Chapter 2

The Diffusion Equation and the Steady State

We shall now study the equations which govern the neutron field in a reactor. These equations are based on the concept of local neutron balance, which takes into account the reaction rates in an element of volume and the net leakage rates out of the volume. The reaction rates are written in terms of the local cross sections, assumed known from a pre-processed data base (e.g., ENDF/B-VI). The starting equation is the Maxwell-Boltzmann transport equation, in its integro-differential form. The various approximations required to go from the transport equation to the neutron diffusion equation will first be presented, because all finite-reactor calculations are based on the diffusion approximation. We shall then discuss the multi-group formalism of the diffusion equations and study the mathematical properties of these equations in steady state. That preliminary step will allow us to derive in a more accurate way, in the next chapter, the reactor point-kinetics equations.

In the diffusion approximation, neutrons diffuse from regions of high concentration to regions of low concentration, just as heat diffuses from regions of high temperature to those of low temperature, or rather as gas molecules diffuse to reduce spatial variations in concentration.

While it is sufficiently accurate to treat the transport of gas molecules as a diffusion process, this approach is too limiting for neutron transport. In contrast to a gas, where collisions are very frequent, the cross sections for the interaction of neutrons with nuclei are relatively small, as we saw in chapter 1 (of the order of barns, i.e., 10^{-24} cm^2). This implies that neutrons traverse appreciable distances (of the order of a centimetre) between collisions. This relatively long neutron mean free path, together with the heterogeneity of the physical medium, requires that a more complete treatment be carried out, taking account of variations in the angular distribution of neutron speed in the vicinity of highly absorbing regions (such as the fuel). The Boltzmann transport equation allows an accurate treatment of neutron leakage in the presence of large heterogeneities. While we shall not directly tackle the solution of the transport equations, the derivation of the diffusion equation from the transport equation will allow us to appreciate the degree of approximation of the methods used in finite-reactor calculations.

2.1 Neutron Balance in a Reactor

From a fundamental point of view, the individual fate of neutrons cannot be defined in a deterministic manner. The Heisenberg uncertainty principle and quantum mechanics teach us that only the *probability* of a given fate can be calculated. Thus, if the total number of neutrons in the system under observation is relatively small, fluctuations will be observed in the number and energies of neutrons at a given point. We shall assume here that the neutron density is sufficiently high that one can neglect these statistical variations and predict the *average behaviour of the neutron field* in a deterministic manner. We shall assume in addition that the neutron density is not so high that neutron-neutron interactions must be taken into account. The starting equation for our analysis will be that which describes deterministically the interaction of the neutron field with the field of nuclei., i.e., the Maxwell-Boltzmann neutron transport equation.

2.1.1 Transport Equation

The transport equation, in its integro-differential form, will allow us to describe the neutron balance in an elemental volume in phase space. The fundamental quantity is the angular density of neutrons, $n(\mathbf{r},E,\vec{\Omega},t)$ defined so that $n(r,E,\vec{\Omega},t)\, d^3r\, d^2\Omega\, dE$ represents the number of neutrons at time t in an element of volume $d^3\mathbf{r}$ around point $\mathbf{r}$. These neutrons have energies between E and $E + dE$; if a sphere of unit radius is drawn around point $\mathbf{r}$, the neutrons travel in a direction inside the solid angle $d^2\Omega$ around the radius vector $\vec{\Omega}$ (the vector $\vec{\Omega}$ is thus of unit length). The angular co-ordinates are shown in Figure 2.1.

Neutrons propagate at scalar speed v, function of E:

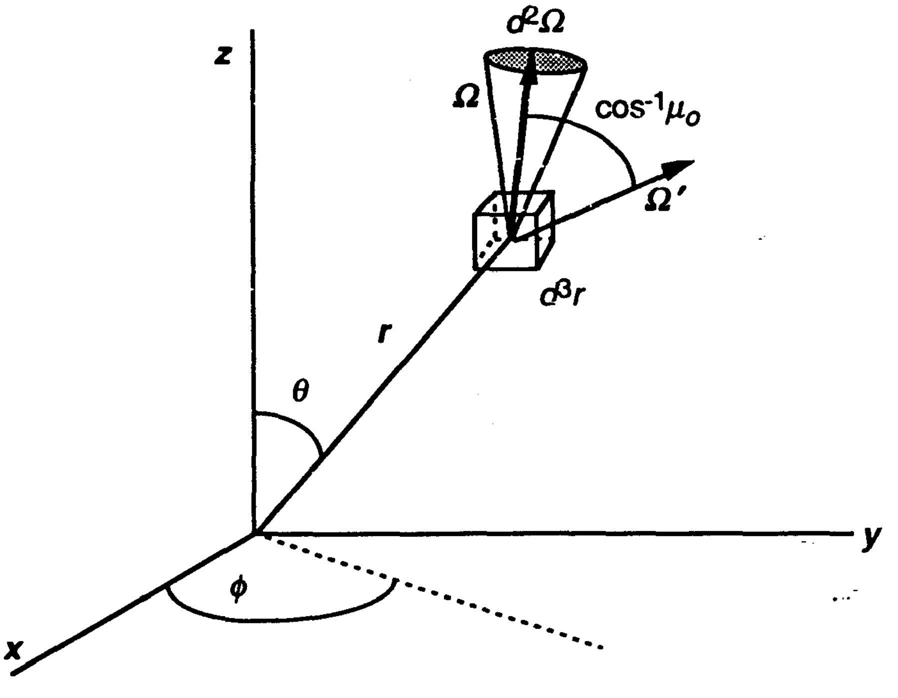
$$v(E) = \sqrt{\frac{2E}{m_0}} \tag{2-1}$$

Given the direction of travel $\vec{\Omega}$ of the neutrons, the velocity *vector* $\vec{v}$ can be written

$$\vec{v}(E) = \vec{\Omega} v(E) \tag{2-2}$$

The density n is continuous, which means that $n(r+s\vec{\Omega},E,\vec{\Omega},t+s/v)$ must be a continuous function of s at all points $\mathbf{r}$ in the domain.

Fig. 2.1 Spherical Coordinates in Transport Calculations



We define also the scalar angular-flux density $\Phi\,(r,E,\vec{\Omega},t)$, and the vector angular-current density $j\,(r,E,\vec{\Omega},t)$, as follows:

$$\Phi\,(r,E,\vec{\Omega},t) = v\;n(r,E,\vec{\Omega},t) \tag{2-3}$$

and

$$j\,(r,E,\vec{\Omega},t) = \vec{\Omega}\,\Phi\,(r,E,\vec{\Omega},t) = \vec{v}\;n(r,E,\vec{\Omega},t) \tag{2-4}$$

The other quantities related to the neutron density are defined in Table 2.1.

Consider now the neutron balance in an element of volume in the 7-dimensional phase space with co-ordinates x, y, z, E, Ω_φ, Ω_θ, and t. The rate of change of the neutron density in the element of volume will of necessity be the result of a difference between the rates of production and removal of neutrons.

The removal of neutrons from the volume element comes about as the result of collisions between the neutrons and the nuclei in the volume, or as the result of the leakage of neutrons out of the volume. Indeed, we assume that if there is a collision and the neutron is not captured by the target, the neutron's final velocity will be different from v and its energy will be different from E, so that the neutron exits from the "hypervolume" element. Consequently, as soon as there is a collision, the neutron disappears from the element of volume.

On the other hand, the production of neutrons within the volume element can result either from collisions or from an independent (external) source q. In order to evaluate the production of neutrons from collisions, one must integrate over all incident speeds and directions, and retain only the collisions which lead to speed v (or energy E) and angle $\vec{\Omega}$. The "collision source" therefore includes neutrons born from fissions[1]. We shall assume that all neutrons emerging from a collision appear instantaneously. That is, we shall neglect delayed-neutron emission for the moment.

Using the notation of Table 2.1, the transport equation *in the absence of delayed neutrons* can be written:

$$\boxed{\begin{aligned}\frac{1}{v}\frac{\partial}{\partial t}\Phi\,(r,E,\vec{\Omega},t) \;=\;& -\Sigma(r,E,t)\,\Phi\,(r,E,\vec{\Omega},t) - \vec{\Omega}\cdot\vec{\nabla}\,\Phi\,(r,E,\vec{\Omega},t)\\ &+ \int_0^\infty dE' \int_0^{4\pi} d^2\Omega'\; g(r;E'\to E,\vec{\Omega}'\to\vec{\Omega})\,\Sigma(r,E',t)\,\Phi(r,E',\vec{\Omega}',t)\\ &+ q(r,E',\vec{\Omega},t)\end{aligned}}$$

(2-5)

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[1] Some authors prefer to treat the fission source separately, by including it for instance in the independent source term.

Referring back to equation 2-3, we see that the left-hand side of equation 2-5 is the time variation of the neutron density.

Let us now consider each term on the right-hand side.

1) Neutrons removed by collision

We have seen in chapter 1 (equation 1-5) that the rate of collisions per unit volume is equal to the product of the total cross section Σ and the flux. The total macroscopic cross section includes neutron scattering and absorption, as in equation 1-7. We shall omit the index t in order to simplify the notation and to avoid confusion with the time dependence of the cross sections (due, for example, to a perturbation or to temperature variations). *We shall assume that cross sections have been averaged with respect to the motion of nuclei.* The dependence of the cross sections on E (the neutron energy, rather than the speed of neutrons relative to the nuclei) will therefore have an implicit dependence on the temperature of the medium.

2) Neutrons removed by leakage

The second term measures neutron loss by leakage in direction $\bar{\Omega}$, by projecting the gradient of the angular-flux density on the direction of propagation Ω. This term gives the number of neutrons which escape from the element of volume without collision. As mentioned previously, this term is large in neutron transport because of the relatively long mean free path of neutrons in matter.

3) Neutrons produced by collisions

Scattering cross sections give no information on the fate of the neutron after a collision. In order to track neutron histories, one needs more information on the post-collision direction and energy of neutrons. This information is provided by the *differential cross section.* We shall use a generalized form for the differential cross sections, viz. $g_x(r; E' \to E, \Omega' \to \Omega)$, i.e., the probability that a neutron of energy E' moving in direction $\bar{\Omega}$, entering in an interaction of type x at point r, will emerge from the collision in a solid angle $d^2\Omega$ around Ω and with an energy between E and $E+dE$. The normalization of g_x is such that:

a) elastic collisions:

$$\int_0^\infty dE \int_0^{4\pi} d^2\Omega\, g_e(\mathrm{r};\, \mathrm{E}' \to \mathrm{E}, \bar{\Omega}' \to \bar{\Omega}) = 1 \tag{2-6}$$

The probability of locating a neutron regardless of its energy E and its direction $\bar{\Omega}$ is thus exactly unity, by definition of elastic (or inelastic) collision.

b) inelastic collisions

$$\int_0^\infty dE \int_0^{4\pi} d^2\Omega\, g_i(\mathrm{r};\, \mathrm{E}' \to \mathrm{E}, \bar{\Omega}' \to \bar{\Omega}) = 1 \tag{2-7}$$

c) radiative capture (n,γ):

$$\int_0^\infty dE \int_0^{4\pi} d^2\Omega\, g_\gamma(\mathbf{r}; E' \to E, \vec{\Omega}' \to \vec{\Omega}) = 0 \tag{2-8}$$

d) (n,2n), (n,3n), ..., reactions:

$$\int_0^\infty dE \int_0^{4\pi} d^2\Omega\, g_{2n,3n...}(\mathbf{r}; E' \to E, \vec{\Omega}' \to \vec{\Omega}) = 2, 3... \tag{2-9}$$

e) fission:

We can assume that fission neutrons are born in isotropic fashion (i.e., with a uniform angular distribution) because, following the formation of the compound nucleus, the incident direction is "forgotten". We saw in chapter 1 that the average number of neutrons emerging from fission is a function of the incident energy *E'*, and that their distribution in energy is given by a spectrum function, $\chi(E)$. We therefore have, *for each fissionable nuclide* at *r*:

$$g_f(E' \to E, \vec{\Omega}' \to \vec{\Omega})d^2\Omega\, dE = \frac{1}{4\pi}\nu(E')\chi(E)\, d^2\Omega\, dE \tag{2-10}$$

Since the spectrum $\chi(E)$ is normalized, we have

$$\int_0^\infty dE \int_0^{4\pi} d^2\Omega\, g_f(E' \to E, \vec{\Omega}' \to \vec{\Omega}) = \nu(E') \tag{2-11}$$

The variation of g_f with *r* originates from the fact that there is in general more than one type of fissionable nuclide at point *r*; g_f depends therefore on the material composition.

Since $\Sigma(r,E)$ is the total cross section, we finally get

$$\int_0^\infty dE \int_0^{4\pi} d^2\Omega\, g_f(E' \to E, \vec{\Omega}' \to \vec{\Omega}) = \frac{\Sigma_e(r,E') + \Sigma_i(r,E') + 2\Sigma_{2n}(r,E') + \nu\Sigma_f(r,E')}{\Sigma(r,E')} \tag{2-12}$$

4) <u>Source Term</u>

The term $q(r,E,\vec{\Omega},t)$ represents a neutron source *independent* of the neutron density in the system (for example, spontaneous fission or an external source).

We note that phase space is 7-dimensional. Equation 2-5 is much too complicated to be solved analytically, except for extremely simple cases. Numerical methods based on discretization of the angular variable (discrete-ordinate method) or methods based on the integral form of the equation (collision-probability methods) allow the numerical solution of the transport equation by computer (Sanchez, 1982; Stamm'ler, 1983; Roy, 1989). However, on account of the highly heterogeneous geometry of reactors and of the complex neutron-energy dependence of the cross sections, transport theory cannot yet be used in finite-reactor analysis.

It is therefore not possible in practice to study the space-time behaviour of neutrons in the entire reactor with transport theory. Instead, it will be necessary to use the Wigner-Seitz approximation, which consists in identifying unit cells in the reactor, in which it is possible to use transport theory to generate average properties (homogeneous macroscopic cross sections). These homogeneous cell properties are then used in diffusion theory to solve for the macroscopic distribution of neutrons in the reactor. That is, the power distribution in a reactor of large size is calculated accurately with diffusion theory, using a pre-processing with transport theory to calculate homogeneous properties (cell calculations).

