phi(\boldsymbol{r}) = \frac{1}{k_{\mathrm{eff}}}\nu\Sigma_{\mathrm{f}}\Phi(\boldsymbol{r}) \tag{103}$$

As pointed out in Lectures 2 and 3, the solution to the criticality eigenvalue problem is not equivalent with the solution to the time-dependent problem, but rather to a modified problem in which the balance between source and loss rates is attained by artificially scaling the number of emitted fission neutrons.

Point-kinetics and eigenvalue equation

Since in the general case k_{eff} differs from unity, the dimensions defined by the geometry buckling B_0^2 from the solution of the Helmholtz equation are not the critical dimensions of the modified system.

These dimensions are instead characterized by another parameter, B_{m}^2, called the material buckling. When $B_0^2 \neq B_{\mathrm{m}}^2$, the flux shape given by be solution to the criticality eigenvalue equation (103) differs from that of the time-dependent equation (55), as expected. This also defines another condition for criticality as:

$$B_0^2 = B_{\mathrm{m}}^2 \tag{104}$$

The material buckling is defined as:

$$B_{\mathrm{m}}^2 = \frac{\nu\Sigma_{\mathrm{f}} - \Sigma_{\mathrm{a}}}{D} = \frac{k_\infty - 1}{M^2} \tag{105}$$

where the infinite multiplication factor is written as:

$$k_\infty = \frac{\nu\Sigma_{\mathrm{f}}}{\Sigma_{\mathrm{a}}} \tag{106}$$

and the migration area (62):

$$M^2 = \frac{D}{\Sigma_{\mathrm{a}}} \tag{107}$$

These results are next generalized for other geometries and multi-group diffusion theory.

