The Multigroup Neutron Balance Equation

Introduction

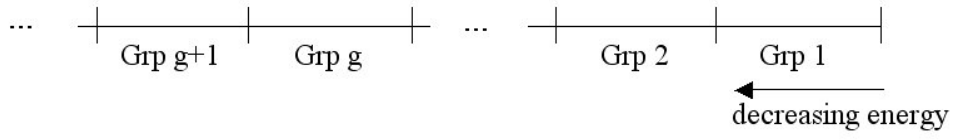
The neutron balance equation represents a fundamental relationship between the various production and loss mechanisms (absorption, fission, scattering, leakage, etc.) that can occur in a nuclear system. To aid in visualizing the various processes involved, it helps to have a good understanding of the basic life cycle of a neutron. In particular, in a thermal reactor, the source neutrons from fission are born at high energies, these neutrons slow down via elastic and inelastic scattering to thermal energies, and it is these thermal neutrons that cause most of the fissions which, in turn, start the cycle over again. Of course there are other important reactions, such as neutron capture and neutron leakage out of the volume of interest, that also affect the life cycle of a neutron.

In describing all these processes quantitatively, one needs to keep track of all the neutron production and loss mechanisms at each energy and spatial point of interest. This is a rather difficult job, especially if both space and energy are treated as continuous variables. In practice, of course, both variables are usually discretized in most realistic applications. For the present development, however, we will only discretize the energy variable, resulting in the multigroup formulation for the space-continuous neutron balance equation. The continuous spatial variable is retained at this point so that some analytical solutions, for a variety of simple geometries, can be obtained. Thus, our focus for this lecture is the development of the multigroup neutron balance equation. Future lectures will deal with various applications/uses of the equations developed here.

Also developed here is the operator form of the diffusion theory representation to the steady state neutron balance equation. This notation is convenient in many situations, especially when a concise shorthand notation helps simplify and explain certain concepts more readily. In particular, we will conclude this section of Lecture Notes on the Multigroup Neutron Balance Equation by discussing the most common situations where this equation is used -- and here the operator notation is really quite useful.

The Multigroup Formulation

Within the multigroup formulation, the full energy domain is broken into a finite number of energy bins. An arbitrary energy bin or interval is usually given the symbol g and the groups are numbered from high energy to low energy. Thus, the energy scale in the multigroup formulation can be represented as shown below:



Since the full space-energy treatment is simply too complex for most realistic situations, our goal becomes one of finding out what happens, on the average, in each energy interval, E_{g+1} to E_g, which is referred to as group g (note that there are G+1 energy boundaries for G total energy groups). Thus, a neutron balance will be performed for an arbitrary energy group g. This

balance will be applied to each interval resulting in a set of G coupled differential equations. For practical reasons, only 1 or 2-group problems are solved analytically. When G becomes large, numerical solution techniques integrated within large production computer codes are employed almost exclusively.

In the multigroup formulation, the flux for energy group g is given as

$$\phi_g = \int_{E_{g+1}}^{E_g} \phi(E)dE \tag{1}$$

where it should be noted that this is an energy integrated value. With this definition, several of the reaction rates that will be needed in writing the neutron balance equation are given as

$$\text{absorption rate} = \int_{E_{g+1}}^{E_g} \Sigma_a(E)\phi(E)dE = \Sigma_{ag}\phi_g = \begin{array}{c}\#\text{ of absorptions/cm}^3\text{-sec} \\ \text{within energy interval g}\end{array} \tag{2}$$

$$\text{where} \quad \Sigma_{ag} = \frac{\int_{E_{g+1}}^{E_g} \Sigma_a(E)\phi(E)dE}{\int_{E_{g+1}}^{E_g} \phi(E)dE} \tag{3}$$

$$\text{total collision rate} = \int_{E_{g+1}}^{E_g} \Sigma_t(E)\phi(E)dE = \Sigma_{tg}\phi_g = \begin{array}{c}\#\text{ of interactions/cm}^3\text{-sec} \\ \text{within energy interval g}\end{array} \tag{4}$$

$$\text{where} \quad \Sigma_{tg} = \frac{\int_{E_{g+1}}^{E_g} \Sigma_t(E)\phi(E)dE}{\int_{E_{g+1}}^{E_g} \phi(E)dE} \tag{5}$$

$$\text{fission rate} = \int_{E_{g+1}}^{E_g} \Sigma_f(E)\phi(E)dE = \Sigma_{fg}\phi_g = \begin{array}{c}\#\text{ of fissions/cm}^3\text{-sec} \\ \text{within energy interval g}\end{array} \tag{6}$$

$$\text{where} \quad \Sigma_{fg} = \frac{\int_{E_{g+1}}^{E_g} \Sigma_f(E)\phi(E)dE}{\int_{E_{g+1}}^{E_g} \phi(E)dE} \tag{7}$$

etc. for all types of reactions. If we desire the energy integrated reaction rate, then

$$\int_{\substack{\text{all} \\ \text{energy}}} \Sigma_a(E)\phi(E)dE = \sum_{g=1}^{G} \Sigma_{ag}\phi_g = \#\text{ of absorptions/cm}^3\text{-sec} \tag{8}$$

$$\int_{\substack{\text{all} \\ \text{energy}}} \Sigma_t(E)\phi(E)dE = \sum_{g=1}^{G} \Sigma_{tg}\phi_g = \#\text{ of interactions/cm}^3\text{-sec} \tag{9}$$

$$\int_{\substack{\text{all} \\ \text{energy}}} \Sigma_f(E)\phi(E)dE = \sum_{g=1}^{G} \Sigma_{fg}\phi_g = \#\text{ of fissions/cm}^3\text{-sec} \tag{10}$$

The above reactions (absorption, total, fission, etc.) are sometimes called one-dimensional (1-D) processes. Neutron scattering, on the other hand, is a 2-D process, since we must consider the

final neutron energy as well as the initial neutron energy. For example, the scattering rate from energy E' to energy interval dE can be written as

$$\begin{pmatrix}\text{scattering rate}\\ \text{from E' to dE}\end{pmatrix} = \left(\begin{matrix}\text{scattering rate}\\ \text{at E'}\end{matrix}\right)\left(\begin{matrix}\text{probability of}\\ \text{scattering into dE}\end{matrix}\right) = \Sigma_s(E')\phi(E')f(E'\rightarrow E)dE \qquad (11)$$