The transition from transport to diffusion theory, and the condensation and homogenization of cross sections, play a central role in reactor physics. These topics will not be discussed in detail here (see the bibliography). We shall instead assume that homogeneous, macroscopic, multi-group cross sections are known for all regions of the reactor (each fuel bundle, each control mechanism, etc.). This data will be the starting point for our analysis.

2.1.2 Continuity Equation

The independent variable required for the calculation of reaction rates (the power) in a reactor is the scalar flux, not the angular flux density. The scalar flux density $\phi(r,E,t)$ is defined such that $\phi(r,E,t)\,dE$ gives the average number of neutrons at time t with energy between E and $E+dE$ at point r (average over all directions of travel). Formally, the scalar flux density, which allows the evaluation of the reaction rates, is simply the average of the angular flux density, obtained from the transport equation. Thus we have

$$\phi(r,E',t) = \int_0^{4\pi} \Phi(r,E,\vec{\Omega},t) \tag{2-13}$$

This equation suggests that an equation for $\phi(r,E,t)$ can be obtained by integrating transport equation 2-5 over all solid angles Ω (i.e., over 4π).

Let us first consider the collision term. We find easily

$$\int_0^{4\pi} \Sigma(r,E,t)\Phi\,(r,E,\vec{\Omega},t)\;d^2\Omega = \Sigma(\,r,E,t)\phi(r,E,t) \tag{2-14}$$

For the leakage term, we find

$$\int_0^{4\pi} d^2\Omega\,(\vec{\Omega}\cdot\vec{\nabla}\,\Phi) = \vec{\nabla}\cdot\int_0^{4\pi} d^2\Omega\,(\vec{\Omega}\,\Phi) = \vec{\nabla}\cdot\vec{J}\,(r,E,t) \tag{2-15}$$

Let us now consider the integral in the third term on the right-hand side of the transport equation 2-5.

$$I_3 = \int_0^{4\pi} d^2\Omega\,\left[\int_0^{4\pi} dE'\int_0^{4\pi} d^2\Omega'\,g(E'\rightarrow E,\vec{\Omega}'\rightarrow\vec{\Omega})\Sigma(r,E',t)\Phi(r,E',\Omega',t)\right]$$

We note first that the differential scattering cross sections do not depend on the angle of incidence, but on the angle of scattering. Thus, the function g depends only on the angle between directions $\vec{\Omega}$ and $\vec{\Omega}'$. This implies that

$$\int_0^{4\pi} d^2\Omega\, g(E'\to E, \vec{\Omega}'\to \vec{\Omega}) = 2\pi \int_{-1}^{1} d\mu_0\, g(E'\to E, \mu_0) \equiv g(E'\to E) \tag{2-16}$$

where, per Figure 2.1,

$$\mu_0 = \cos\theta_0 = \vec{\Omega}'\cdot\vec{\Omega}$$

By changing the order of integration, we then get

$$\begin{aligned} I_3 &= \int_0^\infty dE'\; g(E'\to E)\, \Sigma(r,E',t) \int_0^{4\pi} d^2\Omega\, \Phi(r,E',\vec{\Omega},t) \\ &= \int_0^\infty dE'\; g(E'\to E)\, \Sigma(r,E',t)\, \phi(r,E',t) \\ &= I_f + I_s \end{aligned} \tag{2-17}$$

This term measures the production rate of all neutrons of energy E from all collisions, since the summation is taken over all incident energies E'. We distinguish between neutrons emerging from fission and those "produced" by (elastic or inelastic) scattering, I_s.

As for this scattering term, we shall simplify the notation by writing

$$I_s = \int_0^\infty dE'\; \Sigma_s(r,E'\to E,t)\, \phi(r,E',t) \tag{2-18}$$

We can assume that the fission source is isotropic, as in equation 2-10. Let $\nu_{pi}(E')$ be the average number of *prompt* neutrons per fission of nuclide i induced by incident neutrons of energy E'. Let also $\chi_{pi}(E)$ be the energy spectrum of these fission neutrons from nuclide i. We get

$$I_f = \sum_i \chi_{pi}(E) \int_0^\infty dE'\, \nu_{pi}(E')\Sigma_{fi}(r,E',t)\, \phi(r,E',t) \tag{2-19}$$

We saw in chapter 1 that the prompt-neutron emission spectrum does not depend strongly on the fissionable nuclide. If we neglect such dependence on the nuclide, we can simplify equation 2-19 and find

$$I_f = \chi_p(E) \int_0^\infty dE'\, \nu_p(E')\Sigma_{fi}(r,E',t)\, \phi(r,E',t) \tag{2-20}$$

where the macroscopic cross section satisfies

$$\nu_p(E)\Sigma_f(r,E,t) = \sum_i \nu_{pi}(E)\Sigma_{fi}(r,E,t) \tag{2-21}$$

The notation $\nu\Sigma_f$ will therefore henceforth, in the rest of this book, imply summation over all fissionable nuclides.

We know that a fraction of neutrons emerging from fission are delayed. Similarly to prompt neutrons, we can consider the delayed-neutron source to be isotropic. We shall suppose for the moment that there exists at time t a certain density $S_d(r,E,t)$ defined so that $S_d(r,E,t)dE$ *gives the number of delayed neutrons appearing at time t with energy between E and E + dE.* The relationship between the delayed-neutron source and the scalar flux will be discussed later.

If we use the equations above and gather all terms, we arrive at the *continuity equation*, which describes neutron conservation in the system:

$$\boxed{\begin{aligned}\frac{1}{v}\frac{\partial}{\partial t}\phi(r,E,t) = & -\Sigma(r,E,t)\phi(r,E,t) - \vec{\nabla}\cdot\vec{J}(r,E,t) + \int_0^\infty dE'\,\Sigma_s(r,E'\rightarrow E,t)\,\phi(r,E',t) \\ & + \chi_p(E)\int_0^\infty dE'\,\nu_p(E')\Sigma_{fi}(r,E',t)\,\phi(r,E',t) + S_d(r,E,t) + S(r,E,t)\end{aligned}} \tag{2-22}$$

where

$$S(r,E,t) = \int_0^{4\pi} d^2\Omega\, q(r,E',\vec{\Omega},t) \tag{2-23}$$

We note that this equation now contains two unknowns, $\phi(r,E,t)$ and $\vec{J}(r,E,t)$, in contrast with the transport equation, which contained only one, the angular flux density $\Phi(r,E,t)$. The presence of the leakage term in the transport equation has led to the appearance of a new independent variable in the continuity equation, the *net current* $\vec{J}(r,E,t)$, itself related to the angular density:

$$\vec{J}(r,E,t) = \int_0^{4\pi} d^2\Omega\,\vec{\Omega}\,\Phi(r,E',\vec{\Omega},t) \tag{2-24}$$

This quantity is *independent of* $\phi(r,E,t)$. It is required to complete the information lost on integrating the transport equation 2-5 over all directions $\vec{\Omega}$.

It is important to note that the continuity equation contains no approximation. It only expresses the neutron balance in terms of the scalar flux and of the current, rather than in terms of the angular density only. However, in order to obtain a solution we shall need to derive an additional relation between $\phi(r,E,t)$ and $\vec{J}(r,E,t)$, to take into account the angular dependence of $\Phi(r,E,t)$. Indeed, *it is not sufficient to integrate over* $\vec{\Omega}$ *to eliminate the effect of dependence with angle.*

It is in actual fact not possible to express $\vec{J}(r,E,t)$ as a function of $\phi(r,E,t)$ exactly. From the definition of the net current in equation 2-24, one could be tempted to try to obtain a relation for $\vec{J}(r,E,t)$ by multiplying the transport equation by $\vec{\Omega}$ before integrating over all angles. Since $\vec{\Omega}$ is a vector, one would need in fact to multiply the equation by each component of $\vec{\Omega}$, i.e., Ω_x, Ω_y, and Ω_z, and then integrate over the 4π solid angle. One would obtain three equations, one for each component of the vector $\vec{J}(r,E,t)$ (Duderstadt, 1976).

Table 2.1 Independant Variables in Neutron Transport

Neutron Speed	$\vec{v} = v\vec{\Omega}$
Angular Flux Density	$\Phi(\mathbf{r},E,\vec{\Omega},t) = v\, n(\mathbf{r},E,\vec{\Omega},t)$
Angular Current Density	$\vec{j}(\mathbf{r},E,\vec{\Omega},t) = \vec{\Omega}\Phi = \vec{v}n$
Scalar Flux Density (cm^{-2}·s^{-1}·eV^{-1})	$\phi(\mathbf{r},E,t) = \int_{4\pi}\Phi(\mathbf{r},E,\vec{\Omega},t)\,d^2\Omega = \langle\Phi\rangle_{\vec{\Omega}}$
Net Current	$\vec{J}(r,E,t) = \langle\vec{j}\rangle_{\vec{\Omega}} = \langle\vec{\Omega}\Phi\rangle_{\vec{\Omega}}$
Scalar Flux (group *g*) (cm^{-2}·s^{-1})	$\phi_g(\mathbf{r},t) = \int_{E_{g-1}}^{E_g}\phi(\mathbf{r},E,t)\,dE = \langle\phi\rangle_{\Delta E_g}$
Scalar Flux (total) (cm^{-2}·s^{-1})	$\phi(\mathbf{r},t) = \int_0^{\infty}\phi(\mathbf{r},E',t)dE' = \langle\phi\rangle_E = \langle\Phi\rangle_{\vec{\Omega},E}$
Total Flux (cm·s^{-1})	$\hat{\phi}(t) = \int\phi(r,t)d^3r = \langle\phi\rangle_{E,V} = \langle\Phi\rangle_{\vec{\Omega},E,V}$
Total Number of Neutrons (population)	$n(t) = \frac{1}{v}\hat{\phi}(t) = \langle n\rangle_{\vec{\Omega},E,V}$
Average Neutron Speed (cm·s^{-1})	$\bar{v} = \dfrac{\langle vn\rangle_{\vec{\Omega},E,V}}{\langle n\rangle_{\vec{\Omega},E,V}}$

The problem with this approach is that the leakage term leads to the appearance of still another unknown, in addition to the current density $\vec{J}(r,E,t)$, viz. the tensorial product

$$\bar{\bar{\Pi}}(\mathrm{r},\mathrm{E},\mathrm{t}) = \int_0^{4\pi} d^2\Omega\ \vec{\Omega}\,\vec{\Omega}\,\Phi(\mathrm{r},\mathrm{E},\vec{\Omega},\mathrm{t}) \tag{2-25}$$

This variable is independent of ϕ and of the current $\vec{J}$. It contains 9 components (whereas the current contains 3). The only way to close the system is to introduce an approximation for the angular variation of the solution, so as not to introduce a new variable each time one integrates the leakage term in the transport equation. It is precisely such an approximation which will lead to the diffusion equation.

2.2 Diffusion Equation

We have seen that an approximation is needed for the angular variation of the angular density in order to express the neutron balance in terms of the scalar flux only, thus allowing the easy calculation of reaction rates from the cross sections (which are assumed known). One would therefore like to limit the angular variation of Φ. An elegant way of limiting the angular variation of the flux is to expand the angular distribution Φ in spherical harmonics, and then limit the sum to a few terms only. Retaining the first $(N+1)$ terms in the expansion gives the P_N approximation to the transport equation. The diffusion approximation corresponds to the P_1 approximation, in which only the first two terms are kept.

2.2.1 P_1 Approximation

In the P_1 approximation, one can show (Bell, 1970) that

$$\Phi(r,E,\vec{\Omega},t) = \frac{1}{4\pi}[\phi(r,E,t) + 3\ \vec{\Omega}\cdot\vec{J}(r,E,t)] \tag{2-26}$$

Substituting equation 2-26 into the transport equation, multiplying by $\vec{\Omega}$ and integrating over all angles, one finds (Duderstadt, 1976)

$$\frac{1}{v}\frac{\partial}{\partial t}\vec{J}(r,E,t) + \frac{1}{3}\vec{\nabla}\phi(r,E,t) + \Sigma(r,E,t)\vec{J}(r,E,t) = \int_0^{\infty} dE'\,\Sigma_{s1}(r,E'\rightarrow E,t)\vec{J}(r,E',t) \tag{2-27}$$

There is no source term in this equation, because of the isotropy of the fission sources (prompt and delayed).

Using the P_1 approximation, one finds therefore two equations, continuity equation 2-22 and equation 2-27, with two unknowns, $\phi(r,E,t)$ and $\vec{J}(r,E,t)$. The system is thus closed. The problem now consists in eliminating $\vec{J}(r,E,t)$, so as to obtain a single equation, in $\phi(r,E,t)$. In order to get there, more approximations will be needed.

Consider first the term in the time derivative, $v^{-1}\partial J / \partial t$. This term will be negligible with respect to the others if we can show that

$$\frac{1}{|\vec{J}|}\frac{\partial|\vec{J}|}{\partial t} \ll v\,\Sigma(r,E,t) \tag{2-28}$$

This is equivalent to saying that the rate of change of the current density is much smaller than the frequency of collisions, $v\Sigma$. The latter being of the order of 10^5 s^{-1} or greater, the rate of change of the current would have to be extremely high to invalidate inequality 2-28. In fact one can show, in mono-energetic transport theory (Weinberg, 1958), that in the absence of approximation 2-28 one obtains not the diffusion equation, but rather a second-order equation (the "telegraph" equation) which displays the properties of a wave equation in addition to those of a diffusion equation. Hypothesis 2-28 is tantamount to neglecting the wavefront which propagates from a perturbation at speed v, and to suppose that *the perturbation is felt instantaneously throughout the reactor*. Given the great speed of neutrons (thermal neutrons of energy 0.0625 eV travel at 2,200 m/s) and the relatively small dimensions of reactors, it is in fact a very short delay time which is neglected.

