# Reactor Physics: Multigroup Diffusion

prepared by
Wm. J. Garland, Professor, Department of Engineering Physics,
McMaster University, Hamilton, Ontario, Canada

More about this document

***Summary:***
*The multigroup from of the neutron diffusion equation is developed and explored with the aim to relate the mathematics to the physical meaning.*

## Table of Contents



## List of Figures

# 1 Introduction

## 1.1 Overview

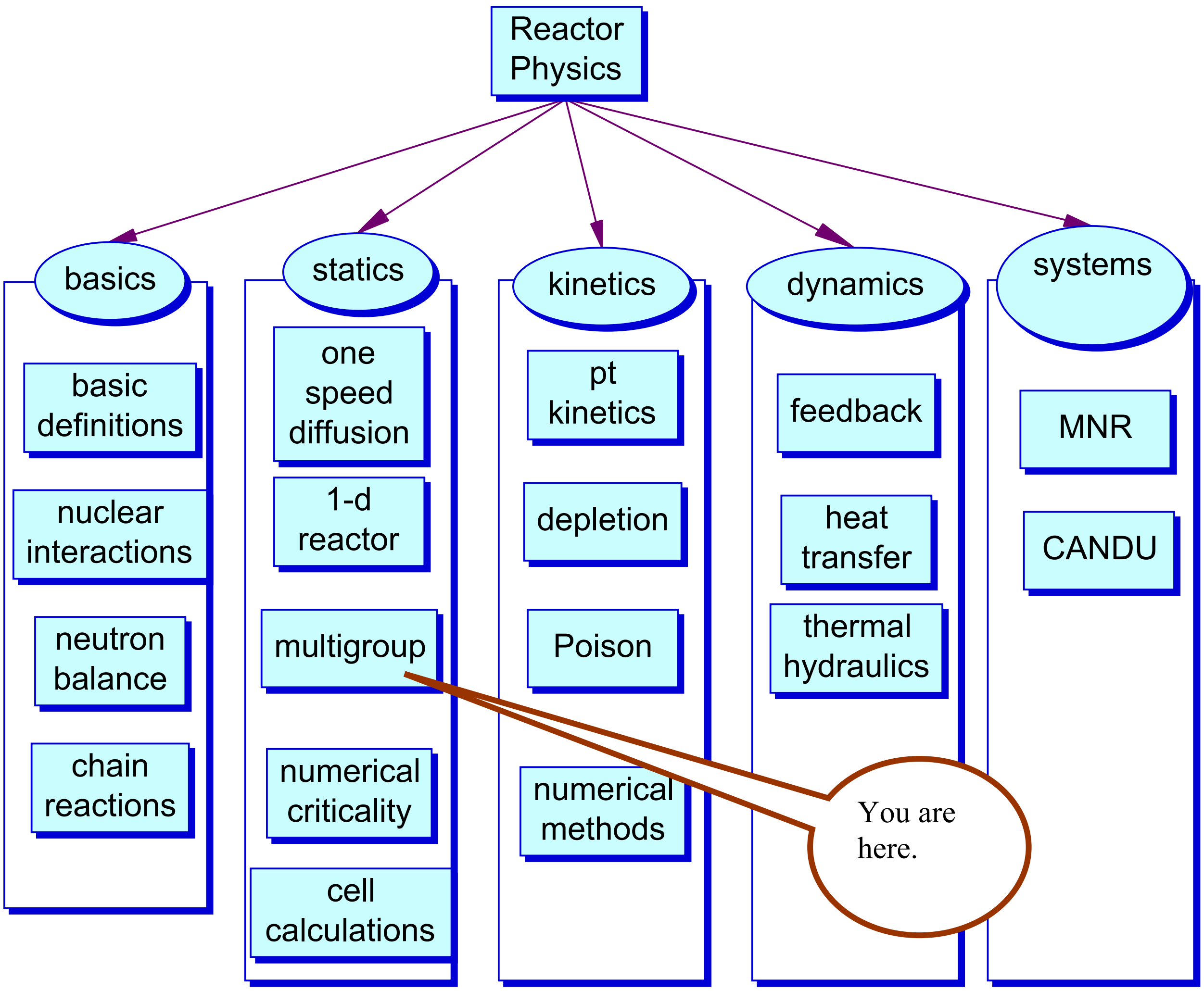


**Figure 1 Course Map.**

## 1.2 Learning Outcomes

The goal of this chapter is for the student to understand:

- The physical meaning of the multigroup equations
- The mathematical expressions that form the multigroup equations
- How to simplify the general forms
- How to model a reactor using the multigroup form
- How to solve the equations.

# 2 Why We Need the Multigroup Model

Neutrons have a wide energy spectrum, ranging from a fraction of an eV to a few MeV. The cross sections vary over decades in this range so we can hardly expect the one group approximation to be very accurate. To illustrate this, consider a simple cell model as shown in figure 2 for a tank type experimental reactor:

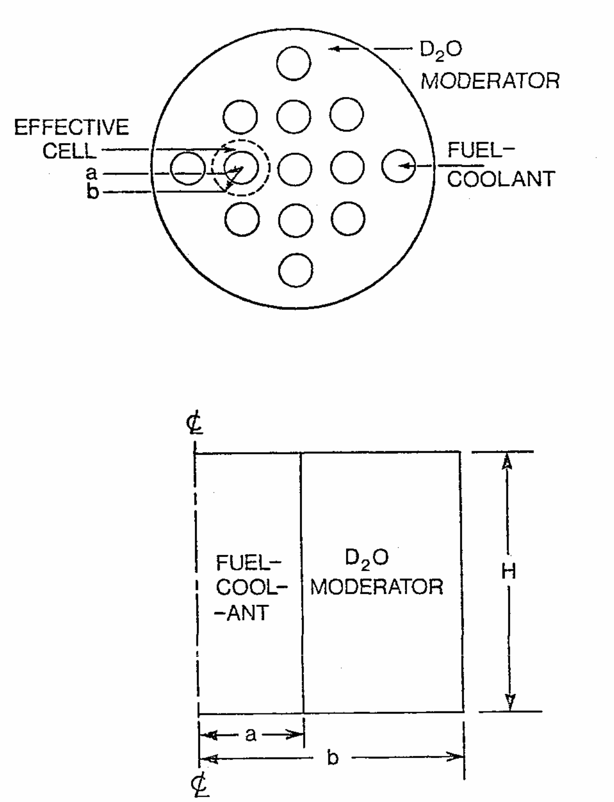


**Figure 2 Schematic of the nuclear reactor model showing the top view of the lattice structure of fuel bundles and a side view of the two-region cell.**

The height, H, of the D2O moderator was varied to achieve criticality. Then a void was introduced in the coolant by bubbling air into it. The height, H, of the moderator was again varied to keep the reactor critical. A range of void fraction was introduced. Figure 3 gives the experimental results (Buckling, $\left(\pi/H\right)^2$ vs. void fraction, $\alpha$) and the predictions of a number of simple reactor models. One group theory does not come close to predicting the buckling, even if the cross sections are varied within their experimental error. The semi-two-group theory does better and the two-group model does better still.

