# **CHAPTER 4**

# **Reactor Statics**

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#### Summary:

This chapter is devoted to the calculation of the neutron flux in a nuclear reactor under special steady-state conditions in which all parameters, including neutron flux, are constant in time. The main calculation method explored in this chapter is the neutron-diffusion equation. Analytical solutions are derived for simple neutron-diffusion problems in one neutron energy group in systems of simple geometry. Two-group diffusion theory and the approximate representation of the diffusion equation using finite differences applied to a discrete spatial mesh are introduced. The rudimentary reactor-physics design of CANDU reactors is presented. The two-step approach to neutronics calculations is presented: multi-group lattice transport calculations, followed by full-core, few-group diffusion calculations. Finally, the chapter covers fuel-property evolution with fuel burnup and specific features of CANDU neutronics resulting from on-line refuelling.

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# 1 Introduction

### 1.1 Overview

This chapter is devoted to the calculation of the neutron flux<sup>1</sup> in a nuclear reactor under special steady-state conditions in which all parameters, including neutron flux, are constant in time. The position-, energy-, and angle-dependent steady-state neutron-transport equation is derived by writing the detailed neutron-balance equation. This is done in Chapter 3 of the book. However, it is also done here for completeness. The steady-state diffusion equation is subsequently derived using a linear approximation of the angular dependence of the neutron flux. Multi-group neutron-energy discretization is also introduced.

Analytical solutions are derived for simple neutron diffusion problems. First, the one-group diffusion equation is solved for a uniform non-multiplying medium in simple geometries. Subsequently, the one-group diffusion equation is solved for a uniform multiplying medium (a homogeneous "nuclear reactor") in simple geometries. The importance of neutron leakage and the concepts of criticality and the neutron cycle are introduced.

Of course, real reactors are almost never homogeneous, and rarely can neutron energies be accurately represented by a single energy group. However, two energy groups are often sufficient to represent neutron diffusion in a thermal reactor because most of the fissions are induced by thermal neutrons. This chapter therefore proceeds to introduce two-group diffusion theory and the approximate representation of the diffusion equation using finite differences applied to a discrete spatial mesh. The latter enables the treatment of non-uniform reactor cores.

Following this treatment of the basic theory of neutron transport and diffusion, the rudimentary reactor-physics design of CANDU reactors is presented, and the associated neutron energy spectrum is discussed. Subsequently, more general core modelling concepts are presented, including the two-step approach to neutronics calculations: multi-group lattice transport calculations, followed by full-core, few-group diffusion calculations. The final section in the chapter concentrates on fuel-property evolution with fuel burnup and specific features of CANDU neutronics resulting from on-line refuelling.

### **1.2 Learning Outcomes**

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

- The neutron transport resulting from the detailed neutron balance;
- The neutron-diffusion equation resulting from the linear approximation of the angular dependence of the neutron flux;
- Analytical solutions of the diffusion equation in simple geometries for both multiplying and non-multiplying media;

<sup>1</sup> In this document, the term "neutron flux" is used to denote the quantity  $\phi = nv$ , where *n* is neutron density and v is neutron speed. The units of flux are  $1 \cdot \text{cm}^{-2} \cdot \text{s}^{-1}$  or  $1 \cdot \text{m}^{-2} \cdot \text{s}^{-1}$ . Some newer texts use the term flux density or fluence rate. All three terms refer to the same physical quantity.

- The concepts of neutron cycle, criticality, and buckling;
- Energy discretization of the diffusion equation using neutron energy groups and spatial discretization using finite differences;
- The two steps of neutronics calculations: lattice-cell transport calculations and fullcore diffusion calculations; and
- Basic design elements of CANDU reactors and their implications for the physical attributes of such reactors.

# 2 Neutron Diffusion Theory

# 2.1 Time-Independent Neutron Transport

The time-independent neutron-transport equation is an equation in six variables: three variables  $\vec{r}$  for the position of the neutron in the reactor, two variables  $\hat{\Omega}$  for the direction of neutron motion, and one variable *E* for neutron energy (we could also use neutron speed v instead of *E*, because there is a one-to-one relationship between v and *E*).

Because we are dealing with time independence (i.e., reactor statics), the neutron-transport equation expresses the fact that the number of neutrons at any position, moving in any direction, and with any energy, is unchanging over time. In other words, if we consider a differential volume in the six-dimensional variable space, i.e.,  $d\vec{r}d\hat{\Omega}dE$  about  $(\vec{r},\hat{\Omega},E)$ , the rate of neutrons "entering" the differential volume must be equal to the rate of neutrons "exiting" the differential volume.

To write the equation, we must therefore consider all phenomena by which neutrons enter or exit the differential volume or are created or destroyed within the volume. The phenomena which we must consider are:

- Neutron production by nuclear fission;
- Neutron scattering, which can change the neutron's energy and/or its direction of motion;
- Neutron absorption;
- Neutron spatial leakage into or out of the differential volume.

[Note: Another process for neutron production is the (n, 2n) nuclear reaction. However, this reaction produces many fewer neutrons than fission and is neglected here.]

The rates at which neutrons enter or exit the differential volume by virtue of these various phenomena, expressed per unit differential volume per second, are given one by one in the following equations.

The rate of birth of neutrons by fission is given by:

$$\frac{\chi(E)}{4\pi} \int_{E'\hat{\Omega}'} v \Sigma_f(\vec{r}, E') \phi(\vec{r}, \hat{\Omega}', E') d\hat{\Omega}' dE', \qquad (1)$$

where

•  $v\Sigma_f(\vec{r}, E')$  is the neutron-yield cross section at position  $\vec{r}$  for fissions induced by neutrons of energy E';

- $\phi(\vec{r}, \hat{\Omega}', E')$  is the angular flux of neutrons at position, of energy E', and moving in direction  $\hat{\Omega}'$ ; and
- $\chi(E)$  is the fraction of all fission neutrons born with energy *E*. Note: In this chapter, for simplicity, a single fission spectrum  $\chi(E)$  is used for fissions induced in all nuclides, whereas in reality the fission spectrum should be taken as different for different nuclides. This fully correct treatment is what is done in Chapter 3.

Note: In the above equation, delayed neutrons are not referred to separately. The neutron production rate includes both prompt and delayed neutrons. This is acceptable because it can be shown that in (true) steady state, accounting separately for delayed-neutron production reduces in any case to the above expression.

The rate of production of neutrons from an "external" source (not related to fissions in the reactor fuel) is given by:

$$S(\vec{r},E),$$
 (2)

where  $S(\vec{r}, E)$  is the external source strength for neutrons of energy *E* at position  $\vec{r}$ .

Note: We will assume that the source is isotropic.

The rate of neutron gain from neutrons entering the differential volume by scattering from other neutron directions of motion or other neutron energies is given by:

$$\int_{E'\hat{\Omega}'} \Sigma_{s} \left( \vec{r}, E' \to E, \hat{\Omega}' \to \hat{\Omega} \right) \phi \left( \vec{r}, \hat{\Omega}', E' \right) d\hat{\Omega}' dE',$$
(3)

where  $\Sigma_s(\vec{r}, E' \to E, \hat{\Omega}' \to \hat{\Omega})$  is the cross section for scattering neutrons from energy E' to energy E and from direction  $\hat{\Omega}'$  to direction  $\hat{\Omega}$ .

The rate of neutron loss from absorption and from neutrons exiting the differential volume by scattering is given by:

$$\Sigma_{t}(\vec{r},E)\phi(\vec{r},\hat{\Omega},E), \qquad (4)$$

where  $\Sigma_t(\vec{r}, E)$ , the total cross section at position  $\vec{r}$  for neutrons of energy  $E_r$ 

$$= \Sigma_{a} \left( \vec{r}, E \right) + \iint \Sigma_{s} \left( \vec{r}, E \to E', \hat{\Omega} \to \hat{\Omega}' \right) d\hat{\Omega}' dE',$$

where  $\Sigma_a(\vec{r}, E)$  is the absorption cross section.

The net rate of neutron spatial leakage (i.e., diffusion) out of the differential volume is given by:

$$\vec{\nabla} \cdot \vec{J}\left(\vec{r},\hat{\Omega},E\right)$$
, (5)

where  $\vec{J}(\vec{r}, \hat{\Omega}, E)$  is the angular current at position  $\vec{r}$  of neutrons moving in direction  $\hat{\Omega}$  with energy *E*.

Note: Because  $\vec{J}(\vec{r}, \hat{\Omega}, E) = \phi(\vec{r}, \hat{\Omega}, E)\hat{\Omega}$ , the neutron leakage [Eq. (5)] can also be written as:

$$\hat{\Omega} \cdot \vec{\nabla} \phi \left( \vec{r}, \hat{\Omega}, E \right). \tag{6}$$

Taking into account all the above rates, the neutron balance can then be expressed in the time-

independent neutron-transport equation as follows:

$$\frac{1}{4\pi}S(\vec{r},E) + \frac{\chi(E)}{4\pi} \int_{E'\hat{\Omega}'} \nabla\Sigma_f(\vec{r},E')\phi(\vec{r},\hat{\Omega}',E')d\hat{\Omega}'dE' + \int_{E'\hat{\Omega}'} \Sigma_s(\vec{r},E' \to E,\hat{\Omega}' \to \hat{\Omega})\phi(\vec{r},\hat{\Omega}',E')d\hat{\Omega}'dE' - \Sigma_t(\vec{r},E)\phi(\vec{r},\hat{\Omega},E) - \vec{\nabla}\cdot\vec{J}(\vec{r},\hat{\Omega},E) = 0.$$
(7)

Note again that for simplicity a single fission spectrum  $\chi(E)$  has been used here. See Chapter 3 for the fully correct treatment. The second term of the equation can be simplified because the fission cross section does not depend on  $\hat{\Omega}'$ , so that the integral over  $\hat{\Omega}'$  in the second term reduces to the angle-integrated flux, and Eq. (7) becomes:

$$\frac{1}{4\pi}S(\vec{r},E) + \frac{\chi(E)}{4\pi} \int_{E'} v\Sigma_f(\vec{r},E')\phi(\vec{r},E')dE' + \int_{E'\hat{\Omega}'} \sum_{S} (\vec{r},E' \to E,\hat{\Omega}' \to \hat{\Omega})\phi(\vec{r},\hat{\Omega}',E')d\hat{\Omega}'dE' - \Sigma_t(\vec{r},E)\phi(\vec{r},\hat{\Omega},E) - \vec{\nabla}\cdot\vec{J}(\vec{r},\hat{\Omega},E) = 0,$$

$$(7)'$$

where  $\phi(\vec{r}, E') = \int_{\hat{\Omega}'} \phi(\vec{r}, \hat{\Omega}', E') d\hat{\Omega}'$  is the total (angle-integrated) flux of neutrons with energy *E* 

at position  $\vec{r}$  .

The neutron-transport equation (7) or (7)' is an exact statement of the general steady-state neutron-balance problem. However, it can immediately be seen that it is very complex: in addition to its dependence on six independent variables, it is an integrodifferential equation. Because of its complexity, this equation cannot be solved analytically except for problems in the very simplest geometries, and real problems require numerical solution by computer.

Note that when there is no external source *S*, the equation appears to be a linear homogeneous equation, which does not generally have a solution (except a trivial zero solution for the flux) for arbitrary values of the nuclear properties. In this case, a solution can be found by modifying the nuclear properties. Mathematically, this can be done by modifying the yield cross section  $v\Sigma_f$  by dividing it by a quantity,  $k_{eff}$ , which can be selected to ensure a non-trivial solution. This quantity  $k_{eff}$  is called the multiplication constant.

Two general categories of codes exist to solve the neutron-transport equation: **deterministic codes** (which solve the equation directly by numerical means) and **Monte Carlo codes** (where stochastic methods are used to model a very large number—typically millions or even hundreds of millions—of neutron births and their travel and event histories, from which the multiplication constant and flux and power distributions can be evaluated using appropriate statistics of these histories). Although the application of either type of transport computer code to full-core reactor models requires very significant computer resources and execution time to achieve a high degree of accuracy, both methods, especially Monte Carlo codes, have seen much greater application in whole-reactor analysis in the last decade or so. While core-wide pin-power reconstruction and time-dependent kinetics calculations are still beyond reach, static eigenvalue calculations and global flux and power distributions can now be carried out routinely using Monte Carlo codes. However, detailed discussion of either type of transport code will not be covered in the present work.

The traditional way of attacking neutronics problems in reactors has been to solve the transport equation numerically in relatively small regions (such as a basic lattice cell or a small collection

of cells) to compute region-averaged properties, and then to use these to solve the full-core reactor problem with a simplified version of the transport equation, the neutron-diffusion equation. This computational scheme is discussed in greater detail in Section 9.

#### 2.2 Fick's Law and Time-Independent Neutron Diffusion

To derive a simplified version of the neutron-transport equation, we note that, because the fission and total cross sections do not depend on the neutron direction of motion  $\hat{\Omega}$  (i.e., "nuclei do not care from which direction neutrons interact with them"), and also because the most important quantity in reactor physics is the fission rate (which determines power production), it may be very effective to try to obtain an equation which is independent of  $\hat{\Omega}$  and which involves only the angle-integrated flux  $\phi(\vec{r}, E)$  [also called the integral flux].