With the neglect of the first term in equation 2-27, the latter can be rewritten

$$\Sigma(r,E,t)\,\vec{J}\,(r,E,t) - \int_0^\infty dE'\,\Sigma_{s1}(r,E'\to E,t)\,\vec{J}\,(r,E',t) = -\,\frac{1}{3}\vec{\nabla}\,\phi(r,E,t) \tag{2-29}$$

Other assumptions on the anisotropy of the collision law are necessary to isolate $\vec{J}\,(r,E,t)$. One can then write (Duderstadt, 1976)

$$\boxed{\vec{J}\,(r,E,t) = -\,D(r,E)\,\vec{\nabla}\,\phi(r,E,t)} \tag{2-30}$$

where D is the diffusion coefficient, which can be expressed as

$$D(r,E,t) = \frac{1}{3\left[\Sigma(r,E,t) - \overline{\mu}_0\Sigma_s(r,E,t)\right]} = \frac{1}{3\Sigma_{tr}(r,E,t)} \tag{2-31}$$

with μ_0 the average cosine of the scattering angle. In this equation we have also introduced the transport cross section, Σ_{tr}.

We find thus that in certain situations the current density is proportional to the flux gradient. This result is analogous to many other phenomena in physics, and is known as *Fick's Law*. The negative sign in equation 2-30 indicates that neutrons tend to diffuse from high-density regions to low-density regions, just as a gas through a porous partition.

Using equation 2-30 to eliminate $\vec{J}\,(r,E,t)$ in the continuity equation, we finally obtain the *energy- and time-dependent diffusion equation*

$$\boxed{\begin{aligned}\frac{1}{v}\frac{\partial}{\partial t}\phi(r,E,t) = & -\Sigma(r,E,t)\phi(r,E,t) + \vec{\nabla}\cdot D(r,E)\vec{\nabla}\,\phi(r,E,t)\\ & + \int_0^\infty dE'\,\Sigma_s(r,E'\rightarrow E,t)\,\phi(r,E',t)\\ & + \chi_p(E)\int_0^\infty dE'\,\nu_p(E')\Sigma_f(r,E',t)\phi(r,E',t)\\ & + S_d(r,E,t) + S(r,E,t)\end{aligned}} \tag{2-32}$$

We shall simplify the notation by making use of the following linear operators:

- *prompt-neutron production:*

$$F_p\phi = \chi_p(E)\int_0^\infty dE'\,\nu_p(E')\Sigma_f(r,E',t)\phi(r,E',t) \tag{2-33}$$

- *neutron removal (interactions and leakage):*

$$\begin{aligned}M\phi = & -\vec{\nabla}\cdot D(r,E)\vec{\nabla}\,\phi(r,E,t) + \Sigma(r,E,t)\phi(r,E,t)\\ & - \int_0^\infty dE'\,\Sigma_s(r,E'\rightarrow E,t)\,\phi(r,E',t)\end{aligned} \tag{2-34}$$

The diffusion equation can then be cast in the form

$$\boxed{\frac{1}{v}\frac{\partial\phi}{\partial t} = (F_p - M)\phi + S_d(r,E,t) + S(r,E,t)} \tag{2-35}$$

We note that $M\phi$ measures the *net* loss of neutrons. Indeed, by convention we include the elastic-scattering term in the operator M, with a negative sign, indicating it is a gain of neutrons of energy E at point r.

The term $F_p\phi$ measures the rate of production of *prompt* neutrons at time t. It thus does not include the ν_d delayed neutrons due to fissions occurring at time t, these neutrons will appear later. Nor in fact does it include delayed neutrons from earlier fissions. The rate of production of delayed neutrons is taken into account via the term $S_d(r,E,t)$, which we shall discuss in section 2.2.3.

2.2.2 Diffusion Approximation

Let us return for now to the diffusion approximation. The main approximations which were made leading to the diffusion equation are the following:

- the angular flux has only one linear component of anisotropy (P_1 approximation, Eq. 2-26);
- neutron sources, including fission, are isotropic;
- the current density varies slowly, relative to the collision frequency (no neutron waves).

The first of these approximations is the most stringent. It is natural to ask in what circumstances the angular flux varies sufficiently slowly with angle to ensure the validity of the diffusion approximation. Comparisons with transport-theory solutions show that the assumption of a weak angular dependence is invalidated in the following cases (Larsen, 1991; Rulko, 1991):

- near external boundaries of the domain, and near interfaces at which properties change suddenly;
- in the vicinity of localized sources;
- in highly absorbing media.

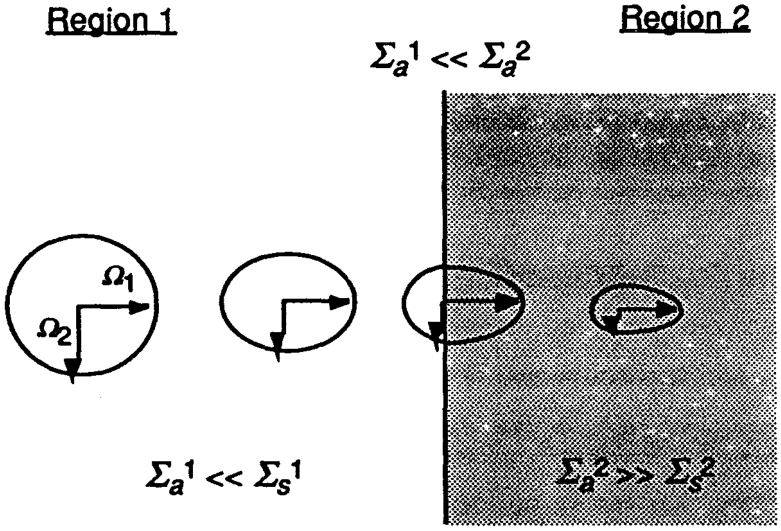
This is illustrated in Figure 2.2, which shows the polar diagram of $n(r,E, \bar{\Omega})$ near an interface between two materials. We assume that the region on the left is of weak absorption and large scattering cross section, while the region on the right is of high absorption.

Let us look first at region 2. Neutrons are strongly absorbed there. Consequently, few neutrons will travel from region 2 to region 1, whereas a large number of neutrons will travel from region 1 to region 2. Near the interface then, $n(r,E, \Omega)$ must be large for those directions Ω pointing towards the interface (e.g., Ω_1). The density $n(r,E, \bar{\Omega})$ will continue to decrease rapidly as one moves away from the interface. Also, the neutron current in the direction from left to right will continue to be greater than that in the opposite direction, even though both currents have diminished due to absorption.

In region 1, where $\Sigma_a \ll \Sigma_s$ neutron scattering will reduce the angular dependence of the current and, at a distance of a few mean free paths, Fick's Law will become a good approximation.

In summary, the diffusion equation applies a few mean free paths inside regions where $\Sigma_s(r,E)$ and $\Sigma_a(r,E)$ do not vary rapidly with position, and in which $\Sigma_a(r,E) \ll \Sigma_s(r,E)$.

Fig. 2.2 Polar Plot of $n(r,E,\vec{\Omega})$ near an Interface



It is natural then to wonder about the applicability of the diffusion equation to finite-reactor calculations, with its strongly absorbing regions such as the fuel and the control mechanisms. One must however remember that the diffusion equation is used to calculate the *macroscopic* flux distribution in the reactor, utilizing properties previously homogenized (by means of transport theory calculations) over unit cells with dimensions much greater than the neutron mean free path. The goal of diffusion calculations is thus, by evaluating the neutron diffusion from cell to cell, to compute the distribution of cell-average reaction rates throughout the reactor.

2.2.3 Delayed-Neutron Source

We note that the delayed-neutron source, $S_d(r,E,t)$ in equation 2-35, is not really independent of the flux, since it depends on the earlier flux level in the reactor ($t'<t$).

We saw in chapter 1 that the delayed-neutron source is directly related to the concentration of the precursor fission products, and that a limited number of precursor groups is sufficient to characterise the source.

Let $C_k(r,t)$ be the concentration of group-k precursors at point r and time t, and let K be the total number of delayed-neutron-precursor groups used (generally 6 for each fissionable isotope and 9 for the photoneutrons). As the delayed neutrons originate from the natural decay of the precursors, the delayed-neutron source can simply be written

$$\boxed{S_d(r,E,t) = \sum_{k=1}^{K} \lambda_k C_k(r,t)\, \chi_{dk}(E)} \tag{2-36}$$

where $\chi_{dk}(E)$ is the normalized spectrum of group-k delayed neutrons. To simplify the notation, and without much error, we have neglected the dependence of the delayed-neutron spectrum χ_{dk}, and of the decay constants λ_k, on the isotope. In addition, we shall use a common set of decay constants to for all isotopes (the yields have to be defined accordingly). The data is found in Tables 1.8, 1.9, and 1.10 of chapter 1.

In order to complete the system of equations, we must now write equations for the evolution of the precursors, which will allow us to calculate the $C_k(r,t)$ in equation 2-36. Since each precursor yields only one neutron and each fission produces ν_{dk} precursors of group k, the evolution of the precursors is governed by

$$\frac{\partial C_k}{\partial t} = -\lambda_k C_k(r,t) + \int_0^\infty dE'\, \nu_{dk}\Sigma_f(r,E',t)\phi(r,E',t) \quad (k = 1,2\ldots K) \tag{2-37}$$

where the sum over fissionable isotopes i is implicit:

$$\nu_{dk}\Sigma_f(r,E,t) = \sum_i \nu_{dki}\Sigma_{fi}(r,E,t) \tag{2-38}$$

The diffusion equation 2-35 is coupled to the precursor evolution equations 2-37. The kinetics problem then reduces to the solution of the system of (K+1) equations 2-35 and 2-37, supplemented by boundary conditions for ϕ and initial conditions for ϕ and the C_k.

2.2.4 Boundary Conditions

Since the diffusion equation 2-35 includes both space and time derivatives, it will be necessary to specify both initial conditions and boundary conditions to complete the description of the problem. The diffusion equation being an approximation to the transport equation, the boundary conditions for the latter will guide the choice of the boundary conditions for the diffusion equation.

a) Initial Conditions

Ideally, initial conditions for the angular flux density must be specified on the entire domain:

$$\Phi(\mathbf{r},E,\vec{\Omega},0) = \Phi_0(\mathbf{r},E,\vec{\Omega}) \tag{2-39}$$

Integrating the initial conditions over solid angles, we obtain easily the initial conditions for the diffusion equation:

$$\phi(r,E,0) = \phi_0(r,E) \tag{2-40}$$

There will also be analogous initial conditions for the precursor concentrations, which will allow the specification of the initial delayed-neutron source in equation 2-35. The two most important types of boundary conditions are those which apply at interfaces between distinct material regions inside the domain, and those which apply at external surfaces of the domain.

b) Conditions at Interfaces

Neutron travel across an interface does not involve the continuity of the angular density. Consider for instance an interface S between two material regions of different cross sections (Figure 2.3). Let Φ_1 and Φ_2 be the flux densities in regions 1 and 2 respectively. The continuity condition on the angular neutron density demands that the following relationship hold at all points r_S on S and for all directions $\vec{\Omega}$:

$$\Phi_1(r_s,E,\vec{\Omega},t) = \Phi_2(r_s,E,\vec{\Omega},t) \tag{2-41}$$

But this condition cannot be satisfied exactly in diffusion theory. Since the latter involves only the first two moments of the angular flux, it will be possible to impose only

$$\int_0^{4\pi} d^2\Omega\ \Phi_1(\mathbf{r}_s,E,\vec{\Omega},t) = \int_0^{4\pi} d^2\Omega\ \Phi_2(\mathbf{r}_s,E,\vec{\Omega},t)$$

that is,

$$\phi_1(r_s,E,t) = \phi_2(r_s,E,t) \tag{2-42}$$

In the same way, multiplying equation 2-41 by $\vec{\Omega}$ and integrating, we get

$$\int_0^{4\pi} d^2\Omega\ \vec{\Omega}\,\Phi_1(r_s,E,\vec{\Omega},t) = \int_0^{4\pi} d^2\Omega\ \vec{\Omega}\,\Phi_2(r_s,E,\vec{\Omega},t)$$

$$\vec{J}_1(r_s,E,t) = \vec{J}_2(r_s,E,t) \tag{2-43}$$

Utilizing equation 2-30, we finally get

$$-D_1\ \nabla\phi_1(r_s,E,t) = -D_2\ \nabla\phi_2(r_s,E,t) \tag{2-44}$$

Therefore, in diffusion theory, the continuity conditions at an interface are simply those which ensure the *continuity of the flux and of the current.* This implies, in particular, that if $D_1 \neq D_2$, the first derivative of the flux will be discontinuous at the interface.

c) External Boundaries (Free surfaces)

Now suppose that S represents the external surface of the domain. In general, we shall assume that the domain is convex. Then, in the absence of a source of neutrons outside the domain, any neutron escaping from the system will not be able to re-enter. The external boundary is a "free surface".

Let $\hat{e}_S$ be the unit out-going vector normal to the surface at a point r_S on the surface (Figure 2.4). Any neutron at the surface travelling in a direction such that $\hat{e}_S \cdot \Omega > 0$ is out-going, while one with $\hat{e}_S \cdot \Omega < 0$ is incoming.

