22.05 Reactor Physics - Part Fifteen

Group Diffusion Method

1. Background:

Thus far, we have examined neutron life cycle analysis, one-velocity theory, and modified one-velocity theory. Next we will consider the group diffusion method which leads to both the "few group" and the "multi-group" calculations. The driving force for changing from the earlier modes of analysis to group techniques was the desire for greater accuracy and the availability of increased computational capability. Group methods dominated reactor physics from the mid-1960s to the late 1990s when Monte Carlo techniques began their ascendancy.

2. Goal:

The goal remains to determine the neutron flux as a function of both energy and position. That is, to calculate $\phi(r,E)$. We began the effort with life cycle analysis which provided some information on criticality as well as an understanding of important phenomena including fast fission, resonance escape, thermal utilization, and leakage. Next we considered one-velocity theory. This allowed us to obtain flux as a function of position but provided no information on the energy dependence because we assumed mono-energetic neutrons. It also ignored scattering which is the process whereby energy dependence arises. Then we examined modified one-velocity theory which assumed two energy ranges and allowed for scattering from one range to the other. This gives us a means of deciding if one-velocity theory will be valid. But it did not truly address energy dependence. Group theory is about energy-dependence. It achieves this by treating neutron scattering properly. Once the energy dependence is resolved, group theory also allows us to investigate spatial dependence. Thus, we can obtain $\phi(r,E)$. The following chart compares the one-velocity and group approaches in terms of the processes that each includes in its derivations.

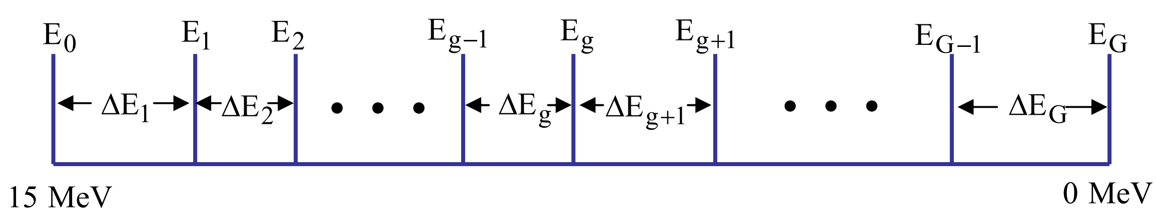
Method	Process			
	Fission	Absorption	Leakage	Scatter
One Velocity	Yes	Yes	Yes	No
Modified One-Velocity	Yes	Yes	Yes	Limited
Group (Initial)	Yes	Yes	No	Yes
Group (Final)	Yes	Yes	Yes	Yes

It is important to recognize the difference in the sequence. For one-velocity, we considered fission, absorption, and leakage in order to get a spatial dependence. We ignored scattering and energy dependence. In the group approach, we will first consider fission, absorption, and scattering in order to get the energy dependence. We will initially ignore leakage and spatial dependence. Once we have determined ϕ (E) accurately, we will then incorporate leakage and obtain spatial effects as well, thereby achieving our goal of ϕ (r,E).

3. **Energy Groups:**

The basic idea is to divide the allowable energy range (1-10 MeV) of fission-produced neutrons into a set of G groups. G could be as large as 3000. Hence, one is no longer limited to treating neutrons as mono-energetic. Within each group, all neutrons are treated as having the same energy and group properties (diffusion, absorption, fission, scatter cross-sections) are averaged over each energy range. The process is entirely straight forward with the biggest challenge being one of nomenclature. We use that given by A. Henry (pp. 66-71).

The figure below shows the partitioning of the energy range (0-15 MeV). The idea is to subdivide it into G groups of width ΔE_G so that each corresponds to a region over which the neutron cross-sections are flat. Group width (the ΔE_G) need not be the same. Thus, many groups of narrow width would be used in the resonance region and fewer groups of broader width in the fast region where cross-sections are often smooth. Groups are labeled in increasing order from high to low energy. Thus, E_0 is 15 MeV and E_G is 0 MeV. ΔE_1 is the group just below 15 MeV. ΔE_{G-1} is the group just above 0 MeV.



