# CHAPTER 3 MULTIGROUP METHOD AND CRITICALITY CALCULATION

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Presume that one wishes to sustain a stable fission chain reaction and thereby reach a steady rate of fission energy production. Therefore, one must design a nuclear reactor in such a way that the rates of neutron absorption and leakage are compensated by the rate of fission neutron production. In this chapter, the multigroup method will be introduced to simplify and reduce the general transport equation into the multigroup equations. Then, readers will be presented with the most vital calculation in reactor physics, that is, the criticality calculation. At this point, the criticality calculation of a nuclear system will allow us to evaluate the stability of the fission chain reaction. At the end of this chapter, the alternative form of the time-independent multigroup diffusion equations will be established. Also, these equations form a matrix expression which is known as the k-eigenvalue equation and it will be used to accomplish a criticality calculation. Briefly, a criticality calculation at first gathers all parameters related to the reactor design, nuclear fuel properties and the reactor core configuration. At the end of the calculation, nuclear engineers will be able to quantitatively estimate the stability of the reactor using the multiplication factor, k.

## 3.1 Interaction Probability

Consider a monodirectional and monoenergetic neutron beam with energy E is targeted along the direction  $\hat{\Omega}$  towards a material of thickness R, with an initial beam flux magnitude  $\phi_0$ . Also, the region outside the material is considered vacuum, and a neutron detector is placed at some distance behind the material. Hence, every neutron

that interacts in the material is lost from the beam and leaving only neutrons that do not interact to reach the detector.



Figure 3.1: Measurement of neutrons that have not interacted with the target.

At this instance, it is convenient to define  $\phi(r)$  as the flux of the neutron beam after penetrating the distance r into the material. After travelling at an additional distance dr, the decrease of the flux is given by,

$$-d\phi(r) = \Sigma_{\rm t}(r) \,\phi(r) \,dr \tag{3.1}$$

Assuming that the target material is homogeneous, and henceforth, the total neutron cross section is constant at all locations within the material,

$$-d\phi(r) = \Sigma_{\rm t} \phi(r) \, dr \tag{3.2}$$

The probability of neutrons that will subsequently interact in the next additional distance dr after penetrating the material at the distance r is given by  $P_1$ ,

$$P_1(r) = \frac{d\phi(r)}{\phi(r)} \tag{3.3}$$

Hence, rearranging Eq. (3.2) and substituting into Eq. (3.3) yields,

$$P_1(r) = -\Sigma_t dr \tag{3.4}$$

Solving the separable differential equation in Eq. (3.2) yields,

$$\phi(r) = \phi_0 e^{-\Sigma_{\rm t} r} \tag{3.5}$$

The probability of the neutrons to penetrate the material until the distance r without any interactions is given by  $P_2$ ,

$$P_2(r) = \frac{\phi(r)}{\phi_0} = e^{-\Sigma_{\rm t} r}$$
(3.6)

Next, the probability of a neutron to have its first interaction in the distance dr, P(r), is given by,

$$P(r) = P_1(r) \times P_2(r) = \Sigma_t e^{-\Sigma_t r} dr$$
(3.7)

Finally, the probability density function of the distance to the next interaction, p(r), is given by,

$$p(r) = \Sigma_{\rm t} e^{-\Sigma_{\rm t} r} \tag{3.8}$$

#### 3.2 Fick's Law

As pointed out in the previous section, solving the neutron transport equation is rather cumbersome. However, it is possible to impose certain conditions so that the neutron flux,  $\phi$ , and current, **J**, are related in a simple way. Thus, the relation can be used to simplify the complicated form of the transport equation which will ease the process of solving the equation. Now, it is practical to derive the relationship between  $\phi$  and **J** by calculating the neutron current density at any location within a medium.



Figure 3.2: An illustration for deriving Fick's law.

The location at which the neutron current density is calculated is defined to be the origin of a coordinate system shown in Fig. 3.2. Most importantly, the three vector components of **J** must be evaluated. It is convenient to begin with  $J_z$  and consider the rate at which neutrons flow through the area  $dA_z$  spanning over the xy-plane at the origin. Note also that there are no neutron sources exist in the medium. Correspondingly, all neutrons that pass through  $dA_z$  have just arrived from a scattering collision. Equally important, all scattering collisions that occur above the xy-plane will always cause some of the outgoing neutrons to flow downward through  $dA_z$  and vice versa.

At this point, it is useful to begin calculating the number of scattering collisions that occur per second in the volume element dV at point **r**. By using the theorems explained in Section 2.4, one can deduce that this number is equal to

$$\Sigma_{\rm s}\phi(\mathbf{r})\,dV\tag{3.9}$$

Based on the assumption that the scattering process is isotropic in the laboratory frame of reference, the fraction of outgoing neutrons that are scattered in the direction of  $dA_z$  is given by

$$\frac{dA_z \cos\theta}{4\pi r^2} \times \Sigma_{\rm s} \phi(\mathbf{r}) \, dV \tag{3.10}$$

Inescapably, a fraction of these scattered neutrons will not succeed in reaching  $dA_z$  where they are absorbed en route. As discussed in the previous section, the fraction of neutrons which able to reach  $dA_z$  per second is given by,

$$\frac{dA_z \cos\theta}{4\pi r^2} \times \Sigma_{\rm s} \phi(\mathbf{r}) \ dV \times e^{-\Sigma_{\rm t} r} \tag{3.11}$$

At this instance, the z-component of neutron current density,  $J_z$  is just the integral of the fraction given by Eq. (3.11) divided by  $dS_z$  over the entire volume. With dV written in spherical coordinates, where,  $dV = r^2 \sin \theta \, dr \, d\theta \, d\varphi$ , thus,

$$J_{z} = \frac{\Sigma_{\rm s}}{4\pi} \int_{r=0}^{\infty} \int_{\theta=0}^{\pi} \int_{\varphi=0}^{2\pi} \phi(\mathbf{r}) \, e^{-\Sigma_{\rm t} r} \cos\theta \sin\theta \, d\varphi \, d\theta \, dr \tag{3.12}$$

At this point of calculation, much of the attention was given to the z-component of **J**, where it is expressed in terms of the equivalent spherical coordinates. Most importantly, the orientation of the spherical coordinate system is symmetric, thus, the form of the right-hand side of Eq. (3.12) also applies to the x-component and ycomponent of **J**. Suppose that the component of interest is denoted with  $\mu \in \{x, y, z\}$ . In general, the three components of **J** in a Cartesian coordinate system can be written in the form of,

$$J_{\mu} = \frac{\Sigma_{\rm s}}{4\pi} \int_{r=0}^{\infty} \int_{\theta_{\mu}=0}^{\pi} \int_{\varphi_{\mu}=0}^{2\pi} \phi(\mathbf{r}_{\mu}) \ e^{-\Sigma_{\rm t} r} \cos\theta_{\mu} \ \sin\theta_{\mu} \, d\varphi_{\mu} d\theta_{\mu} dr \tag{3.13}$$

where  $\theta_{\mu}$  and  $\varphi_{\mu}$  are the polar angle and the azimuthal angle respectively with the zenith of the spherical coordinate system lies along the  $\mu$ -axis of the Cartesian coordinate system.