Assuming no re-entrant neutrons, we then have

$$\Phi(\mathbf{r}_s,\mathrm{E},\vec{\Omega},\mathrm{t}) = 0 \quad \text{for } \mathbf{r}_s \in \mathrm{S} \quad \text{and} \quad \vec{\Omega}\cdot\hat{\mathrm{e}}_s < 0 \tag{2-45}$$

Once again, diffusion theory allows only an approximation to this boundary condition (called Marshak's boundary condition). Since the condition applies locally to only half the solid angle, it will be approximated in an integral sense by the following condition:

$$\mathrm{J}_-(\mathbf{r}_s,\mathrm{E},\mathrm{t}) = \int_0^{2\pi} \mathrm{d}^2\Omega\ \hat{\mathrm{e}}_s\cdot\vec{\Omega}\,\Phi(\mathbf{r}_s,\mathrm{E},\vec{\Omega},\mathrm{t}) = 0 \tag{2-46}$$

In diffusion theory, the P_1 approximation for the partial current gives (Bell, 1970):

$$J_-(r_s,E,t) = \frac{1}{4}\phi(r_s,E,t) + \frac{D}{2}\ \hat{e}_s\cdot\vec{\nabla}\phi(r_s,E,t) = 0 \tag{2-47}$$

Fig. 2.3 Flux Continuity at interfaces

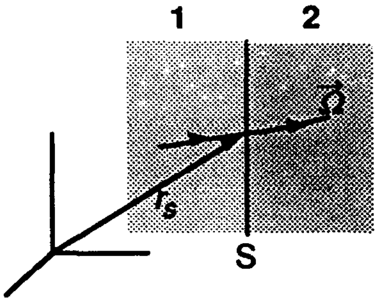
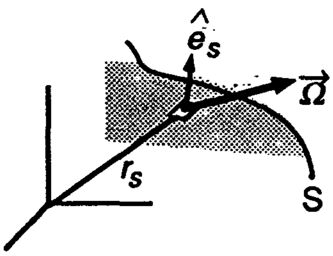


Fig. 2.4 The External Bounddary



This boundary condition can be generalized in the form

$$D(r_s)\,\hat{e}_s \cdot \vec{\nabla}\phi(r_s,E,t) + \frac{1}{2}\left(\frac{1-\alpha}{1+\alpha}\right)\phi(r_s,E,t) = 0 \tag{2-48}$$

where we have introduced the *albedo* α, a positive quantity. The case $\alpha = 0$ reverts to the previous condition. If $\alpha = 1$, we get reflection boundary conditions; these can be used to limit the domain when symmetry exists.

Another form of boundary condition is obtained by demanding that the flux vanish at a certain distance from the physical boundary. By starting from equation 2-47 and extrapolating the flux linearly in the out-going direction, we note that in one dimension it vanishes at the *extrapolation distance*

$$\tilde{x}_s = x_s + 2D = x_s + \frac{2}{3}\lambda_{tr} \tag{2-49}$$

A more detailed treatment (Duderstadt, 1979) gives a more correct value:

$$x_s = x_s + 0.7104\lambda_{tr} \tag{2-50}$$

Finally, it is important to note that the real flux does not go to zero either at the physical boundary or at the extrapolation distance. In fact, in a vacuum, it remains non-zero over an infinite distance. Diffusion theory, using a boundary condition of type albedo (equation 2-48) or of type extrapolation distance (equation 2-50), is valid only within the domain inside a few mean free paths away from the external surface.

2.2.5 Multigroup Formalism

An analytic solution to the time- and energy-dependent diffusion equation is in practice impossible in the large majority of cases. In spite of all the simplifications incorporated in the energy-dependent diffusion equation, the presence of the integral term makes the equation fearsome when applied to finite-reactor calculations. In order to obtain a system of algebraic equations efficiently solvable by computer, it is necessary to further simplify the energy dependence of the diffusion equation, even before considering the spatial discretization of the domain and the application of an appropriate numerical technique for treating differential operators.

We shall briefly describe the multigroup formalism for discretizing the neutron energy domain, which allows the transformation of the energy-dependent diffusion equation into a set of coupled equations in the various energy groups. In this formalism, the operators M and F_p take a matrix form.

Since fission neutrons appear with an energy which can reach 10 MeV, and since they must be slowed to thermal energies (arbitrarily defined as energies $E < 0.625$ eV) before absorption in the fuel, the neutron energy domain spans at least 8 decades, within which cross sections vary in a complex manner. The multigroup formalism consists of reducing the energy dependence to a few energy groups covering the entire domain. It will therefore first be necessary to *condense the cross sections*, in order to reduce their energy dependence to a few group constants.

We have also seen that the diffusion approximation is not valid in the vicinity of a strongly absorbing medium, such as the fuel. It will therefore be necessary to average the cross sections over a larger volume, by including the moderator region, to derive *homogeneous cross sections* allowing the use of diffusion theory.

The approach generally used to perform finite-reactor calculations consists of first effecting a decoupling at the lattice-cell level (with each cell centered around the repeating elements of the lattice, such as the fuel bundles in a CANDU or the fuel clusters in a PWR). Inside the lattice cells, a time-independent transport-theory calculation is performed, assuming reflection boundary conditions (infinite lattice). This calculation provides the microscopic distribution of the neutron flux within the cell, $\psi(r,E)$, which permits the condensation and homogenization of the cross sections *by conserving reaction rates within the unit cells.*

Let us assume that the energy domain has been subdivided into G energy groups. Thus, there will be G energy intervals ΔE_g spanning the neutron energies in the reactor: $E_0 > \ldots > E_g > \ldots > E_G$. Typically, $E_G = 0$ and $E_0 = 15$ MeV. The unknown in the diffusion equation 2-35, the scalar flux density $\phi(r,E,t)$, is interpreted as being the product of a macroscopic scalar flux $\phi(r,t)$, defined over the reactor, and of the microscopic flux $\psi(r,E)$, obtained from the cell calculation:

$$\overbrace{\phi(\mathrm{r},E,t)}^{\substack{\text{scalar flux}\\ \text{density}}} = \overbrace{\phi(\mathrm{r},t)}^{\substack{\text{macroscopic}\\ \text{scalar flux}}} \cdot \overbrace{\psi(r,E)}^{\substack{\text{microscopic}\\ \text{distribution}}} \tag{2-51}$$

The group flux, the solution of the equations to be derived in the multigroup formalism, is formally written

$$\begin{aligned} \phi_g(\mathrm{r},t) &= \int_{E_g}^{E_{g-1}} dE' \ \phi(\mathrm{r},E',t) \\ &= \phi(\mathrm{r},t) \qquad \text{for } E_g < E < E_{g-1} \end{aligned} \tag{2-52}$$

Recall that the group flux $\phi_g(r,t)$ is a scalar quantity, indicating the total *number* of neutrons with energy between E_g and E_{g-1}, while $\phi(r,E,t)$ is a *density*, with $\phi(r,E,t)dE$ giving the number of neutrons between E and $E+dE$. The units of ϕ_g are $cm^{-2}s^{-1}$. In the following, we shall assume that the microscopic flux distribution within the unit cell has been normalized over the cell volume V_{cell}:

$$\frac{1}{V_{cell}}\int_{V_{cell}} d^3r \underbrace{\int_{E_g}^{E_{g-1}} dE'\,\psi(r,E')}_{\psi_g(r)} \qquad = \; 1.0 \tag{2-53}$$

We write all the group fluxes in a column vector $\underline{\Phi}$ of length G (not to be confused with the angular flux):

$$\underline{\Phi} \;=\; \begin{bmatrix} \phi(r,t)_1 \\ \vdots \\ \phi_G(r,t) \end{bmatrix} \qquad \text{(multigroup)} \tag{2-54}$$

In the multigroup formalism, the operators M and F_p in equation 2-35 become GxG matrices. The *neutron removal* operator is

$$M\phi \;=\; [M]\,\underline{\Phi} \;=\; [\mathrm{L}+\mathrm{A}]\,\underline{\Phi} \;=\; L\phi \;+A\phi \tag{2-55}$$

where the leakage operator L and the scattering operator A are

$$L \;=\; \begin{bmatrix} -\nabla\cdot D_1\nabla & 0 & . & 0 \\ 0 & -\nabla\cdot D_2\nabla & . & \vdots \\ \vdots & . & . & 0 \\ 0 & . & 0 & -\nabla\cdot D_G\nabla \end{bmatrix} \tag{2-56a}$$

$$A \;=\; \begin{bmatrix} \Sigma_1 & 0 & \cdot & 0 \\ -\Sigma_{1\to2} & \Sigma_2 & 0 & \cdot \\ \vdots & \cdot & \cdot & \cdot \\ -\Sigma_{1\to G} & -\Sigma_{2\to G} & \cdot & \Sigma_G \end{bmatrix} \tag{2-56b}$$

Note that in the general problem, the cross sections appearing in the matrix operators are all functions of position and of time. Also, the scattering matrix contains no up-scattering terms, i.e., it is assumed neutrons do not gain energy from elastic, or inelastic, collisions.

For the prompt-neutron-production operator, we get

$$F_p\phi \;=\; [\chi_p]\,[F_p]^T\underline{\Phi} \tag{2-57}$$

where the column vector $[\chi_p]$ and the row vector $[F_p]^T$ are

$$[\chi_p] = \begin{bmatrix} \chi_{p1}(r) \\ \vdots \\ \vdots \\ \chi_{pG}(r) \end{bmatrix} \tag{2-58a}$$

and

$$[F_p]^T = [\nu_{p1}\Sigma_{f1}(r,t),\ldots,\ \nu_{pG}\Sigma_{fG}(r,t)] \tag{2-58b}$$

We observe that the prompt fission source (equation 2-57) is the product of a scalar, the rate of production of prompt neutrons, R_f, and a vector, the spectrum χ_p:

$$F_p\phi = [\chi_p]\ \underbrace{\cdot [F_p]^T \underline{\Phi}}_{R_f(r,t) \Rightarrow \text{scalar}} \tag{2-59a}$$

where

$$R_f(r,t) = \sum_{g=1}^{G} \nu_{pg}\Sigma_{fg}(r,t)\phi(r,t) \tag{2-59b}$$

We show a spatial dependence for the spectrum to remember that the fission spectrum is a function of the fuel composition (fissionable isotopes), which can vary with position. We note also that the fission-neutron spectrum is normalized in an analogous fashion with equation 1-15:

$$\sum_{g=1}^{G} \chi_{pg}(r) = 1.0 \tag{2-60}$$

Substituting equation 2-51 into the energy-dependent diffusion equation (equation 2-35), and integrating over energy in each energy group in turn, we obtain the *multigroup diffusion equations*, here shown in matrix form:

$$\boxed{\left[\frac{1}{v}\right]\frac{\partial \underline{\Phi}}{\partial t} = [F_p]\,\underline{\Phi} - [M]\,\underline{\Phi} + \underline{S}_d + \underline{S}} \tag{2-61}$$

where the matrix $[1/v]$ is simply

$$\left[\frac{1}{v}\right] = \begin{bmatrix} \frac{1}{v_1} & 0 & \cdot & 0 \\ 0 & \frac{1}{v_2} & \cdot & \vdots \\ \vdots & \cdot & \ddots & 0 \\ 0 & \cdot & 0 & \frac{1}{v_G} \end{bmatrix} \tag{2-62a}$$

and where the delayed-neutron source $\underline{S}_d$ is the column vector

$$\underline{S}_d = \sum_{k=1}^{K} \lambda_k C_k(r,t) \begin{bmatrix} \chi_{dk1} \\ \vdots \\ \vdots \\ \chi_{dkG} \end{bmatrix} \tag{2-62b}$$

The precursor concentrations are obtained from equation 2-37, with the integral replaced by a sum over the energy groups. The macroscopic group cross sections are derived by *multigroup condensation* in the cell calculation. We shall assume here for simplicity that the microscopic flux distribution $\psi(r,E)$ is known in the lattice cell around r, and that it has been normalized according to equation 2-53. The elements of the matrix operators can the be written:

a) group speeds:

$$\frac{1}{v_g} = \frac{1}{\psi_g(r)} \int_{E_g}^{E_{g-1}} dE \, \frac{\psi(r,E)}{v(E)} \tag{2-63a}$$

b) diffusion coefficient:

$$\nabla \cdot D_g(r) \nabla \psi_g(r) = \int_{E_g}^{E_{g-1}} dE' \; \nabla \cdot D(r,E') \, \nabla \psi(r,E') \tag{2-63b}$$

c) removal cross section:

$$\Sigma_g(r,t) = \frac{1}{\psi_g(r)} \int_{E_g}^{E_{g-1}} dE \left[\Sigma(r,E,t)\psi(r,E) - \int_{E_g}^{E_{g-1}} dE' \, \Sigma_s(r,E' \to E,t)\psi(r,E') \right] \tag{2-63c}$$

d) change-of-energy-group cross section:

$$\Sigma_{h \to g} = \frac{1}{\psi_g(r)} \int_{E_g}^{E_{g-1}} dE \int_{E_h}^{E_{h-1}} dE' \, \Sigma_s(r,E' \to E,t)\psi(r,E') \tag{2-63d}$$

e) production cross section (implicit sum over fissionable isotopes):

$$\nu_p \Sigma_{fg}(r,t) = \frac{1}{\psi(r)} \int_{E_g}^{E_{g-1}} dE \; \nu_p \Sigma_f(r,E,t)\, \psi(r,t) \tag{2-63e}$$

In summary, the multigroup formalism effects a discretization of the quantity E in the energy-dependent diffusion equation. This formalism results in a matrix system of equations (equation 2-61), replacing the integral operator and the continuous energy variable in equation 2-35. From a conceptual point of view, *these two formulations are equivalent.*

In finite-reactor calculations, only a few energy groups are used. For large-size thermal reactors such as the CANDU or the PWR, two energy groups are generally sufficient for design calculations.

Equations 2-61 and 2-37 are continuous in space. They constitute a parabolic system of equations of second order in the partial derivatives, applied to a domain with stepwise-constant properties (the group cross sections having been homogenized over individual cells). The numerical solution of the multigroup equations requires also the discretization of the space variables, leading to a matrix system analogous to the previous one (each element becoming a block matrix). The numerical methods used for space discretization and for the solution of matrix systems will not be discussed in detail here (for the numerical methods, see Nakamura, 1977).

2.3 Time-Independent Equation and Eigenvalue Problem

The neutron balance in the reactor is described by the energy- and time-dependent diffusion equation 2-35, or else by the multigroup equation 2-61. This equation is coupled to the precursor evolution equations 2-37, which allow the tracking of the delayed-neutron source S_d which is present whenever the scalar flux ϕ is non-zero and there is fission. Prior to studying the time-dependent problem in the next chapter, let us now consider the neutron field in a reactor in *steady state*. It will first be necessary to determine whether a steady state is indeed possible, whether in the presence or in the absence of the external source S in the balance equation. This will lead us to introduce the concept of reactor criticality[2].