To simplify the notation slightly, we define the scattering cross section from E' to E as

$$\Sigma_s(E'\rightarrow E) = \Sigma_s(E')f(E'\rightarrow E) \qquad (12)$$

and, with this definition, eqn. (11) becomes

$$\begin{pmatrix}\text{scattering rate}\\ \text{from E' to dE}\end{pmatrix} = \Sigma_s(E'\rightarrow E)\phi(E')dE \qquad (13)$$

Now, when using a discrete energy group notation within the multigroup formulation, we can define the group-to-group scattering cross section as

$$\Sigma_{g'\rightarrow g} = \frac{\int_{E_{g'+1}}^{E_{g'}}\int_{E_{g+1}}^{E_g}\Sigma_s(E'\rightarrow E)\phi(E')dE\,dE'}{\int_{E_{g'+1}}^{E_{g'}}\phi(E')dE'} \qquad (14)$$

and the scattering rate from g' to g as

$$\begin{pmatrix}\text{scattering rate}\\ \text{from g' to g}\end{pmatrix} = \Sigma_{g'\rightarrow g}\phi_{g'} \qquad (15)$$

Note that the total scattering rate out of a particular group g is given as

$$\begin{pmatrix}\text{total scattering}\\ \text{rate out of g}\end{pmatrix} = \sum_{g'\neq g}\Sigma_{g\rightarrow g'}\phi_g \qquad \text{(outscatter rate)} \qquad (16)$$

where the notation and ordering of the g and g' are important. In eqn. (16) the sum is over all groups g' that neutrons in group g can scatter into. The ≠ symbol indicates that group g is not included in the sum. Within group scattering, $\Sigma_{g\rightarrow g}\phi_g$, is not a removal mechanism for neutrons in group g.

Similarly, the total scattering rate into group g is given by

$$\begin{pmatrix}\text{total scattering}\\ \text{rate into g}\end{pmatrix} = \sum_{g'\neq g}\Sigma_{g'\rightarrow g}\phi_{g'} \qquad \text{(inscatter rate)} \qquad (17)$$

Again the precise notation is important. Notice that the reaction takes place in group g' and the neutron after scattering ends up in g. Since we are interested in the total scattering rate into group g, the sum is over all groups, g', that scatter into group g.

Another 2-D neutron production process that is of particular interest is related to the neutrons produced from the fission event. The fission reaction takes place at some neutron energy, E', and the neutrons that are emitted have some different energy, E. The term that describes this process is referred to as the fission source. This term contains information about the fission rate, the average number of neutrons emitted per fission, and the fission spectrum (a function that describes the distribution of energies for the emitted neutrons).

The average number of total neutrons emitted per fission is given the symbol ν_T (usually just ν). The contributions to ν_T are made up from prompt neutrons and delayed neutrons. Prompt neutrons are emitted directly in fission. The delayed component occurs from the neutrons that are released in the decay of certain fission products. These delayed neutron precursors are produced from fission and the neutrons they emit can be thought of as resulting from fission, with a characteristic delay before release.

As discussed previously in the Fundamentals of NSE course, the delayed neutron precursors are usually grouped into six separate groups with effective decay constants, λ_i, and yields, β_i, where

$$\beta_i = \frac{\nu_i}{\nu_T} = \frac{\text{delayed neutrons from precursor i per fission}}{\text{total neutrons emitted per fission}} \tag{18}$$

where β_i is referred to as the delayed neutron fraction for precursor group i.

Note that $\nu_d = \sum_i \nu_i =$ total delayed neutrons per fission (19)

and $\beta = \sum_i \beta_i = \frac{\nu_d}{\nu_T} =$ total delayed neutron fraction (20)

Note also that β is quite small; only about 0.00685 for U235 and about 0.0023 for Pu239.

In writing an expression for the fission neutron source in a reactor, it is important to consider whether the neutrons emitted are prompt or delayed. The total neutrons emitted per cm^3-sec can be written as

$$\frac{\text{total neutrons emitted}}{cm^3 - sec} = \int (1-\beta)\nu_T \Sigma_f(E')\phi(E')dE' + \sum_i \lambda_i C_i \tag{21}$$

The above expression separates the total source into prompt and delayed components, where the production rate of delayed neutrons is represented by the total decay rate of all the precursor groups (C_i here represents the precursor concentration for group i). In writing a neutron balance equation that includes the time variable (i.e. the non steady-state case), this distinction plays an important role. In fact, without the delayed neutrons, we would not be able to control the chain reaction.

The above concepts concerning prompt and delayed neutrons are extremely important. However, our primary focus in this set of Lecture Notes is on developing the steady state neutron balance equation. At steady state, the precursor production rate is identical to the delayed neutron production rate, or

$$\frac{\text{delayed neutrons emitted}}{cm^3 - sec} = \int \beta\nu_T \Sigma_f(E')\phi(E')dE' = \sum_i \lambda_i C_i \qquad \text{(at steady state)} \tag{22}$$

so we can write the steady state neutron production rate as

$$\frac{\text{total neutrons emitted}}{cm^3 - sec} = \int \nu_T \Sigma_f(E')\phi(E')dE' = \int \nu\Sigma_f(E')\phi(E')dE' = \sum_{g'} \nu\Sigma_{fg'}\phi_{g'} \tag{23}$$

where we have replaced ν_T with ν, and the last form shows the discrete multigroup representation (where the spatial dependence of the cross sections and flux has been omitted for convenience and clarity).

Overall, it is important to be aware of the prompt and delayed components of the total neutron source and their role in the control of reactor operations. However, for our current work, we will consider primarily the steady state neutron production rate as given in eqn. (23).