Point-kinetics and eigenvalue equation

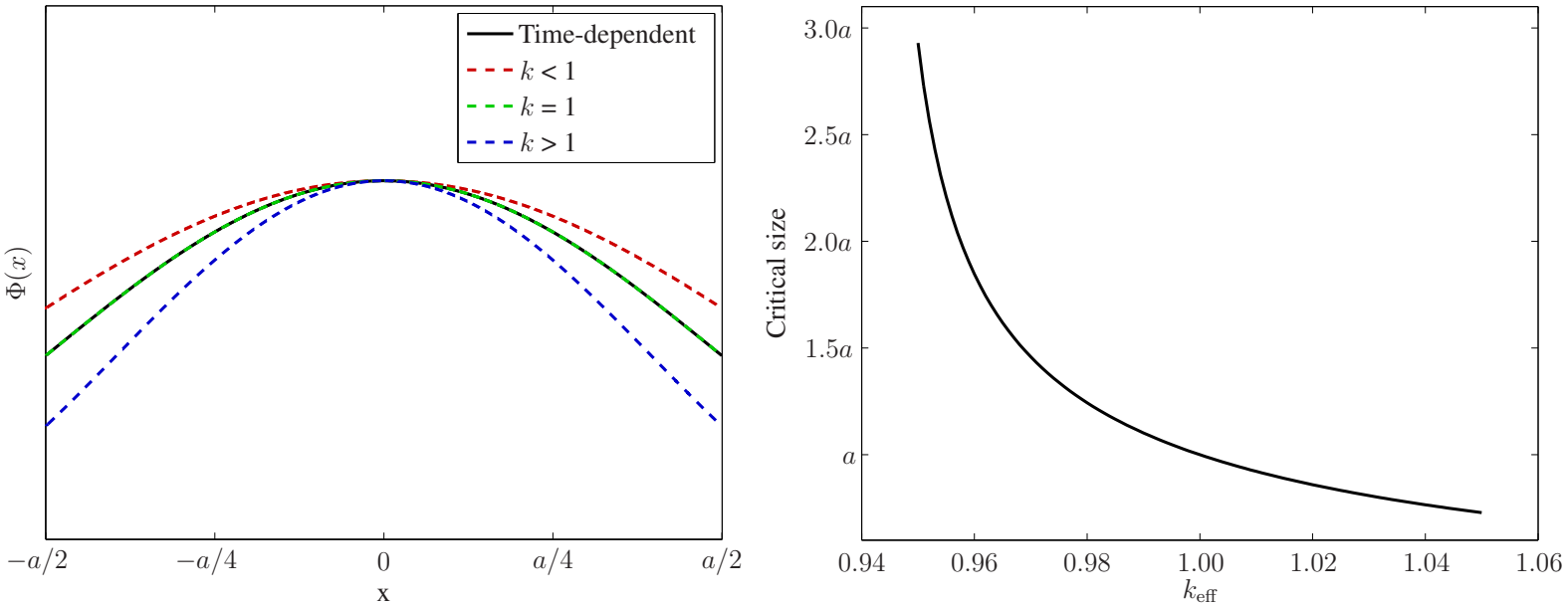


Figure 5 : Left: Spatial flux shape in the infinite bare slab reactor given by the time-dependent solution, and solution to the criticality eigenvalue equation in sub-critical, critical and super-critical state. The change in criticality is invoked by adjusting the absorption cross section. Right: Critical size corresponding to material buckling as function of effective multiplication factor. In the critical state, $B^2_{\text{m}} = B^2_0$, and the critical size corresponds to the physical thickness of the slab. The critical size approaches infinity as $k_\infty \to 1$.

Generalization to other geometries

The periodic cosine shape of the fundamental and transient flux modes was obtained from the solution of the Helmholtz equation in the infinite bare slab geometry. The same principle can be generalized to other one-, two- and three-dimensional geometries as well:

- The flux shape is determined by the solution to the Helmholtz equation, and it depends on the coordinate system and the boundary conditions.
- The solution consists of an infinite number of flux modes, each associated with buckling B_n, which is connected to the inverse period ω_n by Eq. (95).
- The fundamental flux mode represents the asymptotic solution that persists as the transient modes fade away. The corresponding flux shape is determined by the geometry buckling B_0^2.
- The physical parameters determine the material buckling B_{m}^2 in (105), which is associated to the critical dimensions of the system. In critical state $B_{\mathrm{m}}^2 = B_0^2$.

So in addition to the separation of spatial and time dependence, the flux shape is also separated from the physical parameters. This naturally applies only to the case where the geometry is homogeneous.[22]

[22] The flux shape also depends on the presence of other materials via leakage current and boundary conditions, as will pointed out in Lecture 8.

Generalization to other geometries

In three-dimensional Cartesian coordinate system the Laplacian takes the form of:

$$\nabla^2 \Phi = \frac{\partial^2 \Phi}{\partial x^2} + \frac{\partial^2 \Phi}{\partial y^2} + \frac{\partial^2 \Phi}{\partial z^2} \tag{108}$$

The fundamental mode solution in a rectangular parallelepiped with dimensions a, b and c is the product of three terms:

$$\Phi_0(x, y, z) = \Phi_{0,x}(x)\Phi_{0,y}(y)\Phi_{0,z}(z) \tag{109}$$

written separately as:[23]

$$\begin{aligned} \Phi_{0,x}(x) &= C_{0,x} \cos(B_{0,x} x) \\ \Phi_{0,y}(y) &= C_{0,y} \cos(B_{0,y} y) \\ \Phi_{0,z}(z) &= C_{0,z} \cos(B_{0,z} z) \end{aligned} \tag{110}$$

where $C_{0,x}$, $C_{0,y}$ and $C_{0,z}$ are fixed by the boundary conditions, and constants $B_{0,x} = \pi/a$, $B_{0,y} = \pi/b$ and $B_{0,z} = \pi/c$ are defined by the dimensions. The geometry buckling is written as:

$$B_0^2 = B_{0,x}^2 + B_{0,y}^2 + B_{0,z}^2 = \left(\frac{\pi}{a}\right)^2 + \left(\frac{\pi}{b}\right)^2 + \left(\frac{\pi}{c}\right)^2 \tag{111}$$

[23] Assuming that the boundary conditions are symmetric, and the antisymmetric sin-functions disappear.