Alas, the integral in Eq. (3.13) cannot be evaluated because  $\phi(\mathbf{r}_{\mu})$  is unknown. However, if  $\phi(\mathbf{r}_{\mu})$  varies slowly with positions, it can be expressed in Taylor's series. For the case where z-axis as the zenith of the spherical coordinate system ( $\mu \equiv z$ ), the Taylor's expansion of  $\phi(\mathbf{r})$  is given by,

$$\phi(\mathbf{r}) = \phi_0 + x \left(\frac{\partial \phi}{\partial x}\right)_0 + y \left(\frac{\partial \phi}{\partial y}\right)_0 + z \left(\frac{\partial \phi}{\partial z}\right)_0 \dots$$
(3.14)

with  $\mathbf{r} = x\mathbf{e}_x + y\mathbf{e}_y + z\mathbf{e}_z$ ,  $x = r\sin\theta\cos\varphi$ ,  $y = r\sin\theta\sin\varphi$  and  $z = r\cos\theta$ . From Eq. (3.14), it is now clear that the similar form can be used for the other two components of **J**, i.e.  $\mu \equiv x$  and  $\mu \equiv y$ . In general, it is useful to write  $\phi(\mathbf{r}_{\mu})$  as,

φ

$$\int \phi_0 + r \cos \varphi \left(\frac{\partial \phi}{\partial x}\right)_0 + r \sin \theta \cos \varphi \left(\frac{\partial \phi}{\partial y}\right)_0 + r \sin \theta \sin \varphi \left(\frac{\partial \phi}{\partial z}\right)_0, \mu \equiv x \qquad (3)$$

$$= \phi_0 + r\cos\varphi \left(\frac{\partial\phi}{\partial y}\right)_0 + r\sin\theta\cos\varphi \left(\frac{\partial\phi}{\partial z}\right)_0 + r\sin\theta\sin\varphi \left(\frac{\partial\phi}{\partial x}\right)_0, \mu \equiv y \qquad \frac{1}{2}$$

Next, Eq. (3.15) is substituted in Eq. (3.14), and of course, it is found that the terms containing  $\cos \varphi$  and  $\sin \varphi$  will integrate to zero. Thus,  $J_{\mu}$  reduces into,

$$J_{\mu} = \frac{\Sigma_{\rm s}}{4\pi} \int_{r=0}^{\infty} \int_{\theta_{\mu}=0}^{\pi} \int_{\varphi_{\mu}=0}^{2\pi} \left(\phi_{0} + r\cos\varphi_{\mu} \left(\frac{\partial\phi}{\partial\mu}\right)_{0}\right) e^{-\Sigma_{\rm t}r}\cos\theta_{\mu} \sin\theta_{\mu} d\varphi_{\mu} d\theta_{\mu} dr$$
(3.16)

Hence, evaluating the definite integrals in Eq. (3.16) yields,

$$J_{\mu} = -\frac{\Sigma_{\rm s}}{3\Sigma_{\rm t}^2} \left(\frac{\partial\phi}{\partial\mu}\right)_0. \tag{3.17}$$

Finally, the vector **J** is now,

$$\mathbf{J} = J_x \mathbf{e}_x + J_y \mathbf{e}_y + J_z \mathbf{e}_z$$
  
=  $-\frac{\Sigma_s}{3\Sigma_t^2} \nabla \phi.$  (3.18)

In summary, Eq. (3.18) is known as *Fick's law*, which states that the current density vector is proportional to the negative gradient of the flux. It is useful to define the proportionality constant D, which is known as the diffusion coefficient where,

$$D = \frac{\Sigma_{\rm s}}{3\Sigma_{\rm t}^2} \tag{3.19}$$

With this notation, Fick's law can be written as,

$$\mathbf{J} = -D \,\boldsymbol{\nabla}\phi. \tag{3.20}$$

It should be noticed that the derivation of Fick's law in this section is just a prerequisite of the construction of good knowledge and foundation for the research and development of a multigroup Monte Carlo method which will be discussed further in Chapter 4. Readers may find that in the Monte Carlo method, the transport behaviour of neutrons is determined stochastically without the use of Fick's law, as in Eq. (3.20). Here, the diffusion of neutrons within a medium is reproduced via the computer simulation of neutron random walks.

So far, much of the attention has been given to the derivation of Fick's law. However, it is crucial to re-examine the conditions in which this law can be expected to be valid. There are a few assumptions made when deriving Fick's law in reactor calculation. However, most of these assumptions can be relaxed because of some reasons that apply to nuclear reactor conditions. A detailed discussion of these assumptions is given by (Lamarsh & Baratta, 1955). However, the diffusion approximation has to be strictly performed under a number of important assumptions:

- (a) The neutron diffusing medium must be infinite, to allow the integration of Eq. (3.13) over the entire space. Fortunately, the  $e^{-\Sigma_t r}$  term in Eq. (3.13) dies off quickly with distance. Consequently, neutrons streaming from farther distances from the point where **J** is calculated give fewer contributions to **J**, and their effect on the computation of **J** is negligible. Thus, Fick's law is still valid in the interior of a reactor, since the size of a reactor is exceptionally large compared to the diffusion distances of these neutrons. A problem may arise for the case near the outer surface of a reactor because there exists an abrupt change of the material cross section, i.e. between a dense medium (the interior of the reactor) and a vacuous medium (the outer region of the reactor). However, such an issue can be rectified by using a special treatment which is known as the reciprocal logarithmic derivative. A detailed reference of the special treatment is given by (Lamarsh & Baratta, 1955) and (Duderstadt & Hamilton, 1976). It should be noted that this issue is not applicable to Monte Carlo method since the neutron transport behaviour is simulated and purely based on statistical observations.
- (b) The neutron flux is a slowly varying function of position; the Taylor series of the neutron flux,  $\phi(\mathbf{r})$ , given by Eq. (3.15) is only expanded up to the first order. Hence, a rapid change of the neutron flux may compromise the accuracy of the calculation, since it can cause the higher spatial derivative terms of the Taylor expansion of  $\phi(\mathbf{r})$  to be significant and cannot be neglected.
- (c) The neutron flux is a slowly varying function of time; In Eq. (3.13), the neutron flux is assumed to be independent of time. Unfortunately, a neutron needs time to travel from the collision site to the location where J is calculated. As previously discussed, only neutrons streaming from closer distances from the point where J is calculated significantly contributes to J. So, the time taken for neutrons to travel at these close distances is negligible since neutrons travel at high speed. In a nuclear reactor, even the slowest neutrons travel at 1000m/s, thus this assumption can be relaxed.

## 3.3 Multigroup Method

It is well understood that neutron energies typically encountered in a reactor span a range from  $10^{-3}$  eV to  $10^7$  eV. Also, neutron cross sections depend sensitively on energy over most of this range (Duderstadt & Hamilton, 1976). In this section, the continuous neutron energy dependence will be suppressed by assuming that all neutrons can be characterized using a few discrete energy groups. Precisely, the continuous neutron energy range is divided into several energy group intervals. Plus, the energy boundaries of each group interval are defined prior to the neutronic calculation. Subsequently, each individual neutron energy group is assigned to a differential equation known as the *group equation*. Next, a sequence of one-group calculations for each successive energy group is performed.