To achieve this, we can attempt to remove the neutron direction of motion by simply integrating Eq. (7)' over  $\hat{\Omega}$ . Let us see what this gives, term by term. The first two terms in (7)' do not contain  $\hat{\Omega}_{,}$  and because the integral of  $\hat{\Omega}$  over a sphere is  $4\pi$ , their integrals, which we can call  $T_1$  and  $T_2$ , can be written directly as:

$$T_1 = S\left(\vec{r}, E\right) \tag{8}$$

$$T_2 = \chi(E) \int_{E'} v \Sigma_f(\vec{r}, E') \phi(\vec{r}, E') dE'.$$
(9)

Similarly, integrating the fourth term gives a result that depends on the integral flux only:

$$T_4 = \int_{\hat{\Omega}} \Sigma_t(\vec{r}, E) \phi(\vec{r}, \hat{\Omega}, E) d\hat{\Omega} = \Sigma_t(\vec{r}, E) \phi(\vec{r}, E).$$
(10)

Integrating the third term gives a more complex relation:

$$T_{3} = \int_{\hat{\Omega}} \int_{E'\hat{\Omega}'} \Sigma_{s} \left( \vec{r}, E' \to E, \hat{\Omega}' \to \hat{\Omega} \right) \phi \left( \vec{r}, \hat{\Omega}', E' \right) d\hat{\Omega}' dE' d\hat{\Omega}.$$
(11)

We can, however, simplify  $T_3$  by noting that, because no absolute direction in space is "special", the scattering cross section  $\Sigma_s$  cannot depend on the absolute directions  $\hat{\Omega}$  and  $\hat{\Omega}'$ , but only on the scattering angle between the directions of the incoming and scattered neutrons, or even more specifically on the cosine  $\mu$  of that angle, i.e., on  $\mu \equiv \hat{\Omega}' \cdot \hat{\Omega}$ . Using this fact, we can then simplify the integral in Eq. (11) by integrating over  $\hat{\Omega}$  first (actually over  $\mu$ , because  $\Sigma_s$  does not depend on the "azimuthal" angle of scattering, and integrating over that azimuthal angle simply gives  $2\pi$ ). The result is then a product of two integrals:

$$T_{3} = \int_{E'\hat{\Omega}'} \oint \left(\vec{r}, E' \to E, \hat{\Omega}'\right) d\hat{\Omega}' \int_{\mu} 2\pi \Sigma_{s} \left(\vec{r}, E' \to E, \mu\right) d\mu dE'$$
  
$$= \int_{E'} \oint \left(\vec{r}, E'\right) \Sigma_{s} \left(\vec{r}, E' \to E\right) dE',$$
(12)

where we have defined

$$\Sigma_{s}\left(\vec{r}, E' \to E\right) = 2\pi \int_{\mu} \Sigma_{s}\left(\vec{r}, E' \to E, \mu\right) d\mu.$$
(13)

Equation (12) is a useful result because it depends on the integral flux  $\phi(\vec{r}, E')$  only.

For the fifth term, we get:

$$T_{5} = \int_{\hat{\Omega}} \vec{\nabla} \cdot \vec{J} \left( \vec{r}, E, \hat{\Omega} \right) d\hat{\Omega} \left[ = \int_{\hat{\Omega}} \hat{\Omega} \cdot \nabla \phi \left( \vec{r}, E, \hat{\Omega} \right) d\hat{\Omega} \right]$$
  
$$= \vec{\nabla} \cdot \vec{J} \left( \vec{r}, E \right),$$
(14)

where

$$\vec{J}\left(\vec{r},E\right) = \int \vec{J}\left(\vec{r},E,\hat{\Omega}\right) d\hat{\Omega}$$
(15)

is the current of neutrons of energy E at position  $\vec{r}$  .

Unfortunately, this result is not at all of the form we would like, i.e., it is not at all expressible in terms of the integral flux, because it is clear that integrating a function of the vector quantity  $\vec{J}(\vec{r}, E, \hat{\Omega})$  over  $\hat{\Omega}$  will obviously give in general a result totally unrelated to the integral flux  $\phi(\vec{r}, E)$ !

In summary, integrating Eq. (7)' over  $\hat{\Omega}$  gives:

$$S(\vec{r}, E) + \chi(E) \int_{E'} v \Sigma_f(\vec{r}, E') \phi(\vec{r}, E') dE' + \int_{E'} \Sigma_s(\vec{r}, E' \to E) \phi(\vec{r}, E') dE' - \Sigma_t(\vec{r}, E) \phi(\vec{r}, E) - \vec{\nabla} \cdot \vec{J}(\vec{r}, E) = 0,$$
(16)

but the last term on the left-hand side (the leakage term) has thwarted our efforts to achieve an equation in the integral flux only.

However, one approximation which is often used in diffusion problems (diffusion of one material through another) can help us here. This approximation, called Fick's Law, applies in lowabsorption media if the angular flux varies at most linearly with angle and if the neutron source is isotropic [already assumed in writing Eq. (7)]. Under these conditions it states that **the current**  $\vec{J}(\vec{r}, E)$  is in the direction in which the integral flux  $\phi(\vec{r}, E)$  decreases most rapidly, i.e., it is proportional to the negative gradient of  $\phi(\vec{r}, E)$ :

$$\vec{J}(\vec{r},E) = -D(\vec{r},E)\nabla\phi(\vec{r},E), \qquad (17)$$

where the quantity  $D(\vec{r}, E)$  is called the diffusion coefficient and can be written as  $1/(3\Sigma_{tr})$ , with  $\Sigma_{tr}$  being the neutron transport cross section.

The reader is referred to Appendix A (Reactor Statics) of this chapter for the derivation of Fick's Law. Here, we will continue to derive the final form of the neutron-diffusion equation.

Equation (17), when substituted into Eq. (16), finally gives an equation in the integral flux only, **the time-independent neutron-diffusion equation**:

$$S(\vec{r}, E) + \chi(E) \int_{E'} v \Sigma_f(\vec{r}, E') \phi(\vec{r}, E') dE' + \int_{E'} \Sigma_s(\vec{r}, E' \to E) \phi(\vec{r}, E') dE' - \sum_i (\vec{r}, E) \phi(\vec{r}, E) + \vec{\nabla} \cdot D(\vec{r}, E) \nabla \phi(\vec{r}, E) = 0$$
(18)

The time-independent neutron-diffusion equation is much simpler than the neutron-transport equation and can be used to solve for the flux in specially prepared full-core reactor models. Note that the out-leakage term (the last term on the left-hand side) has a positive sign, even though this term nominally represents a loss of neutrons; the + sign arises as a result of the – sign in relationship (17) between the current vector and the flux gradient.

Before the diffusion equation can be used, it is important to understand that Fick's Law is only an approximation; it is valid only in low-neutron-absorption media, when the integral flux does not vary too quickly and when angular flux varies weakly with angle (at most linearly). Therefore, Fick's Law is not an especially good approximation in the vicinity of strong absorbers, where the spatial flux variation is very large, or, for the same reason, near interfaces between regions with large variations in nuclear properties or near external surfaces.

### 2.3 Diffusion Boundary Condition with Vacuum at a Plane Boundary

To solve the diffusion equation, which is a second-order partial differential equation, throughout the reactor volume, we need to define boundary conditions at the surface of the reactor.

The vacuum boundary conditions in transport theory are quite clear: the angular current (or angular flux) at the boundary must be zero for any direction pointing to the inside of the reactor (assuming that the reactor has no re-entrant surface):

$$\phi\left(\vec{r},\hat{\Omega},E\right) = 0 \tag{19}$$

for  $\vec{r}$  at the boundary and any  $\hat{\Omega}$  such that  $\mu \equiv \hat{\Omega} \cdot \hat{e} < 0$ , where  $\hat{e}$  is the unit outgoing normal at  $\vec{r}$ .

This condition cannot be applied in diffusion theory, which depends on the integral flux only, because we have lost all the directional information of the angular flux. In diffusion theory, we need boundary conditions, at most, on the integral flux and its gradient. The conditions can be generalized to demand that the **total rate of incoming neutrons** be zero. We will now proceed to derive the boundary conditions used in diffusion theory.

We first derive a general relationship between the angular flux and the current using the approximation that the angular flux is linear in angle. Linearity in angle means that the angular flux can be written as a linear function of the *x*-, *y*-, and *z*-components of the angle  $\hat{\Omega}$ :

$$\phi(\hat{\Omega}) = a + b_x \Omega_x + b_y \Omega_y + b_z \Omega_z, \qquad (20)$$

where a,  $b_x$ ,  $b_y$ ,  $b_z$  are constants which can be determined in terms of the integral flux and current.

Let us first consider the integral flux  $\phi = \int_{\Omega} \phi(\hat{\Omega}) d\hat{\Omega}$ . From Eq. (20),

$$\phi = a \int_{\Omega} d\hat{\Omega} + b_x \int_{\Omega} \Omega_x d\hat{\Omega} + b_y \int_{\Omega} \Omega_y d\hat{\Omega} + b_z \int_{\Omega} \Omega_z d\hat{\Omega}.$$
 (21)

The first integral in Eq. (21) has value  $4\pi$ , whereas the others have value 0 (it is clear that in integrating a single component of the angle over all solid angles, the + and – components cancel out). This means that  $\phi = 4\pi a$ , which implies that

$$a = \frac{\phi}{4\pi} . \tag{22}$$

Now let us consider the current:

$$\vec{J} = \int_{\Omega} \phi(\hat{\Omega}) \hat{\Omega} d\hat{\Omega} \,. \tag{23}$$

From Eq. (20),

$$\vec{J} = a \int_{\Omega} \hat{\Omega} d\hat{\Omega} + b_x \int_{\Omega} \Omega_x \hat{\Omega} d\hat{\Omega} + b_y \int_{\Omega} \Omega_y \hat{\Omega} d\hat{\Omega} + b_z \int_{\Omega} \Omega_z \hat{\Omega} d\hat{\Omega}.$$
 (24)

It is clear that the first integral in Eq. (24) is zero, for the same reason that the + and – components cancel out. Consider the other integrals in Eq. (24), for instance,  $\int_{\Omega} \Omega_x \hat{\Omega} d\hat{\Omega}$ . This is a vector integral, and only the *x*-component will survive because  $\int_{\Omega} \Omega_x \Omega_y (or \ \Omega_z) d\hat{\Omega} = 0$ , for the same reason, cancellation.

On the other hand, the *x*-component gives  $\int_{\Omega} \Omega_x^2 d\hat{\Omega}$ , which can easily be shown to be equal to  $4\pi/3$  [by symmetry, it must be equal to  $\int_{\Omega} \Omega_z^2 d\hat{\Omega} = 2\pi \int_{-1}^1 \mu^2 d\mu = \frac{2\pi}{3} \mu^3 \Big|_{-1}^1 = \frac{4\pi}{3}$ ].

Therefore, we can conclude that

$$\vec{J} = \frac{4\pi}{3} \left( b_x \hat{i} + b_y \hat{j} + b_z \hat{k} \right),$$
(25)

i.e.,

$$b_x = \frac{3}{4\pi} J_x \tag{26}$$

(and similarly for y and z).

Now, substituting Eqs. (22) and (26) into Eq. (20),

$$\phi(\hat{\Omega}) = \frac{\phi}{4\pi} + \frac{3}{4\pi} \left( J_x \Omega_x + J_y \Omega_y + J_z \Omega_z \right) = \frac{\phi}{4\pi} + \frac{3}{4\pi} \vec{J} \cdot \hat{\Omega}.$$
(27)

Let us now apply Eq. (27) at a plane boundary with vacuum. Assume that the boundary plane is perpendicular to the *z*-axis and the polar axis is the outward normal to the boundary, i.e., the unit vector  $\hat{k}$  in the positive *z*-direction. The total rate of incoming neutrons is:

$$\int_{\Omega^{-}} \vec{J}\left(\hat{\Omega}\right) \cdot \hat{k} d\hat{\Omega},\tag{28}$$

where the integral over the "half-space"  $\Omega$  means integrating over the entire azimuthal angle  $\alpha$  (i.e., over  $2\pi$ ), but only over half the polar angle  $\theta$ , i.e., over  $\theta$  from  $\pi/2$  to  $\pi$  (or over  $\mu \equiv \cos \theta$  from -1 to 0).

Using Eq. (27), the total rate of incoming neutrons is:

$$\int_{\Omega^{-}} \phi(\hat{\Omega}) \hat{\Omega} \cdot \hat{k} d\hat{\Omega} = \int_{\Omega} \left( \frac{\phi}{4\pi} + \frac{3}{4\pi} \vec{J}(\hat{\Omega}) \cdot \hat{\Omega} \right) \hat{\Omega} \cdot \hat{k} d\hat{\Omega}.$$
 (29)

Because  $\hat{\Omega} \cdot \hat{k} = \Omega_z = \mu$ , then, in the integral of the second term, only the part involving  $\Omega_z$  will

survive (for the same reason stated before), and:

Total rate of incoming neutrons = 
$$\frac{\phi}{4\pi} * 2\pi * \int_{-1}^{0} \mu d\mu + \frac{3}{4\pi} * 2\pi * \vec{J} \cdot \hat{k} * \int_{-1}^{0} \mu^2 d\mu = -\frac{\phi}{4} + \frac{\vec{J} \cdot \hat{k}}{2}$$

Applying Fick's Law and setting the total rate of incoming neutrons to 0 gives:

$$-\frac{\phi}{4} - \frac{D}{2}\vec{\nabla}\phi \cdot \hat{k} = 0, \text{ i.e., } -\frac{D}{2}\frac{d\phi}{dz} - \frac{\phi}{4} = 0$$

$$\Rightarrow \frac{1}{\phi}\frac{d\phi}{dz}\Big|_{boundary} = -\frac{1}{2D},$$
(30)

which can be written as

$$-\frac{1}{d_{extr}}$$

which leads to

$$d_{extr} = 2D = \frac{2}{3\Sigma_{tr}},\tag{31}$$

$$d_{extr} = 2D = \frac{2}{3\Sigma_{tr}},\tag{32}$$

where  $\Sigma_{tr}$  is the transport cross section.

