22.211 Lecture 14

Diffusion coefficients

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Outline

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Objectives

- Diffusion Equation
- 1 group approximation
- Analytical solutions to non-multiplying problems
- Diffusion area

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P_1 Approximation

$$\nabla \cdot J(\mathbf{r}, E) + \Sigma_t(\mathbf{r}, E)\phi(\mathbf{r}, E) = \int_0^\infty dE' \Sigma_{s0}(\mathbf{r}, E' \to E)\phi(\mathbf{r}, E') + \chi(E) \int_0^\infty dE' \nu\Sigma_f(\mathbf{r}, E')\phi(\mathbf{r}, E') + S(\mathbf{r}, E)$$

$$\frac{\nabla\phi(\mathbf{r}, E)}{3} + \Sigma_t(\mathbf{r}, E)J(\mathbf{r}, E) = \int_0^\infty dE' \Sigma_{s1}(\mathbf{r}, E' \to E)J(\mathbf{r}, E')$$

We now have 2 equations and 2 unknowns

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Out-Scatter Approximation

In a weakly absorbing media, the in-scatter rate will approximately balance the out-scatter rate.

$$\int_0^\infty \Sigma_{s1}(\mathbf{r}, E' \to E) J(\mathbf{r}, E') dE' \approx \int_0^\infty \Sigma_{s1}(\mathbf{r}, E \to E') J(\mathbf{r}, E) dE'$$

which can be written as

$$\int_0^\infty \Sigma_{s1}(\mathbf{r}, E \to E') J(\mathbf{r}, E) dE' = \mu_0 \Sigma_s(\mathbf{r}, E) J(\mathbf{r}, E)$$

DO NOT USE FOR HYDROGEN-BASED SYSTEMS!

Fick's Law

Using

$$J(\mathbf{r}, E) = -D(\mathbf{r}, E)\nabla\phi(\mathbf{r}, E)$$

where

$$D(\mathbf{r}, E) = \frac{1}{3(\Sigma_t(\mathbf{r}, E) - \mu_0\Sigma_s(\mathbf{r}, E))} = \frac{1}{3\Sigma_{tr}(\mathbf{r}, E)}$$

In-scatter Approximation

$$D(\mathbf{r}, E) = \frac{1}{3\left(\Sigma_t(\mathbf{r}, E) - \frac{\int_0^\infty \Sigma_{s,1}(\mathbf{r}, E' \to E) J(\mathbf{r}, E') dE'}{J(\mathbf{r}, E)}\right)}$$

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Diffusion Equation

$$-\nabla.D(x,E)\nabla\phi(x,E)+\Sigma_t(x,E)\phi(x,E)=$$
$$\int_0^\infty \Sigma_{s0}(x,E'\rightarrow E)\phi(x,E')dE'+$$
$$\chi(E)\int_0^\infty \nu\Sigma_f(x,E')\phi(x,E')+S(x,E)$$

Notes on Diffusion Equation

Main assumptions:

- Angular flux only has a linear angular component
- Neutron sources are isotropic (external sources and fission sources)
- Most events happen in a weakly absorbing media (balance of in-scatter and out-scatter rates)

It breaks down:

- Near external boundaries of the system (vacuum BC)
- Abrupt changes in material properties
- Close to localized sources
- Close to strongly absorbing media (e.g. control rods)

Things to note

- $\chi(E)$ is isotope dependent
- $\chi(E)$ is also incoming energy dependent, i.e. $\chi(E' \to E)$
- In the steady-state form, $\chi(E)$ must include both prompt and delayed components.
- Out-scatter approximation is not valid for reactors with lots of hydrogen.

Partial Currents

$$J^{\pm}(\mathbf{r_s}, E) = \frac{1}{4}\phi(\mathbf{r_s}, E) \mp \frac{D}{2}\nabla\phi(\mathbf{r_s}, E)$$

Boundary Conditions

1. Vacuum $J^{\pm} = 0$
2. Vacuum - Extrapolated distance $\phi(x_s + 2D) = 0$
3. Reflective $J^{+} = J^{-}$
4. Albedo

$$\alpha = \frac{J^{\mp}}{J^{\pm}}$$

Recap

- Scattering kernel can be represented by an orthogonal polynomial expansion
- Scattering kernels are commonly stored in terms of Legendre polynomials
- Angular flux and source can also be expressed in terms of Legendre polynomials
- This expresses all angular dependence from the set of equations as flux moments
- The linear approximation is also known as the Diffusion equation

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Diffusion Equation

General form of the steady-state diffusion equation

$$-\nabla \cdot D(\vec{r}, E)\nabla\phi(\vec{r}, E) + \Sigma_t(\vec{r}, E)\phi(\vec{r}, E) = \int_0^\infty dE'\Sigma_s(\vec{r}, E' \to E)\phi(\vec{r}, E') + \chi(E)\int_0^\infty \nu\Sigma_f(\vec{r}, E')\phi(\vec{r}, E') + S(\vec{r}, E)$$

It represents a balance of neutrons in a volume element.