2.3.1 Steady State and Criticality

Let us first consider the role of each term in the diffusion equation, which we can rewrite as

$$\frac{1}{v}\frac{\partial\phi}{\partial t} = \overbrace{\underbrace{F_p\phi}_{\text{Prompt}} + \underbrace{S_d}_{\text{Delayed}} + S}^{\text{Production}} - \overbrace{M\phi}^{\text{Removal}} \tag{2-64}$$

It is obvious that a steady state can exist in a reactor only if the rate of production of neutrons is exactly equal to the rate of removal at each point of the domain. Indeed, it is evident from equation 2-64 that if the neutron production (including prompt neutrons, delayed neutrons, and neutrons from the external source) at a point r is greater than the neutron removal (by absorption and leakage), the density of neutrons of energy E around r will increase. By summing over all energies and over the entire volume, it can be verified whether the global population of neutrons (i.e., the fission rate and the reactor power) increases or decreases. A steady state therefore implies that the balance is satisfied *at each point of the domain.*

Let us assume for now that there is no external neutron source in the reactor, i.e., that $S(r,E,t) = 0$. Let us also hypothesize that a steady state exists. The cross sections which enter the operators M and F are constant, as is the scalar flux:

$$\frac{1}{v}\frac{\partial\phi}{\partial t} = 0$$

$$\phi(r,E,t) = \phi_0(r,E) \tag{2-65}$$

In the absence of an external source, the diffusion equation 2-35 becomes

$$(F_{p0} - M_0)\,\phi_0(r,E) + S_{d0}(r,E) = 0 \tag{2-66}$$

with

$$F_{p0}\,\phi_0 = \chi_p(E)\int_0^{\infty} dE'\,\nu_p\Sigma_f(r,E')\phi_0(r,E') \tag{2-67}$$

$$\begin{aligned} M_0\,\phi_0 = {} & -\vec{\nabla}\cdot D(r,E)\vec{\nabla}\phi_0(r,E) + \Sigma(r,E)\phi_0(r,E) \\ & - \int_{E'} dE'\,\Sigma_s(r,E'\rightarrow E)\phi_0(r,E') \end{aligned} \tag{2-68}$$

and

$$S_{d0}(r,E) = \sum_{k=1}^{K} \lambda_k C_{k0}(r)\chi_{dk}(E) \tag{2-69}$$

---

[2] In the following we shall use the "continuous" notation of equation 2-35.

The steady-state delayed-neutron source can be found by setting the derivative in equation 2-37 to zero:

$$\frac{\partial C_k}{\partial t} = 0 \Rightarrow \lambda_k C_{k0}(r) = \int_0^\infty dE' \nu_{dk} \Sigma_f(r,E') \phi_0(r,E') \tag{2-70}$$

Substituting this result in equation 2-69, we get

$$\begin{aligned} S_{d0}(r,E) &= \sum_{k=1}^{K} \chi_{dk}(E) \int_0^\infty dE' \nu_{dk} \Sigma_f(r,E') \phi_0(r,E') \\ &= F_{d0}\phi_0 \end{aligned} \tag{2-71}$$

In order to simplify the notation, we shall drop the subscript *0*, since all terms are time-independent. The fission-source term can then be written

$$\begin{aligned} F\phi = (F_p + F_d)\,\phi = {} & \chi_p(E) \int_0^\infty dE' \nu_p \Sigma_f(r,E') \phi(r,E') \\ & + \sum_{k=1}^{K} \chi_{dk}(E) \int_0^\infty dE' \nu_{dk} \Sigma_f(r,E') \phi(r,E') \end{aligned} \tag{2-72}$$

We can simplify further by writing the fission operator as a function of the total spectrum. Neglecting the dependence of ν_p and ν_{dk} on the energy E' of the incident neutron - but not their dependence on the fissionable isotope, implicit in the previous equations 2-21 -we define the *total spectrum*:

$$\chi(E) = \frac{\nu_p \chi_p(E) + \sum_{k=1}^{K} \nu_{dk} \chi_{dk}(E)}{\nu} \tag{2-73}$$

or, using the definition of delayed-neutron fraction,

$$\chi(E) = (1-\beta)\chi_p(E) + \sum_{k=1}^{K} \beta_k \chi_k(E) \tag{2-74}$$

The *total steady-state fission source* can therefore be expressed as follows in terms of the total spectrum and of the production cross section $\nu\Sigma_f$:

$$F\phi = \chi(E) \int_0^\infty dE' \nu \Sigma_f(r,E') \phi(r,E') \tag{2-75}$$

Note that the form of equation 2-75 has been simplified to lighten the notation. It is not an approximation, as we could use the exact form 2-72 of the equation, in which we would show the sum over all fissionable isotopes.

In steady state and *in the absence of an external source*, the diffusion equation reduces to

$$\overbrace{\mathbf{M}\,\phi}^{\text{Losses}} = \overbrace{\mathbf{F}\,\phi}^{\text{Production}} \tag{2-76}$$

From the point of view of physics, this equation simply states the following:

- For a steady state to exist in a reactor in the absence of an external source of neutrons, the number of neutrons produced *at each point of the domain* must be exactly equal to the number of neutrons removed, including leakage to other regions or to the exterior of the domain. In such a case, the reactor is said to be *critical.*

The importance of equation 2-76 is that it allows us to verify this statement for a particular case, to the extent that the geometry and the properties of the reactor are well known. Indeed, everything we have learned to this point is limited to counting neutrons according to the rules which govern the transport of neutrons in matter. A reactor will therefore be critical, in the absence of an external source, if the production of neutrons is equal to their removal. If the production is greater than the removal, the flux level will increase and equation 2-76 does not apply. In this case the reactor is *supercritical,* and the only way to predict the neutron behaviour will be to solve the time-dependent diffusion equation 2-59. If in contrast the production is smaller than the removal, the reactor is *subcritical.*

From the mathematical point of view, the time-independent diffusion equation 2-76 is a *homogeneous equation* which has only a trivial solution ($\phi = 0$), unless the reactor is critical, that is, unless its properties are such as to ensure neutron balance. Since the operators M and F are *linear,* this critical condition translates mathematically to a discretized matrix with a zero determinant. The linearity of the operators[3] also implies that *the neutron flux level in a critical reactor is arbitrary.* The criticality of a reactor is thus defined solely by its properties, in the absence of an external source. It does not depend on the flux level in the reactor, although it is necessary to solve the diffusion equation and calculate the flux distribution to verify criticality.

Let us now consider the case where there is an external source. If we hypothesize a steady state, we find once again the time-independent diffusion equation 2-76, only with an additional source term. If ϕ_S is the steady-state flux, we have

$$\overbrace{\mathbf{F}\,\phi_S}^{\text{Fission}} + \overbrace{S}^{\substack{\text{Independent}\\ \text{Source}}} = \overbrace{\mathbf{M}\,\phi_S}^{\text{Losses}} \tag{2-77}$$

Equation 2-77 leads to two important observations:

- For a reactor steady state to exist *in the presence of an external source,* the reactor must necessarily be *subcritical.* The neutron production by fission then being smaller than the neutron removal, the difference will be compensated exactly by neutrons from the external source.
- The *flux level* in a steady-state subcritical reactor, ϕ_S, *is not arbitrary,* in contrast to the critical state in the absence of an external source. In the subcritical reactor, the steady-state flux level is proportional to the intensity of the external source, which will also influence the flux distribution.

In summary, a steady state is possible in a reactor only in one of two distinct situations: either there is no external source and the reactor is critical, or there is an external source and the reactor is subcritical. On the other hand, if the reactor is supercritical, the neutron flux increases indefinitely, with or without an external source. If the reactor is subcritical and there is no external source, the flux eventually vanishes.

---

[3] It is easy to show that $M(a\phi) = aM(\phi)$ and $F(a\phi) = aF(\phi)$, where a is any constant.

2.3.2 Effective Multiplication Constant and Static Reactivity

Power reactors generally do not use external neutron sources. Consequently, *in normal operation, power reactors are in general critical.* It is then easy to understand the reactor designer's desire to be able to verify *a priori* (before construction) that the configuration selected for the reactor corresponds indeed to a critical state.

Let us consider for example the calculation for a particular reactor, without an external source. This reactor is characterized by a set of cross sections, $\Sigma(r)$. One cannot know in advance whether criticality will be satisfied, unless one solves equation 2-76 for this reactor. Solving the time-independent problem of equation 2-76 therefore implicitly assumes that the physical properties of the reactor allow criticality. However, a small difference between the production and removal of neutrons would lead to a neutron population changing with time. That small difference can indeed reflect a real situation. In such a case, either the model of the reactor is incomplete or the reactor design is incorrect. Or else the difference could be due to uncertainties in the values of the cross sections, even if the reactor is in fact critical.

In order to ensure that we get a non-trivial solution whenever we solve equation 2-76, we introduce a constant, λ, called the ***eigenvalue***, which will be used as a multiplier on the fission-source term. We adjust this constant artificially so that the neutron balance corresponding to criticality is satisfied. In practical terms, this is equivalent to varying artificially the number of neutrons emitted per fission until the neutron production is equal to the removal. Any system containing fissionable material can be made critical by arbitrarily varying the number of neutrons emitted per fission. There must therefore always be a positive solution for ϕ and for λ. The modified equation is thus

$$\boxed{M\phi = \lambda F \phi} \tag{2-78}$$

Note that the *same* constant λ is applied at *all* points of the domain, and that it is necessarily positive (since the neutron flux must be positive).

Mathematically speaking, there may be a large number of *distinct eigenvalues* which satisfy equation 2-78. To these distinct eigenvalues are associated *distinct eigenfunctions*[4]. For greater generality, we should thus write the time-independent diffusion equation as

$$\boxed{M\phi_{(n)} = \lambda_{(n)} F \phi_{(n)}} \tag{2-79}$$

Here the $\phi_{(n)}$ are the eigenvalues (harmonics) of the problem. Only the *fundamental mode* $\phi_{(0)}$ is everywhere positive, and it is the only one which represents a physical quantity (the scalar flux). In the following, the scalar flux of equation 2-78 thus corresponds to the fundamental mode of equation 2-79:

$$\phi(r,E) = \phi_{(0)}(r,E) \tag{2-80}$$

We note also that the harmonics appear in the following *natural order*:

$$\lambda_{(0)} < \lambda_{(1)} < \lambda_{(2)} \tag{2-81}$$

---

[4] In the case of degeneracy, several eigenfunctions may possess the same eignevalue.

The *flux distribution* in a critical reactor can therefore be obtained by solving equation 2-79 for $\phi_{(n)}$. Recall that this equation does not allow the determination of the absolute value of the flux. An additional condition is needed to normalize ϕ. As far as the eigenvalue and the flux distribution go, the normalization is arbitrary. To obtain the absolute flux value, one often uses normalization to the total reactor power P_0. To illustrate, if κ is the average energy released per fission, the *normalization condition* would be written

$$P_0 = \int_V d^3r \int_0^\infty dE'\, H(r,E')\phi(r,E') \tag{2-82}$$

where

$$H(r,E) = \kappa \Sigma_f(r,E) \tag{2-83}$$

The physical meaning of the eigenvalue λ is important. It can be shown that the eigenvalue is simply the inverse of the *effective multiplication constant* k_{eff}, a quantity which springs from the consideration of successive generations of neutrons in fundamental reactor theory.

Intuitively, think of a reactor where the flux level is maintained constant in time, *on average*, by a chain reaction. Under such conditions, k_{eff} is defined as the ratio of the number of neutrons in successive generations, with fission the event separating generations (Lamarsh, 1965). In a critical reactor, the chain reaction is maintained on the strength of k_{eff} being equal to 1.0. Let us now see how the value of k_{eff} can be obtained from diffusion theory, using the approach employed by Bell (1970) with transport theory.

Consider a multiplying medium in which is introduced a pulse source $S(r,E,t)$ at $t=0$. We assume there are no neutrons in the system initially. If δ represents the Dirac delta function, we write

$$S(r,E,t) = S_1(r,E)\delta(t) \tag{2-84}$$

The neutrons from the pulse source constitute the neutrons of the first generation, which we shall denote $\phi_1(r,E,t)$. All the neutrons of each generation will disappear either by absorption (including that leading to fission) or by leakage out of the system. The neutrons produced by fissions induced by first-generation neutrons are the neutrons of the second generation, and so on. Thus, the first-generation neutrons, ϕ_1, will satisfy equation 2-64, where fission appears within the absorption term:

$$\frac{1}{v}\frac{\partial \phi_1}{\partial t} = S(r,E,t) - M\phi(r,E,t) \tag{2-85}$$

Neutrons from the pulse source diffuse throughout the system and eventually disappear. Integrating equation 2-85 over all time, the left-hand side becomes

$$\begin{aligned} \int_0^\infty \frac{\partial \phi_1}{\partial t} dt &= \phi_1(r,E,\infty) - \phi_1(r,E,0) \\ &= 0 \end{aligned} \tag{2-86}$$

Let φ_1 denote the total neutron flux in the first generation:

$$\varphi_1(r,E) = \int_0^\infty \phi_1(r,E,t)dt \tag{2-87}$$

Integration of equation 2-85 over time thus gives

$$M\varphi_1(r,E) = S_1(r,E) \tag{2-88}$$

The neutron source in the second generation can be obtained by integrating appropriately over neutrons of the first generation:

$$\begin{aligned} S_2(r,E) &= \int_0^\infty dt[F_p\phi_1(r,E,t) + S_{dl}(r,E,t)] \\ &= F\varphi_1(r,E) \end{aligned} \tag{2-89}$$

Indeed, integrating the delayed-neutron source over all time gives the steady-state emission spectrum (equation 1-28). This source can therefore be used to find the neutrons of the second generation and those of the third generation. There is in fact here an iterative procedure which allows the calculation of the neutron flux in any generation from the flux in the previous one:

$$M\varphi_i(r,E) = F\varphi_{i-1}(r,E) \tag{2-90}$$

From this recursion relation 2-90, we can expect that the neutron density will increase from one generation to the next if the system is supercritical, that it will decrease if the system is subcritical, and will become constant if the system is critical. In any case, we can expect the ratio of densities (fluxes) in successive generations to become constant, independent of r and of E:

$$\begin{aligned} \lim_{i\to\infty} \frac{\varphi_i(r,E)}{\varphi_{i-1}(r,E)} &= \text{constant} \\ &= k_{eff} \end{aligned} \tag{2-91}$$

Comparing equations 2-90 and 2-78, we find

$$\lambda = \frac{1}{k_{eff}} \tag{2-92}$$

Equations 2-90 and 2-91 serve in fact in general as an iterative procedure for the calculation of the eigenvalue (by the *method of powers*). It will thus be easy to verify whether the multiplying system is critical by calculating the eigenvalue λ and comparing it to 1.0. The difference between λ and 1 is a measure of the non-criticality of the medium. This difference is called the *static reactivity*, ρ_S:

$$\boxed{\rho_s = 1 - \lambda = \frac{k_{eff} - 1}{k_{eff}}} \tag{2-93}$$

The static reactivity is thus a measure of the degree of adjustment which would have to made to the system to make it critical (for instance, by the insertion of the reactor control mechanisms). This quantity is of great interest in reactor studies. In the following section, we shall study the sensitivity of this quantity to various perturbations or modifications which can be made to the system.

