

Derivation of Continuous Energy Diffusion Equation

The transport equation is made up of four terms, the time-rate of change in neutron density, the streaming term, the removal term and the source term q , as seen below [1]. The streaming term is the amount of neutrons that traveled into or out of the system during time t . The removal term, also referred to as a collisions term, is the amount of neutrons lost or added to the system due to collisions, and the source term is the number of neutrons added to the system from within the system. This term is then split between external source Q , the flux-dependent scattering source S , and the fission source F . Since there is no external source, Q will go to zero. In these equations, v is the neutron speed, ψ is the angular neutron flux, \mathbf{r} is the spatial variable, $\hat{\Omega}$ is the unit vector regarding the direction of travel, and E is the neutron energy. Time is t , ν is the mean number of neutrons created from fission, χ is the neutrons born at a certain energy, ϕ is the scalar flux, Σ_f is the macroscopic fission cross-section, and Σ_s is the macroscopic scattering cross-section. E' and $\hat{\Omega}'$ represent new direction and energy neutrons are scattering towards.

$$\frac{1}{v} \frac{\partial}{\partial t} \psi(\mathbf{r}, \hat{\Omega}, E, t) + \hat{\Omega} \cdot \nabla \psi(\mathbf{r}, \hat{\Omega}, E, t) + \Sigma(\mathbf{r}, E) \psi(\mathbf{r}, \hat{\Omega}, E, t) = q(\mathbf{r}, \hat{\Omega}, E, t) \quad (1)$$

$$q(\mathbf{r}, \hat{\Omega}, E, t) = Q(\mathbf{r}, \hat{\Omega}, E, t) + S(\mathbf{r}, \hat{\Omega}, E, t) + F(\mathbf{r}, \hat{\Omega}, E, t) \quad (2)$$

$$S(\mathbf{r}, \hat{\Omega}, E, t) = \int_0^{4\pi} \int_0^\infty \Sigma_s(\mathbf{r}, \hat{\Omega}' \rightarrow \hat{\Omega}, E' \rightarrow E) \psi(\mathbf{r}, \hat{\Omega}', E', t) d\hat{\Omega}' dE' \quad (3)$$

$$F(\mathbf{r}, \hat{\Omega}, E, t) = \frac{\chi(E)}{4\pi} \int_0^\infty \nu \Sigma_f(\mathbf{r}, E') \phi(\mathbf{r}, E', t) dE' \quad (4)$$

To derive the diffusion equation, I will have to integrate out the $\hat{\Omega}$ term of the transport equation. Below I have broken up the terms individually and integrated each one accordingly. The unit vector is integrated from 0 to 4π because it is in spherical coordinates. Energy is integrated from 0 to ∞ to get all the possible energy values. The time-rate of change in neutron density is:

$$\frac{1}{v} \frac{\partial}{\partial t} \psi(\mathbf{r}, \hat{\Omega}, E, t) \quad (5)$$

$$\int_0^{4\pi} \frac{1}{v} \frac{\partial}{\partial t} \psi(\mathbf{r}, \hat{\Omega}, E, t) d\hat{\Omega} \quad (6)$$

$$\frac{1}{v} \frac{\partial}{\partial t} \int_0^{4\pi} \psi(\mathbf{r}, \hat{\Omega}, E, t) d\hat{\Omega} \quad (7)$$

Given that $\phi(\mathbf{r}, E) = \int_0^{4\pi} \psi(\mathbf{r}, \hat{\Omega}, E) d\hat{\Omega}$, I can set

$$\int_0^{4\pi} \psi(\mathbf{r}, \hat{\Omega}, E, t) d\hat{\Omega} = \phi(\mathbf{r}, E, t) \quad (8)$$

$$\int_0^{4\pi} \frac{1}{v} \frac{\partial}{\partial t} \psi(\mathbf{r}, \hat{\Omega}, E, t) d\hat{\Omega} = \frac{1}{v} \frac{\partial}{\partial t} \phi(\mathbf{r}, E, t) \quad (9)$$