Actually, a more advanced analysis gives a slightly higher, more correct value for  $d_{extr}$ :

$$d_{extr} = 2.1312 D = \frac{2.1312}{3\Sigma_{tr}} = \frac{0.7104}{\Sigma_{tr}}.$$
(33)

Equations (30)-(33) result in a zero net incoming current at the physical boundary.

The geometric interpretation of Eq. (30) is that the relative neutron flux near the plane boundary has a slope of  $-1/d_{extr}$ , i.e., the flux would extrapolate linearly to 0 at a distance  $d_{extr}$  beyond the boundary. This is often stated as "the flux goes to 0 at an extrapolation distance  $d_{extr}$ beyond the boundary". Such an interpretation is not literally correct: the flux cannot go to zero in a vacuum, because there are no absorbers to remove the neutrons; the flux only **appears** to be heading to the zero value at the extrapolation point. In fact, instead of using the "slope" version (30), the boundary condition is often applied by "extending" the reactor model to the extrapolation point and demanding a zero flux at that point.

Now, typical values for the diffusion coefficients *D* in CANDU reactors are  $\cong$  1 cm, and therefore the extrapolation distance  $d_{extr}$  is of the order of 2–3 cm. For systems of large dimension, e.g., large power reactors which are several metres in size, the extrapolation distance is sometimes neglected if a slightly approximate answer is sufficient.

[Note: Equation (33) applies in principle to plane boundaries only. Slightly different formulas for the extrapolation distance would apply to curved boundaries; however, the difference is small unless the radius of curvature of the boundary is of the same order of magnitude as  $d_{extr}$ .]

## 2.4 Energy Discretization: The Multi-Group Diffusion Equation

Neutron energy *E* is of course a continuous variable. However, the diffusion equation (18) with continuous *E* is not usually solved as is. Instead, the equation is rewritten in "multi-group" form by subdividing the energy range into a number *G* of intervals, called energy "groups" and labelled with *g* from 1 to *G* (*g* =1 corresponding to the interval with the highest energies and *g* = *G* to the interval with the lowest energies). In each group *g*, the continuous flux  $\phi(\vec{r}, E)$  is replaced by an average group flux,  $\phi_{g}(\vec{r})$ .

The nuclear cross sections in each group are assumed to have been appropriately averaged over the corresponding energy intervals. In multi-group notation, the cross sections and variables are written as follows:

$$S(\vec{r}, E) \Rightarrow S_{g}(\vec{r})$$
  

$$\chi(E) \Rightarrow \chi_{g}$$
  

$$v\Sigma_{f}(\vec{r}, E) \Rightarrow v\Sigma_{f,g}(\vec{r})$$
  

$$\Sigma_{s}(\vec{r}, E' \rightarrow E) \Rightarrow \Sigma_{s,g' \rightarrow g}(\vec{r})$$
  

$$\Sigma_{t}(\vec{r}, E) \Rightarrow \Sigma_{t,g}(\vec{r})$$
  

$$D(\vec{r}, E) \Rightarrow D_{g}(\vec{r}).$$

The multi-group diffusion equation then takes the form:

$$S_{g}(\vec{r}) + \chi_{g} \sum_{g'=1}^{G} \nu \Sigma_{f,g'}(\vec{r}) \phi_{g'}(\vec{r}) + \sum_{g'=1}^{G} \Sigma_{s,g' \to g}(\vec{r}) \phi_{g'}(\vec{r}) - \Sigma_{t,g}(\vec{r}) \phi_{g}(\vec{r}) + \vec{\nabla} \cdot D_{g}(\vec{r}) \nabla \phi_{g}(\vec{r}) = 0, \ g = 1,...,G$$

# 3 One-Group Diffusion in a Uniform Non-Multiplying Medium

We will start the analysis of systems with simple systems and increase complexity gradually. Assume that all neutrons are lumped into a single energy group, i.e., G = 1. There is then no need for the subscript g. With a single energy group, the notion of scattering **across** groups has no meaning, and the "incoming scattering" term in  $\Sigma_s$  cancels the "outgoing scattering" term inherent in the total cross section  $\Sigma_t$  (another way of saying this is that the "out-scattering" and "in-scattering" terms cancel one another if there is only one group). This means that we can drop the second term in the diffusion equation and write  $\Sigma_a$  instead of  $\Sigma_t$  in the third term.

In this section, we will deal with neutron diffusion in non-multiplying media, i.e., in media where the fission cross section is zero and the neutron flux is driven by an external neutron source. This type of problem is sometimes called a "source-sink" problem. We will assume that the medium is uniform outside the source, and also that it is infinite in size. Uniform properties also mean that the diffusion coefficient can be taken outside the divergence operator. With these assumptions, the diffusion equation becomes:

$$S(\vec{r}) - \Sigma_a \phi(\vec{r}) + D \nabla \cdot \nabla \phi(\vec{r}) = 0,$$
  
or  $S(\vec{r}) - \Sigma_a \phi(\vec{r}) + D \nabla^2 \phi(\vec{r}) = 0.$  (34)

### 3.1 Plane Source

We take the source as an infinite plane source, which we can place, without loss of generality, in the *y*-*z* plane. In this case, the flux is a function of *x* only,  $\phi(x)$ , and the Laplacian can be written as:

$$\nabla^2 = \frac{d^2}{dx^2}.$$

The diffusion equation **outside the source**, i.e., for any *x* different from 0, becomes:

$$D\frac{d^2\phi(x)}{dx^2} - \Sigma_a\phi(x) = 0.$$
(35)

We can simplify this equation by dividing by D. If we define

$$L^2 = \frac{D}{\Sigma_a},\tag{36}$$

called the diffusion area (and L called the diffusion length), the equation becomes:

$$\frac{d^2\phi(x)}{dx^2} - \frac{1}{L^2}\phi(x) = 0.$$
(37)

For x > 0, Eq. (37) has mathematical solutions  $\exp(x/L)$  and  $\exp(-x/L)$ , which give a general solution:

$$\phi(x) = Ae^{x/L} + Ce^{-x/L}.$$

However, the term  $e^{x/L}$  goes to  $\infty$  as  $x \to \infty$  and therefore cannot be part of a physically acceptable solution for x > 0. The solution for x > 0 must then be  $\phi(x) = Ce^{-x/L}$ .

By left-right symmetry, we can see that the full solution for any x must be

$$\phi(x) = Ce^{-|x|/L},\tag{38}$$

with C being a constant which we can determine from the boundary condition at x = 0.

If S is the source strength per unit area of the plane, then the number of neutrons crossing outwards per unit area in the positive x-direction must tend to S/2 as  $x \rightarrow 0$ . Therefore,

$$\lim_{x \to 0} \left[ J(x) \right] = \frac{S}{2}$$
$$\Rightarrow \lim_{x \to 0} \left[ -D \frac{d\phi(x)}{dx} \right] = \frac{S}{2}$$
$$\Rightarrow \lim_{x \to 0} \left[ \frac{CD}{L} e^{-x/L} \right] = \frac{S}{2}$$
$$\Rightarrow \frac{CD}{L} = \frac{S}{2}, i.e., C = \frac{SL}{2D}.$$

The neutron flux outside the source is then finally:

$$\phi(x) = \frac{SL}{2D} e^{-|x|/L}.$$
(39)

It is interesting to try to interpret the "physical" meaning of the diffusion area  $L^2$ . Let us calculate the **mean square distance** that a neutron travels in the *x*-direction from the source (at x = 0) to its absorption point. We can do this by averaging  $x^2$  with the absorption rate  $\Sigma_a \phi$  as a weighting function:

$$\overline{x}^2 = \frac{\int\limits_{0}^{\infty} x^2 \Sigma_a \phi dx}{\int\limits_{0}^{\infty} \Sigma_a \phi dx}.$$

With the form (39) for the flux, we can evaluate the integrals and show that

$$< x^{2} >= 2L^{2}$$
.

i.e., we can interpret  $L^2$  as one-half the square of the average distance (in one dimension) between the neutron's birth point and its absorption point.

### 3.2 Point Source

Let us now take the source as a single point source, assumed isotropic. Without loss of generality, we can place the source at the origin of co-ordinates,  $\vec{r} = 0$ .

To solve for the flux in this geometry, we need to write the Laplacian  $\nabla^2$  in spherical coordinates. In view of the spherical symmetry of the problem, there is no dependence on angle (whether polar or azimuthal), the flux is a function of radial distance r only, i.e.,  $\phi(r)$ , and the Laplacian is then:

$$\nabla^2 \equiv \frac{1}{r^2} \frac{d}{dr} \left( r^2 \frac{d}{dr} \right) = \frac{d^2}{dr^2} + \frac{2}{r} \frac{d}{dr}.$$
 (40)

The diffusion equation outside the source, i.e., for all points except the origin, is then:

$$D\nabla^{2}\phi(r) - \Sigma_{a}\phi(r) = 0,$$
  
*i.e.*, 
$$D\left[\frac{d^{2}\phi}{dr^{2}} + \frac{2}{r}\frac{d\phi}{dr}\right] - \Sigma_{a}\phi(r) = 0,$$
 (41)

$$D\nabla^{2}\phi(r) - \Sigma_{a}\phi(r) = 0,$$
  
*i.e.*, 
$$D\left[\frac{d^{2}\phi}{dr^{2}} + \frac{2}{r}\frac{d\phi}{dr}\right] - \Sigma_{a}\phi(r) = 0,$$
 (42)

$$\frac{d^2\phi(r)}{dr^2} + \frac{2}{r}\frac{d\phi(r)}{dr} - \frac{1}{L^2}\phi(r) = 0.$$
(43)

To solve this equation, we can write  $\phi$  in the form  $\phi(r) = \frac{\psi(r)}{r}$ . Then, in terms of  $\psi$ , Eq. (43) becomes:

$$\frac{\frac{d\psi(r)}{dr}}{r} - \frac{\psi(r)}{r^2},$$

$$\frac{\frac{d^2\psi(r)}{dr^2}}{\frac{d^2\psi(r)}{dr^2}} - \frac{\frac{d\psi(r)}{dr}}{r^2} - \frac{\frac{d\psi(r)}{dr}}{r^2} + \frac{2\psi(r)}{r^3}.$$

Substituting these forms into Eq. (43) results in the simpler form:

$$\frac{d^{2}\psi(r)}{dr^{2}} - \frac{1}{L^{2}}\psi(r) = 0.$$
(44)

Equation (44) has mathematical solutions  $\exp(r/L)$  and  $\exp(-r/L)$ , which give a general solution:

$$\psi(r) = Ae^{r/L} + C e^{-r/L}$$
$$\Rightarrow \phi(r) = A \frac{e^{r/L}}{r} + C \frac{e^{-r/L}}{r}$$

Now, the term  $\frac{e^{r/L}}{r} \rightarrow \infty$  as  $r \rightarrow \infty$  and therefore cannot be part of a physically acceptable solution. The solution must then be

$$\phi(r) = C \frac{e^{-r/L}}{r},\tag{45}$$

with C being a constant which remains to be determined. To determine C, we can use the continuity condition at the origin.

If S is the source strength, then the number of neutrons crossing the surface of a small sphere outwards must tend to S as the sphere's radius tends to 0, and therefore:

$$\lim_{r \to 0} \left[ 4\pi r^2 J(r) \right] = S$$
  

$$\Rightarrow \lim_{r \to 0} \left[ 4\pi r^2 \left( -D \frac{d\phi}{dr} \right) \right] = S$$
  

$$\Rightarrow \lim_{r \to 0} \left[ 4\pi r^2 \left( -CD \left( \frac{-\frac{r}{L} e^{-r/L} - e^{-r/L}}{r^2} \right) \right) \right] = S$$
  

$$\Rightarrow 4\pi CD = S, i.e., C = \frac{S}{4\pi D}.$$

The neutron flux outside the source is then, finally:

$$\phi(r) = \frac{S}{4\pi D} \frac{e^{-r/L}}{r}.$$
(46)

Again, it is interesting to interpret the physical meaning of the diffusion area  $L^2$ . Let us calculate the mean square distance that a neutron travels outwards from the source (at r = 0) to its

absorption point. We can do this by averaging  $r^2$  with the absorption rate  $\Sigma_a \phi$  as a weighting function:

$$\overline{r^2} = \frac{\int\limits_0^\infty r^2 \Sigma_a \phi 4\pi r^2 dr}{\int\limits_0^\infty \Sigma_a \phi 4\pi r^2 dr}.$$

With the form (46) for the flux, we can evaluate the integrals and show that

$$\langle r^2 \rangle = 6L^2, \tag{47}$$

i.e., we can interpret  $L^2$  as one-sixth of the square of the average distance outwards between the neutron's birth point and its absorption point.