Not only is it important to determine the number of neutrons emitted per fission, but we also need to know the energy of these neutrons. Fission neutrons are emitted with a continuous energy spectrum that is Maxwellian in nature but shifted in energy such that the peak of the curve is around 1 MeV and the average energy is about 2 MeV (this profile is sometimes referred to as the Watt fission spectrum). This distribution of fission neutron energies is known as the prompt fission spectrum (this is called the prompt fission spectrum because the delayed neutrons are also emitted with a characteristic spectrum, which is somewhat softer that the prompt fission spectrum -- but we will not go into all this detail here). The prompt fission spectrum is denoted by $\chi(E)$, where

$$\chi(E)dE = \begin{array}{c}\text{probability that a fission neutron will} \\ \text{be born with an energy in dE around E}\end{array} \tag{24}$$

Also since this must be a properly normalized distribution function (i.e. probability of finding the neutron energy between 0 and ∞ is unity), then

$$\int_0^\infty \chi(E)dE = 1 \tag{25}$$

In a multigroup formulation, χ_g is defined as

$$\chi_g = \int_{E_{g+1}}^{E_g} \chi(E)dE \tag{26}$$

and

$$\sum_g \chi_g = 1 \tag{27}$$

If we combine the discussion of the neutron energy with the treatment of the number of neutrons emitted per fission, we can define the steady state fission source as

$$\begin{array}{c}\text{neutrons emitted per} \\ \text{cm}^3\text{-sec in interval dE}\end{array} = \chi(E)dE\int \nu\Sigma_f(E')\phi(E')dE' \tag{28}$$

$$\begin{array}{c}\text{neutrons emitted per} \\ \text{cm}^3\text{-sec in group g}\end{array} = \chi_g \sum_{g'} \nu\Sigma_{fg'}\phi_{g'} \tag{29}$$

This latter expression [eqn. (29)] will be the term that makes it into the final steady state neutron balance equation.

Neutron Leakage

In the multigroup formulation, neutrons that exist within group g can ultimately

1. be absorbed within group g (via capture, fission, or any other absorption-type reaction),
2. scatter out of group g, or
3. leak out of the spatial element of interest (while in energy group g).

From the above definitions and equations, we know how to describe the absorption and scattering rates, but we have not yet looked at the third loss mechanism, neutron leakage. To start this process, let's define the net neutron current, $\vec{J}(\vec{r},E)$, as

$$\vec{J}(\vec{r},E)=\int_{\substack{\text{all}\\ \text{angles}}} n(\vec{r},E,\hat{\Omega})\,\vec{v}(E)\,d\hat{\Omega}=\int_{\substack{\text{all}\\ \text{angles}}} n(\vec{r},E,\hat{\Omega})\,v(E)\hat{\Omega}\,d\hat{\Omega} \tag{30}$$

where n is the neutron density, v is the neutron speed, and $\hat{\Omega}$ is a unit vector that describes the direction of travel. Since $\phi = nv$, we can also write eqn. (30) as

$$\vec{J}(\vec{r},E)=\int_{\substack{\text{all}\\ \text{angles}}} \hat{\Omega}\,\phi(\vec{r},E,\hat{\Omega})\,d\hat{\Omega}=\int_{\substack{\text{all}\\ \text{angles}}} \vec{J}(\vec{r},E,\hat{\Omega})\,d\hat{\Omega} \tag{31}$$

Note that $\vec{J}(\vec{r},E)$, or $\vec{J}_g(\vec{r})$ if one integrates over energy interval $\Delta E_g = E_g - E_{g+1}$, is a vector quantity. It is the net neutron current density, since $\vec{J}(\vec{r},E,\hat{\Omega})$ has been integrated over all angles. The direction of $\vec{J}_g(\vec{r})$ is not that of any specific collection of neutrons; it has the direction of the net flow of neutrons. Note also that the units of net neutron current are the same as neutron flux, neutrons/cm^2-sec. However, the current density is a vector quantity, and it describes the net directional behavior of the neutrons.

Since $\vec{J}_g$ is associated with the net flow of neutrons in energy group g, then

$$\vec{J}_g\bullet d\vec{A}=\vec{J}_g\bullet\hat{n}\,dA=\begin{array}{c}\text{net rate at which neutrons in group g}\\ \text{pass through a surface area dA normal}\\ \text{to the outward pointing unit vector}\end{array} \tag{32}$$

where we note that the units of current density times area is neutrons/second -- that is, a neutron flow rate across differential area dA.

With this interpretation, we can now define neutron leakage as the net number of neutrons/sec that leave a given volume V enclosed by surface area A, or

$$\begin{array}{c}\text{leakage rate out}\\ \text{of volume V for}\\ \text{energy group g}\end{array}=\int_A \vec{J}_g\bullet\hat{n}\,dA \tag{33}$$

At times it is convenient to convert the surface integral in eqn. (33) to a volume integral over V. This can be accomplished with the well-known Divergence Theorem (see any Calculus text). Therefore,

$$\begin{array}{c}\text{leakage rate}\\ \text{from V and g}\end{array}=\int_A \vec{J}_g\bullet\hat{n}\,dA=\int_V \vec{\nabla}\bullet\vec{J}_g\,d\vec{r} \tag{34}$$

The surface and volume integral formulations for neutron leakage can be used interchangeably. In practice, the volume integration is used primarily in the formulation of the pointwise neutron balance equation and the surface integral form is used to evaluate leakage once $\vec{J}_g$ is known. However, the choice in any application is simply a matter of convenience.

The Neutron Balance Equation

We now have all the tools required to write the general multigroup neutron balance equation. For some arbitrary volume V and energy group g, one has (accumulation rate = production rate – loss rate), or

$$\begin{array}{ccccc} \text{rate of change} \\ \text{of neutrons} \\ \text{within V and g} \end{array} = \begin{array}{c} \text{production rate} \\ \text{of neutrons} \\ \text{within V and g} \end{array} - \begin{array}{c} \text{loss rate} \\ \text{of neutrons} \\ \text{within V and g} \end{array} \qquad (35)$$

$$\text{(Term 1)} = \text{(Term 2)} - \text{(Term 3)}$$

where the production terms are:

1. External source (independent of neutron flux)
2. Fission source
3. Inscatter source

and the loss terms are:

1. Leakage
2. Absorption
3. Outscatter

where the last two loss components are often combined into the removal term (i.e. Removal = Absorption + Outscatter).