In the multigroup method, the entire continuous neutron energy within a specific thermal nuclear reactor is divided into G energy groups. Suitably, the highest energy that can be attained by a neutron in a nuclear system is  $E_0 = \infty$ . A neutron group is assigned with an index,  $g \in \{1,2,3,\ldots,g-1,g,g+1,\ldots,G-1,G\}$  where it has a predefined neutron energy range covering from  $E_g$  to  $E_{g-1}$ , where  $E_{g-1} > E_g$ . In this work, each neutron group is assigned to a pre-set energy boundary values given in *Appendix A*. To derive the diffusion equation for the energy group g, several group constants for the energy group need to be defined.

Right now, it is favourable to simplify the neutron transport equation given by Eq. (2.30) using Fick's law and the multigroup method. It is beneficial to go through each term of the neutron transport equation and simplify each of these terms accordingly. Consider a system, typically an infinitesimal volume dV of a homogeneous fissile material. To begin with, the energy variable in the neutron transport equation is eliminated by integrating Eq. (2.30) over the  $g^{\text{th}}$  energy group defined within the energy range  $(E_g, E_{g-1})$ . Plus, the neutron direction,  $\hat{\Omega}$ , in the neutron transport equation can be eliminated by integrating the transport equation over the entire neutron directions, i.e.  $[0,4\pi)$ . Thus,

$$\underbrace{\int_{4\pi} \int_{E_g}^{E_{g-1}} \frac{1}{v} \frac{\partial}{\partial t} \psi(\mathbf{r}, E, \hat{\Omega}, t) dE d\hat{\Omega}}_{\text{Time rate of change}} + \underbrace{\int_{4\pi} \int_{E_g}^{E_{g-1}} \hat{\Omega} \cdot \nabla \psi(\mathbf{r}, E, \hat{\Omega}, t) dE d\hat{\Omega}}_{\text{Streaming term}} + \underbrace{\int_{4\pi} \int_{E_g}^{E_{g-1}} \Sigma_{t}(\mathbf{r}, E) \psi(\mathbf{r}, E, \hat{\Omega}, t) dE d\hat{\Omega}}_{\text{Disappearance term}} - \underbrace{\int_{4\pi} \int_{E_g}^{E_{g-1}} \int_{4\pi} \int_{0}^{\infty} \Sigma_{s}(\mathbf{r}, E' \to E, \hat{\Omega}' \to \hat{\Omega}) \psi(\mathbf{r}, E', \hat{\Omega}', t) dE' d\hat{\Omega}' dE d\hat{\Omega}}_{\text{In-scattering term}} + \underbrace{\int_{4\pi} \int_{E_g}^{E_{g-1}} \int_{4\pi} \int_{0}^{\infty} \frac{\chi(E)}{4\pi} v(E') \Sigma_{f}(\mathbf{r}, E', \hat{\Omega}', t) dE' d\hat{\Omega}' dE d\hat{\Omega}}_{\text{In-scattering term}}} - \underbrace{\int_{4\pi} \int_{E_g}^{E_{g-1}} \int_{4\pi} \int_{0}^{\infty} \frac{\chi(E)}{4\pi} v(E') \Sigma_{f}(\mathbf{r}, E', \hat{\Omega}', t) dE' d\hat{\Omega}' dE d\hat{\Omega}}_{\text{In-scattering term}} - \underbrace{\int_{4\pi} \int_{E_g}^{E_{g-1}} \int_{4\pi} \int_{0}^{\infty} \frac{\chi(E)}{4\pi} v(E') \Sigma_{f}(\mathbf{r}, E', \hat{\Omega}', t) dE' d\hat{\Omega}' dE d\hat{\Omega}}_{\text{In-scattering term}}} - \underbrace{\int_{4\pi} \int_{E_g}^{E_{g-1}} \int_{4\pi} \int_{0}^{\infty} \frac{\chi(E)}{4\pi} v(E') \Sigma_{f}(\mathbf{r}, E', \hat{\Omega}', t) dE' d\hat{\Omega}' dE d\hat{\Omega}}_{\text{In-scattering term}}} - \underbrace{\int_{4\pi} \int_{E_g}^{E_{g-1}} \int_{4\pi} \int_{0}^{\infty} \frac{\chi(E)}{4\pi} v(E') \Sigma_{f}(\mathbf{r}, E', \hat{\Omega}', t) dE' d\hat{\Omega}' dE d\hat{\Omega}}_{\text{In-scattering term}}} - \underbrace{\int_{4\pi} \int_{E_g}^{E_{g-1}} \int_{4\pi} \int_{0}^{\infty} \frac{\chi(E)}{4\pi} v(E') \Sigma_{f}(\mathbf{r}, E', \hat{\Omega}', t) dE' d\hat{\Omega}' dE d\hat{\Omega}}_{\text{In-scattering term}}} - \underbrace{\int_{4\pi} \int_{0}^{\infty} \frac{\chi(E)}{4\pi} v(E') \Sigma_{f}(\mathbf{r}, E', \hat{\Omega}', t) dE' d\hat{\Omega}' dE' d\hat{\Omega}' dE' d\hat{\Omega}}_{\text{In-scattering term}}} - \underbrace{\int_{4\pi} \int_{0}^{\infty} \frac{\chi(E)}{4\pi} v(E') \Sigma_{f}(\mathbf{r}, E', \hat{\Omega}', t) dE' d\hat{\Omega}' dE' d\hat{\Omega}' dE' d\hat{\Omega}}_{\text{In-scattering term}}} - \underbrace{\int_{0}^{\infty} \frac{\chi(E)}{4\pi} v(E') \Sigma_{f}(\mathbf{r}, E', \hat{\Omega}', t) dE' d\hat{\Omega}' dE' d\hat{\Omega}' dE' d\hat{\Omega}}_{\text{In-scattering term}} - \underbrace{\int_{0}^{\infty} \frac{\chi(E)}{4\pi} v(E') \Sigma_{f}(\mathbf{r}, E', \hat{\Omega}', t) dE' d\hat{\Omega}' dE' d\hat{\Omega}' dE' d\hat{\Omega}' dE' d\hat{\Omega}}_{\text{In-scattering term}} - \underbrace{\int_{0}^{\infty} \frac{\chi(E)}{4\pi} v(E') \Sigma_{f}(\mathbf{r}, E', \hat{\Omega}', t) dE' d\hat{\Omega}' dE' d\hat{\Omega$$

Fission term

In addition, all integrations with respect to the neutron direction,  $\hat{\Omega}$ , over the entire solid angle,  $4\pi$ , will relax our focus on dealing with  $\hat{\Omega}$ . Remark that the study of the behaviour of neutrons regardless of its direction is in focus instead.