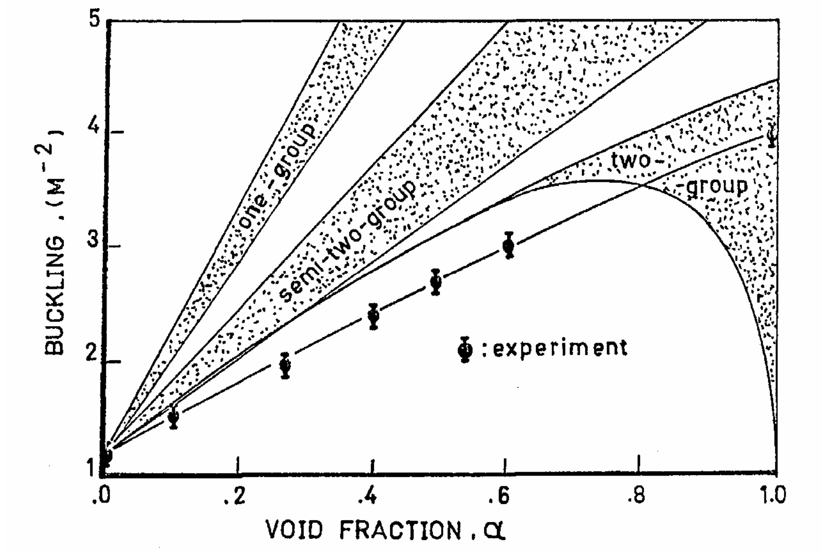


**Figure 3 Comparison between experimentally observed and calculated buckling.**

The two-group model can be further improved by using energy-averaged cross sections obtained by a comprehensive cell code that employs a detailed energy structure. The improved comparison is shown in figure 4 shows what can be achieved with a few-group model (in this case, two) if the 'appropriate' average cross sections can be found that represent the cell in question. We shall see that we can only get good values if we first perform a many-group model calculation.

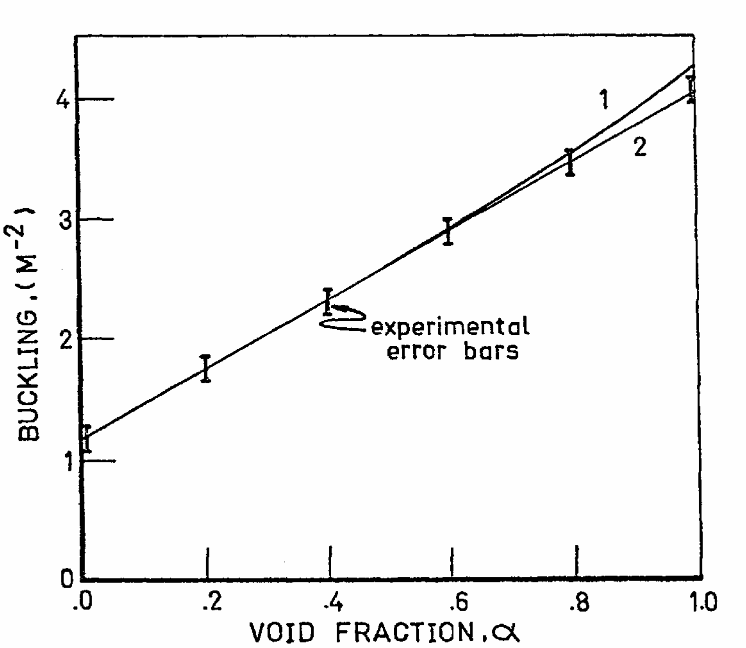


**Figure 4 Comparison of experimentally observed buckling and predictions of the two-group model using adjusted parameters.**

This work is detailed in [GARLAND1975] but for the present discussion, the main point to note is the inadequacy of the one-group model or even the two-group model since the appropriate cross sections are not explicitly available and since these low order models do not come close to capturing the energy structure. Accurate cell calculations are done typically with up to 150 neutron energy groups to obtain cell-averaged cross sections. Then, few-group approximations are used for the full core calculation based on the cell averaged cross sections. Few-group calculations can be successfully done but only if they are backed up by detailed multigroup cell calculations.

This chapter is all about the governing equations for the multigroup model that are the essence of all these calculations.

# 3 The Multigroup Equations

To form the multigroup neutron diffusion equations we first divide the energy range for the neutrons up into groups as shown in figure 5.

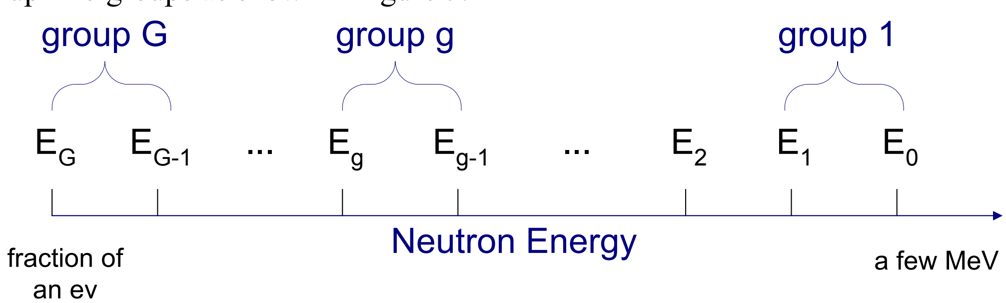


**Figure 5 Neutron energy group numbering scheme.**

Thus we have:

$$\phi_g(\underline{r},t) \text{ for } E \in \left(E_{g,}E_{g-1}\right) \text{ where } E_g < E < E_{g-1} \tag{3.1}$$

The multigroup form of the neutron diffusion equation is:

$$\begin{aligned}\frac{1}{v_g}\frac{\partial}{\partial t}\phi_g(\underline{r},t) = {} & \underbrace{\nabla\cdot D_g(r)\nabla\phi_g(\underline{r},t)}_{\text{leakage}} - \underbrace{\Sigma_{ag}(r)\phi_g(\underline{r},t)}_{\substack{\text{loss by}\\\text{absorption}}} - \underbrace{\Sigma_{sg}(r)\phi_g(\underline{r},t)}_{\substack{\text{removal by}\\\text{scattering}}} + \underbrace{\sum_{g'=1}^{G}\Sigma_{sg'g}(r)\phi_{g'}(\underline{r},t)}_{\text{scattering into group g}} \\ & + \underbrace{\chi_g}_{\substack{\text{fraction}\\\text{appearing}\\\text{in group g}}} \underbrace{\sum_{g'=1}^{G}\nu_{g'}\Sigma_{fg'}(\mathbf{r})\phi_{g'}(\underline{r},t)}_{\substack{\text{total fission}\\\text{production}}} \underbrace{+S_g^{ext}}_{\text{external source}}\end{aligned} \tag{3.2}$$

Note that the neutrons are born with no knowledge of their parents. Thus we write the total fission production as a sum that is independent of the index g. From there, we split out the fraction, $\chi_g$, that appear in group g.

Recall that the cross sections and flux can vary greatly as a function of neutron energy, E. Figure 6 shows an illustrative 5 group approximation. So we will have to use some average flux and cross section that have been averaged over the property in the group energy range in question.