Generalization to other geometries

Laplacian in the cylindrical coordinates is written as:

$$\nabla^2\Phi = \frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial\Phi}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2\Phi}{\partial\vartheta^2} + \frac{\partial^2\Phi}{\partial z^2} \tag{112}$$

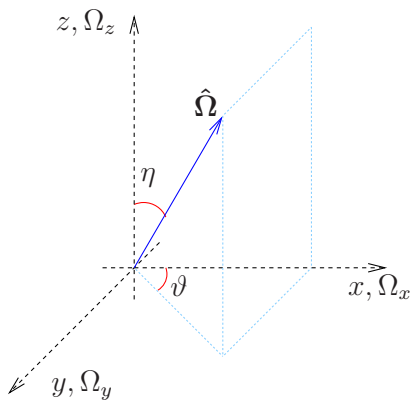
The radial solutions are ordinary Bessel's functions of the first and second kind and axial solutions trigonometric functions.

In spherical system the Laplacian is written as

$$\nabla^2\Phi = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\Phi}{\partial r}\right) + \frac{1}{r^2\sin\vartheta}\frac{\partial}{\partial\vartheta}\left(\sin\vartheta\frac{\partial\Phi}{\partial\vartheta}\right) + \frac{1}{r^2\sin^2\vartheta}\frac{\partial^2\Phi}{\partial\eta^2} \tag{113}$$

where $\vartheta \in [0, \pi]$ is the polar and $\eta \in [0, 2\pi]$ the azimuthal angle. The radial solution takes form:

$$\Phi(r) = C_1\frac{\sin Br}{r} + C_2\frac{\cos Br}{r} \tag{114}$$



Separation of variables for the multi-group equation

The previous results can be generalized to multi-group diffusion theory, and separation of space-, energy- and time-dependence leads to very similar equations. The separation can be written as:

$$\Phi_g(\boldsymbol{r},t) = \Phi_g \mathcal{R}(\boldsymbol{r})\mathcal{T}(t) \tag{115}$$

Starting with time dependence, the substitution of (115) into the multi-group diffusion equation (52) yields:

$$\frac{1}{v_g}\frac{\partial}{\partial t}\Phi_g \mathcal{R}(\boldsymbol{r})\mathcal{T}(t) - D_g\nabla^2\Phi_g\mathcal{R}(\boldsymbol{r})\mathcal{T}(t) + \Sigma_{\mathrm{r},g}\Phi_g\mathcal{R}(\boldsymbol{r})\mathcal{T}(t) = \sum_{g'\neq g}\Sigma_{\mathrm{s},g'g}\Phi_{g'}\mathcal{R}(\boldsymbol{r})\mathcal{T}(t) + \chi_g\sum_{g'}\nu\Sigma_{\mathrm{f},g'}\Phi_{g'}\mathcal{R}(\boldsymbol{r})\mathcal{T}(t) \tag{116}$$

or by re-grouping the terms:

$$\Phi_g\mathcal{R}(\boldsymbol{r})\frac{1}{v_g}\frac{\partial}{\partial t}\mathcal{T}(t) = \mathcal{T}(t)\left[D_g\nabla^2\Phi_g\mathcal{R}(\boldsymbol{r}) - \Sigma_{\mathrm{r},g}\Phi_g\mathcal{R}(\boldsymbol{r}) + \sum_{g'\neq g}\Sigma_{\mathrm{s},g'g}\Phi_{g'}\mathcal{R}(\boldsymbol{r}) + \chi_g\sum_{g'}\nu\Sigma_{\mathrm{f},g'}\Phi_{g'}\mathcal{R}(\boldsymbol{r})\right] \tag{117}$$