Subsequently, several formal definitions of multigroup constants will be introduced. At this instance, the group flux,  $\phi_g$ , is defined as the flux integrated over the entire energy range defined for the group, g, i.e.  $(E_g, E_{g-1})$ 

$$\phi_g(\mathbf{r},t) = \int_{4\pi} \int_{E_g}^{E_{g-1}} \psi(\mathbf{r}, E, \widehat{\mathbf{\Omega}}, t) \, dE \, d\widehat{\mathbf{\Omega}}.$$
(3.22)

The time rate of change term in Eq. (3.21) can be further simplified into,

$$\begin{cases} \text{Time rate} \\ \text{of change} \\ \text{of neutrons} \end{cases} = \int_{4\pi} \int_{E_g}^{E_{g-1}} \frac{1}{v} \frac{\partial}{\partial t} \psi(\mathbf{r}, E, \hat{\mathbf{\Omega}}, t) \, dE \, d\hat{\mathbf{\Omega}} \\ = \frac{1}{v_g} \frac{\partial \phi_g(\mathbf{r}, t)}{\partial t} \end{cases}$$
(3.23)

where the inverse neutron speed characterizing group g is given by

$$\frac{1}{v_g} = \frac{1}{\phi_g(\mathbf{r}, t)} \int_{4\pi} \int_{E_g}^{E_{g-1}} \frac{1}{v} \psi(\mathbf{r}, E, \hat{\mathbf{\Omega}}, t) \, dE \, d\hat{\mathbf{\Omega}}$$
(3.24)

Next, the *streaming term* in Eq. (3.21) can be further simplified in terms of the angular neutron current density,  $\mathbf{j}(r, E, \hat{\Omega}, t)$ , via Eqs. (2.5), (2.6) and (2.7),

$$\int_{4\pi} \int_{E_g}^{E_{g-1}} \widehat{\Omega} \cdot \nabla \psi(\mathbf{r}, E, \widehat{\Omega}, t) \, dE \, d\widehat{\Omega}$$

$$= \int_{4\pi} \int_{E_g}^{E_{g-1}} \nabla \cdot \widehat{\Omega} \psi(\mathbf{r}, E, \widehat{\Omega}, t) \, dE \, d\widehat{\Omega}$$

$$= \int_{4\pi} \int_{E_g}^{E_{g-1}} \nabla \cdot \mathbf{j}(\mathbf{r}, E, \widehat{\Omega}, t) \, dE \, d\widehat{\Omega}$$

$$= \int_{E_g}^{E_{g-1}} \nabla \cdot \mathbf{J}(\mathbf{r}, E, t) \, dE$$
(3.25)

Since Fick's law establishes the relationship between the flux and the current density,  $J(\mathbf{r}, E, t)$  can be approximated by substituting Eq. (3.20) into Eq. (3.25), giving,

$$\int_{E_g}^{E_{g-1}} \nabla \cdot \mathbf{J}(\mathbf{r}, E, t) \, dE = \int_{E_g}^{E_{g-1}} \nabla \cdot \left(-D(\mathbf{r}, E) \nabla \phi(\mathbf{r}, E, t)\right) \, dE$$

$$= -\nabla \cdot \int_{E_g}^{E_{g-1}} D(\mathbf{r}, E) \, \nabla \phi(\mathbf{r}, E, t) \, dE$$
(3.26)

With some simple mathematical manoeuvres, the group diffusion coefficient,  $D_g(\mathbf{r}, t)$ , is defined as

$$D_{g}(\mathbf{r},t) = \frac{\int_{E_{g}}^{E_{g-1}} D(\mathbf{r}, E) \nabla \phi(\mathbf{r}, E, t) \, dE}{\int_{E_{g}}^{E_{g-1}} \nabla \phi(\mathbf{r}, E, t) \, dE}$$
(3.27)

The group diffusion coefficient as defined in Eq. (3.27) permits us to write the multigroup net leakage term as,

$$\begin{cases} \text{Net} \\ \text{leakage} \end{cases} = -\nabla \cdot D_g(\mathbf{r}, t) \,\nabla \phi_g(\mathbf{r}, t)$$
 (3.28)

Subsequently, the total macroscopic group cross section  $\Sigma_t^g(\mathbf{r}, t)$  is defined as

$$\Sigma_{t}^{g}(\mathbf{r},t) = \frac{1}{\phi_{g}(\mathbf{r},t)} \int_{4\pi} \int_{E_{g}}^{E_{g-1}} \Sigma_{t}(\mathbf{r},E) \psi(\mathbf{r},E,\hat{\mathbf{\Omega}},t) \, dE \, d\hat{\mathbf{\Omega}}$$

$$= \frac{1}{\phi_{g}(\mathbf{r},t)} \int_{E_{g}}^{E_{g-1}} \Sigma_{t}(\mathbf{r},E) \phi(\mathbf{r},E,t) \, dE \qquad (3.29)$$

Therefore, the rate at which neutrons from energy group g interacts with the homogeneous fissile material and disappear from the energy group g (also known as the disappearance term) can be simply written as,

$$\begin{cases} \text{Group} \\ \text{disappearance} \\ \text{term} \end{cases} = \Sigma_{t}^{g}(\mathbf{r}, t) \phi_{g}(\mathbf{r}, t)$$
(3.30)

Recall that some neutrons from other energy groups, g', will experience scattering collision with the homogeneous fissile material. Such a scattering collision changes the neutron energy, which also implies the change of the energy group. Consequently, some of these scattered neutrons will fall into group g, and this phenomenon is often coined as in-scattering. Of course, scattering collision can also remove neutrons from energy group g, which is termed as out-scattering. However, it is important to stress that the rate of out-scattering reaction has been included in Eq. (3.30) since it is equivalent to the removal of neutrons from energy group g. To this point, the *macroscopic transfer group cross section* is defined as

$$\Sigma_{s}^{g' \to g}(\mathbf{r}, t) = \frac{1}{\phi_{g'}(\mathbf{r}, t)} \int_{4\pi} \int_{E_{g}}^{E_{g-1}} \int_{4\pi} \int_{E_{g'}}^{E_{g'-1}} \Sigma_{s}(\mathbf{r}, E' \to E, \widehat{\mathbf{\Omega}}' \to \widehat{\mathbf{\Omega}}) \Psi(\mathbf{r}, E', \widehat{\mathbf{\Omega}}', t) \, dE' \, d\widehat{\mathbf{\Omega}}' \, dE \, d\widehat{\mathbf{\Omega}}$$

$$= \frac{1}{\phi_{g'}(\mathbf{r}, t)} \int_{E_{g'}}^{E_{g'-1}} \Sigma_{s}(\mathbf{r}, E' \to E) \phi(\mathbf{r}, E', t) \, dE'$$
(3.31)

where  $\phi^{g'}(\mathbf{r}, t)$  is defined similarly according to Eq. (3.22). Be aware of the special notation, i.e.  $g' \to g$ , where it indicates the transfer of neutrons from group g' into group g. The in-scattering rate from energy group g' into g can be written as,

$$\begin{cases} \text{Group} \\ \text{in-scattering} \\ \text{term} \end{cases} = \Sigma_{s}^{g' \to g}(\mathbf{r}, t) \phi_{g'}(\mathbf{r}, t)$$
(3.32)

Of course, the contribution of the neutron in group g is caused by the in-scattering of neutrons from all energy groups into the energy group g. Such a total contribution can be represented as the summation of the right-hand-side of Eq. (3.32) over the entire incident neutron energy groups,  $g' = \{1, 2, 3, ..., G\}$ . Thus, the total in-scattering rate can be written as,

$$\Sigma_{s}^{1 \to g}(\mathbf{r}) \phi_{1}(\mathbf{r}, t) + \Sigma_{s}^{2 \to g}(\mathbf{r}) \phi_{2}(\mathbf{r}, t) + \dots + \Sigma_{s}^{G \to g}(\mathbf{r}) \phi_{G}(\mathbf{r}, t)$$

$$= \sum_{g'=1}^{G} \Sigma_{s}^{g' \to g}(\mathbf{r}) \phi_{g'}(\mathbf{r}, t)$$
(3.33)