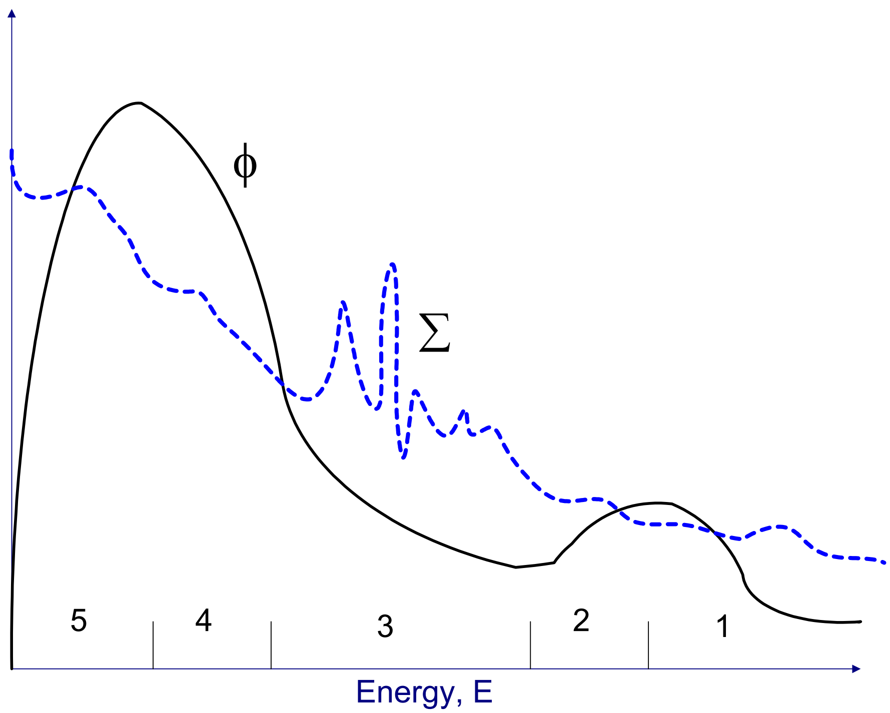


**Figure 6 Illustrative flux and cross section variation with energy.**

We'll see how to do this soon but for now, we want to concentrate on each of the terms in equation 3.2 to make sure you understand what each term represents in a physical sense.

The fission terms are:

$$\underbrace{\sum_{g'=1}^{G} \nu_{g'} \Sigma_{f\,g'}(\mathbf{r})\phi_{g'}(\underline{r},t)}_{\text{total fission production}} = \underbrace{\nu_5 \Sigma_{f\,5}\,\phi_5 + \nu_4 \Sigma_{f\,4}\,\phi_4}_{\text{thermal fissions (about 97\%)}} + \underbrace{\nu_3 \Sigma_{f\,3}\,\phi_3 + \nu_2 \Sigma_{f\,2}\,\phi_2 + \nu_1 \Sigma_{f\,1}\,\phi_1}_{\text{fast fissions (about 3\%)}} \quad (3.3)$$

These fission neutrons, arising mostly from the fissions that are induced by thermal neutrons, have energies in the MeV range, for the most part. Figure 7, illustrates this.

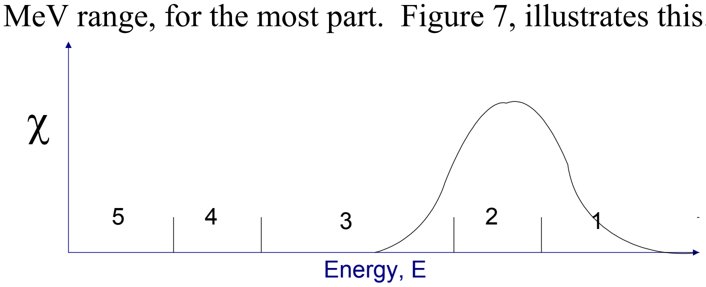


**Figure 7 Fission neutron energy spectrum.**

So, for the illustrated 5 group example, $\chi_5 = \chi_4 = 0$ , and the other $\chi$ 's are non-zero. So, for the thermal groups (ie groups 5 and 4), there are no fission source neutrons. The summation term contains contributions from all 5 fission terms but the biggest contributors are from the thermal group. This sum of fission neutrons will only show up as sources for groups 1, 2 and 3.

**Now would be a good time to look back at the governing equations and write them out for the 5 group case. It is important that you get it right.**

Now, let's look at the scattering terms. These are new. They add complexity but, taken step by step, they are not that hard to understand. In previous chapters, which assumed mono-energetic neutrons, we did not have to consider the loss and gain of neutrons by the scattering process because when a scattering event occurs, the neutron is simply deflected. It is not absorbed, hence it there is no gain or loss of neutrons **in total** because of scattering. But, now that we have subdivided the neutrons up into groups, the scattered neutrons emerge from the scattering process at some energy different, in all likelihood, from the incident energy.

The scattering removal term in equation 3.2 is straightforward. It says that all the neutrons in group g scatter to some other energy and, so, disappear from the g$^{th}$ neutron balance equation. Some of the scattered neutrons will emerge with a new energy that is within the range of the energies represented by group g. So we have to add those back in. We'll do that via the scattering 'in term', discussed next.

The 'scattering in' term is

$$\sum_{g'=1}^{G} \Sigma_{sg'g}(r)\phi_{g'}(\underline{r},t) = \Sigma_{s1g}\phi_1 + \Sigma_{s2g}\phi_2 + \Sigma_{s3g}\phi_3 + \Sigma_{s4g}\phi_4 + \Sigma_{s5g}\phi_5 \tag{3.4}$$

that is, neutrons are scattered into group g from all the 5 groups. Note that we have a term representing scattering from group g to group g, ie the ones that stay in the group even after scatter. This effectively adds back in the neutrons that were erroneously subtracted by the scattering removal term of the previous paragraph. Figure 8 illustrates the process.

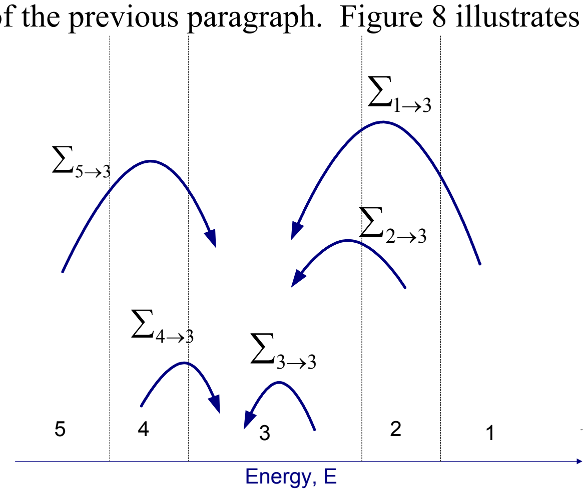


**Figure 8 Scattering into group 3.**

Of course, the total scattering out of group 3 is just the sum total of all the scattering out processes, ie:

$$\Sigma_{s3}\phi_3 = \Sigma_{s31}\phi_3 + \Sigma_{s32}\phi_3 + \Sigma_{s33}\phi_3 + \Sigma_{s34}\phi_3 + \Sigma_{s35}\phi_3 = \left(\sum_{g'=1}^{G}\Sigma_{s3g'}(r)\right)\phi_3\left(\underline{r},t\right) \tag{3.5}$$

or for the general group g:

$$\Sigma_{sg}\phi_g = \Sigma_{sg1}\phi_g + \Sigma_{sg2}\phi_g + \Sigma_{sg3}\phi_g + \Sigma_{sg4}\phi_g + \Sigma_{sg5}\phi_g = \left(\sum_{g'=1}^{G}\Sigma_{sgg'}(r)\right)\phi_g\left(\underline{r},t\right) \tag{3.6}$$

This is illustrated in figure 9.