The collision term is expressed as:

$$\Sigma(\mathbf{r}, E) \psi(\mathbf{r}, \hat{\Omega}, E, t) \quad (10)$$

$$\int_0^{4\pi} \Sigma(\mathbf{r}, E) \psi(\mathbf{r}, \hat{\Omega}, E, t) d\hat{\Omega} = \Sigma(\mathbf{r}, E) \int_0^{4\pi} \psi(\mathbf{r}, \hat{\Omega}, E, t) d\hat{\Omega} \quad (11)$$

$$\int_0^{4\pi} \psi(\mathbf{r}, \hat{\Omega}, E, t) d\hat{\Omega} = \phi(\mathbf{r}, E, t) \quad (12)$$

$$\int_0^{4\pi} \Sigma(\mathbf{r}, E) \psi(\mathbf{r}, \hat{\Omega}, E, t) d\hat{\Omega} = \Sigma(\mathbf{r}, E) \phi(\mathbf{r}, E, t) \quad (13)$$

The streaming term is:

$$\hat{\Omega} \cdot \nabla \psi(\mathbf{r}, \hat{\Omega}, E, t) \quad (14)$$

$$\hat{\Omega} \cdot \nabla \psi(\mathbf{r}, \hat{\Omega}, E, t) = \nabla \cdot \hat{\Omega} \psi(\mathbf{r}, \hat{\Omega}, E, t) \quad (15)$$

Given that $\hat{\Omega}\psi(\mathbf{r}, \hat{\Omega}, E, t) = \mathbf{j}(\mathbf{r}, \hat{\Omega}, E, t)$, where \mathbf{j} is the angular current density per time. Therefore:

$$\nabla \cdot \hat{\Omega}\psi(\mathbf{r}, \hat{\Omega}, E, t) = \nabla \cdot \mathbf{j}(\mathbf{r}, \hat{\Omega}, E, t) \quad (16)$$

$$\int_0^{4\pi} \nabla \cdot \mathbf{j}(\mathbf{r}, \hat{\Omega}, E, t) d\hat{\Omega} = \nabla \cdot \int_0^{4\pi} \mathbf{j}(\mathbf{r}, \hat{\Omega}, E, t) d\hat{\Omega} \quad (17)$$

Given that $\int_0^{4\pi} \mathbf{j}(\mathbf{r}, \hat{\Omega}, E, t) d\hat{\Omega} = \mathbf{J}(\mathbf{r}, E, t)$ and where \mathbf{J} is the neutron current density per time. In other words, the neutron current is the total number of neutrons crossing a specific point for a given period of time. Therefore:

$$\int_0^{4\pi} \nabla \cdot \mathbf{j}(\mathbf{r}, \hat{\Omega}, E, t) d\hat{\Omega} = \nabla \cdot \mathbf{J}(\mathbf{r}, E, t) \quad (18)$$

Moving to the left hand side of the equation, I also have to integrate out the $\hat{\Omega}$ term. Due to the fact that the fission term was not written with angular dependence, that term will remain the same. The scattering term is dependent on $\hat{\Omega}$, however, since there is an integration with respect to $\hat{\Omega}'$, the cosine of the scattering angle μ will be used. This is because the double-differential scattering cross section depends only on the angle between the two directions. μ is the angle between the new and old directions and is integrated from -1 to 1 as that is the range for the cosine function.

$$S(\mathbf{r}, \hat{\Omega}, E, t) = \int_0^{4\pi} \int_0^\infty \Sigma_s(\mathbf{r}, \hat{\Omega}' \rightarrow \hat{\Omega}, E' \rightarrow E) \psi(\mathbf{r}, \hat{\Omega}', E', t) d\hat{\Omega}' dE' \quad (19)$$

$$\int_0^{4\pi} \left[\int_0^{4\pi} \int_0^\infty \Sigma_s(\mathbf{r}, \hat{\Omega}' \rightarrow \hat{\Omega}, E' \rightarrow E) \psi(\mathbf{r}, \hat{\Omega}', E', t) d\hat{\Omega}' dE' \right] d\hat{\Omega} \quad (20)$$

$$\int_0^{4\pi} \int_0^\infty \left[\int_{-1}^1 \Sigma_s(\mathbf{r}, E' \rightarrow E) \psi(\mathbf{r}, \mu, E', t) d\mu \right] \psi(\mathbf{r}, \hat{\Omega}', E', t) d\hat{\Omega}' dE' \quad (21)$$