Multigroup constants

The diffusion coefficient should be weighted by gradient of the flux

$$D_g(\vec{r}) = \frac{\int_{E_g}^{E_{g-1}} D(\vec{r}, E)\nabla\phi(\vec{r}, E)dE}{\int_{E_g}^{E_{g-1}} \nabla\phi(\vec{r}, E)dE} \approx \frac{\int_{E_g}^{E_{g-1}} D(\vec{r}, E)\phi(\vec{r}, E)dE}{\int_{E_g}^{E_{g-1}} \phi(\vec{r}, E)dE}$$

The fission spectrum is expressed as

$$\chi_g = \int_{E_g}^{E_{g-1}} \chi(E)$$

However, if you have many isotopes and/or trying to compute an effective χ, you need to weight χ by the fission rates.

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Multigroup Diffusion Equation

$$
\begin{aligned}
-\nabla \cdot D_g(\vec{r})\nabla\phi_g(\vec{r}) + \Sigma_{t,g}(\vec{r})\phi_g(\vec{r}) &= \sum_{g'=1}^{G} \Sigma_{s,g'\to g}(\vec{r})\phi_{g'}(\vec{r}) \\
&+ \chi_g \sum_{g'=1}^{G} \nu\Sigma_{f,g}(\vec{r})\phi_{g'}(\vec{r}) + S_g(\vec{r})
\end{aligned}
$$

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One group equation

$$-\nabla \cdot D(\vec{r})\nabla\phi(\vec{r}) + \Sigma_t(\vec{r})\phi(\vec{r}) = \Sigma_s(\vec{r})\phi(\vec{r}) + \nu\Sigma_f(\vec{r})\phi(\vec{r}) + S(\vec{r})$$

which can be simplified to

$$-\nabla \cdot D(\vec{r})\nabla\phi(\vec{r}) + \left(\Sigma_a(\vec{r}) - \nu\Sigma_f(\vec{r})\right)\phi(\vec{r}) = S(\vec{r})$$

Non-multiplying with constant parameters

We will further simplify by assuming that $\Sigma_f = 0$ and that the macroscopic cross sections are constant in space.

$$-D\nabla^2\phi(\vec{r}) + \Sigma_a\phi(\vec{r}) = S(\vec{r})$$

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Laplacian

In 1D Cartesian

$$\nabla^2 = \frac{\partial^2}{\partial x^2} \qquad dV = 1cm^2 \cdot dx$$

In 1D Cylindrical

$$\nabla^2 = \frac{1}{r}\frac{\partial}{\partial r} r \frac{\partial}{\partial r} \qquad dV = 1cm \cdot 2\pi r dr$$

In 1D Spherical

$$\nabla^2 = \frac{1}{r^2}\frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r} \qquad dV = 4\pi r^2 dr$$

General Solution - 2^{nd} order ODEs

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

where the general solution takes the form

$$y(x) = e^{rx}$$

with roots of $r^2 + B^2 = 0$. If $B^2 < 0$, the roots are real

$$r = \pm B$$

with an homogeneous solution

$$y(x) = c_1 e^{Bx} + c_2 e^{-Bx}$$

General Solution - 2^{nd} order ODEs

If $B^2 > 0$, the roots are complex

$$r = \pm iB$$

with an homogeneous solution

$$y(x) = c_1 e^{iBx} + c_2 e^{-iBx}$$

Knowing the relation $e^{i\theta} = cos\theta + isin\theta$ and $e^{-i\theta} = cos\theta - isin\theta$, we can express the solution as

$$y(x) = c_1 cos(Bx) + c_2 sin(Bx)$$

General Solutions - 2^{nd} order ODEs

General form

$$\frac{d^2}{dx^2}y(x) - b^2 y(x) = S(x)$$

General solution

$$y(x) = y_{hom}(x) + y_p(x)$$

Homogeneous solution

$$y_{hom}(x) = C_1 e^{-bx} + C_2 e^{bx}$$

General form

$$\frac{d^2}{dx^2}y(x) + a^2 y(x) = S(x)$$

General solution

$$y(x) = y_{hom}(x) + y_p(x)$$

Homogeneous solution

$$y_{hom}(x) = C_1 \sin(ax) + C_2 \cos(ax)$$

Multidimension

In a multi-dimensional problem, we assume separability of spatial variables which implies that B^2 is represented by a sum of the terms in each direction.

$$B^2 = B_x^2 + B_y^2 + B_z^2$$

Then each direction is solved independently, thus some directions can have a positive buckling term and others a negative buckling term.