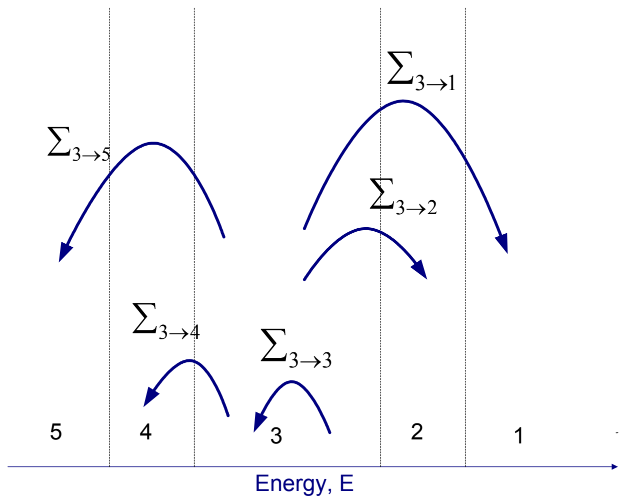


**Figure 9 Scattering out of group 3.**

So we can plug equations 3.4 and 3.6 into 3.2 using group 3 as an example to get:

$$\begin{aligned}\frac{1}{v_3}\frac{\partial}{\partial t}\phi_3\left(\underline{r},t\right) = \; & \underbrace{\nabla\cdot D_3\;(r)\nabla\phi_3\left(\underline{r},t\right)}_{\text{leakage}} - \underbrace{\Sigma_{a3}(r)\phi_3\left(\underline{r},t\right)}_{\text{loss by absorption}} \\ & -\underbrace{\left(\Sigma_{s31}\phi_3 + \Sigma_{s32}\phi_3 + \cancel{\Sigma_{s33}\phi_3} + \Sigma_{s34}\phi_3 + \Sigma_{s35}\phi_3\right)}_{\text{scattering out}} \\ & +\underbrace{\left(\Sigma_{s13}\phi_1 + \Sigma_{s23}\phi_2 + \cancel{\Sigma_{s33}\phi_3} + \Sigma_{s43}\phi_4 + \Sigma_{s53}\phi_5\right)}_{\text{scattering in}} \\ & + \underbrace{\chi_3}_{\text{fraction appearing in group g}} \underbrace{\sum_{g'=1}^{G}\nu_{g'}\Sigma_{fg'}(\mathbf{r})\phi_{g'}\left(\underline{r},t\right)}_{\text{total fission production}} \underbrace{+S_3^{ext}}_{\text{external source}}\end{aligned} \tag{3.7}$$

Notice how the ‘in group’ scattering terms cancel.

Just to confuse matters a bit more, the **removal cross section** is often used. It is defined as, for group 3:

$$\Sigma_{r3} \equiv \Sigma_{a3} + \Sigma_{s3} - \Sigma_{s33} = \Sigma_{a3} + \Sigma_{s31} + \Sigma_{s32} + \Sigma_{s34} + \Sigma_{s35} = \Sigma_{a3} + \sum_{\substack{g'=1 \\ g'\neq 3}}^{G} \Sigma_{s3g'}(r) \tag{3.8}$$

ie, it is the net removal of neutrons from group 3 by scattering and absorption. If we use this definition, the governing equation becomes:

$$\frac{1}{v_g}\frac{\partial}{\partial t}\phi_g(\underline{r},t) = \underbrace{\nabla\cdot D_g(r)\nabla\phi_g(\underline{r},t)}_{\text{leakage}} - \underbrace{\Sigma_{rg}(r)\phi_g(\underline{r},t)}_{\text{removal}} - \underbrace{\Sigma_{sgg}(r)\phi_g(\underline{r},t)}_{\substack{\text{in-group} \\ \text{scattering}}} + \underbrace{\sum_{g'=1}^{G}\Sigma_{sg'g}(r)\phi_{g'}(\underline{r},t)}_{\text{scattering into group g}}$$
$$+ \underbrace{\chi_g}_{\substack{\text{fraction} \\ \text{appearing} \\ \text{in group g}}} \underbrace{\sum_{g'=1}^{G} \nu_{g'}\Sigma_{fg'}(\mathbf{r})\phi_{g'}(\underline{r},t)}_{\substack{\text{total fission} \\ \text{production}}} \underbrace{+S_g^{ext}}_{\text{external source}} \tag{3.9}$$

or, more simply,

$$\frac{1}{v_g}\frac{\partial}{\partial t}\phi_g(\underline{r},t) = \underbrace{\nabla\cdot D_g(r)\nabla\phi_g(\underline{r},t)}_{\text{leakage}} - \underbrace{\Sigma_{rg}(r)\phi_g(\underline{r},t)}_{\text{removal}} + \underbrace{\sum_{\substack{g'=1 \\ g'\neq g}}^{G}\Sigma_{sg'g}(r)\phi_{g'}(\underline{r},t)}_{\text{net scattering into group g}}$$
$$+ \underbrace{\chi_g}_{\substack{\text{fraction} \\ \text{appearing} \\ \text{in group g}}} \underbrace{\sum_{g'=1}^{G} \nu_{g'}\Sigma_{fg'}(\mathbf{r})\phi_{g'}(\underline{r},t)}_{\substack{\text{total fission} \\ \text{production}}} \underbrace{+S_g^{ext}}_{\text{external source}} \tag{3.10}$$

Personally, I find the use of the removal form to be un-necessarily confusing. I prefer to jut remember equation 3.2. Everything else discussed above flows readily from that equation. There is no need to memorize any of this. If you take the time to visualize the processes that are occurring, then you should be able to state equation 3.2 as you go through the accounting of the sinks and sources of neutrons. **Try it! Don't be afraid to spend some time making sure that you have it clear in your mind. It is a milestone concept in reactor physics and the subject won't make sense unless you grasp it.**

# 4 Generating the Coefficients

The raw cross section data is available in libraries like ENDF/B in the public domain. This data gives the experimental values as a function of energy in far too much detail for our multigroup model. We need to come up with good estimates of the group-averaged cross sections. To do that we step back and use the more general form of the neutron diffusion equation, one that has energy represented as a continuum, rather than as discrete bins:

$$\frac{1}{v}\frac{\partial \phi}{\partial t} = \underbrace{\nabla \cdot D(r)\nabla\phi}_{\text{leakage}} - \underbrace{\Sigma_a(r)\phi}_{\substack{\text{loss by}\\ \text{absorption}}} - \underbrace{\Sigma_s(r)\phi}_{\substack{\text{removal by}\\ \text{scattering}}} + \underbrace{\int_0^\infty \Sigma_s(E'\to E)\phi(\underline{r},E',t)\,dE'}_{\text{scattering into } E\to E+dE \text{ range}}$$

$$+ \underbrace{\chi(E)}_{\substack{\text{fraction}\\ \text{appearing}\\ E\to E+dE\\ \text{range}}} \underbrace{\int_0^\infty \nu(E')\Sigma_f(E')\phi(\underline{r},E',t)}_{\substack{\text{total fission}\\ \text{production}}} \underbrace{+S^{ext}}_{\text{external source}} \tag{4.1}$$

$$\text{Note}: \phi = \phi(\underline{r},E,t)$$

The term $\Sigma_s(E'\to E)dE'$ is the cross section for neutrons at energy E' scattering to energy E. Note that $\Sigma_s(E'\to E)dE'$ has units of $cm^{-1}$ so $\Sigma_s(E'\to E)$ as units of $cm^{-1}$ $ev^{-1}$.