$$\int_0^{4\pi} \int_0^\infty \Sigma_s(\mathbf{r}, E' \rightarrow E) \psi(\mathbf{r}, \hat{\Omega}', E', t) d\hat{\Omega}' dE' \quad (22)$$

$$\int_0^\infty \Sigma_s(\mathbf{r}, E' \rightarrow E) \left[\int_0^{4\pi} \psi(\mathbf{r}, \hat{\Omega}', E', t) d\hat{\Omega}' \right] dE' \quad (23)$$

Given $\phi(\mathbf{r}, E) = \int_0^{4\pi} \psi(\mathbf{r}, \hat{\Omega}, E) d\hat{\Omega}$

$$\int_0^\infty \Sigma_s(\mathbf{r}, E' \rightarrow E) \left[\int_0^{4\pi} \psi(\mathbf{r}, \hat{\Omega}', E', t) d\hat{\Omega}' \right] dE' = \int_0^\infty \Sigma_s(\mathbf{r}, E' \rightarrow E) \phi(\mathbf{r}, E', t) dE' \quad (24)$$

The fission source term is

$$F(\mathbf{r}, \hat{\Omega}, E, t) = \frac{\chi(E)}{4\pi} \int_0^\infty \nu \Sigma_f(\mathbf{r}, E') \phi(\mathbf{r}, E', t) dE' \quad (25)$$

$$\int_0^{4\pi} \left[\frac{\chi(E)}{4\pi} \int_0^\infty \nu \Sigma_f(\mathbf{r}, E') \phi(\mathbf{r}, E', t) dE' \right] d\hat{\Omega} \quad (26)$$

$$F(\mathbf{r}, E, t) = \chi(E) \int_0^\infty \nu \Sigma_f(\mathbf{r}, E') \phi(\mathbf{r}, E', t) dE' \quad (27)$$

Combining the simplified terms from Equations (9), (13), (18), (24), and (27) and substitute into Equation (1) to get:

$$\begin{aligned} & \frac{1}{v} \frac{\partial}{\partial t} \phi(\mathbf{r}, E, t) + \Sigma(\mathbf{r}, E) \phi(\mathbf{r}, E, t) + \nabla \cdot \mathbf{J}(\mathbf{r}, E, t) \\ & = \int_0^\infty \Sigma_s(\mathbf{r}, E' \rightarrow E) \phi(\mathbf{r}, E', t) dE' + \chi(E) \int_0^\infty \nu \Sigma_f(\mathbf{r}, E') \phi(\mathbf{r}, E', t) dE' \end{aligned} \quad (28)$$

Now that the diffusion equation, known as the neutron continuity equation in this form, is in regards to time, energy, and space, we have to discretize the energy variable. This can be accomplished when the energy

component is divided between G groups with boundaries E_{g-1} and E_g where E_0 is the largest energy. The next steps show how the different components in the above equation have energy integrated out.

$$\int_{E_g}^{E_{g-1}} \frac{1}{v} \frac{\partial}{\partial t} \phi(\mathbf{r}, E, t) dE = \frac{1}{v_g} \frac{\partial}{\partial t} \phi_g(\mathbf{r}, t) \quad (29)$$

$$\int_{E_g}^{E_{g-1}} \nabla \cdot \mathbf{J}(\mathbf{r}, E, t) dE = \nabla \cdot \mathbf{J}_g(\mathbf{r}, t) \quad (30)$$

$$\int_{E_g}^{E_{g-1}} \Sigma(\mathbf{r}, E) \phi(\mathbf{r}, E, t) dE = \Sigma_g \phi_g(\mathbf{r}, t) \quad (31)$$

For the scattering and fission sources, the integrals are converted to summations with respect to E' and then integrated through by E , as seen below.