4. **Neutron Balance Equation:**

The starting point is to assume an infinite, homogeneous, critical reactor. What do these assumptions imply:

- **Infinite:** **No leakage**
- **Homogeneous:** **No spatial dependence of material properties such as cross-sections within the core**
- **Critical:** **Steady-state**

Our balance equation for a given energy group then becomes:

Removal = Production

Absorption + Scattering Out = Fission + Scattering In

We can now write expressions for each process for some energy interval dE and some volume element dV. However, before doing so, it is appropriate to designate a notation for describing neutron energies. There are three rates that we wish to describe: removal of neutrons from dE, the appearance of neutrons in dE as a result of fissions caused by neutrons of any energy, and the appearance of neutrons in dE as the result of scattering from any energy. We therefore need to distinguish between the current neutron energy and that which existed before the fission and/or scattering event. We will use the symbols E and dE for the former and E' and dE' for the latter. With this distinction, we can now write the desired expressions:

a) Interaction rate of neutrons by all processes within dVdE

$$\Sigma_t(E)\phi(E)dEdV$$

Where Σ_t includes absorption and scattering. Specifically, $\Sigma_t = \Sigma_a + \Sigma_s$ and is called the "total" cross-section. If we wanted removal only, it would be this total rate minus scattering within the group. (See p. 10 of these notes.)

b) Production rate of neutrons from fission in dVdE

$$\chi(E)dE\left[\int_0^\infty \nu\Sigma_f(E')\phi(E')dE'\right]dV$$

Where $\chi(E)$ is the fission energy spectrum, ν, is the average number of neutrons emitted per fission, Σ_f is the fission cross-section, and $\phi(E')$ is the neutron flux. What does this expression mean? The cross-section for the fission of U-235 (and also of those of the other fissile nuclides) is non-zero for all neutron energies. So, there is some probability that any neutron, regardless of its energy, may cause a fission that in turn produces a neutron that appears in dE. We denote the energy of the neutrons before they cause a fission by E'. Thus, $\Sigma_f(E')\phi(E')$ is the fission rate per unit energy per unit volume. We integrate over all energies E' to obtain the total fission rate and multiply by number of neutrons per fission (ν) to get the total number of neutrons produced from fission. The fraction of those so produced that appear in the energy interval E to (E+dE) is obtained by multiplying by χ(E)dE.

c) Appearance rate of neutrons in dVdE by scattering from dE'

$$dE\left[\int_0^\infty \Sigma_s(E' \rightarrow E)\phi(E')dE'\right]dV$$

Where Σ_s is the cross-section for scattering from energy E' to energy E. What does this expression mean? The quantity $\Sigma_s(E' \rightarrow E)\phi(E')$ is the rate per unit energy per unit volume at which neutrons scatter from any energy E' into an energy between E and (E+dE). E' denotes the neutron energy before the scattering event. Thus, we integrate over all energies E' to obtain the total scattering rate. From the discussion of the kinematics of neutron scattering (Part 14 of these notes) we know that the probability of a scattered neutron's appearing in a given energy interval is proportional to the width of that interval. Therefore, we multiply by dE to obtain the appearance rate in an interval E to (E+dE) from scattering.

Upon combining the above, we obtain the steady-state neutron balance relation:

$$\begin{aligned}\Sigma_t(E)\phi(E)dEdV = \chi(E)dE\left[\int_0^\infty \nu\Sigma_f(E')\phi(E')dE'\right]dV \\ + dE\left[\int_0^\infty \Sigma_s(E' \rightarrow E)\phi(E')dE'\right]dV\end{aligned} \tag{1}$$

The above expression can be written in a more compact manner by noting that the integral over dE' is common to both the fission and scattering process. Thus, one obtains:

$$\Sigma_t(E)\phi(E) = \int_0^\infty dE'\left[\chi(E)\nu\Sigma_f(E') + \Sigma_s(E' \rightarrow E)\right]\phi(E') \tag{2}$$

This is the equation as it is normally written in the literature. However, the less compact verion is more appealing in terms of physical understanding. We will continue to work with the less compact version, equation (1) above.