We define the group flux as:

$$\phi_g(\underline{r},t) \equiv \int_{E_g}^{E_{g-1}} \phi(\underline{r},E,t)\,dE \tag{4.2}$$

This prompts us to perform the same integral for each term of equation 4.1 and to equate what we get to equation 3.2 to generate a rigorous definition of the group-averaged cross sections. Thus equation 4.1 becomes, term by term:

$$\frac{\partial}{\partial t}\left(\int_{E_g}^{E_{g-1}} \frac{1}{v(E)}\phi(\underline{r},E,t)\,dE\right) \equiv \frac{\partial}{\partial t}\left(\frac{\phi_g}{v_g}\right) = \frac{1}{v_g}\frac{\partial \phi_g}{\partial t}$$

$$\text{where } \frac{1}{v_g} \equiv \frac{\displaystyle\int_{E_g}^{E_{g-1}} \frac{1}{v(E)}\phi(\underline{r},E,t)\,dE}{\displaystyle\int_{E_g}^{E_{g-1}} \phi(\underline{r},E,t)\,dE} \tag{4.3}$$

Notice how the coefficient, $1/v_g$, is determined simply as the flux weighted integral over the group energy range. As we go through the integral term by term, we will see the same pattern.

Now for the diffusion coefficient:

$$\nabla\bullet\left(\int_{E_g}^{E_{g-1}} D(E)\nabla\phi(\underline{r},E,t)\,dE\right)\equiv\nabla\bullet D_g\nabla\phi_g$$

$$\text{ie. } D_g\equiv\frac{\int_{E_g}^{E_{g-1}} D(E)\nabla\phi(\underline{r},E,t)\,dE}{\int_{E_g}^{E_{g-1}}\nabla\phi(\underline{r},E,t)\,dE}\tag{4.4}$$

This time, the weighting is $\nabla\phi$ since that is how the flux factor appears in the term.

The absorption term is just:

$$\int_{E_g}^{E_{g-1}}\Sigma_a(E)\phi(\underline{r},E,t)\,dE\equiv\Sigma_{a\,g}\,\phi_g$$

$$\text{ie. } \Sigma_{a\,g}\equiv\frac{\int_{E_g}^{E_{g-1}}\Sigma_a(E)\phi(\underline{r},E,t)\,dE}{\int_{E_g}^{E_{g-1}}\phi(\underline{r},E,t)\,dE}\tag{4.5}$$

The scattering removal term is similar.

The scattering down term is a bit messier:

$$\begin{aligned}\int_{E_g}^{E_{g-1}}\left(\int_0^{\infty}\Sigma_s(E'\to E)\phi(\underline{r},E',t)\,dE'\right)dE&=\int_{E_g}^{E_{g-1}}\left(\sum_{g'=1}^{G}\int_{E_{g'}}^{E_{g'-1}}\Sigma_s(E'\to E)\phi(\underline{r},E',t)\,dE'\right)dE\\&=\sum_{g'=1}^{G}\int_{E_g}^{E_{g-1}}\left(\int_{E_{g'}}^{E_{g'-1}}\Sigma_s(E'\to E)\phi(\underline{r},E',t)\,dE'\right)dE\qquad(4.6)\\&\equiv\sum_{g'=1}^{G}\Sigma_{s\,g'g}\,\phi_{g'}\end{aligned}$$

So we have:

$$\Sigma_{s\,g'g}=\frac{1}{\phi_{g'}}\int_{E_g}^{E_{g-1}}\left(\int_{E_{g'}}^{E_{g'-1}}\Sigma_s(E'\to E)\phi(\underline{r},E',t)\,dE'\right)dE\tag{4.7}$$

The fission term is:

$$
\begin{aligned}
\int_{E_g}^{E_{g-1}} \chi(E) \int_0^{\infty} \nu(E')\Sigma_f(E')\phi(\underline{r},E',t)\,dE'\,dE &= \int_{E_g}^{E_{g-1}} \chi(E)dE \int_0^{\infty} \nu(E')\Sigma_f(E')\phi(\underline{r},E',t)\,dE' = \\
&= \chi_g \int_0^{\infty} \nu(E')\Sigma_f(E')\phi(\underline{r},E',t)\,dE' \text{ where } \chi_g \equiv \int_{E_g}^{E_{g-1}} \chi(E)\,dE \\
&= \chi_g \sum_{g'=1}^{G} \int_{E_g}^{E_{g-1}} \nu(E')\Sigma_f(E')\phi(\underline{r},E',t)\,dE' \\
&\equiv \chi_g \sum_{g'=1}^{G} \nu_{g'}\Sigma_{f\,g'}\phi_{g'}
\end{aligned}
\tag{4.8}
$$

Dropping the summation, we finally arrive at:

$$
\begin{aligned}
\nu_{g'}\Sigma_{f\,g'} &\equiv \frac{1}{\phi_{g'}} \int_{E_g}^{E_{g-1}} \nu(E')\Sigma_f(E')\phi(\underline{r},E',t)\,dE' \\
\chi_g &= \int_{E_g}^{E_{g-1}} \chi(E)\,dE
\end{aligned}
\tag{4.9}
$$

The accuracy of the multigroup model depends very much on the group constants chosen.

Note that the constants depend on $\phi$ which depends on the constants. This is a circular argument. To compensate, the typical practice is to follow a scheme as outlined in figure 10.

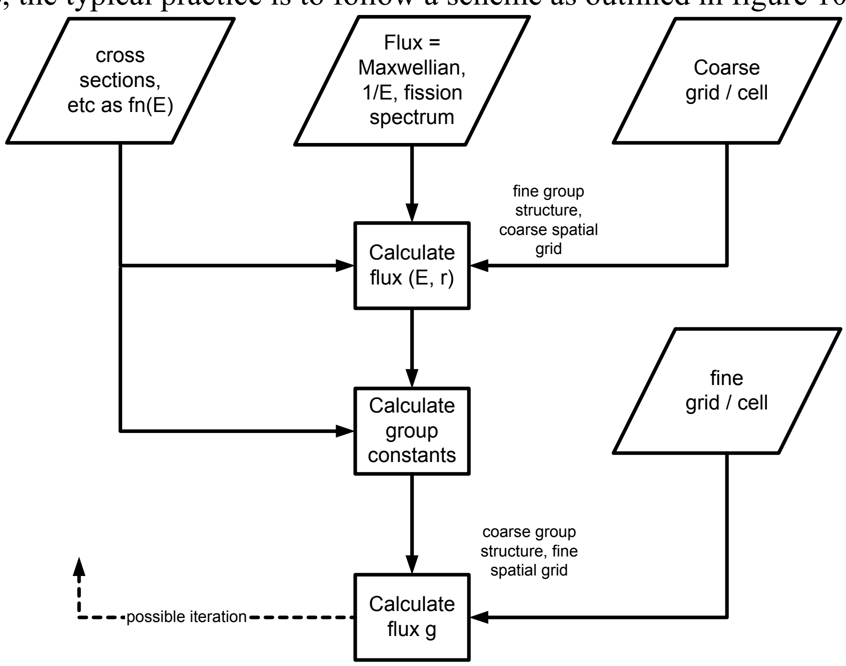


**Figure 10 Typical calculation scheme.**

A fine energy structure (many groups, perhaps of the order of 100 or more) is assumed by taking the flux as Maxwellian in the thermal range, 1/E in the mid-range and a fission spectrum for the high end. A coarse spatial grid is assumed or a small representative region is chosen (usually a representative cell). The multigroup equations can then be solved numerically (high G, small number of spatial mesh points). This yields $\phi_g$ for the cell, g =1, 100 (say). This flus can be used to calculate weighted cross sections and other constants for a coarse energy structure, perhaps G=5 or so. Now, with a manageable number of neutron equations per spatial mesh point, the whole core (or a typical cell) can be numerically solved with a large number of spatial mesh points, giving good spatial detail, albeit with a coarse energy resolution. Once these calculations are done, there is the possibility that a re-weighting of the group constants might have to be done to account for flux dependent effects like Xe, burnup, temperature, control rod position, etc. So, iteration might be required.