Separation of variables for the multi-group equation

Division of Eq. (117) by $\Phi_g \mathcal{R}(\boldsymbol{r})\mathcal{T}(t)$ yields:

$$\frac{1}{\mathcal{T}(t)}\frac{\partial}{\partial t}\mathcal{T}(t) = \frac{v_g}{\Phi_g \mathcal{R}(\boldsymbol{r})}\Bigg[D_g \nabla^2 \Phi_g \mathcal{R}(\boldsymbol{r}) - \Sigma_{\mathrm{r},g}\Phi_g \mathcal{R}(\boldsymbol{r}) + \sum_{g' \neq g} \Sigma_{\mathrm{s},g'g}\Phi_{g'}\mathcal{R}(\boldsymbol{r}) + \chi_g \sum_{g'} \nu\Sigma_{\mathrm{f},g'}\Phi_{g'}\mathcal{R}(\boldsymbol{r})\Bigg] \tag{118}$$

Since the LHS Eq. (118) depends only on time and the RHS on spatial coordinates and energy, both sides must be equal to a constant, independent of all variables.

When this constant is written as ω, the LHS of (118) becomes:

$$\frac{1}{\mathcal{T}(t)}\frac{\partial}{\partial t}\mathcal{T}(t) = \omega \tag{119}$$

or:

$$\frac{\partial}{\partial t}\mathcal{T}(t) - \omega\mathcal{T}(t) = 0 \tag{120}$$

with solution identical to that for the one-group equation (79):

$$\mathcal{T}(t) = \mathcal{T}(0)e^{\omega t} \tag{121}$$

Separation of variables for the multi-group equation

The RHS Eq. (118) is written as:

$$D_g \nabla^2 \Phi_g \mathcal{R}(\boldsymbol{r}) - \Sigma_{\mathrm{r},g} \Phi_g \mathcal{R}(\boldsymbol{r}) + \sum_{g' \neq g} \Sigma_{\mathrm{s},g'g} \Phi_{g'} \mathcal{R}(\boldsymbol{r}) + \chi_g \sum_{g'} \nu \Sigma_{\mathrm{f},g'} \Phi_{g'} \mathcal{R}(\boldsymbol{r}) = \frac{\omega}{v_g} \Phi_g \mathcal{R}(\boldsymbol{r}) \tag{122}$$

By re-grouping the terms, Eq. (122) can be written as:

$$D_g \Phi_g \nabla^2 \mathcal{R}(\boldsymbol{r}) = \mathcal{R}(\boldsymbol{r}) \left[\Sigma_{\mathrm{r},g} \Phi_g - \sum_{g' \neq g} \Sigma_{\mathrm{s},g'g} \Phi_{g'} - \chi_g \sum_{g'} \nu \Sigma_{\mathrm{f},g'} \Phi_{g'} + \frac{\omega}{v_g} \Phi_g \right] \tag{123}$$

Division of Eq. (123) by $\Phi_g \mathcal{R}(\boldsymbol{r})$ yields:[24]

$$\frac{1}{\mathcal{R}(\boldsymbol{r})} \nabla^2 \mathcal{R}(\boldsymbol{r}) = \frac{1}{D_g \Phi_g} \left[\Sigma_{\mathrm{r},g} \Phi_g - \sum_{g' \neq g} \Sigma_{\mathrm{s},g'g} \Phi_{g'} - \chi_g \sum_{g'} \nu \Sigma_{\mathrm{f},g'} \Phi_{g'} + \frac{\omega}{v_g} \Phi_g \right] \tag{124}$$

Since the LHS of the equation depends only on the spatial coordinates and the RHS on energy, both sides must be equal to a constant, independent of all variables.

[24] It is assumed here that the boundary conditions are the same for each energy group.

Separation of variables for the multi-group equation

When this constant is denoted by $-B^2$, the LHS of (124) is written as:

$$\frac{1}{\mathcal{R}(\boldsymbol{r})}\nabla^2\mathcal{R}(\boldsymbol{r}) = -B^2 \tag{125}$$

or:

$$\nabla^2\mathcal{R}(\boldsymbol{r}) + B^2\mathcal{R}(\boldsymbol{r}) = 0 \tag{126}$$

which is the Helmholtz equation, identical to that derived for the one-group theory (84).