So far, intense work on deriving the group flux, multigroup inverse neutron speed, multigroup streaming term, multigroup disappearance term and multigroup inscattering has been completed. In a fissile medium, one must include a mathematical term that accounts for the neutron production due to fission reaction in the neutron transport equation. Originally, such a mathematical term is the fission term which is given by Eq. (2.28). The multigroup form of the fission term can be derived by first considering the production rate of fission neutrons with energy E and direction  $\hat{\Omega}$  due to fission reactions induced by an incident neutron with energy E' and direction  $\hat{\Omega}'$ . This is given by,

$$S_{\rm f}(\mathbf{r}, E, \widehat{\mathbf{\Omega}}, t) = \frac{\chi(E)}{4\pi} \int_{4\pi} v(E') \Sigma_{\rm f}(\mathbf{r}, E') \psi(\mathbf{r}, E', \widehat{\mathbf{\Omega}}', t) \, d\widehat{\mathbf{\Omega}}'$$
(3.34)

In the above equation, the integration with respect to  $d\hat{\Omega}'$  over the entire solid angle,  $4\pi$ , simply indicates that  $S_f(\mathbf{r}, E, \hat{\Omega}, t)$  considers all possible incident neutron directions. Bear in mind that it is assumed that the fission neutrons are emitted isotropically. Put differently, the probability of ejecting fission neutrons isotropically via fission caused by an incident neutron of any direction is equal. Suppose that isotropic fission is implied, the total birth rate of fission neutrons in energy group g cause by fission reactions induced by incident neutron regardless of their energy and direction is given by,

$$S_{f}(\mathbf{r}, E, t) = \frac{\chi(E)}{4\pi} \int_{4\pi} \int_{4\pi} v(E') \Sigma_{f}(\mathbf{r}, E') \psi(\mathbf{r}, E', \widehat{\mathbf{\Omega}}', t) \, d\widehat{\mathbf{\Omega}}' \, d\widehat{\mathbf{\Omega}}$$
  
$$= \frac{\chi(E)}{4\pi} v(E') \Sigma_{f}(\mathbf{r}, E') \int_{4\pi} d\widehat{\mathbf{\Omega}} \, \int_{4\pi} \psi(\mathbf{r}, E', \widehat{\mathbf{\Omega}}', t) \, d\widehat{\mathbf{\Omega}}'$$
  
$$= \chi(E) v(E') \Sigma_{f}(\mathbf{r}, E') \phi(\mathbf{r}, E', t) \qquad (3.35)$$

where,

$$\int_{4\pi} d\widehat{\mathbf{\Omega}} = 4\pi \tag{3.36}$$

The multigroup form of  $S_f(\mathbf{r}, E, t)$  can be derived by integrating it with respect to the incident neutron energy, E' and the outgoing fission neutron energy E over the entire energy range characterizing group g' and g respectively,

$$\int_{E_g}^{E_{g-1}} dE \, S_{\rm f}(\mathbf{r}, E, t) = \int_{E_g}^{E_{g-1}} \int_{E_{g'}}^{E_{g'-1}} \chi(E) \nu(E') \Sigma_{\rm f}(\mathbf{r}, E') \phi(\mathbf{r}, E', t) \, dE' \, dE$$
(3.37)

To further simplify the group fission term given in Eq. (3.37), several group constants of the fission term are defined. The group fission spectrum is defined as,

$$\chi_g = \int_{E_g}^{E_{g-1}} \chi(E) dE \tag{3.38}$$

and the group neutron production cross section is defined as,

$$v_{g'} \Sigma_{\rm f}^{g'} = \frac{1}{\phi_{g'}(\mathbf{r},t)} \int_{E_{g'}}^{E_{g'-1}} v(E') \Sigma_{\rm f}(\mathbf{r},E') \phi(\mathbf{r},E',t) \, dE'$$
(3.39)

Consequently, Eq. (3.37) can be simplified into,

$$\int_{E_g}^{E_{g-1}} S_{\mathbf{f}}(\mathbf{r}, E, t) \, dE = \chi_g v_g \Sigma_{\mathbf{f}}^{g'}(\mathbf{r}) \phi_{g'}(\mathbf{r}, t) \tag{3.40}$$

Correspondingly, the total production of fission neutrons in group g can be obtained by considering the sum of the fission neutrons production induced by incident neutrons from all groups. Thus, using Eq. (3.40), the group fission term can be written as:

$$\begin{cases} \text{Group} \\ \text{fission} \\ \text{term} \end{cases} = \chi_g v_1 \Sigma_f^1(\mathbf{r}) \phi_1(\mathbf{r}, t) + \chi_g v_2 \Sigma_f^2(\mathbf{r}) \phi_2(\mathbf{r}, t) + \cdots \\ + \chi_g v_G \Sigma_f^G(\mathbf{r}) \phi_G(\mathbf{r}, t) \\ = \chi_g \sum_{g'=1}^G v_{g'} \Sigma_f^{g'}(\mathbf{r}) \phi_{g'}(\mathbf{r}, t) \end{cases}$$
(3.41)

Perhaps, the most direct way of deriving the multigroup neutron diffusion equation is to apply the concept of neutron balance to a given energy group. Base on this notion, the mechanisms in which neutrons enter and leave the energy group g are balanced. Mathematically, the neutron balance equation can be written as,



Now, Eqs. (3.23), (3.28), (3.30), (3.32) and (3.41) are substituted into Eq. (3.42), which will then yield the general form of the *multigroup equations*,

$$\frac{1}{v_g} \frac{\partial \phi_g(\mathbf{r}, t)}{\partial t} = -\nabla \cdot D_g(\mathbf{r}, t) \nabla \phi_g(\mathbf{r}, t) - \Sigma_t^g(\mathbf{r}, t) \phi_g(\mathbf{r}, t) + \sum_{g'=1}^G \Sigma_s^{g' \to g}(\mathbf{r}, t) \phi_{g'}(\mathbf{r}, t) + \chi_g \sum_{g'=1}^G v_{g'} \Sigma_f^{g'}(\mathbf{r}, t) \phi_{g'}(\mathbf{r}, t) g = 1, 2, 3, \dots, G$$
(3.43)

Several remarks on these equations are essential and need be clearly stated before proceeding to the next step of reactor calculation. The general form of multigroup diffusion equations given in Eq. (3.43) are reasonably exact since the following group constants were introduced,

$$\frac{1}{\nu_g}, D_g, \Sigma_t^g, \Sigma_s^{g' \to g}, \chi_g, \nu_{g'}, \Sigma_f^{g'}$$