$$\int_0^\infty \Sigma_s(\mathbf{r}, E' \rightarrow E) \phi(\mathbf{r}, E', t) dE' = \sum_{g'} \Sigma_{s,g'} \phi(\mathbf{r}, t) \quad (32)$$

$$\int_{E_g}^{E_{g-1}} \sum_{g'} \Sigma_{s,g'} \phi(\mathbf{r}, t) dE = \sum_{g'} \Sigma_{s,g'} \phi(\mathbf{r}, t) \quad (33)$$

$$\chi(E) \int_0^\infty \nu \Sigma_f(\mathbf{r}, E') \phi(\mathbf{r}, E', t) dE' = \chi(E) \sum_{g'} \nu \Sigma_{f,g'} \phi_{g'}(\mathbf{r}, t) \quad (34)$$

$$\int_{E_g}^{E_{g-1}} \chi(E) \sum_{g'} \nu \Sigma_{f,g'} \phi_{g'}(\mathbf{r}, t) dE = \chi_g \sum_{g'} \nu \Sigma_{f,g'} \phi_{g'}(\mathbf{r}, t) \quad (35)$$

Taking Equations (29)-(31), (33), and (35), and substituting into Equation (28), we can get the diffusion equation with respect to distance and time. I will first simplify the equation by using Fick's law to convert the flux gradient to a more manageable neutron current density form.

$$\frac{1}{v_g} \frac{\partial}{\partial t} \phi_g(\mathbf{r}, t) + \nabla \cdot \mathbf{J}_g(\mathbf{r}, t) + \Sigma_g \phi_g(\mathbf{r}, t) = \chi_g \sum_{g'} \nu \Sigma_{f,g'} \phi_{g'}(\mathbf{r}, t) + \sum_{g'} \Sigma_{s,g'} \phi(\mathbf{r}, t) \quad (36)$$

Given the fact that $\mathbf{J}_g(\mathbf{r}, t) = -D_g \nabla \phi_g(\mathbf{r}, t)$,

$$\nabla \cdot \mathbf{J}_g(\mathbf{r}, t) = -\nabla \cdot D(\mathbf{r}) \nabla \phi(\mathbf{r}, t) \quad (37)$$

$$\frac{1}{v_g} \frac{\partial}{\partial t} \phi_g(\mathbf{r}, t) - \nabla \cdot D(\mathbf{r}) \nabla \phi(\mathbf{r}, t) + \Sigma_g \phi_g(\mathbf{r}, t) = \chi_g \sum_{g'} \nu \Sigma_{f,g'} \phi_{g'}(\mathbf{r}, t) + \sum_{g'} \Sigma_{s,g'} \phi(\mathbf{r}, t) \quad (38)$$

$$\int_{t^n}^{t^{n+1}} \frac{1}{v_g} \frac{\partial}{\partial t} \phi_g(\mathbf{r}, t) dt = \frac{1}{v} (\phi_g^{n+1}(\mathbf{r}) - \phi_g^n(\mathbf{r})) \quad (39)$$

The first term was simple to integrate out the time variable, however, for the rest of the terms, the backward Euler method will be used [2]. In this method, $y^{n+1} = y^n + \Delta t f(y^{n+1}, t^{n+1})$, which will be used below for integrating the terms from t^n to t^{n+1} below.

$$\phi^{n+1}(\mathbf{r}) = \phi^n(\mathbf{r}) + \Delta t \phi^{n+1}(\mathbf{r}) \quad (40)$$

$$\int_{t^n}^{t^{n+1}} -\nabla \cdot D(\mathbf{r}) \nabla \phi(\mathbf{r}, t) dt = -\nabla \cdot D_g(\mathbf{r}) \nabla (\phi^{n+1}(\mathbf{r}) - \phi^n(\mathbf{r})) \quad (41)$$

$$= -\nabla \cdot D_g(\mathbf{r}) \nabla (\phi^n(\mathbf{r}) + \Delta t \phi^{n+1}(\mathbf{r}) - \phi^n(\mathbf{r})) \quad (42)$$

$$= -\Delta t (\nabla \cdot D_g(\mathbf{r}) \nabla \phi^{n+1}(\mathbf{r})) \quad (43)$$

$$\int_{t^n}^{t^{n+1}} \Sigma_g \phi_g(\mathbf{r}, t) dt = \Sigma_g [\phi_g^{n+1}(\mathbf{r}) - \phi_g^n(\mathbf{r})] \quad (44)$$