The objective is now to solve the neutron balance equation by integrating it over each energy group ΔE_g. The process is straightforward for the removal term. One integrates from E_g to E_{g-1} to obtain the total removal rate per unit volume of all neutrons from ΔE_g. Thus, the result is

$$\int_{E_g}^{E_{g-1}} \Sigma_t(E)\phi(E)dE$$

Next consider the fission term. There are three separate steps to the procedure. First, integrate $\nu\Sigma_f(E')\phi(E')dE'$ over an energy group $\Delta E_{g'}$. This gives the fission rate in a particular energy group. Second, sum over all such groups to obtain the total fission rate caused by neutrons of all energies. Third, integrate over ΔE_g to obtain the rate of appearance of fission neutrons at energies between E_g and E_{g-1}. Thus,

$$\underbrace{\int_{E_g}^{E_{g-1}} \chi(E)dE \left[\underbrace{\sum_{g'=1}^{G} \underbrace{\int_{E_{g'}}^{E_{g'-1}} \nu\Sigma_f(E')\phi(E')dE'}_{\text{Integrate over } \Delta E_{g'}}}_{\text{Sum over all groups } \Delta E_{g'}} \right]}_{\text{Integrate over } \Delta E_g}$$

Finally, consider the scatter term. Here, there is also an integral over dE' that must be replaced by a sum of integrals over $\Delta E_{g'}$. Thus,

$$\int_{E_g}^{E_{g-1}} dE \left[\sum_{g'=1}^{G} \int_{E_{g'}}^{E_{g'-1}} \Sigma_s(E' \to E)\phi(E')dE' \right]$$

The final result is obtained by equating the removal to the fission and scatter terms. Thus,

$$\int_{E_g}^{E_{g-1}} \Sigma_t(E)\phi(E)dE = \int_{E_g}^{E_{g-1}} \chi(E)dE \left[\sum_{g'=1}^{G} \int_{E_{g'}}^{E_{g'-1}} \nu\Sigma_f(E')\phi(E')dE' \right]$$
$$+ \int_{E_g}^{E_{g-1}} dE \left[\sum_{g'=1}^{G} \int_{E_{g'}}^{E_{g'-1}} \Sigma_s(E' \to E)\phi(E')dE' \right]$$

The above can be written in a more compact form by noting that the summation is common to both the fission and scatter terms. Thus,

$$\int_{E_g}^{E_{g-1}} \Sigma_t(E)\phi(E)dE = \sum_{g'=1}^{G} \left[\int_{E_g}^{E_{g-1}} \chi(E)dE \int_{E_{g'}}^{E_{g'-1}} \nu\Sigma_f(E')\phi(E')dE' \right.$$

$$\left. + \int_{E_g}^{E_{g-1}} dE \int_{E_{g'}}^{E_{g'-1}} \Sigma_s\left(E' \to E\right)\phi(E')dE' \right] \quad (g = 1,2,...,G).$$

This is the equation that we need to solve. Two insights that are obtainable by physical arguments are that $\phi(E)$ will be zero at both high and low energies. It is zero at high energies because the fission process produces few neutrons with energies above 10 MeV (and none above 15 MeV). It approaches zero at low energies (well below 0.025 eV) because absorption cross-sections exhibit 1/v behavior as $E \to 0$. Hence, most neutrons are absorbed.

5. **<u>Group Constants</u>**:

We now have the neutron balance equation written for each energy group ΔE_g. These are averages of the quantity in question (a flux, $\chi(E)$, a cross-section) over the energy interval. We define these averages as:

$$\Phi_g \equiv \int_{E_g}^{E_{g-1}} \phi(E)dE$$

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

$$\Sigma_{tg} \equiv \frac{\int_{E_g}^{E_{g-1}} \Sigma_t(E)\phi(E)dE}{\Phi_g}$$

$$\nu\Sigma_{fg'} \equiv \frac{\int_{E_{g'}}^{E_{g'-1}} \nu\Sigma_f(E')\phi(E')dE'}{\Phi_{g'}}$$

$$\Sigma_{gg'} \equiv \frac{\int_{E_g}^{E_{g-1}} dE \int_{E_{g'}}^{E_{g'-1}} \Sigma_s(E' \to E)\phi(E')dE'}{\Phi_{g'}}$$

"Note the order of the subscripts in $\Sigma_{gg'}$: the scattering is *from* group g' to group g. The balance then becomes:

$$\Sigma_{tg}\Phi_g = \sum_{g'=1}^{G} \left[\chi_g \nu \Sigma_{fg'} + \Sigma_{gg'}\right]\Phi_{g'} \quad (g = 1, 2, ..., G).$$

The quantity Φ_g is called the group flux. Note that it is not a density in energy, and thus it has dimensions different from $\phi(E)$. Physically Φ_g is the number of neutrons per unit volume in the energy range ΔE_g multiplied by their average speed.