We could use the same basic equation (ie equation 3.2) for both the fine energy calculation and the fine spatial mesh calculation. The more typical route, however, is to <u>not</u> use diffusion based calculation for the fine energy mesh / cell calculation because diffusion theory is not accurate near interfaces that involve large changes in cross sections (like water / control rod interfaces, for instance). Rather, a transport-based code such as WIMS is used. The fine spatial mesh / core calculations typically <u>do</u> use the diffusion approximation propped up by the group-averaged coefficients based on transport calculations. Herein, we will assume that the proper flux weighted coefficients have been found and we explore some simplifications and criticality calculations.

# 5 Simplifications

Most neutrons lose energy when they scatter. Only the low energy thermal neutrons experience any significant upscatter (that's what the Maxwellian is all about, after all). So it is a reasonable approximation to assume that all groups do not upscatter if the thermal breakpoint is kept above ~1 eV. That will keep the thermal upscatter restricted to itself. Thus:

$$\Sigma_{sg'g} \approx 0 \text{ for } g'>g \quad \textbf{no upscatter assumption} \tag{5.1}$$

This simplifies the group in-scattering term:

$$\underbrace{\sum_{g'=1}^{G} \Sigma_{sg'g}(r)\phi_{g'}(\underline{r},t)}_{\text{scattering into group g}} \rightarrow \sum_{g'=1}^{g-1} \Sigma_{sg'g}(r)\phi_{g'}(\underline{r},t) + \underbrace{\Sigma_{sgg}(r)\phi_g(\underline{r},t)}_{\substack{\text{can lump this into} \\ \text{the removal term}}} \tag{5.2}$$

We can also sometimes assume that scattering down is to the next lowest group only, ie no groups are skipped when scattering down. Thus:

$$\underbrace{\sum_{g'=1}^{G} \Sigma_{sg'g}(r)\phi_{g'}(\underline{r},t)}_{\text{scattering into group g}} \rightarrow \Sigma_{sg-1g}(r)\phi_{g-1}(\underline{r},t) + \Sigma_{sgg}(r)\phi_g(\underline{r},t) \tag{5.3}$$

This is called **"directly coupled"**.

Recall that in a scattering event:

$$E_f = \alpha E_i, \qquad \alpha \equiv \left(\frac{A-1}{A+1}\right)^2 \tag{5.4}$$

Therefore, if we maintain a group separation such that

$$\frac{E_g}{E_{g-1}} \le \alpha \tag{5.5}$$

then the scattered neutron cannot have a final energy that is below the next group down. For hydrogen, which has A=1, there is a problem because $\alpha$=0. But it can be shown that, even then, the error is < 1% if $E_g/E_{g-1}$ < 1/150.

# 6 Criticality

The criticality calculation follows the same itinerary as the one speed neutron case except that we now have to sweep through the energy groups as well as through space. The basic steady state equation to solve is (assuming no up-scatter):

$$-\nabla \cdot D_g(r)\nabla\phi_g(\underline{r},t) + \underbrace{\Sigma_{rg}(r)\phi_g(\underline{r},t)}_{\text{removal}} - \sum_{g'=1}^{G}\Sigma_{sg'g}(r)\phi_{g'}(\underline{r},t) = \frac{1}{k}\chi_g \sum_{g'=1,g\neq g}^{G} \nu_{g'}\Sigma_{fg'}(\mathbf{r})\phi_{g'}(\underline{r},t) \tag{6.1}$$

Note that $\Sigma_{rg} = \Sigma_{tg} - \Sigma_{sgg} = \Sigma_{ag} + \Sigma_{sg} - \Sigma_{sgg}$. We can write this in a matrix form:

$$M\phi = \frac{1}{k}F\phi \tag{6.2}$$

where

$$\underline{\underline{M}} = \begin{pmatrix} -\nabla\bullet D_1\nabla + \Sigma_{r1} & 0 & 0 & \cdots \\ -\Sigma_{S12} & -\nabla\bullet D_2\nabla + \Sigma_{r2} & 0 & \\ -\Sigma_{S13} & & -\nabla\bullet D_3\nabla + \Sigma_{r3} & \\ \vdots & \vdots & \vdots & \end{pmatrix} \tag{6.3}$$

$$\underline{\phi} = \begin{bmatrix} \phi_1 \\ \phi_2 \\ \phi_3 \\ \vdots \end{bmatrix} \tag{6.4}$$

$$\underline{\underline{F}} = \begin{pmatrix} \chi_1\nu_1\Sigma_{f1} & \chi_1\nu_2\Sigma_{f2} & \chi_1\nu_3\Sigma_{f3} & \cdots \\ \chi_2\nu_1\Sigma_{f1} & \chi_2\nu_2\Sigma_{f2} & \chi_2\nu_3\Sigma_{f3} & \\ \chi_3\nu_1\Sigma_{f1} & \chi_3\nu_2\Sigma_{f2} & \chi_3\nu_3\Sigma_{f3} & \\ \vdots & \vdots & \vdots & \end{pmatrix} \tag{6.5}$$

Please note that the span is over the groups, not space. Imbedded in the diffusion term is the space mesh. Two dimensional paper cannot do justice to the complexity of the structure in matrix form. With the assumption of no up-scatter, the M matrix is lower triangular. If we further assume that the neutrons are directly coupled, M would be 2-striped, ie:

$$M = \underbrace{\begin{bmatrix} x & & & \\ x & x & & \\ x & x & x & \\ x & x & x & x \end{bmatrix}}_{\text{no up-scatter}} = \underbrace{\begin{bmatrix} x & & & \\ x & x & & \\ & x & x & \\ & & x & x \end{bmatrix}}_{\text{directly coupled}} \tag{6.6}$$

Solution, numerically, proceeds are for the one speed case. The right hand side (RHS) of equation 6.2 is evaluated from a guess at the flux in space and energy. The RHS is the source term. The flux is found using Gauss-Seidel or SOR to complete the inner iteration for the first iteration. Typically, the spatial grip is swept sequentially, starting with the equation for group 1, then 2, …G since the faster neutrons are essentially the source terms for the slower neutrons, but I suspect that it really doesn't matter what order the equations are swept.

Next, the source terms and k are updated and the iteration is repeated until both k and the flux have converged. It is a straightforward procedure; just be careful to properly account for all the scattering terms.

# 7 Group Collapsing

Herein we will collapse the multigroup equations to 1 group just to show that the two forms are consistent with each other. Then we will look at the 2 group approximation because it is commonly used and it is illustrative without being overly complex.