The RHS of (124) is written as:

$$\frac{\omega}{v_g}\Phi_g + D_g B^2\Phi_g + \Sigma_{\mathrm{r},g}\Phi_g = \sum_{g'\neq g}\Sigma_{\mathrm{s},g'g}\Phi_{g'} + \chi_g\sum_{g'}\nu\Sigma_{\mathrm{f},g'}\Phi_{g'} \tag{127}$$

This corresponds to Eq. (85) in one-group theory.

In other words, the multi-group diffusion equation (52) is now separated into an exponential time-dependent amplitude function (79), the Helmholtz equation (126) describing the spatial dependence and G algebraic equations (127) describing the energy dependence. These equations are coupled by two constants ω and B for each flux mode n.

Separation of variables for the multi-group equation

With two energy groups, the energy-separated equations are written as:

$$\begin{aligned} \frac{\omega}{v_1}\Phi_1 - D_1 B^2 \Phi_1 + \left(\Sigma_{\mathrm{a},1} + \Sigma_{\mathrm{rem}}\right)\Phi_1 &= \nu\Sigma_{\mathrm{f},1}\Phi_1 + \nu\Sigma_{\mathrm{f},2}\Phi_2 \\ \frac{\omega}{v_2}\Phi_2 - D_2 B^2 \Phi_2 + \Sigma_{\mathrm{a},2}\Phi_2 &= \Sigma_{\mathrm{rem}}\Phi_1 \end{aligned} \tag{128}$$

or in k-eigenvalue form:

$$\begin{aligned} -D_1 B^2 \Phi_1 + \left(\Sigma_{\mathrm{a},1} + \Sigma_{\mathrm{rem}}\right)\Phi_1 &= \frac{1}{k_{\mathrm{eff}}}\left[\nu\Sigma_{\mathrm{f},1}\Phi_1 + \nu\Sigma_{\mathrm{f},2}\Phi_2\right] \\ -D_2 B^2 \Phi_2 + \Sigma_{\mathrm{a},2}\Phi_2 &= \Sigma_{\mathrm{rem}}\Phi_1 \end{aligned} \tag{129}$$

Material buckling is written similar to the one-group case (105):

$$B_{\mathrm{m}}^2 = \frac{k_\infty - 1}{M^2} \tag{130}$$

but the migration area is divided into fast and thermal diffusion areas:

$$M^2 = L_1^2 + L_2^2 = \frac{D_1}{\Sigma_{\mathrm{rem}} + \Sigma_{\mathrm{a1}}} + \frac{D_2}{\Sigma_{\mathrm{a2}}} \tag{131}$$

Separation of variables for the multi-group equation

The infinite multiplication factor is written as:

$$k_\infty = \frac{\Sigma_{\mathrm{a},2}\nu\Sigma_{\mathrm{f},1}(L_2^2B_0^2+1)+\nu\Sigma_{\mathrm{f},2}\Sigma_{\mathrm{rem}}}{\Sigma_{\mathrm{a},2}\Sigma_{\mathrm{a},1}(L_2^2B_0^2+1)+\Sigma_{\mathrm{a},2}\Sigma_{\mathrm{rem}}} \tag{132}$$

the effective multiplication factor as:

$$k_{\mathrm{eff}} = \frac{1}{\Sigma_{\mathrm{a},1}+\Sigma_{\mathrm{rem}}}\left[\frac{\nu\Sigma_{\mathrm{f},1}}{L_1^2B_0^2+1}+\frac{\Sigma_{\mathrm{rem}}\nu\Sigma_{\mathrm{f},2}}{\Sigma_{\mathrm{a},2}\left(L_1^2B_0^2+1\right)\left(L_2^2B_0^2+1\right)}\right] \tag{133}$$

and flux ratio as:

$$\frac{\Phi_1}{\Phi_2} = \frac{\Sigma_{\mathrm{a},2}(L_2^2B_0^2+1)}{\Sigma_{\mathrm{rem}}} \tag{134}$$

Boundary conditions

The diffusion flux solution is determined by:

- The physical reaction cross sections: group-transfer, absorption, fission neutron production
- Diffusion coefficient, characterizing distance of neutron migration in homogeneous medium
- Initial conditions, determining the flux shape at $t = 0$ (in time-dependent problems)
- Boundary conditions, fixing the value of Φ at the outer boundary

Some of the most common boundary conditions are introduced in the following. In most cases, the formulation is straightforward in transport theory with angular flux and current density, but the use of diffusion theory, and integration over full solid angle requires additional approximations.