The physical meaning of the above relation is that the total rate at which neutrons are removed from energy group g (per unit volume in an infinite, homogeneous, critical reactor) equals the sum of the rate at which they appear in group g because of fissions in all groups plus the rate at which they appear because of scattering from all groups (including group g itself)." (From Henry pp. 69-70)

The above equation can be solved algebraically and hence its solution is far simpler than that of the original integral equation. In order to get $\phi(E)$, one assembles the group fluxes. As the ΔE_g get small, the approximation to $\phi(E)$ improves.

However, there is a major problem in that we do not know the group parameters and in order to obtain them we first have to know $\phi(E)$, which of course is what we are trying to find. We can resolve this problem by assuming a particular shape for $\phi(E)$ in each energy group. Thus, "we make the following approximation:

$$\phi(E) = \text{constant} = C_g \text{ for } E_g < E \le E_{g-1} \qquad (g = 1, 2, \ldots, G).$$

In words, we approximate $\phi(E)$ within each energy group ΔE_g by a constant. For G large and the locations of the partition energies carefully chosen, this approximation is an excellent one. (Computer programs that can handle many thousand energy groups are currently in operation, although, for most applications, use of fewer than 100 groups provides satisfactory results.)

With $\phi(E)$ constant within each ΔE_g, the flux-dependent "group cross sections" become:

$$\Sigma_{tg} \equiv \frac{\int_{E_g}^{E_{g-1}} \Sigma_t(E)dE}{\Delta E_g}$$

$$\nu\Sigma_{fg'} \equiv \frac{\int_{E_{g'}}^{E_{g'-1}} \nu\Sigma_f(E')dE'}{\Delta E_{g'}}$$

$$\Sigma_{gg'} \equiv \frac{\int_{E_g}^{E_{g-1}} dE \int_{E_{g'}}^{E_{g'-1}} \Sigma_s(E' \to E)dE'}{\Delta E_{g'}}$$

These parameters, along with χ_g can be obtained directly from the basic nuclear data and material concentrations in the medium. As a result, we can solve for the Φ_g without first having to know $\phi(E)$. Moreover, insofar as the approximate group constants are close to the exact group constants, we expect that these approximate constants, when used in the group equations will yield values of Φ_g that are close to those of the exact Φ_g**."** (From Henry p. 70)

It is convenient to write the entire set of G energy group equations in matrix form. Thus, for three energy groups, we have:

$$\begin{bmatrix} \Sigma_{t1} - \Sigma_{11} - \chi_1\nu\Sigma_{f1} & -\chi_1\nu\Sigma_{f2} & -\chi_1\nu\Sigma_{f3} \\ -\chi_2\nu\Sigma_{f1} - \Sigma_{21} & \Sigma_{t2} - \Sigma_{22} - \chi_2\nu\Sigma_{f2} & -\chi_2\nu\Sigma_{f3} \\ -\Sigma_{31} & -\Sigma_{32} & \Sigma_{t3} - \Sigma_{33} \end{bmatrix} \begin{bmatrix} \Phi_1 \\ \Phi_2 \\ \Phi_3 \end{bmatrix} = 0$$

Where any term that is zero is not shown. (We will discuss which are zero and why shortly. For now, we examine the matrix.) Matrix equations can be daunting. It is therefore useful to expand the above to show the individual equations.

Group	Equations
1	$(\Sigma_{t1} - \Sigma_{11} - \chi_1 \nu \Sigma_{f1})\phi_1 - \chi_1 \nu \Sigma_{f2}\phi_2 - \chi_1 \nu \Sigma_{f3}\phi_3 = 0$ or $(\Sigma_{t1} - \Sigma_{11})\phi_1 - \chi_1 \nu \Sigma_{f1}\phi_1 - \chi_1 \nu \Sigma_{f2}\phi_2 - \chi_1 \nu \Sigma_{f3}\phi_3 = 0$
2	$(-\chi_2 \nu \Sigma_{f1} - \Sigma_{21})\phi_1 + (\Sigma_{t2} - \Sigma_{22} - \chi_2 \nu \Sigma_{f2})\phi_2 - \chi_2 \nu \Sigma_{f3}\phi_3 = 0$ or $-\chi_2 \nu \Sigma_{f1}\phi_1 - \Sigma_{21}\phi_1 + (\Sigma_{t2} - \Sigma_{22})\phi_2 - \chi_2 \nu \Sigma_{f2}\phi_2 - \chi_2 \nu \Sigma_{f3}\phi_3 = 0$
3	$-\Sigma_{31}\phi_1 - \Sigma_{32}\phi_2 + (\Sigma_{t3} - \Sigma_{33})\phi_3 = 0$