Writing Term 1 in full detail gives

$$\text{Term 1} = \frac{d}{dt}\int_V\int_E n(\vec{r},E,t)d\vec{r}dE = \frac{d}{dt}\int_V\int_E \frac{n(\vec{r},E,t)v(E)d\vec{r}dE}{v(E)} \qquad (36)$$

or

$$\text{Term 1} = \frac{d}{dt}\int_V \frac{1}{v_g}\phi_g(\vec{r},t)d\vec{r} = \int_V \frac{1}{v_g}\frac{\partial}{\partial t}\phi_g(\vec{r},t)d\vec{r} \qquad (37)$$

where the last equality (taking the derivative inside the integral) requires a stationary volume element, and the group-averaged inverse velocity is given by

$$\frac{1}{v_g} = \frac{\int_{E_{g+1}}^{E_g}\frac{1}{v(E)}\phi(E)dE}{\int_{E_{g+1}}^{E_g}\phi(E)dE} \qquad (38)$$

Also writing Terms 2 and 3 in detail gives

$$\text{Term 2} = \int_V Q_g(\vec{r})d\vec{r} \quad + \quad \chi_g \sum_{g'} \int_V \nu\Sigma_{fg'}(\vec{r})\phi_{g'}(\vec{r})d\vec{r} \quad + \quad \sum_{g'\neq g} \int_V \Sigma_{g'\to g}(\vec{r})\phi_{g'}(\vec{r})d\vec{r} \qquad (39)$$

external source fission source inscatter source

and

$$\text{Term 3} = \int_V \vec{\nabla}\bullet\vec{J}_g(\vec{r})d\vec{r} \quad + \quad \int_V \Sigma_{ag}(\vec{r})\phi_g(\vec{r})d\vec{r} \quad + \quad \sum_{g'\neq g} \int_V \Sigma_{g\to g'}(\vec{r})\phi_g(\vec{r})d\vec{r} \qquad (40)$$

leakage absorption outscatter

where we note that Term 2 (the production term) includes the steady state fission source expression [not valid for a time dependent problem -- see discussion related to the difference between eqns. (21) and (23) on page 4].

Since the integrals in Terms 1-3 are over the same arbitrary volume element, one can simply equate the integrands to obtain a pointwise or space continuous neutron balance equation (per unit volume) for group g,

$$\vec{\nabla}\bullet\vec{J}_g(\vec{r}) + \Sigma_{Rg}(\vec{r})\,\phi_g(\vec{r}) - S_g(\vec{r}) = -\frac{1}{v_g}\frac{\partial}{\partial t}\phi_g(\vec{r}) \qquad (41)$$

where $\Sigma_{Rg}(\vec{r}) = \Sigma_{ag}(\vec{r}) + \sum_{g'\neq g} \Sigma_{g\to g'}(\vec{r})$ (42)

$$S_g(\vec{r}) = Q_g(\vec{r}) + \chi_g \sum_{g'} \nu\Sigma_{fg'}(\vec{r})\,\phi_{g'}(\vec{r}) + \sum_{g'\neq g} \Sigma_{g'\to g}(\vec{r})\,\phi_{g'}(\vec{r}) \qquad (43)$$

Notice that eqn. (41) has been multiplied by -1. The reason for this is simply for consistency of notation for steady state cases (i.e. when $\partial\phi_g/\partial t = 0$). Also note that eqns. (42) and (43) define the removal cross section and total steady state neutron source, respectively. Equations (41)-(43) completely describe the general neutron balance equation (for no delayed neutrons).

The time derivative term in eqn. (41) was introduced and retained up to this point for generality. However, the balance equation developed here is usually applied to steady state systems (since the fission source given here is not valid for time dependent problems). For steady state, the temporal derivative vanishes and eqn. (41) reduces to

$$\vec{\nabla}\bullet\vec{J}_g(\vec{r}) + \Sigma_{Rg}(\vec{r})\,\phi_g(\vec{r}) = S_g(\vec{r}) \qquad (44)$$

This simply states that, in steady state, the loss rate (leakage + removal) exactly matches or balances the production rate on a per unit volume basis -- that is, the production and loss terms must balance out at every spatial point and energy group. Equation (44) [along with the definitions given in eqns. (42) and (43)] is the desired steady state multigroup neutron balance equation.

Transport vs. Diffusion Theory

Before we can solve the steady state equation for a specific system, something needs to be done to relate the neutron current, $\vec{J}_g$, to the neutron flux, ϕ_g, since we now have a single equation with two dependent variables. There are two approaches for doing this -- one leading to the ***Transport Equation*** and the other giving the ***Diffusion Equation***.

The ***Transport Equation*** is derived by using the basic definition of neutron current as implied in eqn. (31). In its basic form, the angular current density is given by

$$\vec{J}(\vec{r}, E, \hat{\Omega}) = \hat{\Omega}\,\phi(\vec{r}, E, \hat{\Omega}) \tag{45}$$

Therefore, the $\vec{\nabla}\bullet\vec{J}_g$ term in eqn. (44) becomes

$$\vec{\nabla}\bullet\vec{J}_g = \vec{\nabla}\bullet\hat{\Omega}\phi_g = \hat{\Omega}\bullet\vec{\nabla}\phi_g \tag{46}$$

Also note that, if self scattering is included in both the inscatter and outscatter terms (so that the balance equation is unaffected), then the removal cross section becomes the total cross section,

$$\Sigma_{tg} = \Sigma_{Rg} + \Sigma_{g\to g} = \Sigma_{ag} + \sum_{g'} \Sigma_{g\to g'} \tag{47}$$

With these substitutions, the steady state Boltzmann transport equation becomes

$$\hat{\Omega}\bullet\vec{\nabla}\phi_g(\vec{r}, \hat{\Omega}) + \Sigma_{tg}(\vec{r})\,\phi_g(\vec{r}, \hat{\Omega}) = S_g(\vec{r}, \hat{\Omega}) \tag{48}$$

where

$$S_g(\vec{r}, \hat{\Omega}) = Q_g(\vec{r}, \hat{\Omega}) + \chi_g \sum_{g'} \int_{4\pi} \nu\Sigma_{fg'}(\vec{r})\,\phi_{g'}(\vec{r}, \hat{\Omega}')d\hat{\Omega}' + \sum_{g'} \int_{4\pi} \Sigma_{g'\to g}(\vec{r}, \hat{\Omega}' \to \hat{\Omega})\,\phi_{g'}(\vec{r}, \hat{\Omega}')d\hat{\Omega}' \tag{49}$$

This expression takes into account the angular dependence of the scattering cross sections and the neutron flux. The formal solution of eqn. (48) for realistic applications is relatively complicated. Discrete Ordinates, Monte Carlo, or Integral Transport Theory methods are usually employed for the solution of eqn. (48) (or one of its many equivalent representations). However, a discussion of these methods is beyond the scope of the introductory treatment given here. Thus, for the present discussion, the existence of the Boltzmann transport equation and its distinction from diffusion theory are the key points of interest.