Nevertheless, these group constants are still undetermined and need to be calculated. From the definitions of the group constants given by Eqs. (3.24), (3.27), (3.29), (3.31), (3.38) and (3.39), it is apparent that the flux  $\phi(\mathbf{r}, E, t)$  must be known prior to the calculation of the group constants. However,  $\phi(\mathbf{r}, E, t)$  is just the function that needs to be solved in the first place by discretizing the neutron energy into groups. This seems that the development of the multigroup method has been quite circular. Note also that the group constants are also dependent on the space and time which makes the problem even more cumbersome. Indeed, the group constants will be rigorously constant only if  $\phi(\mathbf{r}, E, t)$  is of the separable form,

$$\phi(\mathbf{r}, E, t) = F(\mathbf{r}, t)G(E) \tag{3.44}$$

For such a scenario, the group constants will reduce to group averages over the flux energy spectrum G(E). Alas, this is not the case in a nuclear reactor where the flux is usually not separable in energy. To rectify the problem, one may attempt to guess and approximate the intragroup flux characterizing each neutron energy group, i.e.  $\phi(\mathbf{r}, E, t) \cong \tilde{\phi}(\mathbf{r}, E, t)$ . Hence, the group constants can be calculated by replacing  $\phi(\mathbf{r}, E, t)$  with  $\tilde{\phi}(\mathbf{r}, E, t)$  in their corresponding mathematical definition. For example, the group total neutron cross section can be calculated as averages over these approximate intragroup fluxes,

$$\Sigma_{\rm t}^g(\mathbf{r},t) = \frac{1}{\phi_g(\mathbf{r},t)} \int_{E_g}^{E_{g-1}} \Sigma_{\rm t}(\mathbf{r},E) \tilde{\phi}(\mathbf{r},E,t) \, dE \tag{3.45}$$

with

$$\phi_g(\mathbf{r},t) = \int_{E_g}^{E_{g-1}} \tilde{\phi}(\mathbf{r}, E, t) \, dE.$$
(3.46)

In the next section, the strategy of approximating the flux  $\phi(\mathbf{r}, E, t)$  will be discussed in detail, and thus, the group constants can be directly calculated.

#### **3.4** Fine Group Constants

Recall that in the previous section, intense work has been accomplished to simplify the neutron transport equation via multigroup diffusion method. Along the simplification process, several group constants were introduced. However, these group constants are still dependent on space, energy and time because their calculation requires the flux,  $\phi(\mathbf{r}, E, t)$ , to be known beforehand. Unfortunately, the purpose of solving the transport equation is to compute the flux. Thus, the only way to rectify such issue is by first ignoring the space and time variation of the flux, i.e.,  $\phi(\mathbf{r}, E, t) \sim \phi(E)$ . Then,  $\phi(E)$  is approximated with the intragroup fluxes – a weighing flux as a function of neutron energy characterizing each of the neutron energy group g. Above all, one will be able to do very good multigroup calculations with only a few neutron energy groups provided that a good guess of the shape of  $\phi(E)$  for a nuclear system is made.

Since the nature of the neutron transport equation is separable in time, the flux  $\phi(\mathbf{r}, E, t)$  can be written as

$$\phi(\mathbf{r}, E, t) = F(\mathbf{r}, E)\tau(t) \tag{3.47}$$

As a result, group constants can be averaged over time. In general, the mathematical definitions of the group constants can be generally written as,

$$\Sigma_g = \frac{\int_{E_g}^{E_{g-1}} K\phi(\mathbf{r}, E, t) \, dE}{\int_{E_g}^{E_{g-1}} \phi(\mathbf{r}, E, t) \, dE}$$
(3.48)

where *K* is the integral kernel which maps Eq. (3.48) into various type of group constants, i.e.  $K \in \left\{\frac{1}{v(\mathbf{r},E)}, \Sigma_t(\mathbf{r},E), \Sigma_s(\mathbf{r},E' \to E), \nu \Sigma_f(\mathbf{r},E), \right\}$ . Suppose that the flux is separable in time, it is convenient to eliminate the time variable in our group constants calculation, since,

$$\Sigma_{g} = \frac{\int_{E_{g}}^{E_{g-1}} KF(\mathbf{r}, E)\tau(t) \, dE}{\int_{E_{g}}^{E_{g-1}} F(\mathbf{r}, E)\tau(t) \, dE}$$

$$= \frac{\int_{E_{g}}^{E_{g-1}} KF(\mathbf{r}, E) \, dE}{\int_{E_{g}}^{E_{g-1}} F(\mathbf{r}, E) \, dE}$$
(3.49)

Also, from the definition of the group diffusion coefficient,

$$D_g = \frac{\int_{E_g}^{E_{g-1}} D(\mathbf{r}, E) \nabla^2 F(\mathbf{r}, E) \tau(t) \, dE}{\int_{E_g}^{E_{g-1}} \nabla^2 F(\mathbf{r}, E) \tau(t) \, dE}$$
(3.50)

Since Laplacian operator,  $\nabla^2$ , does not operate on the time variable, the definition of the group diffusion coefficient can be written as

$$D_g = \frac{\int_{E_g}^{E_{g-1}} D(\mathbf{r}, E) \nabla^2 F(\mathbf{r}, E) dE}{\int_{E_g}^{E_{g-1}} \nabla^2 F(\mathbf{r}, E) dE}$$
(3.51)

At this point, it is clear that the group constants are only dependent on position and energy. In the actual reactor calculation practice, one usually works with from two to 20 neutron energy groups. Such few group calculations are only reliable with reasonably accurate estimates of the group constants. Again, accurate estimates of the group constants can only be achieved if the intragroup fluxes,  $\phi(E)$ , are accurately determined. The widely accepted strategy is to perform two multigroup calculations. In the first multigroup calculation, the spatial and time dependence is neglected or very crudely approximated, and a very finely structured multigroup calculation is performed to calculate the fine spectrum fluxes. The group constants for this fine spectrum calculation are usually pre-calculated and represented as a tabulated multigroup cross section data library. Furthermore, the group constants are averaged over each of the fine energy groups. An example of such a library is the IAEA WIMSD formatted data library. The IAEA WIMSD formatted data library offers 69 and 172 fine group structures for nuclear reactor calculations. Fig. 3.3 shows the total cross section of U-235 in 69 and 172 fine energy groups.



**Figure 3.3**: Multigroup neutron cross section plot for U-235. (Plot retrieved from International Atomic Energy Agency (IAEA) website, https://www-nds.iaea.org/wimsd/xsplots.htm)



**Figure 3.4**: An equivalent heterogeneous cell consisting of three different materials, i.e. fissile fuel ( $\Sigma_1$ ), fuel cladding ( $\Sigma_2$ ) and the coolant channel ( $\Sigma_3$ ), is homogenized. The heterogeneous cell is represented with an equivalent homogenized cell with the equivalent cross section  $\Sigma_{eq}$ .

At first sight, a reactor core can be constructed using its basic lattice structures which are known as unit cells. The geometry of each of these unit cells is defined such

that the entire reactor core can be build using repetitions of these unit cells. For instance, the unit cells forming a reactor core are illustrated in Fig. 3.4. Essentially, the spatial dependence of the group constants reflects the fact that the geometry is heterogeneous which compose of discrete uniform material zones. Here, a heterogeneous unit cell is made up of a few separated regions of materials. To be more specific, a fuel cell consists of four different types of heterogeneous regions, i.e. the fuel meat, cladding material and the adjacent coolant channel. Note also that these heterogeneous regions are represented with specific group constants characterizing the material contained in each region.