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Knowing that

$$\phi(r) = \frac{Se^{-r/L}}{4\pi Dr}$$

we can write that the number of neutrons, dN, absorbed per second in a spherical volume, $dV = 4\pi r^2 dr$, located between r and $r + dr$ is equal to

$$dN = \Sigma_a \phi(r) dV = \frac{S}{L^2} r e^{-r/L} dr$$

We can write the probability of a source neutron being absorbed as

$$p(r)dr = \frac{dN}{S} = \frac{1}{L^2} re^{-r/L} dr$$

The second moment of which is equal to

$$\bar{r^2} = \frac{1}{L^2} \int_0^{\infty} r^3 e^{-r/L} dr = 6L^2$$

Thus the diffusion area, defined as L^2 is equal to

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

where $\bar{r^2}$ is the square of the crow flight distance.

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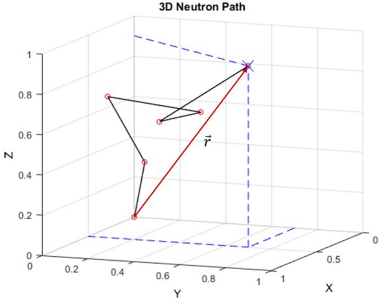
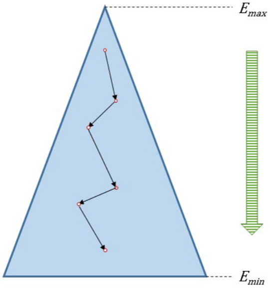
Migration area





Diffusion coefficient - Infinite medium

Thus in the infinite medium, we can define the 1 group diffusion coefficient as

$$D = \frac{\Sigma_a \bar{r}^2}{6}$$

or in terms of the transport mean free path

$$\lambda_{tr} = \frac{\Sigma_a \bar{r}^2}{2}$$

Asymptotic value

The asymptotic value of D can also be calculated for a constant cross section following the derivation in the Lamarsh Reactor Theory book. If a neutron travels in direction x, its first path, x_0, on average is λ. The second path, x_1, will be $\lambda\bar{\mu}$. From the addition theorem, we can calculate the third path, x_2,

$$cos\alpha = cos\theta_1 cos\theta_2 + sin\theta_1 sin\theta_2 cos(\phi_1 - \phi_2)$$

Thus, the third path is equal to $\overline{\lambda \cos\alpha}$, which knowing that $\phi_1 - \phi_2$ is arbitrary between 0 and 2π is equal to $\lambda\bar{\mu}^2$. The sum of the distance travel becomes

$$\bar{x_0} + \bar{x_1} + \bar{x_2} + \cdots = \lambda + \lambda\bar{\mu} + \lambda\bar{\mu}^2 + \cdots = \frac{\lambda}{1-\bar{\mu}} = \lambda_{tr}$$

Cumulative Migration Area

However, cross-sections are not constant, and in H-1, the asymptotic is not reached until significant slowing down as already occurred. It is thus important to properly capture the energy dependence of the slowing down process and migration.

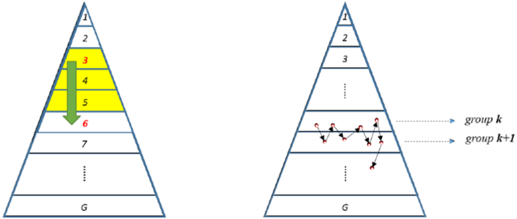


Figure 7. Scenario examples of a neutron's energy transition in a down-scatter reaction (left) and a series of down-scatter and up-scatter reactions (right).

Cumulative Migration Area

The original process computes the migration area from birth to each group boundaries, which provides the diffusion equation from birth to the energy bound if we also know the cumulative removal cross-section

$$(M_g^c)^2 = \frac{1}{6}\bar{r}^2 \qquad (M_g^c)^2 = \frac{D_g^c}{\Sigma_{r,g}^c}$$

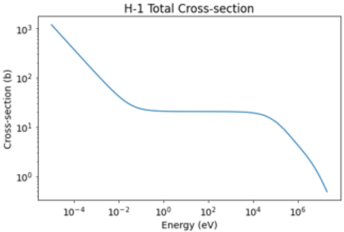
The cumulative diffusion coefficient is then unfolded

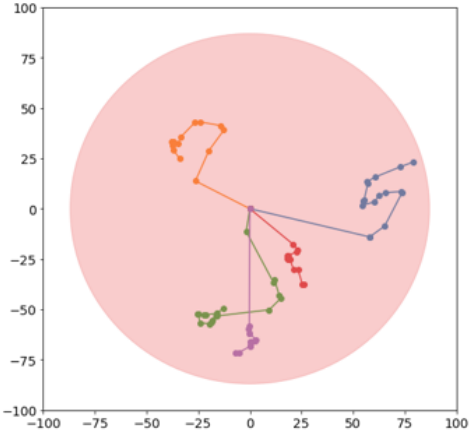
$$D_g^c = \frac{\sum_{g'=1}^{g} D_{g'}\phi_{g'}}{\sum_{g'=1}^{g}\phi_{g'}}$$

Recently, a new equivalent approach was developed only using incremental migration area thus facilitating the process.