The ***Diffusion Equation*** uses an approximate relationship between the neutron flux and net current density based on the observation that neutrons tend to diffuse from regions of high concentration to regions of low concentration. Fick's Law states this in mathematical terms as

$$\vec{J}_g(\vec{r}) = -D_g(\vec{r})\vec{\nabla}\phi_g(\vec{r}) \tag{50}$$

which states that the net neutron current is proportional to the negative gradient of the neutron flux. The variable D_g is the proportionality constant and it is typically called the diffusion coefficient for group g.

Substitution of Fick's Law [eqn. (50)] into the basic steady state neutron balance equation [eqn. (44)] gives the standard multigroup diffusion formulation,

$$-\vec{\nabla}\bullet D_g(\vec{r})\vec{\nabla}\phi_g(\vec{r}) + \Sigma_{Rg}(\vec{r})\,\phi_g(\vec{r}) = S_g(\vec{r}) \tag{51}$$

where the explicit definitions of Σ_{Rg} and S_g are given in eqns. (42) and (43), respectively. Equation (51) is called the ***Diffusion Equation*** -- this will be the starting point for much of the introductory steady-state nuclear reactor theory discussed as part of this series of Lecture Notes.

It should be noted that Fick's Law is only an approximation. In particular, it is not strictly valid

a. in a medium that strongly absorbs neutrons (i.e. near control rods),

b. within a few mean free paths of either a neutron source or the exterior surface of a medium (the neutron flux has a strong angular dependence in these regions), and

c. when the scattering of neutrons is strongly anisotropic (has a strong angular dependence).

In general, when the angular dependence is not extreme, then Fick's Law represents a good approximation for relating the neutron current and neutron flux, and the diffusion equation becomes a reasonable mathematical representation of the neutron behavior within the system of interest. The validity of Fick's Law often weakens as one approaches the core periphery and shield regions, but even in these situations it gives a rough estimation of neutron attenuation. For core physics studies, diffusion theory is used almost exclusively for modeling multidimensional systems for routine analysis. On the other hand, transport theory is usually used for modeling cell and assembly configurations in cross section collapsing codes, and in treating shielding analysis problems. The angular dependence of the neutron flux is usually a key consideration in these applications. However, in large homogenized core regions, where the isotropic fission source is the dominant source of neutrons, the diffusion equation (and Fick's Law) is an adequate approximation.

Before moving on, the diffusion coefficient, which appears in the definition of Fick's Law, needs some further clarification. The diffusion coefficient appears as a proportionality constant in an approximate expression for the neutron current in terms of the neutron flux. Using transport theory methods, one can compute ϕ_g and J_g directly, and then determine appropriate values for D_g. This procedure has been performed many times and it has shown that a good approximation to D_g is

$$D_g = \frac{1}{3\Sigma_{trg}} \tag{52}$$

where

$$\Sigma_{trg} = \Sigma_{tg} - \bar{\mu}_0 \Sigma_{sg} \tag{53}$$

where Σ_{trg} is the transport cross section for group g. The transport cross section is a derived quantity which is written in terms of the total cross section and the scattering cross section. Recall that $\bar{\mu}_0$ is the average value of the scattering angle in the laboratory system for isotropic scattering in the center-of-mass (CM) system (see Refs. 1 and 2).

The diffusion coefficient is written in this fashion primarily because it gives reasonable results compared to transport theory. There are more elaborate ways of computing D_g, but eqn. (52) is the most popular method for introductory studies. In few group cross section libraries, σ_{trg} (note that $\Sigma_{trg} = N\sigma_{trg}$) is usually tabulated with the other basic data (σ_{ag}, σ_{fg}, etc.).

Note that eqn. (53) can be written as $\Sigma_{trg} = \Sigma_{ag} + (1-\bar{\mu}_0)\Sigma_{sg}$ and for $\Sigma_{ag} \ll (1-\bar{\mu}_0)\Sigma_{sg}$, this becomes $\Sigma_{trg} = (1-\bar{\mu}_0)\Sigma_{sg}$. Reference 1 writes Σ_{trg} in this fashion, although eqn. (53) is more accurate. Finally, one should also note that the units of D_g are cm (since Σ_{trg} has units of cm^{-1}), where this definition assures that each term in the diffusion equation has consistent units.

Boundary Conditions

Before we can actually solve the diffusion equation, one must address what happens at the boundaries of the system. The diffusion equation is a second-order differential equation in the spatial variable (because of the leakage term, $-\vec{\nabla}\cdot D_g \vec{\nabla}\phi_g$). Therefore, it requires two boundary conditions to obtain the complete solution for a particular problem situation. Although no explicit solutions are addressed here, we will briefly identify several of the most common boundary conditions -- as preparation for further work that explicitly addresses the solution of the Diffusion Equation for different scenarios.

There are three types of conditions discussed here:

General Boundary Conditions

1. The neutron flux must be real and non-negative.
2. The flux must be finite (except at artificial singular points of a source distribution).
3. The neutron current is zero at symmetry boundaries (no net current across boundary).

Interface Boundary Conditions (between two different or similar media)

1. Continuity of Flux -- the flux must be continuous across a material interface.

   For 1-D Cartesian geometry, this can be written as

$$\lim_{\varepsilon \to 0} \phi(x_o - \varepsilon) = \lim_{\varepsilon \to 0} \phi(x_o + \varepsilon) \tag{54}$$

2. Continuity of Current -- the current must be continuous across a material interface.

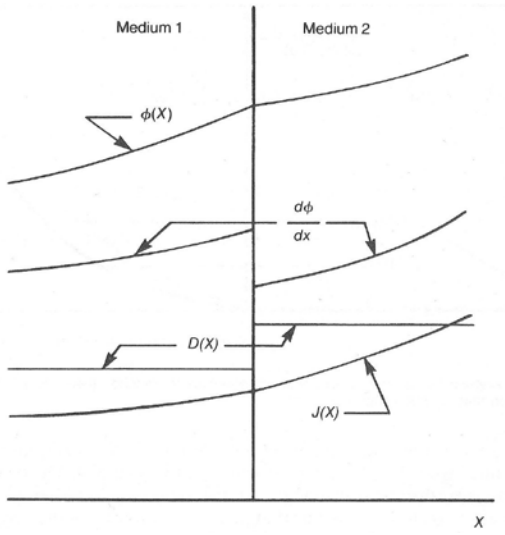
   For 1-D Cartesian geometry, this can be expressed as

$$\lim_{\varepsilon \to 0} J(x_o - \varepsilon) = \lim_{\varepsilon \to 0} J(x_o + \varepsilon) \tag{55}$$

   where x_o is the location of the material interface.