#### 3.3 Flux Curvature in Source-Sink Problems and Neutron In-Leakage

Let us consider the "out-leakage" term (call it *Leak<sub>out</sub>*) in the above examples.

Leak<sub>out</sub>  $\equiv$  leakage out per differential physical volume  $d\vec{r} = \vec{\nabla} \cdot \vec{J} = -\vec{\nabla} \cdot D(\vec{r})\nabla\phi(\vec{r})$ . Applying this to the flux from a plane source (Eq. 39) gives, for x > 0:

$$Leak_{out} = -D\nabla^2 \left(\frac{SL}{2D}e^{-x/L}\right) = -\left(\frac{S}{2L}\right)e^{-x/L} < 0.$$

We can also show that  $Leak_{out} < 0$  for x < 0. If we apply the formula to the flux from a point source (Eq. 46):

$$Leak_{out} = -D\nabla^2 \left(\frac{S}{4\pi D} \frac{e^{-r/L}}{r}\right) = -D\left(\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr}\right) \left(\frac{S}{4\pi D} \frac{e^{-r/L}}{r}\right), \text{ which we can show}$$
$$= -\frac{S}{4\pi L^2} \frac{e^{-r/L}}{r} < 0.$$

We see that in all cases,  $Leak_{out} < 0$ , i.e., the leakage is inwards (in-leakage) at any point outside the source. This can actually be seen in the general case from

$$S(\vec{r}) - \Sigma_a \phi(\vec{r}) + D\nabla^2 \phi(\vec{r}) = 0,$$

stated earlier as Eq. (34), which for any point outside the source gives  $-D\nabla^2 \phi(\vec{r}) = -\Sigma_a \phi(\vec{r}) < 0$ . In other words, we can say that any point outside an external source in a non-multiplying medium sees a positive flux curvature and neutron in-leakage, **i.e.**, any differential volume is a net sink or absorber of neutrons:

Positive flux curvature  $\equiv$  neutron in-leakage.

# 4 One-Group Diffusion in a Uniform Multiplying Medium with No External Source

We will now switch to the analysis of reactor systems with no external source, meaning that all neutrons are produced by neutron-induced nuclear fission. In this section, as in the previous one, we will start by assuming that all neutrons are lumped into a single energy group, i.e., G =

1. There is then, again, no need for the subscript g. Also, as explained in Section 3, we can drop the term in  $\Sigma_s$  and replace  $\Sigma_t$  by  $\Sigma_a$ .

The neutron-diffusion equation in this case is:

$$v\Sigma_f \phi(\vec{r}) - \Sigma_a \phi(\vec{r}) + D\nabla^2 \phi(\vec{r}) = 0.$$
(48)

A very important point to note is that without the external source, this is a linear homogeneous equation in the flux (if the properties are truly constant and independent of the flux). This means that if we find one solution of the equation, then any multiple is also a solution. Therefore, the absolute value of the flux cannot possibly be deduced from the diffusion equation (incidentally, not from the transport equation either). This is totally different from problems with external sources, which drive the absolute value of the flux.

### 4.1 Uniform Infinite Reactor in One Energy Group

Let us first assume a uniform reactor, infinite in size. This assumption makes all points in space "equivalent", which means that the neutron flux  $\phi$  would also have to be constant throughout space. Moreover, there can be no leakage from one point to another; therefore, the leakage term can be dropped from the equation.

The equation in the infinite uniform multiplying medium is then:

$$\nu \Sigma_f \phi - \Sigma_a \phi = 0. \tag{49}$$

This equation is interesting. The only solution is a trivial solution, i.e., a null flux,  $\phi = 0$ , **unless** 

$$\nu \Sigma_f = \Sigma_a. \tag{50}$$

In other words, unless the composition of the medium is exactly balanced so that Eq. (50) is satisfied, the uniform infinite reactor cannot really operate in steady state (except in a trivial zero-flux situation). We can call Eq. (50) the **criticality condition** for a uniform infinite reactor.

What happens if the criticality condition in Eq. (50) is not satisfied? Then there is no non-trivial solution, but is this all that we can say? Actually, we can ensure that there is always a non-trivial solution if we modify Eq. (49) by "tuning" the neutron-yield cross section by dividing it by a new "modifying factor" which we call  $k_{\infty}$ , as in:

$$\frac{v\Sigma_f}{k_{\infty}}\phi - \Sigma_a\phi = 0.$$
(51)

A non-trivial solution of Eq. (51) can always be guaranteed by selecting the value of  $k_{\infty}$  as:

$$k_{\infty} = \frac{\nu \Sigma_f}{\Sigma_a}.$$
 (52)

What this means is that if the composition of the uniform infinite reactor is modified from the original composition by dividing the neutron-yield cross section by  $k_{\infty}$  defined as in Eq. (52), the **modified** uniform infinite reactor can then be operated in steady state with a non-zero flux; this modified reactor is now **critical**. What is the value of the flux? We can see from Eq. (51) that with the modified neutron-yield cross section, the flux can have **any** value; in other words, the critical uniform infinite reactor can operate at any flux (and therefore power) value! This is a direct consequence of the (apparent) homogeneity of the equation (i.e., the equation is of the

form  $F\phi = 0$ , with F an arbitrary operator independent of the flux).

Comparing Eqs. (50) and (51), the criticality condition for a uniform infinite reactor can be seen to be:

$$k_{\infty} \equiv \frac{\nu \Sigma_f}{\Sigma_a} = 1$$
(53)

for criticality. The deviation of  $k_{\infty}$  from 1 tells us **how far** the reactor with the original composition  $(v\Sigma_f, \Sigma_a)$  is from criticality.  $k_{\infty}$  is called the **infinite reactor multiplication constant** and can have the following values:

 $k_{\infty}$  < 1: the infinite reactor is said to be subcritical;

 $k_{\infty}$  = 1: the infinite reactor is critical;

 $k_{\infty} > 1$ : the infinite reactor is said to be supercritical.

The physical interpretation of  $k_{\infty}$  can be stated as follows:

$$k_{\infty} \equiv \frac{\nu \Sigma_f}{\Sigma_a} = \frac{\nu \Sigma_f \phi}{\Sigma_a \phi} = \frac{\text{neutron production rate}}{\text{neutron loss rate}}.$$
 (54)

A quantity related to  $k_{\infty}$ , but "centred" at 0 instead of at 1, is the "reactivity",  $\rho_{\infty}$ , defined as:

$$\rho_{\infty} = 1 - \frac{1}{k_{\infty}}.$$
(55)

Therefore:

 $k_{\infty} < 1 \Rightarrow \rho_{\infty} < 0$ : the infinite reactor is subcritical  $k_{\infty} = 1 \Rightarrow \rho_{\infty} = 0$ : the infinite reactor is critical  $k_{\infty} > 1 \Rightarrow \rho_{\infty} > 0$ : the infinite reactor is supercritical.

Real-life reactors are designed to be operated at critical or very close to critical. Therefore, in most situations, we would expect  $k_{\infty}$  to be very close to 1 and  $\rho_{\infty}$  to be very close to 0. As a result, while  $\rho_{\infty}$  (and  $k_{\infty}$ ) are absolute, dimensionless numbers, a new fractional "unit" of 1 milli-k (or mk) is defined for reactivity, where:

$$1 \text{ mk} = 0.001.$$
 (56)

For example,  $\rho_{\infty} = +2$  mk (or -1 mk) means that  $\rho_{\infty} = +0.002$  (or -0.001). Another reactivity unit, "pcm"  $\equiv 0.01$  mk, is commonly used in Europe.

### 4.2 Uniform Finite Reactors in One Energy Group

We will now analyze uniform reactors of finite size (at least in some dimensions). The nuclear properties are assumed uniform throughout the reactor, but not all points in the reactor are equivalent spatially (some are further from or closer to the reactor boundary), so that the flux is a function of space,  $\phi(\vec{r})$ , and also the leakage term must remain in the diffusion equation:

$$\nu \Sigma_f \phi(\vec{r}) - \Sigma_a \phi(\vec{r}) + D \nabla^2 \phi(\vec{r}) = 0,$$

presented earlier as Eq. (48). This can be rewritten as:

$$-D\nabla^2 \phi(\vec{r}) = v \Sigma_f \phi(\vec{r}) - \Sigma_a \phi(\vec{r}).$$
(57)

The left-hand side of Eq. (57) is the leakage out of the "point"  $\vec{r}$ . If we integrate Eq. (57) over the volume V of the reactor:

$$-\int_{V} D\nabla^{2} \phi(\vec{r}) d\vec{r} = \left( v \Sigma_{f} - \Sigma_{a} \right) \int_{V} \phi(\vec{r}) d\vec{r}.$$
(58)

The left-hand side of Eq. (58) is the **total leakage out of the reactor**. This of course must be positive: neutrons can only go **out of** the reactor, not **into** it, because there are no sources of neutrons outside which can "feed" neutrons into the reactor. Therefore, if Eq. (58) is true as is, the right-hand side must be positive, and because the integral of the flux must also be positive, so must the quantity  $(\nu \Sigma_f - \Sigma_a)$ . We can therefore write Eq. (57) as:

$$-\nabla^{2}\phi(\vec{r}) = \frac{\nu\Sigma_{f} - \Sigma_{a}}{D}\phi(\vec{r})$$
*i.e.*, 
$$-\nabla^{2}\phi(\vec{r}) = B_{g}^{2}\phi(\vec{r}),$$
(59)

where we have defined

$$B_g^2 = \frac{v\Sigma_f - \Sigma_a}{D}.$$
 (60)

The quantity  $B_g^2$ , as it appears in Eq. (59), is called the **geometrical buckling** of the reactor. Its physical meaning can be understood by rewriting Eq. (60) as:

$$B_g^2 = -\frac{\nabla^2 \phi(\vec{r})}{\phi(\vec{r})}.$$
(61)

In other words, the geometrical buckling is the negative relative curvature of the neutron flux. Because we have established that  $B_g^2$  is definitely positive, this means that the flux curvature is negative (see Figure 1), and in fact, in view of Eq. (59), the relative curvature is uniform (and negative) in a homogeneous finite reactor. Note that this statement is strictly true for homogeneous reactors only. In real reactors, the relative flux curvature (and the buckling) can vary and even change sign.



Figure 1 Negative flux curvature in homogeneous reactor

Because the neutron flux curvature/geometrical buckling must "bend" the flux to bring it to 0

almost at the reactor boundary (actually, at an extrapolation distance  $d_{extr}$  beyond the physical boundary), it is clear that the flux curvature will be large for reactors of small dimensions and small if the reactor dimensions are large. Therefore,  $B_g^2$  in Eq. (59) is purely a geometrical quantity.

Returning now to Eq. (57) and using the definition of geometrical buckling, the diffusion equation for homogeneous reactors can be rewritten as:

$$\nu \Sigma_f \phi(\vec{r}) - \Sigma_a \phi(\vec{r}) - DB_g^2 \phi(\vec{r}) = 0.$$
(62)

This equation has the same characteristics as Eq. (49). The only solution is a null flux,  $\phi(\vec{r}) = 0$ , unless

$$v\Sigma_f = \Sigma_a + DB_g^2.$$
(63)

In other words, unless the composition of the reactor is exactly balanced so that Eq. (63) is satisfied, the uniform reactor cannot really operate in steady state (except in a trivial zero-flux situation). We can call Eq. (63) the **criticality condition** for a uniform finite reactor.

What happens if the criticality condition Eq. (63) is not satisfied? Then there is no non-trivial solution. However, just as we did for the infinite medium, we can ensure that there is always a non-trivial solution if we modify Eq. (62) by tuning the neutron-yield cross section by dividing it by a similar parameter, called  $k_{eff}$ , as in:

$$\frac{\nu \Sigma_f}{k_{eff}} \phi(\vec{r}) - \Sigma_a \phi(\vec{r}) - DB_g^2 \phi(\vec{r}) = 0.$$
(64)

A non-trivial solution of Eq. (64) can always be guaranteed by selecting the value of  $k_{eff}$  as:

$$k_{eff} = \frac{V\Sigma_f}{\Sigma_a + DB_g^2},\tag{65}$$

which can also be written as:

$$B_g^2 = \frac{\frac{\nu \Sigma_f}{k_{eff}} - \Sigma_a}{D}.$$
 (66)

This means that if the composition of the uniform reactor is modified from the original composition by dividing the neutron-yield cross section by  $k_{eff}$  defined as in Eq. (65), the **modified** uniform reactor can then operate in steady state (i.e., as a **critical** reactor) with a non-zero flux. Again, as in the infinite medium, the flux in the modified critical reactor can have **any** value, that is, the critical uniform reactor can operate at any flux (and therefore power) value!

In summary, the criticality condition for a uniform finite reactor is:

$$k_{eff} \equiv \frac{v\Sigma_f}{\Sigma_a + DB_g^2} = 1$$
(67)

or

$$B_g^2 = \frac{v\Sigma_f - \Sigma_a}{D} = \frac{\frac{v\Sigma_f}{\Sigma_a} - 1}{\frac{D}{\Sigma_a}} = \frac{k_\infty - 1}{L^2}.$$
(68)

Equation (67) is clearly a generalization of the criticality condition Eq. (53) for the infinite medium, where the buckling was 0, i.e.,  $B_g^2 = 0$  (flat flux). The deviation of  $k_{eff}$  from 1 tells us **how far** the reactor with the original composition ( $v\Sigma_f, \Sigma_a, D$ ) is from criticality.