The most trivial boundary condition is to set the flux zero at the boundary:[25]

$$\Phi(\boldsymbol{r}) = 0 \tag{135}$$

when $\mathbf{r} \in S$ and S is the outer geometry boundary. This boundary condition is somewhat unphysical, as the flux practically never goes to zero immediately beyond the region of interest.

[25] The zero-flux boundary condition is easily confused with the vacuum boundary condition.

Boundary conditions

In transport theory, vacuum boundary implies that the inward current component is zero at the outer boundary:

$$J^- = \int_{-1}^{0} \int_S \int_E \left[\mathbf{j}(\boldsymbol{r}, \hat{\boldsymbol{\Omega}}, E) \cdot \hat{\mathbf{u}} \right] d\mu dS dE = 0 \tag{136}$$

where $\mu = \hat{\boldsymbol{\Omega}} \cdot \hat{\mathbf{u}}$ is the cosine between the neutron direction of motion and the surface normal.[26]

This definition does not apply to diffusion theory, which only deals with the net current. The most common approach to handle vacuum boundaries is to introduce an extrapolation distance that extends the zero-point of flux over the outer boundary. In the infinite slab geometry this would change the geometry buckling (90) into:

$$B_0^2 = \frac{\pi}{a + d_{\mathrm{ex}}} \tag{137}$$

where the extrapolation distance is given by:

$$d_{\mathrm{ex}} = \frac{2}{3}\lambda_{\mathrm{tr}} = \frac{2}{3\Sigma_{\mathrm{tr}}} = 2D \tag{138}$$

The flux solution is not valid outside the slab, but near the boundary this approximation takes into account the fact that flux does not fall to zero in vacuum.

[26] Assuming that $\hat{\mathbf{u}}$ points in the outward direction.

Boundary conditions

In repeated geometries, such as infinite lattices, it is common to describe the repeated structure with reflective or periodic boundary conditions.

Reflection means that each reflected neutron has an equal and opposite contribution to the inward and outward component of net current, which means that the net current at the boundary is reduced to zero:

$$\mathbf{J}(\boldsymbol{r}, E) \cdot d\mathbf{S} = 0 \tag{139}$$

when $\mathbf{r} \in S$. This boundary condition is relatively easy to invoke by applying Fick's law to write the condition for flux gradient. For the slab geometry with flux given by (89) this condition would be written as:[27]

$$\frac{d}{dx}\Big[C_1 \sin(Bx) + C_2 \cos(Bx)\Big]_{x=\frac{a}{2}} = -C_1 \sin(B\frac{a}{2}) + C_2 \cos(B\frac{a}{2}) = 0 \tag{140}$$

In nodal diffusion methods the boundary conditions are obtained from so-called discontinuity factors, which couple the flux solution in adjacent nodes together at the common boundary:

$$f_k^- \Phi_g^-(x_k) = f_k^+ \Phi_g^+(x_k) \tag{141}$$

where k_k is the discontinuity factor at surface k, and $-$ and $+$ refer to the negative and positive side, respectively. This topic will be covered in Lecture 8.

[27] Note that this system may not be critical, in which case B is not given by the geometry configuration alone.