To suppress the spatial dependency of the group constants, the heterogeneous unit cell is replaced with an equivalent homogenized unit cell. Consequently, a homogenized unit cell is defined such that the separated regions are "mixed" thus preserving the integral neutron behaviour. In this context, neutron behaviour is a sequence of events where various neutron-nucleus interactions take place. Thus, after the homogenization process, a set of homogenized group constants characterizing the homogenized material within the unit cell is obtained. A detailed procedure to calculate the homogenized group constants for the case of a TRIGA reactor core will be discussed intensively in Chapter 4.

#### 3.5 Multiplication Factor

Recall that in the previous section, the main working principle of a nuclear reactor is by tapping the energy released in fission reaction via the use of fission chain reaction. Such an essential idea is based on the fact that a fission neutron produced by the previous fission reaction will eventually induce another fission reaction. Thus, the neutrons that induce the fission reactions are known as the chain carriers. In normal nuclear engineering practice, it is desirable to ensure a steady-state chain reaction, which simply means a chain reaction that does not grow or decay away with time. Consequently, a nuclear engineer must design a reactor that is capable of inducing one fission reaction per fission neutrons produced by the previous fission reaction. Plus, certain factors that cause the fission chain reaction to degenerate have to be considered. Specifically, the remaining neutrons produced by the previous fission reaction could either be absorbed by means of disappearance reactions or will leak and escape out from the reactor.

Such a neutron balance requirement can be expressed in mathematical form. To begin with, it is handy to consider the life cycle history of a single neutron. Essentially, the birth of a neutron usually begins as a result of a fission event. Then, the neutron will usually scatter for multiple times within the reactor region until it arrives at the point where its death or disappearance occurs. Also, some of the neutrons that were absorbed by fissionable nuclei will turn out inducing another fission reaction. This leads to the creation of a new generation of fission neutrons. Now, the quantity that describes the balance of neutrons within a nuclear reactor is known as the *effective multiplication factor*, which is defined as,

$$k_{\text{eff}} \equiv \frac{\text{Number of neutrons born in a reactor}}{\text{Number of neutrons loss in a reactor}}$$
  
$$\equiv \frac{\text{Number of neutrons in generation } j}{\text{Number of neutrons in previous generation } j - 1}$$
(3.52)

Note that if  $k_{eff} = 1$ , the number of neutrons produced in a reactor is equal to the number of neutron loss in a reactor. Consequently, the number of neutrons in any two consecutive fission generations will be the same. Plus, the chain reaction will become time-independent. For the case when  $k_{eff} < 1$ , there will be more neutron loss in the reactor since the denominator of Eq. (3.52) is larger than its numerator. Accordingly, the fission chain is expected to die off and the reactor is said to be in the state of subcritical. Finally, if  $k_{eff} > 1$ , the chain reaction is expected to grow exponentially, since more fission neutrons are produced during each successive fission generation. Such a condition is coined as supercritical.

In conclusion, the effective multiplication factor plays an extremely important role in assessing the stability of a nuclear reactor. The calculation of  $k_{eff}$  characterizing a specific reactor configuration and composition is often the main interest of most nuclear engineers. From this point, readers will find the rest of this book will be focusing on the development of various methods and procedures for performing this calculation.

## 3.6 Reactor *k*-Eigenvalue Equation

With the available knowledge of neutron transport, it is now suitable to determine the composition and size of a particular reactor so that the reactor is critical, i.e.  $k_{eff} = 1$ . Such a determination is crucial in the reactor core designing and management process since nuclear engineers will always desire to have a self-sustaining (critical) and a constant power-producing nuclear reactor. Inevitably, the existence of the time derivative in the multigroup equation given by Eq. (3.43) indicates that the number of neutrons in nuclear reactors is not always balanced over time. In reality, the state of a nuclear reactor always fluctuates over time. Therefore, assessing the state of neutron balance in a particular nuclear reactor using the time-dependent transport equation is not practical. Plus, such a practice can cause difficulties during the process of designing a self-sustaining nuclear reactor.

Practically, determining the criticality of a nuclear reactor with a specific geometry and composition requires the time-averaging of the neutron transport equation. Here, *time-averaging* simply means that the average reactor behaviour over time is observed instead. Note also that a time-averaged transport equation is often called the static eigenvalue equation. One of the approaches to create a static eigenvalue equation is to force the time derivative of the transport equation (continuous form or multigroup form) to zero. Next, a scaling factor, 1/k, on the fission term of the transport equation is introduced. To comprehend the reason behind the introduction of the scaling factor 1/k, it is useful to first consider the multigroup diffusion equation is set to zero so that the equation is time-averaged and static. For this reason,

$$\frac{1}{v_g} \underbrace{\frac{\partial \phi_g(\mathbf{r}, t)}{\partial t}}_{g'=1} + \nabla \cdot D_g(\mathbf{r}) \nabla \phi_g(\mathbf{r}) + \Sigma_t^g(\mathbf{r}) \phi_g(\mathbf{r})$$

$$= \sum_{g'=1}^G \Sigma_s^{g' \to g}(\mathbf{r}) \phi_{g'}(\mathbf{r}) + \chi_g \sum_{g'=1}^G v_{g'} \Sigma_f^{g'}(\mathbf{r}) \phi_{g'}(\mathbf{r})$$

$$g = 1, 2, 3, \dots, G$$
(3.53)

Recall that the right-hand side of Eq. (3.53) indicates the gain of neutrons within the reactor and the left-hand side of Eq. (3.53) indicates the loss of neutrons from the reactor. Setting  $\partial \phi_{g'} \partial t = 0$  forces the net gain of neutrons to be equal with the net loss of neutrons from the reactor, and such condition only possible when the reactor is critical. As a result, Eq. (3.53) has no general solution, unless the exact combination of the core composition, geometry and group constants such that the reactor is critical is just happened to hit. The only way to alleviate this issue is to introduce the 1/k factor to the fission term of Eq. (3.53). Henceforth, this will mathematically scale the fission term so that the equation satisfies for any reactor condition, even if the reactor core is not critical, i.e. subcritical or supercritical. Thus,

$$\nabla \cdot D_{g}(\mathbf{r}) \nabla \phi_{g}(\mathbf{r}) + \Sigma_{t}^{g}(\mathbf{r}) \phi_{g}(\mathbf{r})$$

$$= \sum_{g'=1}^{G} \Sigma_{s}^{g' \to g}(\mathbf{r}) \phi_{g'}(\mathbf{r}) + \frac{1}{k} \chi_{g} \sum_{g'=1}^{G} v_{g'} \Sigma_{f}^{g'}(\mathbf{r}) \phi_{g'}(\mathbf{r})$$

$$g = 1, 2, 3, \dots, G$$
(3.54)