Equation (68) is intriguing. The left-hand side,  $B_g^2$ , is a geometrical quantity, as already noted. The right-hand side, on the other hand, is a function of the nuclear properties only and is not a geometrical quantity. It is nonetheless called a "buckling", the **material buckling**:

$$B_m^2 = \frac{k_\infty - 1}{L^2}.$$
 (69)

In view of this, the criticality condition for a uniform reactor in one neutron-energy group can be expressed as:

Geometrical Buckling = Material Buckling,  $B_g^2 = B_m^2$ . (70)

The physical interpretation of  $k_{eff}$  can be obtained from:

$$k_{eff} = \frac{\nu \Sigma_f}{\Sigma_a + DB_g^2} = \frac{\nu \Sigma_f \phi(\vec{r})}{\Sigma_a \phi(\vec{r}) + DB_g^2 \phi(\vec{r})} = \frac{\text{neutron production rate}}{\text{neutron loss rate (by absorption and leakage)}}.$$
 (71)

This ratio of production to loss is **the same at any point in a homogeneous reactor** and is of course then also the same as the ratio of the reactor-integrated production and loss.

Incidentally, Eq. (64), a linear equation with a boundary condition (zero flux at the extrapolation distance beyond the boundary), is mathematically an **eigenvector problem**, which can best be seen by rewriting the equation in the form:

$$\left(\Sigma_{a} + DB_{g}^{2}\right)\phi\left(\vec{r}\right) = \lambda v \Sigma_{f} \phi\left(\vec{r}\right),$$
(72)

where

$$\lambda = \frac{1}{k_{eff}}$$
(73)

is the eigenvalue of the problem.

Eigenvalues of eigenvector problems can take on only distinct, non-continuous values. This tells us that  $k_{eff}$  cannot have just any value, but it can have only a certain number of distinct values. Later, we will see that the "physical"  $k_{eff}$  is the largest of these distinct values.

### 4.3 Uniform Finite Reactors in Various Geometries

Equations (67) and (68) relate the reactor multiplication constant to the reactor properties and to geometrical buckling, but we do not yet have a value for the buckling or for the distribution of the neutron flux in the reactor. In this section, we will solve for the flux distribution and for the value of the reactor multiplication constant  $k_{eff}$  for reactors of various geometries (and we

can therefore also derive the value of the buckling). We will do this by showing how to solve the diffusion equation in the following form [rewritten from Eq. (59)]:

$$\nabla^2 \phi(\vec{r}) + B_g^2 \phi(\vec{r}) = 0. \tag{74}$$

#### 4.3.1 Infinite slab reactor

Let us consider a reactor in the shape of a slab of physical width *a* in the *x*-direction and infinite in the *y*- and *z*-directions. The reactor is centred at *x* = 0; see Figure 2. This is a one-dimensional problem, meaning that  $\phi$  is a function of *x* only. The Laplacian reduces to  $\frac{d^2}{dx^2}$ , and the diffusion equation (74) is now:

$$\frac{d^2\phi(x)}{dx^2} + B_g^2\phi(x) = 0.$$
 (75)

This equation has mathematical solutions  $\phi(x) \propto \sin(B_g x)$  and  $\phi(x) \propto \cos(B_g x)$ . However, by leftright symmetry,  $\sin(B_g x)$  is not a viable solution (because the flux would be negative in half the space). Therefore, the only physical solution must have the form  $\phi(x) = A\cos(B_g x)$ , where A is a constant.

Figure 2 Infinite-slab reactor

However, we must also satisfy the boundary condition for the problem, which is  $\phi\left(\frac{a_{ex}}{2}\right) = 0$ , where  $a_{ex}$  is the "extrapolated width" and  $x = a_{ex}/2$  is the point at which the flux appears to go to zero. Therefore, we must have  $A\cos\left(B_g \frac{a_{ex}}{2}\right) = 0$ , which means that the values of  $B_g$  are limited to  $B_g = \frac{n\pi}{a_{ex}}$ , where n = any odd integer.

While any odd integer value of n gives a mathematical solution of Eq. (75), only n = 1 is a physically acceptable solution, because higher values of n would give cosine functions which would



become negative for some values of x before returning to 0 at  $a_{ex}$  (see Figure 3). Therefore, the final solution for the flux distribution in an infinite slab reactor is

$$\phi(x) = A\cos\left(\frac{\pi x}{a_{ex}}\right),\tag{76}$$

and the buckling is



$$B_g^2 = \left(\frac{\pi}{a_{ex}}\right)^2.$$
 (77)

#### Figure 3 Flux with physical and unphysical values of buckling

Note: The value of buckling which gives the only physical solution is the smallest of the mathematically possible values, and the corresponding value of  $k_{eff}$  for the physical solution is the largest of the mathematically possible values (i.e., the physical eigenvalue is the smallest of the possible values).

Equation (76) gives the flux **distribution** in the reactor. However, the amplitude *A*, which gives the absolute value of the flux, cannot be obtained from the diffusion equation, as noted at the beginning of Section 4. To find *A*, an extraneous condition has to be imposed, for instance the actual value of the flux at a point, or the total power of the reactor, or the power in some region of the reactor.

For example, if we assume a value *P* for the power per unit area of the *y*-*z* plane and note that  $E_f$  is the energy released per fission (typically 200 MeV  $\cong$  3.2\*10<sup>-11</sup> joules), we have:

$$P = E_f \Sigma_f \int_{-a/2}^{a/2} \phi(x) dx = E_f \Sigma_f \int_{-a/2}^{a/2} A_1 \cos\left(\frac{\pi x}{a_{ex}}\right) dx$$
  
i.e.,  $P = \frac{a_{ex}}{\pi} E_f \Sigma_f A \sin\left(\frac{\pi x}{a_{ex}}\right) \Big|_{-a/2}^{a/2} = 2A \frac{a_{ex}}{\pi} E_f \Sigma_f \sin\left(\frac{\pi a}{2a_{ex}}\right)$   
 $\therefore A = \frac{\pi P}{2a_{ex} E_f \Sigma_f \sin\left(\frac{\pi a}{2a_{ex}}\right)},$ 

and the absolute flux in the slab is

$$\phi(x) = \frac{\pi P}{2a_{ex}E_f \Sigma_f \sin\left(\frac{\pi a}{2a_{ex}}\right)} \cos\left(\frac{\pi x}{a_{ex}}\right).$$
(78)

If the extrapolation distance is ignored, i.e.,  $a_{ex} = a$ , this reduces to:

$$\phi(x) = \frac{\pi P}{2aE_f \Sigma_f} \cos\left(\frac{\pi x}{a}\right).$$
(79)

#### 4.3.2 Infinite cylindrical reactor

We now consider a reactor in the shape of a uniform cylinder of physical radius R and of infinite length in the axial (z) direction, as shown in Figure 4. The problem is independent of the azimuthal angle, and the flux is a function of the r variable only.



#### Figure 4 Infinite-cylinder reactor

The Laplacian can now be written as

$$\frac{1}{r}\frac{d}{dr}\left(r\frac{d}{dr}\right),$$

and the diffusion equation (74) becomes:

$$\frac{1}{r}\frac{d}{dr}\left(r\frac{d\phi(r)}{dr}\right) + B_g^2\phi(r) = 0$$

$$i.e., \frac{d^2\phi(r)}{dr^2} + \frac{1}{r}\frac{d\phi(r)}{dr} + B_g^2\phi(r) = 0.$$
(80)

This differential equation is actually well known to mathematicians: it is called Bessel's equation of order 0, and its mathematical solutions are the ordinary Bessel functions of the first and second kind,  $J_{0}(Br)$  and  $Y_{0}(Br)$  respectively; see Figure 5.



Figure 5 Ordinary Bessel functions of first and second kind

From Figure 5, we can see that  $Y_0(Br)$  goes to  $-\infty$  as  $r \rightarrow 0$  and is therefore not acceptable as a physical solution for the neutron flux. The only solution is then:

$$\phi(r) = AJ_0(B_s r). \tag{81}$$

The flux must go to 0 at the extrapolated radial boundary  $R_{ex}$ , i.e., we must have:

$$J_0\left(B_g R_{ex}\right) = 0. \tag{82}$$

Figure 5 shows that  $J_0(r)$  has several zeroes, called  $r_i$ : the first is at  $r_1 \cong 2.405$ , and the second at  $r_2 \cong 5.6$ . However, because the neutron flux cannot have regions of negative values, the only physically acceptable value for  $B_q$  is

$$B_{g} = \frac{2.405}{R_{ex}}.$$
 (83)

As a result, the flux in the infinite cylinder is given by:

$$\phi(r) = AJ_0\left(\frac{2.405r}{R_{ex}}\right),\tag{84}$$

and the buckling for the infinite cylinder is

$$B_g^2 = \left(\frac{2.405}{R_{ex}}\right)^2.$$
 (85)

If we use the reactor power *P* per unit axial height to determine *A* and neglect the extrapolation distance, the following value is obtained:

$$A = \frac{0.738P}{E_f \Sigma_f R^2},\tag{86}$$

and the absolute flux is

$$\phi(r) = \frac{0.738P}{E_f \Sigma_f R^2} J_0\left(\frac{2.405r}{R}\right).$$
(87)

#### 4.3.3 Parallelepiped reactor

We now look at a fully finite reactor geometry (i.e., the reactor is finite in every dimension, and is uniform): the parallelepiped of sides *a*, *b*, *c* (see Figure 6). In this case, we use the Cartesian co-ordinate system, and the flux is written as  $\phi(\vec{r}) \equiv \phi(x, y, z)$ . The diffusion equation becomes:

$$\frac{d^{2}\phi(x, y, z)}{dx^{2}} + \frac{d^{2}\phi(x, y, z)}{dy^{2}} + \frac{d^{2}\phi(x, y, z)}{dz^{2}} + B_{g}^{2}\phi(x, y, z) = 0.$$
(88)

#### Figure 6 Rectangular-parallelepiped reactor

To solve this equation, we try a separable form for the neutron flux, i.e.,

$$\phi(x, y, z) = f(x)g(y)h(z), \tag{89}$$

where f, g, and h are functions to be determined. Substituting form (89) into Eq. (88), we get:

$$\frac{d^2 f(x)}{dx^2} g(y)h(z) + f(x)\frac{d^2 g(y)}{dy^2}h(z) + f(x)g(y)\frac{d^2 h(z)}{dz^2} + B_g^2 f(x)g(y)h(z) = 0.$$
(90)

Dividing the equation by f(x)g(y)h(z):

$$\frac{1}{f(x)}\frac{d^2f(x)}{dx^2} + \frac{1}{g(y)}\frac{d^2g(y)}{dy^2} + \frac{1}{h(z)}\frac{d^2h(z)}{dz^2} = -B_g^2.$$
(91)

The left-hand side of Eq. (91) is a sum of three terms which are functions only of x, y, and z

respectively. The right-hand side is a constant. The only way in which this can happen is if each of the three terms on the left-hand side is a constant on its own, i.e., if we can write:

$$\frac{1}{f(x)}\frac{d^2f(x)}{dx^2} = -B_x^2, \quad \frac{1}{g(y)}\frac{d^2g(y)}{dy^2} = -B_y^2, \quad \frac{1}{h(z)}\frac{d^2h(z)}{dz^2} = -B_z^2, \tag{92}$$

where  $B_x^2$ ,  $B_y^2$ ,  $B_z^2$  are constants and

$$B_x^2 + B_y^2 + B_z^2 = B_g^2.$$
 (93)

Each of the equations in (92), e.g.,

$$\frac{1}{f(x)}\frac{d^2f(x)}{dx^2} = -B_x^2 \Longrightarrow \frac{d^2f(x)}{dx^2} + B_x^2f(x) = 0,$$
(94)

is exactly the same equation as for the slab reactor, with the same solution

$$f(x) \propto \cos(B_x x), \tag{95}$$

where

$$B_x = \frac{\pi}{a_{ex}} \,. \tag{96}$$

The full solution for the neutron flux in the parallelepiped reactor is therefore:

$$\phi(x, y, z) = A\cos\left(\frac{\pi x}{a_{ex}}\right)\cos\left(\frac{\pi y}{b_{ex}}\right)\cos\left(\frac{\pi z}{c_{ex}}\right).$$
(97)

The quantities

$$B_x^2 = \left(\frac{\pi}{a_{ex}}\right)^2, \ B_y^2 = \left(\frac{\pi}{b_{ex}}\right)^2, \ B_z^2 = \left(\frac{\pi}{c_{ex}}\right)^2,$$
 (98)

are called the "partial bucklings" in the three directions, and the total buckling is

$$B_g^2 = \left(\frac{\pi}{a_{ex}}\right)^2 + \left(\frac{\pi}{b_{ex}}\right)^2 + \left(\frac{\pi}{c_{ex}}\right)^2.$$
(99)

If we normalize the flux to the total fission power *P* of the reactor and neglect the extrapolation distance, we can show that the normalization constant, *A*, is given by

$$A = \frac{\pi^3 P}{8abcE_f \Sigma_f}.$$
(100)