Let's start with the Group 3 equation which is the simplest. The term $\Sigma_{31}\phi_1$ represents neutrons that scatter from Group 1 to Group 3. Similarly, $\Sigma_{32}\phi_2$ is neutrons that scatter from Group 2 to Group 3. Next is the $(\Sigma_{t3} - \Sigma_{33})\phi_3$ term. $\Sigma_{t3}\phi_3$ is the group's absorption plus the group's scattering. $\Sigma_{33}\phi_3$ is the portion of the Group 3 scattering (in this case 100% because Group3 is the lowest energy group in this example) that returns to Group 3. So, $(\Sigma_{t3} - \Sigma_{33})\phi_3$ is the total removal (absorption plus scattering out). No fission neutrons appear in Group 3 because $\chi(E)$, the fission spectrum, is zero for the lowest group.

Now consider the group 2 equation. The term $\chi_2 \nu \Sigma_{f1}\phi_1$ represents fissions in Group 1 that produce neutrons in Group 2. The $\Sigma_{21}\phi_1$ term is scattering from Group 1 to 2. The $(\Sigma_{t2} - \Sigma_{22})\phi_2$ is the total removal (absorption plus scattering out) from Group 2. The $\chi_2 \nu \Sigma_{f2}\phi 2$ is fissions in Group 2 that produce neutrons in Group 2 and the $\chi_2 \nu \Sigma_{f3}\phi_3$ is fissions in Group 3 that produce neutrons in Group 3.

The Group 1 equation is similar. $(\Sigma_{t1} - \Sigma_{11})\phi$ is the total removal. The other three terms are the fissions in Groups 1, 2, and 3 respectively that produce neutrons in Group 1.

If instead of writing our matrix equation for three groups, we had kept it completely general so that it covered G groups, it would have the form:

$$\begin{bmatrix} \Sigma_{t1} - \chi_1 \nu \Sigma_{f1} - \Sigma_{11} & -\chi_1 \nu \Sigma_{f2} - \Sigma_{12} & \cdots & -\chi_1 \nu \Sigma_{fG} - \Sigma_{1G} \\ -\chi_2 \nu \Sigma_{f1} - \Sigma_{21} & \Sigma_{t2} - \chi_2 \nu \Sigma_{f2} - \Sigma_{22} & \cdots & -\chi_2 \nu \Sigma_{fG} - \Sigma_{2G} \\ \vdots & \vdots & & \vdots \\ \chi_G \nu \Sigma_{f1} - \Sigma_{G1} & -\chi_G \nu \Sigma_{f2} - \Sigma_{G2} & \cdots & \Sigma_{tG} - \chi_G \nu \Sigma_{fG} - \Sigma_{GG} \end{bmatrix} \begin{bmatrix} \Phi_1 \\ \Phi_2 \\ \vdots \\ \Phi \end{bmatrix} = 0$$

Where all terms, including ones that are zero, are retained for completeness.

Which terms are zero? First, as noted earlier, the spectrum of fission neutrons, $\chi(E)$, is zero at low energies. So, $\chi_g \nu \Sigma_{fg}$ is zero for large values of g. Also up scattering is rarely observed unless the neutrons are in the thermal range. So $\Sigma_{12}, \Sigma_{13}, \ldots \Sigma_{1G}$, are zero.

One final matter of notation is useful. The quantity $\Sigma_{tg} - \Sigma_{gg}$ appears frequently. So, it is given a special name – total removal. Its symbol is Σ_g. Thus

$$\begin{aligned} \Sigma_g &\equiv \Sigma_{tg} - \Sigma_{gg} \\ &= \Sigma_{ag} + \Sigma_{sg} - \Sigma_{gg} \\ &= \Sigma_{ag} + \sum_{g' \neq g} \Sigma_{g'g} \end{aligned}$$