2.4 Perturbation Theory and Flux Adjoint

Power reactors are highly heterogeneous. Let us consider for instance the CANDU 6. This reactor has 380 fuel channels (≈ 10 cm in diameter and 600 cm long), arrayed in a square lattice on a 28.6-cm lattice pitch. The space between channels is filled with heavy water, which serves as the moderator. Reactivity devices are inserted at various locations in the moderator, as part of the reactor regulating system. Each channel contains 12 fuel bundles, which can be moved axially along the channel. The reactor is refuelled on-line, with a small fraction of the fuel load replaced each day on the average. In view of the changes in fuel composition with burnup during reactor operation, each fuel bundle can be considered to have different properties. Finally, the reactor core is surrounded by a radial reflector of thickness ≈ 60 cm, consisting of heavy water only.

Cell calculations can give us homogenized cross sections in two neutron energy groups for each lattice cell (fuel bundle and its surrounding moderator). Transport calculations in 3 dimensions can be performed on supercells defined around the reactivity mechanisms in order to homogenize their properties over the neighbouring lattice cells. The two-energy-group properties of the reflector complete the data set which is used to carry out diffusion-theory calculations for the entire reactor.

The time-independent diffusion equation 2-78 is thus applied over a domain containing a large number of material regions[5], typically of the order of 10,000. In its multigroup form, it is in fact a set of G partial differential (elliptic) equations of second order, with $G \times N$ unknowns, N being the number of variables appearing from the spatial discretization. N is generally greater than the number of material regions, because many variables are introduced in discretizing the leakage term, which contains derivatives. The method used to satisfy the continuity equations 2-42 and 2-44 at the interfaces between the finite elements (material regions) can also govern the number of unknowns.

The number of equations for the discretized system can thus easily reach 50,000. In addition, the eigenvalue problem requires outer iterations on the eigenvalue, as seen earlier (equation 2-89). Even when using convergence acceleration techniques (Hébert, 1985), of the order of 50 iterations will be required. While this type of calculation is easily performed on a computer, its cost (in computer time) is not negligible.

It is important to remember that a reactor design is the end product of a long process. For each core configuration, the diffusion calculation is performed to determine the power distribution that would be obtained *if* the reactor were critical (the reference distribution). This calculation also gives an eigenvalue for each configuration, which is a measure, as we saw earlier, of the reactivity difference between the actual configuration and a critical state. Taking into account the large number of design variables to be optimized, the detailed design of the reactor core can require several thousand diffusion calculations.

In many cases, what is of interest are the variations in k_{eff} due to "perturbations" (minor design variations, small changes in device positions, etc.), whereas the perturbed flux is not really required, because the perturbations to the flux are considered localized or negligible. In this section, we shall discuss perturbation theory, which allows the evaluation of changes in the eigenvalue *without the need for a new diffusion calculation for the perturbed system.*

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[5] In the context of a diffusion calculation, a material region is a sub-volume within which the cross sections are uniform.

Such perturbation calculations give great computational savings. However, what is even more important for us is that perturbation theory introduces intrinsic properties of a critical system which will influence the manner of defining kinetic parameters in the next chapters. Recall indeed that most transients studied in reactor kinetics are those of a reactor which differs only very slightly from criticality.

A mathematical review will allow us to simplify the presentation which will follow.

MATHEMATICAL REVIEW

The vectorial space to which the solutions to the diffusion equation belong consists of the set of real functions which are analytical on the domain $\{r \in V,\ E_G < E < E_0\}$ and which satisfy the flux and current continuity conditions (equations 2-42 and 2-44 respectively) at the interfaces between the material regions which make up the reactor, and the boundary conditions (equation 2-48) at the external surface delimiting the reactor volume V.

Let $f(\mathbf{r},E)$ and $h(\mathbf{r},E)$ be two elements in this vectorial space. In the multigroup formalism (equation 2-61), the elements of the space are the column vectors $\underline{f}$ and $\underline{h}$, whose G components are group spatial distributions defined over volume V.

A function which defines a correspondence between an element or set of elements of the vectorial space and a (real or complex) number is called a functional. One functional of interest isthe internal (or scalar) product of two elements, which is written

$$\langle f,h\rangle = \int_V d^3r \int_0 f(r,E)\cdot h(r,E) \tag{2-94}$$

In matrix notation (multigroup formalism), this is written

$$\begin{aligned}\langle \underline{f},\underline{h}\rangle &= \langle \underline{f}^T \cdot \underline{h}\rangle \\ &= \sum_{g=1}^{G} \int_V f_g(\mathrm{r})\cdot h_g(\mathrm{r})\ d^3r\end{aligned} \tag{2-95}$$

Let A be an operator which transforms a vector into another in this vectorial space. The operator A^* is the *adjoint operator* to A if the following relation is true for all f and h in the space:

$$\boxed{\langle f, Ah\rangle = \langle A^* f, h\rangle} \tag{2-96}$$

It is easy to show that the following rules apply for the construction of an adjoint operator:

- *real matrix:*

$$\begin{aligned}A &= [A] \\ A^* &= [A]^T \qquad \text{(transpose)}\end{aligned}$$

- *differential operator*:

$$A = d^n/dt^n$$

$$A^* = (-1)^n \left(\frac{d^n}{dt^n}\right)$$

Odd-numbered derivatives change sign. When the independent variable is time, initial conditions become final conditions.

- *integral operator*:

$$f(x) = Ah(x) = \int K(x,x')h(x')dx'$$

$$f^*(x) = A^*h(x) = \int K(x'x)h(x')dx'$$

To find the adjoint to an integral operator, one inverts the order of integration (interchanging the arguments of the kernel of the operator).

2.4.1 First-Order Perturbation Theory

The objective of this section is to obtain an expression for the change or the variation in the eigenvalue due to a perturbation or modifications to the material properties of the reactor. The expression is to be a function of the eigenvalue and of the flux, assumed known, in the unperturbed system. The situation envisaged is summarized in Table 2.2.

Table 2.2 Application of a Perturbation

Reference System	Perturbed System
Non-perturbed reactor for which the flux ϕ_o has already been calculated according to: $M_o \phi_o = \lambda_o F_o \phi_o$ (2-97)	Reactor for which we wish to find λ from: $\lambda = \lambda_o + \Delta\lambda$ $M = M_o + \Delta M$ (2-98) $F = F_o + \underbrace{\Delta F}_{\text{Perturbation}}$

The change in the static reactivity which accompanies the perturbation is equal to the change $\Delta\lambda$ in the eigenvalue, but of opposite sign:

$$\begin{aligned}\Delta\lambda &= \lambda - \lambda_o \\ &= \left(1 - \frac{1}{k_{eff,0}}\right) - \left(1 - \frac{1}{k_{eff}}\right) \\ &= \rho_o - \rho \\ &= -\Delta\rho\end{aligned} \tag{2-99}$$

We would like to calculate $\Delta\lambda$ without knowing the flux distribution in the perturbed system, that is, we would like to avoid solving the diffusion equation again for the perturbed system:

$$M\phi = \lambda F\phi \tag{2-100}$$

Note that the operator ΔM in equation 2-98 contains a perturbation to the differential operator $-\vec{\nabla}\cdot D\vec{\nabla}$. For the leakage term, it will thus not be possible to express the perturbation with a simple difference of cross sections only. One will need to write

$$\begin{aligned}\Delta L &= -\vec{\nabla}\cdot D\vec{\nabla} + \vec{\nabla}\cdot D_0\vec{\nabla} \\ &\neq -\vec{\nabla}\cdot(\Delta D)\vec{\nabla}\end{aligned}$$

The notation ΔM must thus be understood as an abbreviation for the operator $(M - M_0)$. ϕ_0 is the known unperturbed flux and ϕ the unknown perturbed flux, solution to equation 2-100. Let us write

$$\phi(r,E) = \phi_0(r,E) + \Delta\phi(r,E) \tag{2-101}$$

and let us substitute equation 2-101 into equation 2-100. Keeping in mind equation 2-99, we get

$$M\phi_0 = \lambda F\phi_0 - (M-\lambda F)\Delta\phi \tag{2-102}$$

We also have

$$\begin{aligned}\lambda F\phi_c &= \lambda(F_0 + \Delta F)\phi_0 \\ &= \lambda F_0\phi_0 + \lambda_0\Delta F\phi_0 + \underbrace{\Delta\lambda\Delta F\phi_0}_{2nd\,order} \\ &\approx \lambda F_0\phi_0 + \lambda_0\Delta F\phi_0\end{aligned} \tag{2-103}$$

Substituting this into equation 2-102, we find

$$M\phi_0 = \lambda F\phi_0 + \lambda_0\Delta F\phi_0 - (M-\lambda F)\Delta\phi \tag{2-104}$$

This relation is true (to first order) at each point of the domain. On the other hand, the quantity we want, $\Delta\lambda$, is a *scalar*. In order to preserve as much generality as possible, we shall use *all* the points of the domain to calculate $\Delta\lambda$, by integrating equation 2-104 over the entire domain (space and neutron energy).

The sensitivity of λ to arbitrary perturbations is not necessarily the same for all points or all energies of the domain. To preserve as much generality as possible in the calculation of $\Delta\lambda$, we multiply equation 2-104 by *an arbitrary weighting function* ϕ^W before integrating over r and E. Thus $\phi^W(r,E)$ will weight the contribution of each point (r,E) in the integral. We assume also that ϕ^W belongs to the same vectorial space as the solution. Integrating the equation and making use of definition 2-94, we find the following relation between the internal products:

$$\left\langle \phi^w, M\phi_0 \right\rangle \approx \lambda\left\langle \phi^w, F_0\phi_0 \right\rangle + \lambda_0\left\langle \phi^w, \Delta F\phi_0 \right\rangle - \left\langle \phi^w, (M-\lambda F)\Delta\phi \right\rangle \qquad (2\text{-}105)$$

From equation 2-97, we have

$$\left\langle \phi^w, M_0\phi_0 \right\rangle = \lambda_0\left\langle \phi^w, F_0\phi_0 \right\rangle \qquad (2\text{-}106)$$

Subtracting this equation from 2-105, we get

$$\left\langle \phi^w, (\Delta M - \lambda_0\Delta F)\phi_0 \right\rangle \approx \Delta\lambda\left\langle \phi^w, F_0\phi_0 \right\rangle - \left\langle \phi^w, (M-\lambda F)\Delta\phi \right\rangle \qquad (2\text{-}107)$$

Note that only the second term on the right is a function of the perturbed flux. The other terms are in the known flux, ϕ_0. Since ϕ^W is arbitrary, there may be a particular choice which makes the second term on the right disappear, *regardless of* $\Delta\phi$. In such a case relation 2-107, from which $\Delta\lambda$ will be derived, will be a function of the known unperturbed flux ϕ_C only. Let us therefore examine the second term in equation 2-107. We note that

$$\begin{aligned}\left\langle \phi^w, (M-\lambda F)\Delta\phi \right\rangle &= \left\langle \phi^w, (M_0-\lambda_0 F_0)\Delta\phi \right\rangle \\ &+ \left\langle \phi^w, (\Delta M-\lambda_0\Delta F-\Delta\lambda F_0)\Delta\phi \right\rangle \quad \text{(2nd order)} \\ &- \Delta\lambda\left\langle \phi^w, \Delta F\Delta\phi \right\rangle \quad \text{(3rd order)}\end{aligned} \qquad (2\text{-}108)$$

Since we limited equation 2-107 to first order, we shall keep only the first term on the right in equation 2-108. This last relation then tells us that we can eliminate the second term on the right in equation 2-107, *if* we can show that

$$\left\langle \phi^w, (M_0-\lambda_0 F_0)\Delta\phi \right\rangle = 0 \qquad (2\text{-}109)$$

But there is indeed a particular choice for the weighting function ϕ^W which satisfies equation 2-109, *regardless of* $\Delta\phi$. This choice is the *adjoint flux*, solution to the adjoint equation for the unperturbed system:

$$M_0^*\phi_0^* = \lambda_0^* F_0^*\phi_0^* \qquad (2\text{-}110)$$

Let us multiply equation 2-97 by ϕ_0^* and equation 2-110 by ϕ_0. Then let us integrate both equations over the entire domain and subtract, to find

$$\begin{aligned}\left\langle \phi_0^*, M_0\phi_0 \right\rangle - \left\langle \phi_0, M_0^*\phi_0^* \right\rangle &= (\lambda_0-\lambda_0^*)\left\langle \phi_0, F_0^*\phi_0^* \right\rangle \\ &= 0\end{aligned} \qquad (2\text{-}111)$$

This result is immediate, by definition of the adjoint operator M_0^*. Since

$$\langle \phi_0, F_0^* \phi_0^* \rangle > 0$$

we have

$$\boxed{\lambda_0^* = \lambda_0} \tag{2-112}$$

It will then be advantageous to choose the adjoint flux as weighting function in equation 2-109:

$$\boxed{\phi^w = \phi_0^*} \tag{2-113}$$

because then equation 2-109 becomes an identity:

$$\langle \phi_0^*, (M_0 - \lambda_0 F_0)\Delta\phi \rangle = \Big\langle \underbrace{(M_0^* - \lambda_0 F_0^*)\phi_0^*}_{0}, \Delta\phi \Big\rangle$$

$$= 0 \tag{2-114}$$

for any value of $\Delta\phi$.