$$= \Delta t [\Sigma_g \phi_g^{n+1}(\mathbf{r})] \quad (45)$$

$$\int_{t^n}^{t^{n+1}} \chi_g \sum_{g'} \nu \Sigma_{f,g'} \phi_{g'}(\mathbf{r}, t) dt = \chi_g \sum_{g'} \nu \Sigma_{f,g'} [\phi_{g'}^{n+1}(\mathbf{r}) - \phi_{g'}^n(\mathbf{r})] \quad (46)$$

$$= \Delta t \left[\chi_g \sum_{g'} \nu \Sigma_{f,g'} \phi_{g'}^{n+1}(\mathbf{r}) \right] \quad (47)$$

$$\int_{t^n}^{t^{n+1}} \sum_{g'} \Sigma_{s,g'} \phi(\mathbf{r}, t) dt = \sum_{g'} \Sigma_{s,g'} [\phi^{n+1}(\mathbf{r}) - \phi^n(\mathbf{r})] \quad (48)$$

$$= \Delta t \left[\sum_{g'} \Sigma_{s,g'} \phi^{n+1}(\mathbf{r}) \right] \quad (49)$$

Taking the terms from (39), (43), (45), (47), and (49), and dividing through by Δt , the result is the diffusion equation in terms of space.

$$\frac{1}{v\Delta t} (\phi_g^{n+1}(\mathbf{r}) - \phi_g^n(\mathbf{r})) - \nabla \cdot D_g(\mathbf{r}) \nabla \phi^{n+1}(\mathbf{r}) + \Sigma_g \phi_g^{n+1}(\mathbf{r}) = \chi_g \sum_{g'} \nu \Sigma_{f,g'} \phi_{g'}^{n+1}(\mathbf{r}) + \sum_{g'} \Sigma_{s,g'} \phi^{n+1}(\mathbf{r}) \quad (50)$$

Since we are looking at steady-state equations, I will insist that $n = 0$ and $\Delta t = 0$, which simplifies to

$$-\nabla \cdot D_g(\mathbf{r}) \nabla \phi(\mathbf{r}) + \Sigma_g \phi_g(\mathbf{r}) = \frac{\chi_g}{k} \sum_{g'} \nu \Sigma_{f,g'} \phi_{g'}(\mathbf{r}) + \sum_{g'} \Sigma_{s,g'} \phi(\mathbf{r}) \quad (51)$$

I added the $1/k$ value above to the fission term as it will serve as the eigenvalue term, thus making this an eigenvalue problem related to the criticality of the diffusion equation. The next step is to discretize the space variable, which will be represented by a grid of I number of cells and $I - 1$ edges. Equation (52) is the cell center, while equations (53) and (54) are the left and right edges of the cell respectively. In this step, I will also convert the diffusion operator to use the diffusion equation for a one-dimensional sphere.

$$r_i = i\Delta r + \frac{\Delta r}{2}, \quad i = 0, 1, \dots, I - 1 \quad (52)$$

$$r_{i-1/2} = i\Delta r, \quad i = 0, 1, \dots, I - 1 \quad (53)$$

$$r_{i+1/2} = (i + 1)\Delta r, \quad i = 0, 1, \dots, I - 1 \quad (54)$$

$$\nabla \cdot D_g(\mathbf{r}) \nabla = \frac{1}{\mathbf{r}^2} \frac{d}{d\mathbf{r}} \mathbf{r}^2 D(\mathbf{r}) \frac{d}{d\mathbf{r}} \quad (55)$$

$$\phi_i = \frac{1}{V_i} \int_{r_{i-1/2}}^{r_{i+1/2}} \phi(\mathbf{r}) dV \quad (56)$$

$$dV = 4\pi \mathbf{r}^2 d\mathbf{r} \quad (57)$$

$$V_i = \frac{4}{3} \pi (r_{i+1/2}^3 - r_{i-1/2}^3) \quad (58)$$

This is where ϕ_i is the average flux in cell i . Therefore, I can then integrate the diffusion equation over the volume, as seen below. I will also set the surface area as $S_{i\pm 1/2} = 4\pi r_{i\pm 1/2}^2$ and simplify the equation. We can also assume that the cell flux average is equal to the cell center which, using the Forward Euler method, I can simplify the d/dr term.