## 7.1 Multigroup → One-Group

We have the general multigroup equation:

$$\frac{1}{v_g}\frac{\partial}{\partial t}\phi_g = \nabla\cdot D_g\nabla\phi_g - \Sigma_{ag}\phi_g - \Sigma_{sg}\phi_g + \sum_{g'=1}^{G}\Sigma_{sg'g}\phi_{g'} + \chi_g\sum_{g'=1}^{G}\nu_{g'}\Sigma_{fg'}\phi_{g'} + S_g^{ext} \tag{7.1}$$

And we had the definitions of the coefficients:

$$\phi_g(\underline{r},t) \equiv \int_{E_g}^{E_{g-1}} \phi(\underline{r},E,t)\,dE \Rightarrow \phi(\underline{r},t) \equiv \int_0^\infty \phi(\underline{r},E,t)\,dE \tag{7.2}$$

$$\frac{1}{v_g} \equiv \frac{\int_{E_g}^{E_{g-1}} \frac{1}{v(E)}\phi(\underline{r},E,t)\,dE}{\int_{E_g}^{E_{g-1}} \phi(\underline{r},E,t)\,dE} \Rightarrow \frac{1}{v} \equiv \frac{\int_0^\infty \frac{1}{v(E)}\phi(\underline{r},E,t)\,dE}{\int_0^\infty \phi(\underline{r},E,t)\,dE} \text{ for one group} \tag{7.3}$$

$$\text{ie. } D_g \equiv \frac{\int_{E_g}^{E_{g-1}} D(E)\nabla\phi(\underline{r},E,t)\,dE}{\int_{E_g}^{E_{g-1}} \nabla\phi(\underline{r},E,t)\,dE} \Rightarrow D \equiv \frac{\int_0^\infty D(E)\nabla\phi(\underline{r},E,t)\,dE}{\int_0^\infty \nabla\phi(\underline{r},E,t)\,dE} \tag{7.4}$$

$$\Sigma_{a\,g} \equiv \frac{\int_{E_g}^{E_{g-1}} \Sigma_a(E)\phi(\underline{r},E,t)\,dE}{\int_{E_g}^{E_{g-1}} \phi(\underline{r},E,t)\,dE} \Rightarrow \Sigma_a \equiv \frac{\int_0^\infty \Sigma_a(E)\phi(\underline{r},E,t)\,dE}{\int_0^\infty \phi(\underline{r},E,t)\,dE} \tag{7.5}$$

The scattering terms are:

$$-\Sigma_{s\,g}\,\phi_g + \sum_{g'=1}^{G} \Sigma_{s\,g'g}(r)\phi_{g'}(\underline{r},t) \to -\Sigma_s\,\phi_g + \Sigma_s\,\phi = 0 \text{ when } G=1 \tag{7.6}$$

The fission term is:

$$\begin{gathered}\chi_g \equiv \int_{E_g}^{E_{g-1}} \chi(E)\,dE \Rightarrow \chi \equiv \int_0^\infty \chi(E)\,dE = 1, \\ \sum_{g'=1}^{G} \nu_{g'}\,\Sigma_{f\,g'}\,\phi_{g'} \Rightarrow \nu\,\Sigma_f\,\phi\end{gathered} \tag{7.7}$$

Putting all these terms together, we get back the one-group equation:

$$\frac{1}{v}\frac{\partial}{\partial t}\phi(\underline{r},t) = \nabla\bullet D(r)\nabla\phi(\underline{r},t) - \Sigma_a(r)\phi(\underline{r},t) + \nu\Sigma_f\,\phi(\underline{r},t) \tag{7.8}$$

## 7.2 Multigroup → Two-Group

The two-group approximation is a common and illustrative one. We divide the neutrons into a thermal group and a fast group with the division at 1 eV, as shown in figure 11.

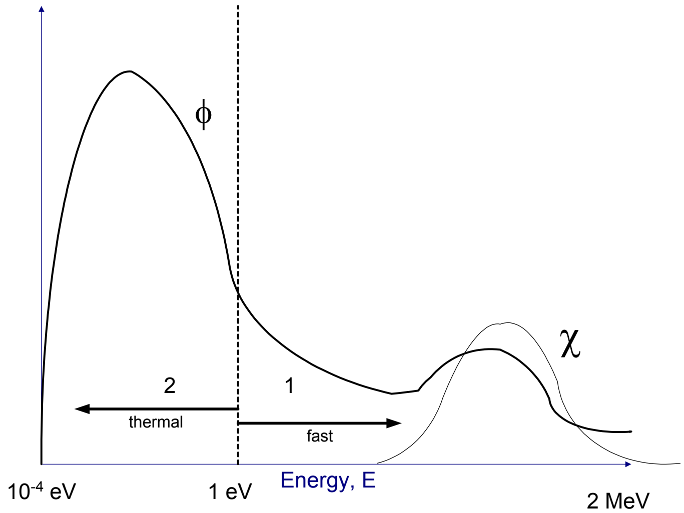


**Figure 11 Two-group approximation.**

Note that

$$\chi_2 = \int_0^{1\text{eV}} \chi(E)dE = 0 \text{ and } \chi_1 = 1 \tag{7.9}$$

Thus the general fission source term

$$S_g = \underbrace{\chi_g}_{\substack{\text{fraction}\\ \text{appearing}\\ \text{in group g}}} \underbrace{\sum_{g'=1}^{G} \nu_{g'} \Sigma_{f\,g'}(\mathbf{r})\phi_{g'}(\underline{r},t)}_{\substack{\text{total fission}\\ \text{production}}} \tag{7.10}$$

for the simple two-group case is:

$$\begin{aligned} S_1 &= \nu_1 \Sigma_{f1} \phi_1 + \nu_2 \Sigma_{f2} \phi_2 \\ S_2 &= 0 \end{aligned} \tag{7.11}$$

There is no up-scattering so:

$$\Sigma_{s21} = 0 \Rightarrow \Sigma_{s2} = \Sigma_{s21} + \Sigma_{s22} \Rightarrow \Sigma_{s2} = \Sigma_{s22} \tag{7.12}$$

Therefore

$$\Sigma_{r2} = \Sigma_{t2} - \Sigma_{s22} = \Sigma_{a2} \tag{7.13}$$

Thus the two-group equations are:

$$\begin{aligned} \frac{1}{v_1}\frac{\partial \phi_1}{\partial t} &= \nabla \cdot D_1 \nabla \phi_1 - \Sigma_{r1}\phi_1 + \nu_1 \Sigma_{f1}\phi_1 + \nu_2 \Sigma_{f2}\phi_2 \quad \text{no up-scatter} \\ \frac{1}{v_2}\frac{\partial \phi_2}{\partial t} &= \nabla \cdot D_2 \nabla \phi_2 - \Sigma_{a2}\phi_2 + \Sigma_{s12}\phi_1 \quad \text{no direct fission source} \end{aligned} \tag{7.14}$$

In steady state, adding the k fudge factor we have:

$$\begin{aligned} -\nabla \cdot D_1 \nabla \phi_1 + \Sigma_{r1}\phi_1 &= \frac{1}{k}\left[\nu_1 \Sigma_{f1}\phi_1 + \nu_2 \Sigma_{f2}\phi_2\right] \quad \text{no up-scatter} \\ -\nabla \cdot D_2 \nabla \phi_2 + \Sigma_{a2}\phi_2 &= \Sigma_{s12}\phi_1 \quad \text{no direct fission source} \end{aligned} \tag{7.15}$$

Notice how the fast flux is the source term for the thermal neutrons (by scattering down in energy), while the thermal flux is the source for the fast neutrons by the fission event. This is illustrated in figure 12.