#### 4.3.4 Finite-cylinder reactor

In the case of a finite-cylinder uniform reactor of radius *R* and height *H* (see Figure 7), we use the cylindrical co-ordinate system to write the flux as  $\phi(\vec{r}) \equiv \phi(r, z)$ . The Laplacian can be written as:

$$\nabla^2 = \frac{d^2}{dr^2} + \frac{1}{r}\frac{d}{dr} + \frac{d^2}{dz^2},$$
 (101)

and the diffusion equation becomes

$$\frac{d^2\phi(r,z)}{dr^2} + \frac{1}{r}\frac{d\phi(r,z)}{dr} + \frac{d^2\phi(r,z)}{dz^2} + B_g^2\phi(r,z) = 0.$$
 (102)



#### **Figure 7 Finite-cylinder reactor**

To solve this equation, we again try a separable form for the neutron flux, i.e.,

$$\phi(r,z) = f(r)g(z), \qquad (103)$$

where f and g are functions to be determined. Substituting Eq. (103) into Eq. (102), we get:

$$\frac{d^{2}f(r)}{dr^{2}}g(z) + \frac{1}{r}\frac{df(r)}{dr} + f(r)\frac{d^{2}g(z)}{dz^{2}} + B_{g}^{2}f(r)g(z) = 0.$$
 (104)

Let us divide this equation by f(r)g(z):

$$\frac{1}{f(r)}\frac{d^{2}f(r)}{dr^{2}} + \frac{1}{f(r)}\frac{1}{r}\frac{df(r)}{dr} + \frac{1}{g(z)}\frac{d^{2}g(z)}{dz^{2}} = -B_{g}^{2}.$$
(105)

The left-hand side of Eq. (105) is the sum of a function of r and a function of z. The right-hand side is a constant. The only way in which this can happen is if the parts in r and z are each individually equal to a constant, i.e., if we can write:

$$\frac{1}{f(r)}\frac{d^{2}f(r)}{dr^{2}} + \frac{1}{f(r)}\frac{1}{r}\frac{df(r)}{dr} = -B_{r}^{2}, \quad \frac{1}{g(z)}\frac{d^{2}g(z)}{dz^{2}} = -B_{z}^{2}, \quad (106)$$

where  $B_r^2$ ,  $B_g^2$  are constants and

$$B_r^2 + B_g^2 = B_g^2. (107)$$

The equations in (106) have been seen before; they are the same equations as for the infinite cylinder and the slab reactor respectively and therefore have the same solutions:

$$f(r) \propto J_0(B_r r), \ g(z) \propto \cos(B_z z),$$
 (108)

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where

$$B_r = \frac{2.405}{R_{ex}}$$
 and  $B_z = \frac{\pi}{H_{ex}}$ , (109)

where  $R_{ex}$  and  $H_{ex}$  are the extrapolated radius and the extrapolated axial dimension of the reactor. The full solution for the neutron flux in the finite-cylinder reactor is therefore:

$$\phi(r,z) = AJ_0\left(\frac{2.405r}{R_{ex}}\right)\cos\left(\frac{\pi z}{H_{ex}}\right),\tag{110}$$

$$B_r^2 = \left(\frac{2.405}{R_{ex}}\right)^2, \ B_z^2 = \left(\frac{\pi}{H_{ex}}\right)^2$$
 (111)

are called the radial and axial bucklings respectively, and the total buckling is

$$B_{g}^{2} = \left(\frac{2.405}{R_{ex}}\right)^{2} + \left(\frac{\pi}{H_{ex}}\right)^{2}.$$
 (112)

If we normalize the flux to the total fission power *P* of the reactor and neglect the extrapolation distance, we can show that the normalization constant is:

$$A = \frac{3.63P}{\pi R^2 H E_f \Sigma_f}.$$
(113)

#### 4.3.5 Spherical reactor

The last geometry we will look at is a spherical uniform reactor of radius *R*. We use the spherical co-ordinate system, and because there is spherical symmetry, the flux can be written as  $\phi(\vec{r}) \equiv \phi(r)$ . The Laplacian can be written as:

$$\nabla^2 = \frac{1}{r^2} \frac{d}{dr} \left( r^2 \frac{d}{dr} \right),\tag{114}$$

and the diffusion equation becomes

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{d\phi(r)}{dr}\right) + B_g^2\phi(r) = 0.$$
(115)

Let us try to represent  $\phi(r)$  in the form

$$\phi(r) = \frac{\psi(r)}{r},\tag{116}$$

where the function  $\psi(r)$  is to be determined. Equation (115) then reduces to:

$$\frac{1}{r^{2}}\left[\frac{d}{dr}\left\{r^{2}\left(-\frac{1}{r^{2}}\psi\left(r\right)+\frac{1}{r}\frac{d\psi\left(r\right)}{dr}\right)\right\}\right]+B_{g}^{2}\frac{\psi\left(r\right)}{r}=0$$
i.e., 
$$\frac{1}{r^{2}}\left[\frac{d}{dr}\left\{-\psi\left(r\right)+r\frac{d\psi\left(r\right)}{dr}\right\}\right]+B_{g}^{2}\frac{\psi\left(r\right)}{r}=0$$
i.e, 
$$\frac{1}{r^{2}}\left[-\frac{d\psi\left(r\right)}{dr}+\frac{d\psi\left(r\right)}{dr}+r\frac{d^{2}\psi\left(r\right)}{dr^{2}}\right]+B_{g}^{2}\frac{\psi\left(r\right)}{r}=0,$$
to
$$\frac{d^{2}\psi\left(r\right)}{dr^{2}}+B_{g}^{2}\psi\left(r\right)=0.$$
(117)

which finally reduces to

The general solution of this equation is:

$$\psi(r) = A\sin(B_g r) + C\cos(B_g r),$$

which gives

$$\phi(r) = A \frac{\sin(B_{g}r)}{r} + C \frac{\cos(B_{g}r)}{r}.$$
(118)

However, the cosine term goes to  $\infty$  as  $r \rightarrow 0$ , which is physically not acceptable, whereas the sine term is acceptable because it has a finite limit as  $r \rightarrow 0$  (as can be verified using L'Hôpital's rule). Therefore, the final solution for the spherical reactor is

$$\phi(r) = A \frac{\sin(B_g r)}{r},$$

where, for the same reason as in the other geometries (to guarantee no negative flux),  $B_g$  must take the lowest allowable value, i.e.,

$$B_g = \frac{\pi}{R_{ex}},\tag{119}$$

so that finally

$$\phi(r) = A \frac{\sin\left(\frac{\pi r}{R_{ex}}\right)}{R}.$$
(120)

If we normalize the flux by imposing a value P for the total fission power of the reactor and neglect the extrapolation distance, we find that:

$$P = 4AR^{2}E_{f}\Sigma_{f}$$
$$\Rightarrow A = \frac{P}{4R^{2}E_{f}\Sigma_{f}}.$$
(121)

### 4.4 Flux Curvature and Neutron Out-Leakage

Let us consider the "out-leakage" term (call it  $Leak_{out}$ ) in the above examples:  $Leak_{out} \equiv$  outleak-

age per differential physical volume  $d\vec{r} = \vec{\nabla} \cdot \vec{J} = -\vec{\nabla} \cdot D(\vec{r}) \nabla \phi(\vec{r})$ . Applying this to the flux in a uniform slab reactor (Eq. 76) gives, for x > 0:

$$Leak_{out} = -D\nabla^2 \left(A\cos\left(\frac{\pi x}{a_{ex}}\right)\right) = +DA\left(\frac{\pi}{a_{ex}}\right)^2 \cos\left(\frac{\pi x}{a_{ex0}}\right) > 0.$$

We can similarly show for all other uniform reactors that  $Leak_{out} > 0$ . This can actually be seen in the general case from  $v\Sigma_f \phi(\vec{r}) - \Sigma_a \phi(\vec{r}) + D\nabla^2 \phi(\vec{r}) = 0$  (presented earlier as Eq. (48)), which for any point in the **uniform** reactor gives  $-D\nabla_2 \phi(\vec{r}) = (v\Sigma_f - \Sigma_a)\phi(\vec{r}) = DB^2\phi(\vec{r}) > 0$ . This means that we can say that any point in a uniform reactor sees neutron out-leakage (i.e., any differential volume is a source of neutrons).

Note again that the above finding applies to uniform reactors, not to all reactors in general. Real reactors may have regions which are net sinks of neutrons, where the flux curvature is positive and where there is a net in-leakage of neutrons. The general rule that we can infer from the above and also from what we learned in source-sink problems is that:

Positive flux curvature = Net neutron in-leakage, while

Negative flux curvature  $\equiv$  Net neutron out-leakage.

# 5 Reactors in Two Neutron-Energy Groups with No External Source

### 5.1 The Neutron Cycle and the Four-Factor Formula

Neutrons born in fission have high energy (see the sketch of their energy distribution in Figure 8).



Figure 8 Energies of fission neutrons

It can be seen that the peak in their energy distribution is ~0.73 MeV. A 1-MeV neutron has a speed of ~13,800 km/s: fission neutrons are **fast** neutrons. There are essentially no fission neutrons born with thermal energies  $\leq$ ~1 eV; the reference thermal energy is 0.025 eV, speed 2,200 m/s, T = 293.6 K.



Figure 9 Sketch of cross section versus neutron energy

However, the probability of neutrons inducing fission in fissile nuclei (such as <sup>235</sup>U) is orders of magnitude larger for thermal neutrons (with energies of a small fraction of 1 eV) than for fast neutrons (see Figure 9). This is why thermal reactors (such as CANDU reactors) use a neutron moderator (such as heavy water in CANDU) to slow neutrons down. This leads to the neutron cycle in thermal reactors: neutrons are born "fast" (i.e., with relatively high energy, typically in the range of MeV) and are "encouraged" to slow down to the thermal range, where they induce more fissions. Of course, fast neutrons do induce a small number of fissions; in fact, only fast neutrons can fission non-fissile nuclides (e.g.,  $^{238}$ U), because there is usually a minimum energy threshold for such fission to occur. Moreover, while following the cycle, neutrons can also escape (leak out of the reactor) or be captured in non-productive absorptions at any energy, in particular in the "resonance range" (between  $\sim 1 \text{ eV}$  and  $\sim 10^5 \text{ eV}$ ), where many strong resonance-absorption peaks (mostly leading to non-productive captures) exist. To reduce resonance capture, most power reactors are designed with the fuel lumped into (mostly) cylindrical elements in fuel-rod assemblies (inside fuel channels in the case of CANDU) surrounded by a moderator. Note also that some up-scattering (increase in neutron energy on collision with a nucleus) can occur in the neutron cycle; this is much less than the rate of down-scattering (moderation) of neutrons, and the up-scattering cross section is sometimes neglected. The neutron cycle in a thermal reactor and with no up-scattering (i.e., scattering from a low-energy group to a high-energy group neglected) is illustrated in Figure 10.



Figure 10 Neutron cycle in thermal reactor

We can derive an equation for the infinite-lattice multiplication constant  $k_{\infty}$  by "following" the various phases of the neutron cycle in the "neutron-generation" view, as follows:

- Imagine that **N** neutrons are born in <u>thermal fissions</u> in one generation (each thermal fission produces about 2.5 neutrons on average).
- There will also be some neutrons born in <u>fast fissions</u> in the same generation. Define ε as the ratio of the total number of fission neutrons born in both fast and thermal fissions to the number born in thermal fissions. ε is called the **fast-fission ratio** (ε > 1). Therefore the total number of fast neutrons is now Nε.
- These neutrons start to slow down, but some are captured in non-productive resonances. If we define *p* as the resonance-escape probability (*p* < 1), the number of neutrons which survive to thermal energies is now *Nɛp*.
- These thermal neutrons can be absorbed in fuel or in non-fuel components of the medium. If we define f as the ratio of thermal neutrons absorbed in fuel nuclides to the total number of thermal neutrons absorbed in this same generation, then the number of neutrons absorbed in fuel in the current generation is *Nepf; f* is called the **fuel utilization** ( $f \le 1$ ).
- Some of the neutrons absorbed in fuel may induce more fissions, and some may not. Define η as the average number of fission neutrons released per thermal absorption event in the fuel. Then the total number of fission neutrons born (in this new generation!) from these thermal fissions is now Nεpfη. η is called the reproduction factor (η > 1).
- We have now gone around the cycle one full time, and we can compare the number of neutrons in the same phase in successive generations: the ratio in successive generations is k<sub>∞</sub>, given by:

$$k_{\infty} = \frac{N\varepsilon pf\eta}{N} = \varepsilon pf\eta.$$
(122)

# 5.2 The Two-Energy-Group Model

The neutron energy range in the neutron cycle is very wide, eight or nine orders of magnitude (from ~10 MeV to ~0.01 eV). From this it is obvious that the one-neutron-energy-group diffusion treatment, while very instructive, cannot be very accurate. Because a very large majority of fissions are induced by thermal neutrons and the fission rate is the most important rate to calculate correctly (because it is essentially the heat-production rate), a two-energy-group treatment is often sufficiently accurate in diffusion calculations. The nuclear properties in two groups must of course be obtained by proper averaging of the detailed many-group properties determined by a transport-theory calculation. Next, we will analyze the two-energy-group model.