Note that although the neutron current and flux are continuous across material boundaries, the flux slope or gradient can be discontinuous if the diffusion coefficient is different on each side of the material interface (since $J = -D\, d\phi/dx$).

These concepts are illustrated nicely in the sketch shown on the right (from **Introductory Nuclear Reactor Statics** by Ott and Bezella -- see Ref. 3), where the flux and current continuity and the possible discontinuity in the flux gradient are highlighted at the interface between two materials. Using the subscript 1 to denote medium 1 and 2 to refer to medium 2, eqn. (55) says that



$$-D_1 \frac{d}{dx}\phi\bigg|_{x_o\,(\text{from left})} = -D_2 \frac{d}{dx}\phi\bigg|_{x_o\,(\text{from right})}$$

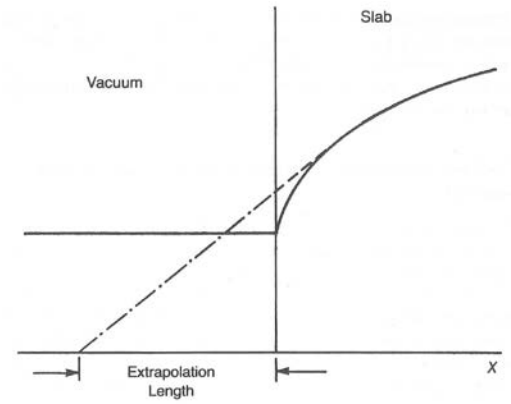
Thus, if $D_1 \neq D_2$, then clearly there must be a discontinuity in the slope of the flux at the interface.

External (or Vacuum) Boundary Conditions

First we note that Fick's Law is not really valid in this situation. The true vacuum boundary condition is one which specifies that there are no reentrant neutrons. For example, using 1-D Cartesian geometry again, this condition can be written mathematically as

$$\phi_g(x,\hat{\Omega})\Big|_{x=x_o} = 0 \quad \text{for } \hat{\Omega} > 0 \text{ for left boundary} \tag{56}$$

Now if we desire to use Fick's Law, one can modify this condition such that the diffusion theory flux approximates the more exact transport theory result. At an external boundary, this is done by assuming that the diffusion theory flux vanishes at some small distance, d, beyond the external surface, where d is referred to as the extrapolation distance. This is illustrated nicely in the diagram (from Ref. 3 again), where the solid line represents the flux computed from transport theory, the dashed line corresponds to the diffusion theory flux, and the dotted-dashed line represents the extrapolation of the diffusion theory flux to zero at a distance d beyond the physical boundary.



Using transport theory as the correct solution, one can show that a good approximation for the extrapolation length (for 1-D Cartesian geometry) is

$$d = 0.71\lambda_{tr} = \frac{0.71}{\Sigma_{tr}} = 0.71(3D) = 2.13D \tag{57}$$

and approximate values of the thermal diffusion coefficient for some common moderators are:

D_{water} = 0.16 cm, $D_{heavy\ water}$ = 0.87 cm, D_{Be} = 0.50 cm, $D_{graphite}$ = 0.84 cm

Therefore, we see that the extrapolation distance, d, is on the order of only a few centimeters or less (note that, for fast neutrons, D will be somewhat larger than illustrated here). However, for large power reactors, d is usually small compared to realistic reactor dimensions (and can often be ignored). For small bare critical systems, d cannot be neglected.

With the above discussion, we can write the vacuum boundary condition for use in diffusion theory as (again, we use 1-D Cartesian geometry to simplify the notation),

$$\phi_g(x)\Big|_{x=x_o \pm d} = 0 \tag{58}$$

or

$$\phi_g(x)\Big|_{x=x_o} = 0 \qquad \text{for } |x_o| \gg d \tag{59}$$

where x_o is the location of the external boundary of the system and $x_o \pm d$ is referred to as the extrapolated boundary (the plus sign is used for a right boundary and the negative sign is used on the left side). Therefore, we see that the standard vacuum boundary condition in diffusion theory is that the flux goes to zero at the extrapolated boundary [this is expressed as eqn. (58)]. When the extrapolation distance is small compared to the dimensions of the system, then it may be

appropriate to simply ignore d and say that the flux goes to zero at the physical boundary [this is expressed as eqn. (59)].

Operator Form of the Diffusion Equation

The multigroup diffusion equation is given by the combination of eqn. (51), which gives the basic balance relationship, and eqns. (42) and (43), which explicitly define the removal cross section and the neutron source terms that appear on the right side of eqn. (51), respectively. Although these are not overly complicated, it becomes a little tedious to write out these relationships in full detail every time one wants to discuss the basic balance equation. In particular, it certainly would be convenient to be able to write the general steady state diffusion equation using some simplified notation. Towards this goal, let's define the following matrix operators,

$$\underline{\underline{L}} = -\vec{\nabla}\cdot\underline{\underline{D}}\vec{\nabla} + \underline{\underline{\Sigma}}_R - \underline{\underline{\Sigma}}_S^I \tag{60}$$

and $$\underline{\underline{F}} = \underline{\underline{\chi}}\,\underline{\underline{\nu\Sigma}}_f \tag{61}$$

where

$$\underline{\underline{D}} = \begin{bmatrix} D_1 & & & 0 \\ & D_2 & & \\ & & \ddots & \\ 0 & & & D_G \end{bmatrix} \qquad \underline{\underline{\Sigma}}_R = \begin{bmatrix} \Sigma_{R1} & & & 0 \\ & \Sigma_{R2} & & \\ & & \ddots & \\ 0 & & & \Sigma_{RG} \end{bmatrix} \tag{62a}$$

$$\underline{\underline{\Sigma}}_S^I = \begin{bmatrix} 0 & \Sigma_{2\to1} & \Sigma_{3\to1} & \cdots & \Sigma_{G\to1} \\ \Sigma_{1\to2} & 0 & \Sigma_{3\to2} & \cdots & \Sigma_{G\to2} \\ \Sigma_{1\to3} & \Sigma_{2\to3} & 0 & \cdots & \Sigma_{G\to3} \\ & & \vdots & & \\ \Sigma_{1\to G} & \Sigma_{2\to G} & \Sigma_{3\to G} & \cdots & 0 \end{bmatrix} \tag{62b}$$