Boundary conditions

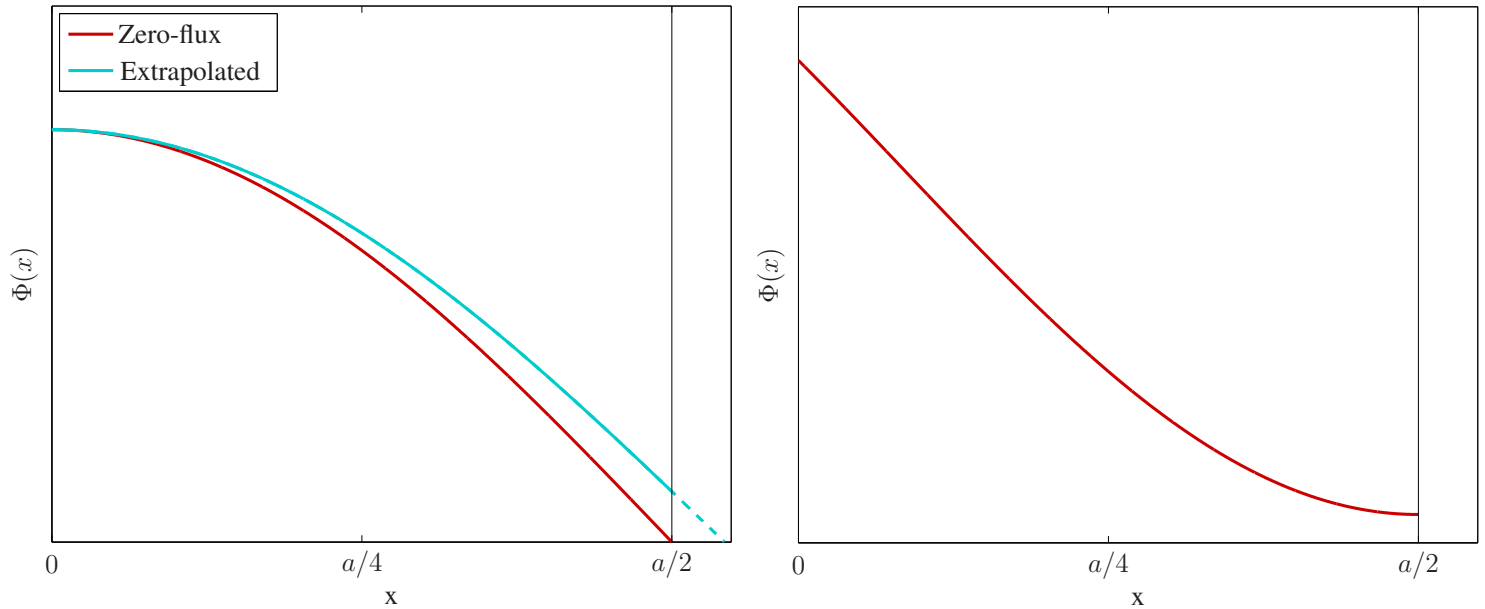


Figure 6 : Left: Zero-flux and vacuum boundary condition using extrapolation distance. The zero-point of flux is extended beyond the boundary to get at better representation inside. Right: Reflective boundary condition, which enforces the flux gradient to zero at the boundary.

Summary of main topics

Diffusion theory is one of the most widely used solution methods in reactor analysis. The main advantage of the method is that neutron balance can be expressed in terms of the scalar flux alone, which makes the resulting diffusion equation easy to solve.

The theory is derived based on a number of seemingly crude assumptions:

- Linearly isotropic flux and isotropic scattering[28]
- No steep flux gradients
- Scattering is the dominant reaction mode

Diffusion approximation fails in heterogeneous geometries, but can be applied with remarkable accuracy when combined with spatial homogenization.

The spatial flux solution can be written using analytical form functions in simple geometries. The solution depends on the geometry, physical reaction cross sections (absorption, group-transfer, fission neutron production), diffusion coefficient and the boundary conditions.

Solution of the two-group diffusion equation in regularly-shaped homogeneous nodes forms the basis of nodal diffusion methods, which are the fundamental calculation tools in full-scale fuel cycle and transient simulations.

[28] The error introduced by isotropic scattering is corrected to some extent in the definition of the diffusion coefficient.

Topics of next lecture

The topic of next lecture (28.3.2018) is burnup calculation, i.e. tracking the isotopic changes in fuel during neutron irradiation.

Specific topics include:

- Effects of fuel burnup on neutronics
- Fission product poisons and xenon oscillations
- Radioactive decay and transmutation reactions
- Formulation and solution of the Bateman depletion equations
- Burnup algorithms
- Burnup calculation as an example of a non-linear coupled problem