# 5.3 Neutron Diffusion Equation in Two Energy Groups

With two energy groups, we will need:

- Two fluxes  $\phi_1(\vec{r})$  and  $\phi_2(\vec{r})$ , with index 1 for the fast (sometimes called the slowingdown) group and index 2 for the thermal group;
- Two absorption cross sections,  $\Sigma_{a1}(\vec{r})$  and  $\Sigma_{a2}(\vec{r})$ ;
- Two neutron-yield cross sections,  $v\Sigma_{f1}(\vec{r})$  and  $v\Sigma_{f2}(\vec{r})$ , acting on the fast and thermal fluxes respectively;
- Down-scattering and up-scattering cross sections,  $\Sigma_{1\to 2}(\vec{r})$  and  $\Sigma_{2\to 1}(\vec{r})$  respectively;
- Two diffusion coefficients,  $D_1(\vec{r})$  and  $D_2(\vec{r})$ .

The diffusion equation for two energy groups is actually two equations, one for each group. There must be neutron balance in each group. As previously indicated, all neutrons are born in the fast group:

$$v\Sigma_{f1}(\vec{r})\phi(\vec{r}) + v\Sigma_{f2}(\vec{r})\phi_{2}(\vec{r}) + \Sigma_{2\to1}(\vec{r})\phi_{2}(\vec{r}) -\Sigma_{a1}(\vec{r})\phi(\vec{r}) - \Sigma_{1\to2}(\vec{r})\phi(\vec{r}) + \vec{\nabla} \cdot D_{1}(\vec{r})\nabla\phi(\vec{r}) = 0,$$
(123)  
$$\Sigma_{1\to2}(\vec{r})\phi(\vec{r}) - \Sigma_{a2}(\vec{r})\phi_{2}(\vec{r}) - \Sigma_{2\to1}(\vec{r})\phi_{2}(\vec{r}) + \vec{\nabla} \cdot D_{2}(\vec{r})\nabla\phi_{2}(\vec{r}) = 0.$$
(124)

# 5.4 Uniform Infinite Medium in Two Energy Groups

As we did in one energy group, let us first assume a uniform reactor, infinite in size. Again, all points in space are "equivalent", which means that the neutron fluxes are constant through space and there is no leakage from one point to another; therefore the leakage terms can be dropped from the equations.

The diffusion equations (123) and (124) in the infinite uniform multiplying medium then become:

$$\begin{split} \nu \Sigma_{f1} \phi_1 + \nu \Sigma_{f2} \phi_2 + \Sigma_{2 \to 1} \phi_2 - \Sigma_{a1} \phi_1 - \Sigma_{1 \to 2} \phi_1 = 0 \\ \Sigma_{1 \to 2} \phi_1 - \Sigma_{a2} \phi_2 - \Sigma_{2 \to 1} \phi_2 &= 0, \end{split}$$

which can be written as a linear homogeneous system of two equations:

$$\left(\nu\Sigma_{f1} - \Sigma_{a1} - \Sigma_{1\to 2}\right)\phi_1 + \left(\nu\Sigma_{f2} + \Sigma_{2\to 1}\right)\phi_2 = 0$$
(125)

$$\Sigma_{1\to 2}\phi_1 - (\Sigma_{a2} + \Sigma_{2\to 1})\phi_2 = 0.$$
 (126)

Now, this system can have a non-trivial flux solution if and only if the determinant of the flux coefficients is zero, i.e.:

$$-\left(\nu\Sigma_{f1} - \Sigma_{a1} - \Sigma_{1\to 2}\right)\left(\Sigma_{a2} + \Sigma_{2\to 1}\right) - \left(\nu\Sigma_{f2} + \Sigma_{2\to 1}\right)\Sigma_{1-2} = 0.$$
(127)

Satisfying the criticality condition, Eq. (127), requires a very fine balance between the nuclear properties. What if that balance is not achieved and Eq. (127) is not satisfied? Then there is no non-trivial solution, i.e., we do not have a real operating infinite-medium reactor. However, we can ensure that there is always a non-trivial solution if we "tune" the neutron-yield cross sections by dividing them by a parameter,  $k_{\infty}$  (to be determined). The diffusion equations then become:

$$\left(\frac{\nu\Sigma_{f1}}{k_{\infty}} - \Sigma_{a1} - \Sigma_{1\to 2}\right)\phi_1 + \left(\frac{\nu\Sigma_{f2}}{k_{\infty}} + \Sigma_{2\to 1}\right)\phi_2 = 0$$
(128)

$$\Sigma_{1\to 2}\phi_1 \qquad -\left(\Sigma_{a2} + \Sigma_{2\to 1}\right)\phi_2 = 0, \qquad (129)$$

and the criticality condition is:

$$\left(\frac{\nu\Sigma_{f1}}{k_{\infty}} - \Sigma_{a1} - \Sigma_{1\to 2}\right) \left(\Sigma_{a2} + \Sigma_{2\to 1}\right) - \left(\frac{\Sigma_{f2}}{k_{\infty}} + \Sigma_{2\to 1}\right) \Sigma_{1\to 2} = 0.$$
(130)

From Eq. (130), we can determine the value that  $k_{\infty}$  must have for criticality:

$$k_{\infty} = \frac{\nu \Sigma_{f1} \left( \Sigma_{a2} + \Sigma_{2 \to 1} \right) + \nu \Sigma_{f2} \Sigma_{1 \to 2}}{\Sigma_{a1} \Sigma_{a2} + \Sigma_{a1} \Sigma_{2 \to 1} + \Sigma_{a2} \Sigma_{1 \to 2}}.$$
(131)

As before, we can define the reactivity as

$$\rho_{\infty} = 1 - \frac{1}{k_{\infty}}.$$

The difference of  $k_{\infty}$  from unity (or of  $\rho_{\infty}$  from 0) tells us how far from critical the original uniform medium is.

When the fast-fission and up-scattering cross sections are neglected, the form obtained for  $k_{\infty}$  is simpler and instructive:

$$k_{\infty,noup-scattering \& no fast fission} = \frac{\nu \Sigma_{f2}}{\Sigma_{a2}} \frac{\Sigma_{1\to 2}}{\Sigma_{a1} + \Sigma_{1\to 2}}.$$
 (132)

The second factor in Eq. (132),

$$\frac{\Sigma_{1\to 2}}{\Sigma_{a1} + \Sigma_{1\to 2}}$$

gives the probability that fast neutrons will down-scatter relative to their probability of being absorbed or down-scattered; i.e., it is the probability of fast neutrons surviving to thermal energies, which is simply the **resonance-escape probability** p in Eq. (122). The first factor in Eq. (132) is the number of fission neutrons produced per thermal absorption, i.e., it is the **reproduction factor**  $\eta$ .

Another important quantity to determine in the two-group model, which has no meaning in the one-group treatment, is the ratio of group fluxes. In the uniform infinite medium, this can be obtained most simply from Eq. (129):

$$\frac{\phi_2}{\phi} = \frac{\Sigma_{1\to 2}}{\Sigma_{a2} + \Sigma_{2\to 1}}.$$
(133)

Note that the criticality condition (130) ensures that the same value would be obtained from Eq. (128).

### 5.5 Uniform Finite Reactors in Two Energy Groups

We now analyze uniform finite reactors. The diffusion equations are now:

$$v\Sigma_{f1}\phi(\vec{r}) + v\Sigma_{f2}\phi_{2}(\vec{r}) + \Sigma_{2\to 1}\phi_{2}(\vec{r}) - \Sigma_{a1}\phi_{1}(\vec{r}) - \Sigma_{1\to 2}\phi(\vec{r}) + D_{1}\nabla^{2}\phi(\vec{r}) = 0$$
(134)

$$\Sigma_{1\to 2}\phi_{1}(\vec{r}) - \Sigma_{a2}\phi_{2}(\vec{r}) - \Sigma_{2\to 1}\phi_{2}(\vec{r}) + D_{2}\nabla^{2}\phi_{2}(\vec{r}) = 0.$$
(135)

We can try to find a solution for the flux which is separable in space and energy, i.e., where the two-row flux vector

$$\Phi(\vec{r}) \equiv \begin{pmatrix} \phi(\vec{r}) \\ \phi_2(\vec{r}) \end{pmatrix}$$

can be written as a group-dependent amplitude times a group-independent flux shape. If we can solve the equation with such a solution, then it is a good solution:

$$\begin{pmatrix} \phi(\vec{r}) \\ \phi_{2}(\vec{r}) \end{pmatrix} = \begin{pmatrix} A_{l}\psi(\vec{r}) \\ A_{2}\psi(\vec{r}) \end{pmatrix}.$$
(136)

Substituting Eq. (136) into Eq. (135), we get:

$$\left(\Sigma_{1\to 2}A_{1} - \Sigma_{a2}A_{2} - \Sigma_{2\to 1}A_{2}\right)\psi(\vec{r}) + D_{2}A_{2}\nabla^{2}\psi(\vec{r}) = 0,$$
(137)

and if we divide by  $\psi(\vec{r})$ :

$$\frac{\nabla^2 \psi\left(\vec{r}\right)}{\psi\left(\vec{r}\right)} = -\frac{\sum_{1\to 2} A_1 - \sum_{a2} A_2 - \sum_{2\to 1} A_2}{D_2 A_2}.$$
(138)

The right-hand side of Eq. (138) is a single number, independent of space, which we can write as  $-B^2$ . [Note: We would have reached a similar conclusion if we had substituted Eq. (136) into Eq. (134).] Equation (138) is analogous to Eq. (61), i.e.,  $B^2$  is a group-independent geometric buckling that is applicable to both the fast and the thermal groups:

$$\nabla^2 \phi_g(\vec{r}) = -B^2 \phi_g(\vec{r}), \ g = 1, 2.$$
(139)

Because this is exactly the same equation as we found with one energy group, the flux distribution in two groups is exactly the same as in one energy group: i.e., a product of cosines in a parallelepiped reactor, an axial cosine times a radial Bessel function in a cylindrical reactor, and a sine-over-r function in a spherical reactor. The only new quantity is the ratio of the group fluxes!

Let us now return to the criticality conditions for a finite reactor. Substituting Eq. (139) into Eqs. (134) and (135) gives a linear homogeneous system, and therefore we can divide the yield cross sections by  $k_{eff}$  as usual to ensure a non-trivial solution:

$$\left(\frac{\nu\Sigma_{f1}}{k_{eff}} - \Sigma_{a1} - \Sigma_{1\to 2} - D_1 B^2\right) \phi\left(\vec{r}\right) + \left(\frac{\nu\Sigma_{f2}}{k_{eff}} + \Sigma_{2\to 1}\right) \phi_2\left(\vec{r}\right) = 0$$
(140)

$$\Sigma_{1\to 2}\phi_1(\vec{r}) - (\Sigma_{a2} + \Sigma_{2\to 1} + D_2 B^2)\phi_2(\vec{r}) = 0.$$
(141)

The criticality condition for finite reactors in two energy groups is found by equating the determinant of this system to zero, which yields:

$$k_{eff} = \frac{\nu \Sigma_{f1} \left( \Sigma_{a2} + \Sigma_{2 \to 1} + D_2 B^2 \right) + \nu \Sigma_{f2} \Sigma_{1 \to 2}}{\left( \Sigma_{a1} + D_1 B^2 \right) \left( \Sigma_{a2} + \Sigma_{2 \to 1} + D_2 B^2 \right) + \Sigma_{1 \to 2} \left( \Sigma_{a2} + D_2 B^2 \right)}.$$
(142)

If we consider the simpler case obtained by neglecting up-scattering and fast fission, as we did following Eq. (131), we get:

$$k_{eff,noup-scattering \& no fast fission} = \frac{v \Sigma_{f2} \Sigma_{1 \to 2}}{\left(\Sigma_{a1} + D_1 B^2\right) \left(\Sigma_{a2} + D_2 B^2\right) + \Sigma_{1 \to 2} \left(\Sigma_{a2} + D_2 B^2\right)}$$

$$= \frac{v \Sigma_{f2} \Sigma_{1 \to 2}}{\left(\Sigma_{a1} + \Sigma_{1 \to 2} + D_1 B^2\right) \left(\Sigma_{a2} + D_2 B^2\right)}.$$
(143)

The ratio of Eq. (143) to Eq. (132) gives the effect of leakage:

$$\frac{k_{eff}}{k_{\infty}} = \frac{\frac{V\Sigma_{f2}\Sigma_{1\to2}}{(\Sigma_{a1} + \Sigma_{1\to2} + D_1B^2)(\Sigma_{a2} + D_2B^2)}}{\frac{V\Sigma_{f2}\Sigma_{1\to2}}{\Sigma_{a2}(\Sigma_{a1} + \Sigma_{1\to2})}} = \frac{\Sigma_{a1} + \Sigma_{1\to2}}{\Sigma_{a1} + \Sigma_{1\to2} + D_1B^2} \frac{\Sigma_{a2}}{\Sigma_{a2} + D_2B^2}.$$
 (144)

The first factor is the ratio of (fast absorption + down-scattering) to (fast absorption + down-scattering + fast leakage). Therefore, the first factor represents the fast non-leakage probability, which we can call  $P_{1NL}$ . In the same way, the second factor represents the thermal non-leakage probability,  $P_{2NL}$ . Therefore, Eq. (144) is equivalent to

$$k_{eff} = k_{\infty} P_{1NL} P_{2NL}, \qquad (145)$$

and the total non-leakage probability is

$$P_{NL} = P_{1NL} P_{2NL}.$$
 (146)

If we use the four-factor formula for  $k_{\infty}$ , then Eq. (146) becomes a **six-factor formula** for  $k_{eff}$ .

$$k_{eff} = \varepsilon p f \eta P_{1NL} P_{2NL}.$$
 (147)

# 6 Solution for Neutron Flux in a Non-Uniform Reactor

For uniform (homogeneous) reactors of various geometries, we were able to solve the diffusion equation analytically and find closed forms for the neutron-flux distribution. However, real reactors are not homogeneous. The steady-state neutron-diffusion equation must then be solved numerically. This section shows one method for doing this in the two-neutron-energy group case.