$$-\frac{1}{V_i} \int_{r_{i-1/2}}^{r_{i+1/2}} \nabla \cdot D_g(\mathbf{r}) \nabla \phi(\mathbf{r}) dV = -\frac{4\pi}{V_i} \left[D_{i+1/2} r_{i+1/2}^2 \frac{d}{dr} \phi(r_{i+1/2}) - D_{i-1/2} r_{i-1/2}^2 \frac{d}{dr} \phi(r_{i-1/2}) \right] \quad (59)$$

$$-\frac{1}{V_i} \int_{r_{i-1/2}}^{r_{i+1/2}} \nabla \cdot D_g(\mathbf{r}) \nabla \phi(\mathbf{r}) dV = -\frac{1}{V_i} \left[D_{i+1/2} S_{i+1/2} \frac{d}{dr} \phi(r_{i+1/2}) - D_{i-1/2} S_{i-1/2} \frac{d}{dr} \phi(r_{i-1/2}) \right] \quad (60)$$

$$\frac{d}{dr} \phi(r_{i+1/2}) = \frac{\phi_{i+1} - \phi_i}{\Delta r} + O(\Delta r^2) \quad (61)$$

$$-\frac{1}{V_i} \int_{r-1/2}^{r+1/2} \nabla \cdot D_g(\mathbf{r}) \nabla \phi(\mathbf{r}) dV = -\frac{1}{V_i} \left[D_{i+1/2} S_{i+1/2} \frac{\phi_{i+1} - \phi_i}{\Delta r} - D_{i-1/2} S_{i-1/2} \frac{\phi_i - \phi_{i-1}}{\Delta r} \right] \quad (62)$$

$$\frac{1}{V_i} \int_{r-1/2}^{r+1/2} \Sigma_g \phi_g(\mathbf{r}) dV = \Sigma_{g,i} \phi_i \quad (63)$$

$$\frac{1}{V_i} \int_{r-1/2}^{r+1/2} \frac{\chi_g}{k} \sum_{g'} \nu \Sigma_{f,g'} \phi_{g'}(\mathbf{r}) dV = \frac{\chi_g}{k} \sum_{g'} \nu \Sigma_{f,g',i} \phi_i \quad (64)$$

$$\frac{1}{V_i} \int_{r-1/2}^{r+1/2} \sum_{g'} \Sigma_{s,g'g} \phi(\mathbf{r}) dV = \sum_{g'} \Sigma_{s,g'g,i} \phi_i \quad (65)$$

Combining the terms in equations (62)-(65), the resultant is

$$-\frac{1}{V_i} \left[D_{i+1/2} S_{i+1/2} \frac{\phi_{i+1} - \phi_i}{\Delta r} - D_{i-1/2} S_{i-1/2} \frac{\phi_i - \phi_{i-1}}{\Delta r} \right] + \Sigma_{g,i} \phi_i = \frac{\chi_g}{k} \sum_{g'} \nu \Sigma_{f,g',i} \phi_i + \sum_{g'} \Sigma_{s,g'g,i} \phi_i \quad (66)$$

Oftentimes, the total macroscopic cross-section and the “self” scattering cross sections are combined into a removal cross section.

$$\Sigma_r = \Sigma_t - \Sigma_{s,i \rightarrow i} \quad (67)$$

$$-\frac{1}{V_i} \left[D_{i+1/2} S_{i+1/2} \frac{\phi_{i+1} - \phi_i}{\Delta r} - D_{i-1/2} S_{i-1/2} \frac{\phi_i - \phi_{i-1}}{\Delta r} \right] + \Sigma_{r,g,i} \phi_i = \frac{\chi_g}{k} \sum_{g'} \nu \Sigma_{f,g',i} \phi_i + \sum_{g' \neq g} \Sigma_{s,g'g,i} \phi_i \quad (68)$$

References

- [1] J. Leppanen. “Diffusion Theory.” *Department of Applied Physics, Aalto University* (2016).
- [2] R. G. McClarren. *Computational Nuclear Engineering and Radiological Science Using Python*. Academic Press (2017).