For simplicity, an operator  $\hat{T}$  is introduced such that,

Finally, Eq. (3.54) can be written into its equivalent matrix form:

$$\operatorname{diag}(\widehat{T}_{1}, \widehat{T}_{2}, \dots, \widehat{T}_{G}) \begin{pmatrix} \phi_{1} \\ \phi_{2} \\ \vdots \\ \phi_{g} \\ \vdots \\ \phi_{G} \end{pmatrix}$$

$$= \begin{pmatrix} \sum_{s}^{1 \to 1} \dots \sum_{s}^{G \to 1} \\ \sum_{s}^{1 \to 2} \dots \sum_{s}^{G \to 2} \\ \vdots \\ \sum_{s}^{1 \to G} \dots \sum_{s}^{G \to G} \end{pmatrix} \begin{pmatrix} \phi_{1} \\ \phi_{2} \\ \vdots \\ \phi_{g} \\ \vdots \\ \phi_{g} \\ \vdots \\ \chi_{G}v_{1}\Sigma_{f}^{1} \dots \chi_{I}v_{G}\Sigma_{f}^{G} \end{pmatrix} \begin{pmatrix} \phi_{1} \\ \phi_{2} \\ \vdots \\ \chi_{2}v_{1}\Sigma_{f}^{1} \dots \chi_{2}v_{G}\Sigma_{f}^{G} \\ \vdots \\ \chi_{G}v_{1}\Sigma_{f}^{1} \dots \chi_{G}v_{G}\Sigma_{f}^{G} \end{pmatrix} \begin{pmatrix} \phi_{1} \\ \phi_{2} \\ \vdots \\ \phi_{g} \\ \vdots \\ \phi_{g} \\ \vdots \\ \phi_{G} \end{pmatrix}$$

$$(3.56)$$

It is also convenient to simplify the form of Eq. (3.56) by introducing several matrix operators, **T**, **S** and **F**, such that

$$\mathbf{\Gamma}\Phi = \mathbf{S}\Phi + \frac{1}{k}\mathbf{F}\Phi \tag{3.57}$$

where,

$$\mathbf{T} \equiv \operatorname{diag}\left(\hat{\mathbf{T}}_{1}, \hat{\mathbf{T}}_{2}, \dots, \hat{\mathbf{T}}_{G}\right)$$
(3.58)

$$\mathbf{S} \equiv \begin{pmatrix} \Sigma_{\mathrm{s}}^{1 \to 1} & \dots & \Sigma_{\mathrm{s}}^{G \to 1} \\ \Sigma_{\mathrm{s}}^{1 \to 2} & \dots & \Sigma_{\mathrm{s}}^{G \to 2} \\ \vdots & \ddots & \vdots \\ \Sigma_{\mathrm{s}}^{1 \to G} & \dots & \Sigma_{\mathrm{s}}^{G \to G} \end{pmatrix}$$
(3.59)

and

$$\mathbf{F} \equiv \begin{pmatrix} \chi_1 v_1 \Sigma_{\mathrm{f}}^1 & \dots & \chi_1 v_G \Sigma_{\mathrm{f}}^G \\ \chi_2 v_1 \Sigma_{\mathrm{f}}^1 & \dots & \chi_2 v_G \Sigma_{\mathrm{f}}^G \\ \vdots & \ddots & \vdots \\ \chi_G v_1 \Sigma_{\mathrm{f}}^1 & \dots & \chi_G v_G \Sigma_{\mathrm{f}}^G \end{pmatrix}$$
(3.60)

Also, the group flux vector,  $\Phi$ , is given by,

$$\Phi \equiv (\phi_1 \quad \phi_2 \quad \dots \quad \phi_G)^{\mathrm{T}} \tag{3.61}$$

Next, it is suitable to re-arrange Eq. (3.57) into,

$$(\mathbf{T} - \mathbf{S})^{-1}\mathbf{F}\Phi = k\Phi \tag{3.62}$$

If the above matrix equation is carefully analysed, the operator  $(\mathbf{T} - \mathbf{S})^{-1}\mathbf{F}$  is a square matrix, which has the dimension of  $G \times G$ . So, Eq. (3.62) is actually an eigen-equation with  $\Phi$ , a column vector identified as the eigenvector and the scalar value k as the eigenvalue. Recall that the whole point of neutron transport theory is to solve the neutron flux, which in this case the eigenvector  $\Phi$ . Plus, the existence of the eigenvalue, k, in Eq. (3.62) allow nuclear engineers to use it as a tool for searching the right combination of reactor composition and geometry such that the reactor is critical.

At this level, the readers might question on how to solve the eigen-equation in Eq. (3.62) so that  $\Phi$  and k are determined. One must also note that the reactor composition and geometry will change the characteristics of the square matrix operator  $(\mathbf{T} - \mathbf{S})^{-1}\mathbf{F}$ . Thus, solving the eigen-equation yields a specific value of k and a specific group flux vector,  $\Phi$ . Essentially, the solution of the eigenvalue problem given by Eq.

(3.62) can be accomplished by using the standard common technique in numerical analysis known as the *power iteration method*.

Recall that in a nuclear reactor, neutrons serve as the fission chain reaction carrier. Additionally, a neutron from the previous generation may induce another fission reaction, creating neutrons of the next fission generation. To begin with, it is customary to introduce an integer denoting the current fission generation number, *j*. Firstly, notice that if the group flux vector of the neutron population from the previous fission generation,  $\Phi^{(j-1)}$  is known, then it is possible to determine the group flux vector of the current fission generation,  $\Phi^{(j)}$  using Eq. (3.62), where,

$$\Phi^{(j)} = \frac{1}{k^{(j-1)}} (\mathbf{T} - \mathbf{S})^{-1} \mathbf{F} \Phi^{(j-1)}$$
(3.63)

Unfortunately, the true value of k is unknown and the true group flux vector of the previous generation is not known. Consequently, the issue is resolved by estimating the initial guess of the group flux vector,  $\Phi^{(0)}$  and the initial guess of the effective multiplication factor,  $k^{(0)}$ . Thus,  $\Phi^{(0)}$  and  $k^{(0)}$  are used to obtain  $\Phi^{(1)}$  using Eq. (3.63) whereas  $k^{(1)}$  is estimated using an equation that will be derived later. This successive generation iteration continues until a sufficiently large number of iterations j so that the  $\Phi^{(j)}$  and  $k^{(j)}$  converge to their corresponding true value. The convergence of  $\Phi^{(j)}$  and  $k^{(j)}$  can be proven mathematically. Throughout the iteration, the value of  $k^{(j)}$  and  $\Phi^{(j)}$  are self-adjusted until the combination of these quantities satisfies the eigenequation in Eq. (3.63). Eventually, this successive generation iteration will guarantee to converge regardless of the value of  $\Phi^{(0)}$  and  $k^{(0)}$  prescribed during the starting point of the iteration. For a large number of iterations,

$$\Phi^{(j)} \cong \frac{1}{k^{(j)}} (\mathbf{T} - \mathbf{S})^{-1} \mathbf{F} \Phi^{(j)}$$
(3.64)

Thus, if Eq. (3.64) is integrated over the entire space, it is reasonable to define the current estimate of the effective multiplication factor,  $k^{(j)}$  as,

$$k^{(j)} \cong \frac{\int (\mathbf{T} - \mathbf{S})^{-1} \mathbf{F} \Phi^{(j)} d^3 r}{\int \Phi^{(j)} d^3 r}$$
(3.65)

Finally, by using the above formula it is now possible to compute a new guess of the effective multiplication factor,  $k^{(j)}$ . In summary, the iterative algorithm of finding the solution of the eigenvalue problem deterministically is given in Fig. 3.5.



Figure 3.5: The summary of power iteration algorithm.

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