Relation 2-114 is important, because it demonstrates that the change in eigenvalue is stationary with respect to arbitrary variations in the flux when the adjoint of the unperturbed flux is used as weighting function in equation 2-107. *The error made in neglecting the change in flux,* $\Delta\phi$*, in the calculation of* $\Delta\lambda$ *is thus minimized if the adjoint flux is used to weight the reaction rates.*

Substituting this result in equation 2-107, we finally obtain the *first-order-perturbation formula* for the change in eigenvalue:

$$\boxed{\Delta\lambda = \frac{\langle \phi_0^*, (\Delta M - \lambda_0 \Delta F)\phi_0 \rangle}{\langle \phi_0^*, F_0 \phi_0 \rangle} + O(\Delta\phi)^2} \tag{2-115}$$

Using the continuous notation, equation 2-115 can be written

$$\Delta\lambda = \frac{\int_V dV \int_E dE\, \phi_0^*(r,E) [\Delta M - \lambda_0 \Delta F] \phi_0(r,E)}{\int_V dV \int_E dE\, \phi_0^*(r,E) F_0 \phi_0(r,E)} \tag{2-116}$$

2.4.2 Perturbation Formulas for the Reactivity

Let us consider a reactor in any state different from the *reference (critical) state*. This may be taken to be the perturbed state defined by equation 2-100. Multiplying equation 2-100 by ϕ_0^* (the reference-state adjoint) and integrating over the entire domain, we readily find the following expression for the eigenvalue:

$$\lambda = \frac{\langle \phi_0^*, M\phi \rangle}{\langle \phi_0^*, F\phi \rangle} \qquad (2\text{-}117)$$

This expression is a much more exact definition of the eigenvalue of the problem than was equation 2-91. It is *Rayleigh's quotient*. We note that it is a homogeneous functional, the ratio of two bilinear functionals.

An interesting property of this functional was pointed out in the previous section. Since the functional is stationary with respect to arbitrary changes in the flux, it will have a minimum value when the exact flux, solution of equation 2-100, is used. In fact, this property is often employed in variational methods for convergence acceleration, in the outer iterations of the flux calculation (Hébert, 1985).

Since the static reactivity is equal to (1 - λ), we obtain the *exact formula for the static reactivity*:

$$\boxed{\rho_s = \frac{\langle \phi_0^*, (F-M)\phi \rangle}{\langle \phi_0^*, F\phi \rangle}} \qquad (2\text{-}118)$$

This formula is exact, because it contains the perturbed flux ϕ, in addition to the perturbed operators M and F.

It is possible in the same way to find an exact expression for $\Delta\lambda$. Let us multiply equation 2-100 by ϕ_0^* and equation 2-110 by ϕ, and then integrate over the domain. We find

$$\langle \phi_0^*, M\phi \rangle = \lambda \langle \phi_0^*, F\phi \rangle \qquad (2\text{-}119)$$

$$\langle \phi, M_0^* \phi_0^* \rangle = \lambda_0 \langle \phi, F_0^* \phi_0^* \rangle \qquad (2\text{-}120)$$

Transposing terms in this equation,

$$\begin{aligned} \langle \phi_0^*, M_0\phi \rangle &= \lambda_0 \langle \phi_0^*, F_0\phi \rangle \\ &= \lambda_0 \langle \phi_0^*, F\phi \rangle - \lambda_0 \langle \phi_0^*, \Delta F\phi \rangle \end{aligned} \qquad (2\text{-}121)$$

Subtracting equation 2-121 from equation 2-119, we get for $\Delta\lambda$:

$$\Delta\lambda^{exact} = \frac{\langle \phi_0^*, \Delta M \phi \rangle - \lambda_0 \langle \phi_0^*, \Delta F \phi \rangle}{\langle \phi_0^*, F\phi \rangle} \tag{2-122}$$

Since $\Delta\rho = -\Delta\lambda$, the following *exact formula for the reactivity change* emerges:

$$\boxed{\Delta\rho^{exact} = \frac{\langle \phi_0^*, (\lambda_0 \Delta F - \Delta M)\phi \rangle}{\langle \phi_0^*, F\phi \rangle}} \tag{2-123}$$

This can be compared to the *first-order-perturbation formula*, taken from equation 2-115:

$$\boxed{\Delta\rho^{(1)} = \frac{\langle \phi_0^*, (\lambda_0 \Delta F - \Delta M)\phi_0 \rangle}{\langle \phi_0^*, F_0\phi_0 \rangle}} \qquad \text{2-124)}$$

The exact formula differs from the first-order formula in the use of the perturbed flux, ϕ, in the bilinear products, and, in the denominator, of the perturbed operator, F, instead of F_0.

We note the following.

- The importance of the perturbation formula is that *it allows the evaluation of changes in reactivity for a large number of perturbations, without a calculation of the perturbed flux in each case,* and to order $O(\Delta\phi)^2$, where $\Delta\phi$ represents the flux error (when using the unperturbed flux).

- The importance of the exact formula 2-122 or 2-123 is that it allows a *more precise evaluation of* $\Delta\lambda$ than that obtained by taking the difference of the eigenvalues of equations 2-97 and 2-100. This stems from the fact that Rayleigh's quotient is stationary with respect to arbitrary variations in ϕ. Thus, *using the adjoint flux in equation 2-118 or 2-123*, even with only an estimate for the perturbed (exact) flux, *the error in* ρ *or in* $\Delta\rho$ *is minimized with respect to* $\Delta\phi$ (error $\approx O(\Delta\phi)^2$).

2.4.3 Adjoint Equation

The exact formula or the perturbation formulas can be used to evaluate the static reactivity for a large number of perturbations once the reference-system (unperturbed) adjoint flux has been calculated. We shall now derive the adjoint diffusion equation, that is, find expressions for the operators M^* and F^* which appear in equation 2-110.

From the definition of an adjoint operator in equation 2-96, we have

$$\left\langle \phi^*, M\phi \right\rangle = \left\langle \phi, M^*\phi^* \right\rangle \qquad \text{(losses)} \qquad (2\text{-}125)$$

$$\left\langle \phi^*, F\phi \right\rangle = \left\langle \phi, F^*\phi^* \right\rangle \qquad \text{(fission source)} \qquad (2\text{-}126)$$

Let us begin with the fission-source term.

FISSION SOURCE

In its integral form, the total-fission-source term, weighted by the adjoint, is written

$$\left\langle \phi^*, F\phi \right\rangle = \int_E \int_V \phi^*(r,E) \overbrace{\chi(E) \int_{E'} \nu\Sigma_f(r,E')\phi(r,E')dE'}^{F\phi} dE d^3r$$

$$= \int_E \int_V \phi(r,E) \underbrace{\nu\Sigma_f(r,E) \int_{E'} \chi(E')\phi^*(r,E')dE'}_{F^*\phi^*} dE d^3r \qquad (2\text{-}127)$$

We can see, by inverting the order of integration in the operator, that the adjoint operator for the fission source can be written as follows in continuous notation:

$$\boxed{F^*\phi^* = \nu\Sigma_f(r,E)\int_{E'} \chi(E')\phi^*(r,E')dE'} \qquad (2\text{-}128)$$

In matrix notation (multigroup formalism), we get

$$\begin{aligned}
\left\langle \underline{\Phi}^* \cdot [\chi][F]^T \underline{\Phi} \right\rangle &= \int_V \sum_g \phi_g^*(r)\chi_g \overbrace{\left[\sum_{g'} \nu_{g'} \Sigma_{fg'}(r)\phi_{g'}(r) \right]}^{[F]^T \underline{\Phi}} d^3r \\
&= \int_V \sum_{g'} \nu_{g'} \Sigma_{fg'}(r)\phi_{g'}(r) \sum_g \chi_g \phi_g^*(r) d^3r \\
&= \int_V \sum_g \nu_g \Sigma_{fg}(r)\phi_g(r) \underbrace{\sum_{g'} \chi_{g'} \phi_{g'}^*(r)}_{[\chi]^T \underline{\Phi}} d^3r \\
&= \left\langle \underline{\Phi} \cdot [F][\chi]^T \underline{\Phi}^* \right\rangle
\end{aligned} \qquad (2\text{-}129)$$

Consequently we find, in matrix notation:

$$\boxed{F^*\phi^* = [F][\chi]^T \underline{\Phi}^*} \tag{2-130}$$

This result is in case immediate, from the observation

$$[F][\chi]^T = \left[[\chi][F]^T\right]^T \tag{2-131}$$

Let us now obtain the adjoint operator for neutron loss.

NEUTRON REMOVAL

The operator M consists of a leakage term, L, and a collision term, A, as we saw in equation 2-55:

$$\left\langle \phi^*, M\phi \right\rangle = \left\langle \phi^*, (L+A)\phi \right\rangle$$

$$= \left\langle \phi^*, L\phi \right\rangle + \left\langle \phi^*, A\phi \right\rangle \tag{2-132}$$

where, in matrix notation:

$$L\phi = -\vec{\nabla} \cdot D(r,E)\vec{\nabla}\phi(r,E) \tag{2-133a}$$

$$A\phi = \Sigma(r,E)\phi(r,E) - \int_{E'} \Sigma_s(r,E' \rightarrow E)\phi(r,E') \tag{2-133b}$$

First consider the *collision term*. We see that

$$\int_V \int_E \phi^*(r,E)\Sigma(r,E)\phi(r,E)dEd^3r = \int_V \int_E \phi(r,E)\Sigma(r,E)\phi^*(r,E)dEd^3r \tag{2-134}$$

Similarly

$$\int_V \int_E \phi^*(r,E)\left[\int_{E'} \Sigma_s(r,E' \rightarrow E)\phi(r,E')dE'\right]dEd^3r$$

$$= \int_V \int_{E'} \phi(r,E')\left[\int_E \Sigma_s(r,E' \rightarrow E)\phi^*(r,E)dE\right]dE'\,d^3r$$

$$= \int_V \int_E \phi(r,E)\left[\int_{E'} \Sigma_s(r,E \rightarrow E')\phi^*(r,E')dE'\right]dEd^3r \tag{2-135}$$

It is then evident that

$$\boxed{A^*\phi^* = \Sigma(r,E)\phi^*(r,E) - \int_{E'} \Sigma_s(r,E \rightarrow E')\phi^*(r,E')dE'} \tag{2-136}$$

The leakage operator L requires closer attention, because it contains derivatives. First, we note the following vector identity, ***which holds at every point*** of the domain (r,E):

$$\vec{\nabla}\cdot\left(\phi^* D\vec{\nabla}\phi\right) = \phi^*\vec{\nabla}\cdot\left(D\vec{\nabla}\phi\right) + D\vec{\nabla}\phi\cdot\vec{\nabla}\phi^* \tag{2-137}$$

We therefore have

$$\int_V\int_E \phi^*\vec{\nabla}\cdot\left(D\vec{\nabla}\phi\right)dE\,d^3r = \int_V\int_E \vec{\nabla}\cdot\left(\phi^* D\vec{\nabla}\phi\right)dE\,d^3r - \int_V\int_E D\vec{\nabla}\phi\cdot\vec{\nabla}\phi^*\,dE\,d^3r \tag{2-138}$$

Let us apply the divergence (Gauss') theorem to the first term on the right-hand side of equation 2-138:

$$\int_E\left[\int_V \vec{\nabla}\cdot\left(\phi^* D\vec{\nabla}\phi\right)d^3r\right]dE = \int_E\left[\int_S \vec{n}\cdot\left(\phi^* D\vec{\nabla}\phi\right)d^2r\right]dE \tag{2-139}$$

where S is the external surface of volume V and $\vec{n}$ is the unit vector $\hat{e}_S$ shown in Figure 2.4.

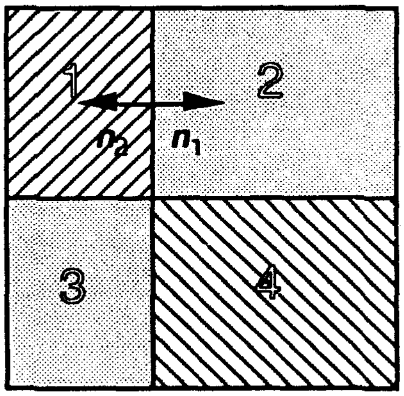
In order for the divergence theorem to apply to equation 2-139, the function $(\phi^* D\vec{\nabla}\phi)$ must be continuous everywhere in volume V. Let us assume the volume consists of sub-volumes Vi, material regions within which the diffusion constant is constant. We can then write

$$\begin{aligned}\int_V \vec{\nabla}\cdot\left(\phi^* D\vec{\nabla}\phi\right)d^3r &= \sum_i \int_{V_i} \vec{\nabla}\cdot\left(\phi^* D\vec{\nabla}\phi\right)d^3r \\ &= \sum_i \int_{S_i} \vec{n}\cdot\left(\phi^* D\vec{\nabla}\phi\right)d^2r \end{aligned}\tag{2-140}$$

where $\vec{n}_i$ is the out-going unit vector normal to surface S_i. The sum in equation 2-140 is over all surfaces, both internal and external. First consider the internal surfaces (interfaces between the material regions), illustrated in Figure 2.5.

For each internal surface, the sum contains two terms, corresponding to the two sides of the surface, with vectors $\vec{n}_i$ of opposite sign (opposite direction).