$$\underline{\underline{\chi}} = \begin{bmatrix} \chi_1 & & & 0 \\ & \chi_2 & & \\ & & \ddots & \\ 0 & & & \chi_G \end{bmatrix} \qquad \underline{\underline{\nu\Sigma}}_f = \begin{bmatrix} \nu\Sigma_{f1} & \nu\Sigma_{f2} & \nu\Sigma_{f3} & \cdots & \nu\Sigma_{fg} \\ \nu\Sigma_{f1} & \nu\Sigma_{f2} & \nu\Sigma_{f3} & \cdots & \nu\Sigma_{fG} \\ \nu\Sigma_{f1} & \nu\Sigma_{f2} & \nu\Sigma_{f3} & \cdots & \nu\Sigma_{fG} \\ & & \vdots & & \\ \nu\Sigma_{f1} & \nu\Sigma_{f2} & \nu\Sigma_{f3} & \cdots & \nu\Sigma_{fG} \end{bmatrix} \tag{62c}$$

Finally, defining the group flux vector, $\underline{\phi}$, and external source vector, $\underline{Q}$, as

$$\underline{\phi} = \begin{bmatrix} \phi_1 \\ \phi_2 \\ \vdots \\ \phi_G \end{bmatrix} \qquad \text{and} \qquad \underline{Q} = \begin{bmatrix} Q_1 \\ Q_2 \\ \vdots \\ Q_G \end{bmatrix} \tag{63}$$

one can write the operator form of the diffusion equation as

$$\left(\underline{\underline{L}} - \underline{\underline{F}}\right)\underline{\phi} = \underline{Q} \tag{64}$$

or

$$\left[-\vec{\nabla}\bullet\underline{\underline{D}}\vec{\nabla} + \underline{\underline{\Sigma}}_R - \underline{\underline{\Sigma}}_S^I\right]\underline{\phi} \; - \; \left[\underline{\underline{\chi\nu\Sigma}}_f\right]\underline{\phi} \; = \; \underline{Q} \tag{65}$$

Recall that a matrix times a vector can be written as $\underline{b} = \underline{\underline{A}}\,\underline{x}$, where each element of $\underline{b}$ is given as

$$b_i = \sum_j a_{ij} x_j \tag{66}$$

Applying this definition of matrix multiplication, one sees that eqn. (64) is just a simplified form of the multigroup equations.

To see that these definitions really work, let's look at the specific case of the 2-group problem. Consider the multigroup diffusion equation in eqn. (51) as the starting point, with full expansion of Σ_{Rg} and S_g via eqns. (42) and (43). For the group 1 equation, let g = 1 and vary g' = 1,2 accordingly. For the group 2 equation, simply let g = 2 and again vary g' over all appropriate groups. Expanding fully, one has

$$-\vec{\nabla}\bullet D_1\vec{\nabla}\phi_1 + \left(\Sigma_{a1} + \Sigma_{1\to 2}\right)\phi_1 - \Sigma_{2\to 1}\phi_2 - \chi_1\left(\nu\Sigma_{f1}\phi_1 + \nu\Sigma_{f2}\phi_2\right) = Q_1 \tag{67}$$

$$-\vec{\nabla}\bullet D_2\vec{\nabla}\phi_2 + \left(\Sigma_{a2} + \Sigma_{2\to 1}\right)\phi_2 - \Sigma_{1\to 2}\phi_1 - \chi_2\left(\nu\Sigma_{f1}\phi_1 + \nu\Sigma_{f2}\phi_2\right) = Q_2 \tag{68}$$

Now, putting these two equations into matrix form gives

$$\begin{bmatrix} -\vec{\nabla}\bullet D_1\vec{\nabla} & 0 \\ 0 & -\vec{\nabla}\bullet D_2\vec{\nabla} \end{bmatrix}\begin{bmatrix}\phi_1 \\ \phi_2\end{bmatrix} + \begin{bmatrix} \Sigma_{a1} + \Sigma_{1\to 2} & 0 \\ 0 & \Sigma_{a2} + \Sigma_{2\to 1}\end{bmatrix}\begin{bmatrix}\phi_1 \\ \phi_2\end{bmatrix} - \begin{bmatrix} 0 & \Sigma_{2\to 1} \\ \Sigma_{1\to 2} & 0\end{bmatrix}\begin{bmatrix}\phi_1 \\ \phi_2\end{bmatrix}$$

$$- \begin{bmatrix}\chi_1 & 0 \\ 0 & \chi_2\end{bmatrix}\begin{bmatrix}\nu\Sigma_{f1} & \nu\Sigma_{f2} \\ \nu\Sigma_{f1} & \nu\Sigma_{f2}\end{bmatrix}\begin{bmatrix}\phi_1 \\ \phi_2\end{bmatrix} = \begin{bmatrix}Q_1 \\ Q_2\end{bmatrix} \tag{69}$$

For most 2-group thermal reactor problems, $\chi_1 = 1.0$ and $\chi_2 = 0.0$ (that is, there is no fission source in group 2) and upscatter is usually negligible (i.e. $\Sigma_{2\to 1} = 0$). With these conditions, the above expressions become $\left(\underline{\underline{L}} - \underline{\underline{F}}\right)\underline{\phi} = \underline{Q}$, where

$$\underline{\underline{L}} = \begin{bmatrix} -\vec{\nabla}\bullet D_1\vec{\nabla} & 0 \\ 0 & -\vec{\nabla}\bullet D_2\vec{\nabla}\end{bmatrix} + \begin{bmatrix}\Sigma_{a1} + \Sigma_{1\to 2} & 0 \\ 0 & \Sigma_{a2}\end{bmatrix} - \begin{bmatrix} 0 & 0 \\ \Sigma_{1\to 2} & 0\end{bmatrix}$$

or $$\underline{\underline{L}} = \begin{bmatrix} -\vec{\nabla}\bullet D_1\vec{\nabla} + \Sigma_{R1} & 0 \\ -\Sigma_{1\to 2} & -\vec{\nabla}\bullet D_2\vec{\nabla} + \Sigma_{a2}\end{bmatrix} \tag{70a}$$

and $$\underline{\underline{F}} = \begin{bmatrix}\nu\Sigma_{f1} & \nu\Sigma_{f2} \\ 0 & 0\end{bmatrix} \tag{70b}$$

Thus, we see that the use of the expression $\left(\underline{\underline{L}} - \underline{\underline{F}}\right)\underline{\phi} = \underline{Q}$ is simply a matter of convenience, as long as one understands the significance and precise meaning of the individual terms. Finally, it should also be noted that in much of the literature, even the formal matrix (two underlines) and vector (one underline) notation is dropped; again simply as a matter of convenience. Thus, many times one will see the diffusion equation simply written as

$$\left(L - F\right)\phi = Q \tag{71}$$

which is certainly much easier to write than all the above expressions -- assuming, of course, that one understands the shorthand notation.