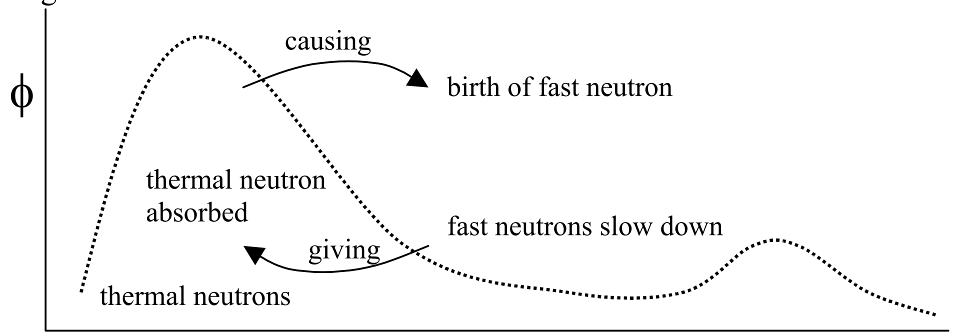


**Figure 12 Thermal - fast exchange.**

So, it follows that you would expect to see an abundance, or peak of fast neutrons in the fuel region (because that is where the fissions take place). They diffuse to the moderator where there is a high probability of slowing down (because of the materials used there for just that purpose). Hence you would expect to see a peak of thermal neutrons in the moderator. This is illustrated in figure 13.

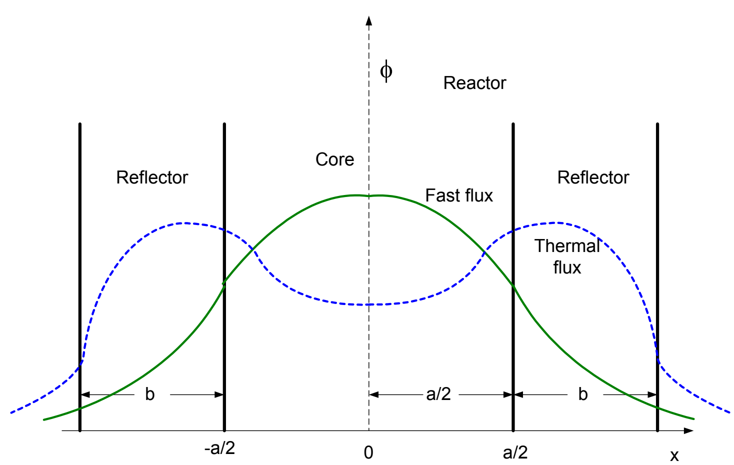


**Figure 13 Spatial distribution of flux.**

Thus the fast and thermal neutrons not only have a vastly different energy distribution, they have different spatial distributions in general.

## 7.3 Two-Group Criticality

We consider the case of a bare (ie, un-reflected) reactor so that we can develop the criticality condition for the two-group case and compare it to the one-speed case developed earlier. Because the moderator and fuel are mixed together, the thermalization and fission processes are not physically separated. We can expect that both the fast and the thermal fluxes will have the same fundamental cosine shape for a simple slab reactor. The basic equations are:

$$\begin{aligned} -\nabla \cdot D_1 \nabla \phi_1 + \Sigma_{r1}\phi_1 &= \frac{1}{k}\left[\nu_1 \Sigma_{f1}\phi_1 + \nu_2 \Sigma_{f2}\phi_2\right] \\ -\nabla \cdot D_2 \nabla \phi_2 + \Sigma_{a2}\phi_2 &= \Sigma_{s12}\phi_1 \end{aligned} \tag{7.16}$$

We write the flux as a product of an amplitude factor and a shape factor:

$$\phi_1(\underline{r}) = \varphi_1 \psi(\underline{r}),\ \ \phi_2(\underline{r}) = \varphi_2 \psi(\underline{r}) \tag{7.17}$$

Defining the buckling as usual:

$$\nabla^2 \psi(\underline{r}) + B^2 \psi(\underline{r}) = 0 \tag{7.18}$$

we find that equation 7.17 becomes:

$$\begin{aligned} +D_1 B^2 \varphi_1 + \Sigma_{r1}\varphi_1 &= \frac{1}{k}\left[\nu_1 \Sigma_{f1}\varphi_1 + \nu_2 \Sigma_{f2}\varphi_2\right] \\ +D_2 B^2 \varphi_2 + \Sigma_{a2}\varphi_2 &= \Sigma_{s12}\varphi_1 \end{aligned} \tag{7.19}$$

or in matrix form:

$$\begin{bmatrix} \left(D_1 B^2 + \Sigma_{r1} - \dfrac{\nu_1 \Sigma_{f1}}{k}\right) & -\dfrac{\nu_2 \Sigma_{f2}}{k} \\ -\Sigma_{s12} & \left(D_2 B^2 + \Sigma_{a2}\right) \end{bmatrix} \begin{bmatrix} \varphi_1 \\ \varphi_2 \end{bmatrix} = 0 \tag{7.20}$$

ie:

$$\underline{\underline{A}}\,\underline{\varphi} = 0 \tag{7.21}$$

which has a non-trivial solution for the flux amplitudes only if:

$$\left|\underline{\underline{A}}\right| = 0 \tag{7.22}$$

Thus:

$$\left(D_1 B^2 + \Sigma_{r1} - \frac{\nu_1 \Sigma_{f1}}{k}\right)\left(D_2 B^2 + \Sigma_{a2}\right) - \frac{\nu_2 \Sigma_{f2} \Sigma_{s12}}{k} = 0 \tag{7.23}$$

Solving for k:

$$
\begin{aligned}
k &= \underbrace{\frac{\nu_1 \Sigma_{f1}}{\Sigma_{r1} + D_1 B^2}}_{\text{fast fission}} + \frac{\Sigma_{s12}}{\left(\Sigma_{r1} + D_1 B^2\right)} \frac{\nu_2 \Sigma_{f2}}{\left(\Sigma_{a2} + D_2 B^2\right)} \\
&= 1 \text{ at criticality}
\end{aligned}
\tag{7.24}
$$

The first term on the R.H.S. is the fast fission contribution. We can lump it into the second term via , , the fast fission factor and recognize that:

- The resonance escape probability is just the ratio of the number of neutrons that successfully scatter down to group 2 over the number that leave group 1.
- Likewise $\eta f$ is just the ratio of neutrons born to the number of thermals absorbed.

Thus we can reconstruct the four factor formula, with additional factors for fast and thermal leakage:

$$
\begin{aligned}
k &= \frac{,\Sigma_{s12}}{\left(\Sigma_{r1} + D_1 B^2\right)} \frac{\nu_2 \Sigma_{f2}}{\left(\Sigma_{a2} + D_2 B^2\right)} \\
&= \frac{,\ \Sigma_{s12} / \Sigma_{r1}}{\left(1 + L_1^2 B^2\right)} \frac{\nu_2\ \Sigma_{f2} / \Sigma_{a2}}{\left(1 + L_2^2 B^2\right)} = \frac{,p}{\left(1 + L_1^2 B^2\right)} \frac{\eta f}{\left(1 + L_2^2 B^2\right)} \\
&= ,p\eta f\, P_{NL1}\, P_{NL2}
\end{aligned}
\tag{7.25}
$$

(Recall that $L^2 \equiv D / \Sigma_a$ .)

# 8 Concluding Remarks

In this chapter we have seen the multigroup formalism that sees extensive use in the nuclear industry. Numerical solutions follow the same procedures as developed for the one-speed case and will be left to a separate chapter.

# About this document:

back to page 1

**Author and affiliation:** Wm. J. Garland, Professor, Department of Engineering Physics, McMaster University, Hamilton, Ontario, Canada

**Revision history:**
Revision 1.0, 2002.07.4, initial creation from hand written notes.
Revision 1.1, 2004.08.17, minor typos.
Revision 1.2, 2005.07.13, minor typos.

Source document archive location: See page footer.

Contact person: Wm. J. Garland

**Notes:**