Fig. 2.5 Internal Surfaces



We can therefore write

$$\int_V \vec{\nabla}\cdot\left(\phi^* D\vec{\nabla}\phi\right)d^3r = \sum_{S_i(\text{int})} \vec{n}_i\cdot\phi^* \overbrace{\left(D_i^-\vec{\nabla}\phi_i^- - D_i^+\vec{\nabla}\phi_i^+\right)}^{\text{Continuity of current}} + \sum_{S_j(ex)} \overbrace{\vec{n}_i\cdot\phi^* D_j^-\vec{\nabla}\phi_j^-}^{\text{Boundary conditions}} \qquad (2\text{-}141)$$

Conservation of neutrons across internal surfaces of the domain requires *continuity of the current* $J = -D\vec{\nabla}\phi$. Consequently, if the solution satisfies the continuity conditions 2-42 and 2-44, the first term on the right-hand side in equation 2-141 vanishes. We then get

$$\vec{J}_i^- = \vec{J}_i^+ \qquad (2\text{-}142)$$

On the reactor's external surfaces, the *boundary conditions* (equation 2-48) can be written in general form as

$$b\phi(r_s) = -\vec{n}\cdot D\vec{\nabla}\phi(r_s) \qquad (2\text{-}143)$$

$$\text{with}\begin{cases} b = 0 \Rightarrow \textit{reflection} \\ b = 1/2 \Rightarrow \textit{vacuum} \end{cases}$$

Analogous boundary conditions will be written for the adjoint flux:

$$b^*\phi^*(r_s) = -\vec{n}\cdot D\vec{\nabla}\phi^*(r_s) \qquad (2\text{-}144)$$

Equation 2-138 then becomes

$$\int_V\int_E \phi^*\vec{\nabla}\cdot\left(D\vec{\nabla}\phi\right)dE\,d^3r = -\int_V\int_E D\vec{\nabla}\phi\cdot\vec{\nabla}\phi^*\,dE\,d^3r + \int_E\int_{S_\infty} b\phi^*\phi\,d^2r\,dE \qquad (2\text{-}145)$$

From this we see that ϕ and ϕ^* can be interchanged without affecting the value of the right-hand-side term. We can thus write

$$\int_V\int_E \phi^*\vec{\nabla}\cdot\left(D\vec{\nabla}\phi\right)dE\,d^3r = \int_V\int_E \phi\vec{\nabla}\cdot\left(D\vec{\nabla}\phi^*\right)dE\,d^3r$$

and consequently

$$\boxed{L^*\phi^* = -\vec{\nabla}\cdot D(r,E)\vec{\nabla}\phi^*(r,E)} \qquad (2\text{-}146)$$

Combining equations 2-136 and 2-146, we finally find for the adjoint M^* of the removal operator

$$\boxed{M^*\phi^* = -\vec{\nabla}\cdot D(r.E)\vec{\nabla}\phi^*(r,E) + \Sigma(r,E)\phi^*(r,E) - \int_{E'}\Sigma_s(r,E\to E')\phi^*(r.E')dE'} \qquad (2\text{-}147)$$

In the multigroup formalism (matrix notation) we easily find

$$\begin{aligned}\left\langle \underline{\Phi}^*,[M]\underline{\Phi}\right\rangle &= \left\langle \underline{\Phi}^*,([L]+[A])\underline{\Phi}\right\rangle \\ &= \left\langle \Phi,\left([L]^T+[A]^T\right)\underline{\Phi}^*\right\rangle \\ &= \left\langle \underline{\Phi},[M]^*\underline{\Phi}^*\right\rangle \qquad (2\text{-}148)\end{aligned}$$

TREATMENT OF THE LEAKAGE TERM IN THE PERTURBATION FORMULAS

The perturbation formulas for the reactivity (equations 2-122, 2-123 and 2-124), which we have derived in the preceding section, each contain a term in ΔM. Since M includes the leakage term, it is necessary to apply the divergence theorem to all internal surfaces to evaluate the perturbation due to the variations in the diffusion coefficient.

Consider the following functional:

$$\Delta_M = \left\langle \phi_0^*,\Delta M\phi\right\rangle = \left\langle \phi_0^*,M\phi\right\rangle - \left\langle \phi_0^*,M_0\phi\right\rangle \qquad (2\text{-}149)$$

On the other hand

$$M = L + A \quad \Rightarrow \quad \Delta_M = \Delta_L + \Delta_A \qquad (2\text{-}150)$$

The Δ_A term poses no great difficulty since it contains no derivative. In contrast, the variation in the leakage term is

$$\Delta_L = -\left\langle \phi_0^*,\vec{\nabla}\cdot D\vec{\nabla}\phi\right\rangle + \left\langle \phi,\vec{\nabla}\cdot D_0\vec{\nabla}\phi_0^*\right\rangle \qquad (2\text{-}151)$$

And using the vector identity 2-137

$$\Delta_L = \overbrace{\left\langle\left(-\vec{\nabla}\cdot\phi_0^*D\vec{\nabla}\phi\right)\right\rangle}^{\delta_L} + \left\langle (D-D_0)\vec{\nabla}\phi\cdot\vec{\nabla}\phi_0^*\right\rangle \qquad (2\text{-}152)$$

Now apply the divergence theorem to δ_L:

$$\begin{aligned}\delta_L &= -\int_E\int_S \vec{n}\cdot\left(\phi_0^*D\vec{\nabla}\phi - \phi D_0\vec{\nabla}\phi_0^*\right)dE\,d^2r \\ &= \int_E\int_{S_{\infty}}\left(b\phi_0^*\phi - b^*\phi_0^*\phi\right)dE\,d^2r = 0 \qquad (2\text{-}153)\end{aligned}$$

If we select $b^* = b$ in equation 2-144, we can write ΔM as a function of the increments of the cross sections only:

$$\boxed{\left\langle \phi_0^*,\Delta M\phi\right\rangle = \left\langle \phi_0^*,\Delta A\phi\right\rangle + \left\langle \Delta D\vec{\nabla}\phi_0^*\cdot\vec{\nabla}\phi\right\rangle} \qquad (2\text{-}154)$$

2.4.4 Importance of Adjoint Weighting

We can understand the importance of adjoint weighting of reaction rates in reactivity calculations by considering the simplified problem shown in Figure 2.6.

Assume we have a slab reactor of width $L = 2a$ in the x direction (and of infinite extent in the other two directions). Assume also a single neutron-energy group, and that the unperturbed reactor is uniform. The reference flux distribution, $\phi_0(x)$, satisfies the equation

$$\left(-D_0\frac{d^2}{dx^2}+\Sigma_{a0}\right)\phi_0(x)=\lambda_0\nu\Sigma_{f0}\phi_0(x) \qquad (2\text{-}155)$$

with the following boundary conditions:

$$\phi_0(x_b)=0 \qquad (x_b=\pm a)$$

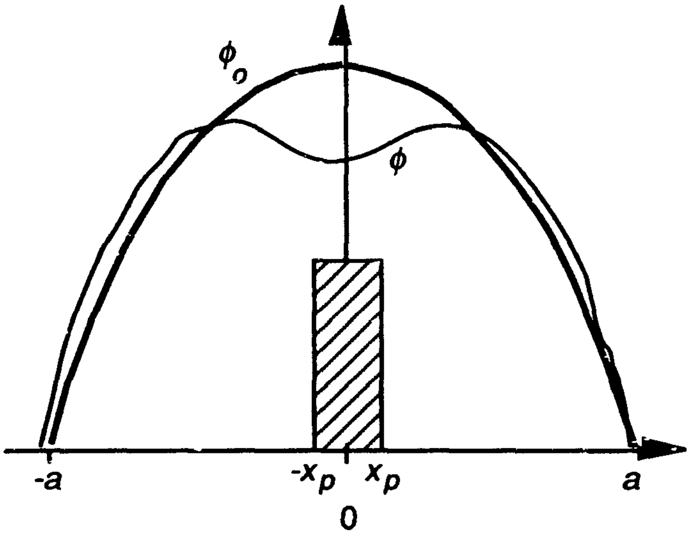
The above equation is of the form

$$\frac{d^2\phi}{dx^2}+B^2\phi=0 \qquad (2\text{-}156)$$

The only solution which is positive throughout the domain and which satisfies the boundary conditions is

$$\phi_0(x)=\phi_0\cos Bx \qquad (2\text{-}157)$$

Fig. 2.6 Localized Perturbation



with the following value for B^2, the *geometric buckling*:

$$B^2=\left(\frac{\pi}{2a}\right)^2 \qquad (2\text{-}158)$$

Now assume that a perturbation is made *in the centre of the reactor*, more specifically, that only the absorption cross section is perturbed, in the interval $x=-x_p$ to $x=+x_p$. That is, only $\Delta\Sigma_a \neq 0$ in the region of the perturbation.

The fundamental eigenvalue for the unperturbed reactor is obtained by substituting $d^2\phi/dx^2$ with $-B^2\phi$ in equation 2-155. Since the reference state is uniform, the same relation applies at all points. We find:

$$k_0 = \frac{1}{\lambda_0} = \frac{\nu\Sigma_{f0}}{D_0 B^2 + \Sigma_{a0}} \qquad \text{(2-159)}$$

From the definition for the adjoint operator, it is easy to see that when a single energy group is used the adjoint equation is identical to the "direct" equation for the flux[6]. We have therefore

$$\phi_0^*(x) = \phi_0(x) \qquad \text{(2-160)}$$

Let us evaluate the change in the reactivity due to this perturbation in two different ways:

- $\Delta\rho^{(0)}$: assuming that all points in the domain have the same importance; there is no weighting ($\phi^*_0 = 1$);
- $\Delta\rho^{(1)}$: first-order approximation (equation 2-124).

If we neglect weighting, we find approximately (taking $\cos Bx \approx 1$) for $-x_p<x<x_p$:

$$\Delta\rho^{(0)} = \frac{-\int_{-x_p}^{x_p} dx\Delta\Sigma_a\phi_0(x)}{\int_{-a}^{a} dx\nu\Sigma_{f0}\phi_0(x)} \approx -\frac{\pi}{2}\left(\frac{\Delta\Sigma_a}{\nu\Sigma_{f0}}\right)\frac{x_p}{a} \qquad \text{(2-161)}$$

Using now the perturbation formula 2-124 and also equation 2-160, we find

$$\Delta\rho^{(1)} = \frac{-\int_{-x_p}^{x_p} dx\Delta\Sigma_a[\phi_0(x)]^2}{\int_{-a}^{a} dx\nu\Sigma_{f0}[\phi_0(x)]^2} \approx -2\left(\frac{\Delta\Sigma_a}{\nu\Sigma_{f0}}\right)\frac{x_p}{a} \qquad \text{(2-162)}$$

The right-hand sides in formulas 2-161 and 2-162 each contain three factors. The second factor, $-\Delta\Sigma_a/\nu\Sigma_{f0}$, is the contribution due to a uniform change in Σ_a. The third factor, x_p/a, is the fraction of the domain affected by the perturbation. The first factor is greater than 1, and takes into account the fact that the perturbation is concentrated at the centre of the reactor, where the flux is higher than on average. When we neglect weighting, this factor is $\pi/2 \approx 1.57$. But with adjoint weighting, this factor becomes equal to 2. There is a *difference of 27 %*.

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[6] This is not the case when using more than one neutron energy group. In general $\phi^*(r,E) \neq \phi(r,E)$.

This difference can be attributed to the fact that *the neutron importance is not uniform in the reactor*. In our example, the neutron importance in the central region is greater than the average by 27 %. In contrast to a neutron born in the centre of the reactor, one born near the core periphery has a greater chance of escaping from the system before being absorbed. Its contribution to the effective multiplication constant will thus be smaller, and its importance reduced relative to a neutron at the centre.

This simplified example illustrates the necessity of taking into account the adjoint-flux distribution in reactivity calculations, because the spatial importance is not the same everywhere. Furthermore, heterogeneities in the energy domain make the use of the importance (adjoint) even more necessary when treating energy groups.

2.5 Conclusion

In this chapter, we have presented the main approximations made to allow the calculation of the scalar-flux distribution in the reactor, using multigroup diffusion theory. We have introduced the concept of criticality of a reactor, and given a rigorous definition of the critical steady state. The static reactivity has been defined relative to the eigenvalue λ emerging from the steady-state diffusion calculation.

Using first-order perturbation theory, we have seen how to calculate the change in static reactivity, $\Delta\rho$, due to a perturbation acting on the reactor, even without the knowledge of the perturbed flux. This calculation actually gives the change in reactivity to second order in the change in flux. Such precision is obtained by *adjoint weighting*, and stems from the stationarity of Rayleigh's quotient.

When using a single neutron energy group, the adjoint is identical to the scalar flux, i.e., $\phi^* = \phi$ (the diffusion operator is hermitean). In reality, one should generally consider the variation of flux with E and adopt the multigroup approach in calculations. In that case

$$\phi_g^*(r) \neq \phi_g(r)$$

$$\phi^*(\boldsymbol{r},\mathrm{E}) \neq \phi(\boldsymbol{r},E)$$

i.e., the adjoint cannot be obtained from the flux itself, but only by actually solving the adjoint equation. Note that the adjoint operator is constructed from a discretized form of the direct operator. The adjoint equation contains therefore the same number of groups, and the finite difference is applied on the same mesh. The adjoint satisfies the same continuity conditions and the same boundary conditions as the flux.

A complete description of a reactor in steady state thus requires the knowledge of the scalar flux, of the eigenvalue, *and* of the adjoint flux, which allows the evaluation of the sensitivity of the eigenvalue to perturbations. Since the starting point of a transient is generally a steady state, our results will have an impact on the exact formulation of the kinetics equations, to be presented in the next chapter.

Finally, we note that the classical approach of perturbation theory can be generalized to functionals of the flux other than the eigenvalue λ. By defining generalized adjoints, variational methods (Stacey, 1974) allow the evaluation of flux functionals with a precision of order $O(\Delta\phi)^2$. The generalized perturbation theory which is derived in that fashion finds application in fuel design and fuel management, where it is important to know the sensitivity of the characteristic functionals of the system (Rozon, 1990).