Energy Dependence

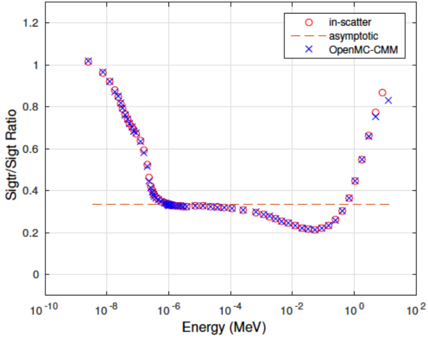
- Fast neutrons tend to travel greater distances and contribute most to the migration area.
- After many interactions, neutrons tend to travel less and lose sight of their initial direction.





Energy dependent transport xs

The first neutron knows nothing about the medium and its asymptotic properties, so it's mean free path should be $1/\Sigma_t$. The reason why simply assuming the asymptotic value with H-1 is a poor approximation is that neutrons can lose lots of energy with few collisions, thus they have already slowed down significantly before reaching that asymptotic. This leads to significantly mispredicting the flow of fast neutrons.



Different diffusion approximations

In-scatter

$$\sigma_{tr,g} = \sigma_{t,g} - \frac{\sum_{g'=1}^{G} \sigma_{s1,g'\rightarrow g} J_{g'}}{J_g}$$

Out-scatter (use average μ but only within the group)

$$\sigma_{tr,g} = \sigma_{t,g} - \frac{\sum_{g'=1}^{G} \sigma_{s1,g\rightarrow g'} J_{g}}{J_g} = \sigma_{t,g} - \bar{\mu}_g \sigma_{s,g}$$

Flux-limited

$$\sigma_{tr,g} = \sigma_{t,g} - \frac{\sum_{g'=1}^{G} \sigma_{s1,g'\rightarrow g} \phi_{g'}}{\phi_g}$$

Asymptotic (same average μ across entire energy range)

$$\sigma_{tr,g} = \sigma_{t,g} - \bar{\mu} \sigma_{s,g}$$

Results

Diffusion coefficients are condensed in energy

$$D_g = \frac{\sum_{h'=1}^{H} D_{h'} \phi_{h'}}{\sum_{h'=1}^{H} \phi_{h'}}$$

Never condense a transport cross-section in energy!

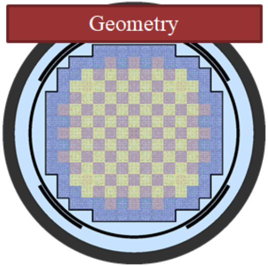
	Fast Group Diffusion Coefficient			
Energy Collapse Weighting	P1 with Inscatter	P1 with Outscatter	B1 with Inscatter	Monte Carlo Cumulative Migration*
Diffusion Coefficient	1.435	1.544	1.393	1.426
Difference From MC	0.6%	8.3%	-2.3%	
Sigma Transport	1.169	1.149	1.397**	
Difference From MC	-18.0%	-19.4%	-2.0%	

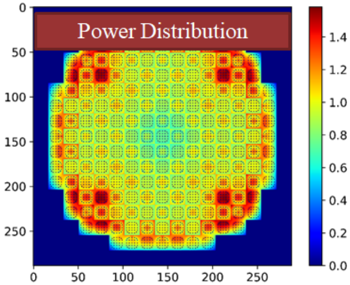
*See Companion Paper by Liu, Smith, and Forget

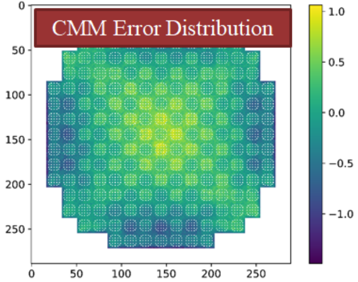
** Lepannen for 2.4% lattice wth 12 Pyrex BP

Impact at core level - Full core PWR

These results are from a transport theory simulation in 70 groups using transport-corrected data (similar to a diffusion coefficient) on a 2D PWR model.







Mispredicting the streaming of fast neutrons leads to large in/out tilts.