Overview of Typical Applications

The above development and notation for the steady state multigroup diffusion equation is quite general. For any specific application, however, only the applicable terms are used. In most cases of interest, one of the following three situations arise:

1. Subcritical non-multiplying systems (no fission source): $L\phi = Q$
2. Subcritical multiplying systems (has both fission and external sources): $(L - F)\phi = Q$
3. Critical systems (no external sources): $(L - \lambda F)\phi = 0$

The first case is applicable primarily in shield design applications (and possibly for non-multiplying fusion blanket design). This situation represents a subcritical geometry with no fission source. The neutron balance equation for this case states that leakage + removal – inscatter = external source. Using our condensed notation, this can be written as $L\phi = Q$.

The second case must be considered in situations where both the fixed source and fission source are important. This is given in equation form as $(L - F)\phi = Q$. The most common situation where this arises is during reactor startup and shutdown periods. Clearly, a reactor core has a substantial fission potential, but it may be arranged in a subcritical configuration (either by having some assemblies missing or by having large amounts of control inserted). Without an external source, there would be no steady state flux in this subcritical arrangement. However, in most fuel (especially fuel that has a substantial amount of burnup), there is an inherent neutron source due to the spontaneous fission and (α,n) reactions that are associated with the higher actinides. The neutrons emitted from these reactions, or from an externally applied fixed source, undergo subcritical multiplication (they cause fission in the fuel material) and give rise to a steady state neutron distribution throughout the system.

Subcritical systems (both multiplying and non-multiplying) with external sources are not particularly difficult to analyze. They are fixed-source problems. In simple cases, one can construct a general solution as a linear combination of homogeneous and particular solutions to the defining equations. In computer computations, one solves the equations using some numerical approximation (finite difference methods, for example). The only consideration here is that without the source, the system must be subcritical for the problem to converge properly (that is, leakage and absorption must dominate neutron production from fission).

The third and probably most important class of problems that arises is the critical reactor problem. In this situation, the leakage and absorption rates exactly balance the neutron production from fission, and any inherent neutron source that may be present in the fuel is totally

dominated by the fission source. Since the fixed source is negligible, it is simply dropped from the defining equations.

We know from the above discussion that, for a steady state critical system, there has to be a very precise balance between the neutron production and loss rates. Any arbitrary mixture of fuel, moderator, structure, and control will not satisfy this constraint. This situation is consistent with the basic nature of the defining equation for a critical system [i.e. eqn. (71) with Q = 0]. This is a homogeneous eigenvalue problem. To emphasize this, one usually includes a mathematical eigenvalue (denoted as λ) before the fission source,

$$\left(L - \lambda F\right)\phi = 0 \tag{72}$$

In a critical operating reactor, λ is unity. In design analysis, however, we often want to know if a particular combination of materials will give a critical reactor. Thus, for any given material distribution, λ is computed as part of the solution procedure. It is allowed to vary from unity so that the equation can be balanced mathematically (i.e. λ * production = loss). This allows considerable insight to be gained from any given reactor material distribution and geometry combination. It should be emphasized, however, that in an operating critical system, λ must be unity.

To see the significance of λ, let's integrate eqn. (72) over all space and energy, giving

$$\left\langle L\phi \right\rangle - \lambda \left\langle F\phi \right\rangle = 0$$

or

$$\lambda = \frac{\left\langle L\phi \right\rangle}{\left\langle F\phi \right\rangle} = \frac{\text{loss rate}}{\text{production rate}} \tag{73}$$

The term $< F\phi >$ represents the total neutron production rate from fission. Also, when performing integration over all energy, the inscatter and outscatter components within the $< L\phi >$ term exactly cancel. Therefore, $< L\phi >$ represents the total loss rate (leakage + absorption). From the definition of the multiplication factor, k,

$$k_{eff} = \frac{\text{production rate}}{\text{loss rate}} \tag{74}$$

we see that

$$\lambda = \frac{1}{k_{eff}} \tag{75}$$

Thus, we see that the addition of the eigenvalue within the defining equation is quite justifiable. At steady state operating conditions, $k_{eff} = 1/\lambda = 1.0$. For any given material configuration, the calculated k_{eff} may not be unity, but this, in fact, tells the designer how far from critical the configuration is, and that some modification is required (control in or out, more or less fuel is required, etc.).

The above discussion and the usefulness of this approach to solving the critical balance equation will become clear as one gains some experience with a variety of simple hand calculations and with the use of various design tools for reactor analysis. However, the discussion of actual solutions for a variety of example problems that involve the three types of applications presented above will have to wait for another day, since our goal in this set of Lecture Notes -- the development and interpretation of the Multigroup Neutron Balance Equation -- is now complete!!!

Summary

This lecture focused on the development of the multigroup neutron balance equation, with special emphasis on the diffusion theory approximation. It first identified all the neutron production and loss mechanisms that can occur within a nuclear system, and then put these together to give the desired steady state neutron balance relationship. A formal notation was developed that allowed one to rigorously define all the important components of the resultant balance equation. In addition, in the last subsection, a shorthand operator notation was also introduced and utilized to overview the three primary classes of problems that can be addressed using the equations developed here.

It should be noted, however, that this material only represents a foundation for further study, since no solutions or example analyses were attempted. The goal here was to develop a strong base to support further work in reactor theory and, hopefully, we were successful in achieving that result. The material from this lecture will be used as a theoretical base for most of the remaining reactor physics topics covered in this course -- so make sure you have a good foundation here before venturing too far into unknown territory…

References

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3. K. O. Ott and W. A. Bezella, ***Introductory Nuclear Reactor Statics***, American Nuclear Society (1983).