We start with the two-group neutron-diffusion-equation system, Eqs. (123) and (124), which we rewrite with the required  $k_{eff}$  added as a divisor to the fission cross sections (6.1):

$$(v\Sigma_{f1}(\vec{r})\phi_{1}(\vec{r}) + v\Sigma_{f2}(\vec{r})\phi_{2}(\vec{r})) / k_{eff} + \Sigma_{2\to1}(\vec{r})\phi_{2}(\vec{r}) - \Sigma_{a1}(\vec{r})\phi_{1}(\vec{r}) - \Sigma_{1\to2}(\vec{r})\phi_{1}(\vec{r}) + \vec{\nabla} \cdot D_{1}(\vec{r})\nabla\phi_{1}(\vec{r}) = 0$$

$$\Sigma_{1\to2}(\vec{r})\phi_{1}(\vec{r}) - \Sigma_{a2}(\vec{r})\phi_{2}(\vec{r}) -$$
(148)

$$\Sigma_{2\to 1}(\vec{r})\phi_{2}(\vec{r}) + \vec{\nabla} \cdot D_{2}(\vec{r})\nabla\phi_{2}(\vec{r}) = 0.$$
(149)

All cross sections in a lattice cell are homogenized (averaged spatially within the cell) and condensed to two groups using a multi-group transport code for each lattice cell, but in a real reactor, they must also incorporate the effects of reactivity devices superimposed upon the basic lattice.

## 6.1 Finite-Difference Form of the Neutron-Diffusion Equation

The simplest method for solving the neutron-diffusion equation in a non-homogeneous reactor starts by developing a finite-difference form of the equations.



Figure 11 Face view of very simple reactor model

Consider a two-dimensional view of a reactor model, where each spatial dimension has been subdivided into intervals (see Figure 11). The model is then a collection of homogeneous cells (which may generally all have different nuclear properties). These cells can be basic lattice cells or subdivisions of these cells. The finite-difference method then consists of solving for the flux distribution at a single point in each cell, the centre of the cell in the mesh-centred formulation, which we will use here.

Let us look at one of these cells (which we label with a superscript C for Central) and its six nearest neighbours in the three directions, labelled with a superscript n = 1 to 6 (1 to 4 in x-y geometry). We get the finite-difference form of the diffusion equation if we integrate Eqs. (148) and (149) over the volume of cell C:

$$\int_{C} \left[ \frac{\nu \Sigma_{f_{1}}^{C} \phi(\vec{r}) + \nu \Sigma_{f_{2}}^{C} \phi_{2}(\vec{r})}{k_{eff}} + \Sigma_{2 \to 1}^{C} \phi_{2}(\vec{r}) - \left(\Sigma_{a1}^{C} + \Sigma_{1 \to 2}^{C}\right) \phi_{1}(\vec{r}) + \vec{\nabla} \cdot D_{1}^{C} \nabla \phi_{1}(\vec{r}) \right] d\vec{r} = 0$$
(150)

$$\int_{C} \left[ \Sigma_{1 \to 2}^{C} \phi_{1}\left(\vec{r}\right) - \left( \Sigma_{a2}^{C} + \Sigma_{2 \to 1}^{C} \right) \phi_{2}\left(\vec{r}\right) + \vec{\nabla} \cdot D_{2}^{C} \nabla \phi_{2}\left(\vec{r}\right) \right] d\vec{r} \qquad = 0.$$
 (151)

where we have dropped the dependence on  $\vec{r}$  for the properties because the cells are homogeneous.

There are two types of integrals in Eqs. (150) and (151). The first type does not involve the divergence operator " $\vec{\nabla}$ ." In these integrals, the (homogeneous) cross sections can be taken out of the integral sign, for example:

$$\int_{C} \Sigma_{a2}^{C} \phi_{2}\left(\vec{r}\right) = \Sigma_{a2}^{C} \int_{C} \phi_{2}\left(\vec{r}\right) dr.$$

For the integral on the right-hand side, the approximation is made that the integral is equal to the value of the flux at the centre of the cell multiplied by the volume  $V^C \equiv \Delta x^C \Delta y^C \Delta z^C$  of the cell ( $\Delta x^C, \Delta y^C, \Delta z^C$  being the dimensions of the cell in *x*, *y*, and *z*). Then:

$$\int_{C} \Sigma_{a2}^{C} \phi_{2}\left(\vec{r}\right) = \Sigma_{a2}^{C} \phi_{2}^{C} V^{C}.$$
(152)

The second type of integral has the divergence operator in the integrand. This type of integral simply represents the leakage out of cell C to its neighbours. By Gauss's theorem, the volume integral over the divergence is equal to a surface integral, for example,

$$\int_{C} \vec{\nabla} \cdot D_{1}^{C} \nabla \phi_{1}\left(\vec{r}\right) d\vec{r} = \int_{S} D_{1}^{C} \nabla \phi_{1}\left(\vec{r}\right) \cdot \hat{n} ds = \int_{S} \vec{J}_{1} \cdot \hat{n} ds,$$
(153)

where S is the surface of the cell,  $\hat{n}$  is the outer normal to the surface, and by Fick's Law,  $J_1$  is the net outward current at a point on the surface of the cell.



Figure 12 Flux in a cell and in immediate neighbours



Figure 13 Linear treatment of flux in central cell and one neighbour

Because the cell has six faces, the surface integral is evaluated over the six interfaces between cell C and its six neighbours, n = 1-6. If we take as an example the face towards the cell with the lowest *x*-value (n = 1) for cell C, we can evaluate the surface integral of the current in the fast group over that face (which we call face C1) as follows. First, denote the group-1 flux at the centre of the face by  $\phi_1^{C1}$  (see Figure 12). Then let us assume that the flux is linear between the centre of the cell and the centre of the face (see Figure 13). Then the group-1 current from cell C to its neighbouring cell 1, at the centre of the face, is:

$$J_{1,C\to 1} = -D_1^C \frac{d\phi_1^C}{dx} = -D_1^C \frac{\left[\phi_1^C - \phi_1^{C1}\right]}{\frac{1}{2}\Delta x^C}.$$
 (154)

Similarly, the group-1 current from cell 1 to cell C is:

$$J_{1,1\to C} = -D_1^1 \frac{\left[\phi_1^{C1} - \phi_1^1\right]}{\frac{1}{2}\Delta x^1}.$$
(155)

However, the current must be continuous at the face, i.e.,

$$J_{1,1\to C} = J_{1,C\to 1}.$$
(156)

Then by equating Eqs. (154) and (155) and solving for the interface flux, we find that:

$$\phi_{1}^{C1} = \frac{D_{1}^{C} \Delta x^{1} \phi_{1}^{C} + D_{1}^{1} \Delta x^{C} \phi_{1}^{1}}{D_{1}^{C} \Delta x^{1} + D_{1}^{1} \Delta x^{C}}.$$
(157)

We can then substitute this into Eq. (155) and calculate the current at the centre of the face:

$$J_{1,C\to 1} = -D_1^C \frac{\left[\phi_1^C - \phi_1^{C1}\right]}{\frac{1}{2}\Delta x^C} = -\frac{2D_1^C D_1^1 \left(\phi_1^C - \phi_1^1\right)}{D_1^C \Delta x^1 + D_1^1 \Delta x^C}.$$
(158)

If we assume that the average current over the face is equal to the current at the centre of the face, the total current over face C1 is:

$$\int_{C1} \vec{J}_1 \cdot \hat{n} ds = -\frac{2D_1^C D_1^1 \Delta y^C \Delta z^C}{D_1^C \Delta x^1 + D_1^1 \Delta x^C} (\phi_1^C - \phi_1^1) \equiv A_1^{C1} (\phi_1^C - \phi_1^1),$$
(159)

where  $A_{l}^{C1}$  is a coupling coefficient:

$$A_{1}^{C1} = -\frac{2D_{1}^{C}D_{1}^{1}\Delta y^{C}\Delta z^{C}}{D_{1}^{C}\Delta x^{1} + D_{1}^{1}\Delta x^{C}}.$$
(160)

A very similar process can of course be performed for all six faces between cell C and its neighbours. The total outward current in Eq. (153) is then:

$$\int_{S} \vec{J}_{1} \cdot \hat{n} ds = \sum_{n=1}^{6} A_{1}^{Cn} \left( \phi_{1}^{C} - \phi_{1}^{n} \right).$$
(161)

Using all the above results, the finite-difference neutron-diffusion Eqs. (150) and (151) then become:

$$\frac{\nu \Sigma_{f1}^{C} \phi_{1}^{C} + \nu \Sigma_{f2} \phi_{2}^{C}}{k_{eff}} V^{C} + \Sigma_{2 \to 1}^{C} \phi_{2}^{C} V^{C} - \left(\Sigma_{a1}^{C} + \Sigma_{1 \to 2}^{C}\right) \phi_{1}^{C} V^{C} + \sum_{n=1}^{6} A_{1}^{Cn} \left(\phi_{1}^{C} - \phi_{1}^{n}\right) = 0$$
(162)

$$\Sigma_{1\to2}^C \phi^C V^C - \left(\Sigma_{a2}^C + \Sigma_{2\to1}^C\right) \phi_2^C V^C + \sum_{n=1}^6 A_2^{Cn} \left(\phi_2^C - \phi_2^n\right) = 0.$$
(163)

These equations couple cell C to its closest neighbours. These and similar equations for all the other cells in the model make up a coupled system of linear homogeneous equations for the fluxes at the centres of the cells. If there are N cells in the model, the system is composed of 2N equations. To solve this coupled system, we need also the boundary conditions at the model edges, which we look at now.

The edge cells have neighbour cells only towards the "interior" of the model. In directions outward from the model, the diffusion boundary condition with vacuum is that the flux goes to zero at the extrapolation distance beyond the boundary.

However, we can express the boundary condition in the same form as Eqs. (162) and (163) by creating a "dummy" neighbour cell of width 2  $d_{extr}$ , where  $d_{extr}$  is the extrapolation length = 2.1312  $D^{C}$  [see Eq. (33)] and forcing the flux to be zero at the extrapolation distance (see Figure 14).



Figure 14 Flux in cell at reactor boundary

# 6.2 Iterative Solution of the Neutron-Diffusion Equation

The finite-difference neutron-diffusion-equation system described above is a coupled set of 2N homogeneous equations, where N is the number of real cells in the model. However, actually we seem to have (2N + 1) unknowns: two values of flux for each of the N cells, plus the value of  $k_{eff}$ . In fact, however, there are only 2N unknowns because the overall flux normalization is arbitrary in the homogeneous diffusion equation and only relative fluxes can be determined. The absolute flux normalization factor must be determined using an extraneous condition such as the total reactor fission power.

In real-life reactors, the number of cells *N* is very large (typically tens of thousands). Consequently, the system of equations can be solved only by iterative techniques. The first step is that a flux guess must be selected; this can be as simple as a "flat" flux distribution, i.e., the same value in all cells. A first guess must also be made for  $k_{eff}$ ; for instance, we can use the guess  $k_{eff} = 1$ .

Once a flux guess has been established, the flux iterations can begin. At each iteration, the computer program progresses from cell to cell in the *x*-direction, the *y*-direction, and finally the *z*-direction, with each cell considered as the central cell C. The two equations (162) and (163) are solved simultaneously to obtain the fluxes in cell C,  $\phi_1^C$  and  $\phi_2^C$ , using the latest values of the fluxes in the neighbouring cells. As the sweep progresses through the cells, all the fluxes are updated and used as the latest flux values when the cells are called upon as neighbours. During this sweep, the value of  $k_{eff}$  is kept constant. However, when a full sweep over all reactor cells (a "full iteration") is completed, the value of  $k_{eff}$  is updated. It can be recalculated from the definition of the reactor multiplication constant:

$$k_{eff} = \frac{\text{Neutron Production}}{\text{Neutron Absorption} + \text{Neutron Leakage}}$$
$$= \frac{\int_{\vec{r}} [v\Sigma_{f1}(\vec{r})\phi_1(\vec{r}) + v\Sigma_{f2}(\vec{r})\phi_2(\vec{r})]d\vec{r}}{\int_{\vec{r}} [\Sigma_{a1}(\vec{r})\phi_1(\vec{r}) + \Sigma_{a2}(\vec{r})\phi_2(\vec{r}) + \vec{\nabla}\cdot\vec{J}_1(\vec{r}) + \vec{\nabla}\cdot\vec{J}_2(\vec{r})]d\vec{r}},$$

where the latest fluxes from the latest iteration are used and the integrals are evaluated as sums over the cells.

One iteration is not sufficient to obtain a self-consistent solution of the entire system of finitedifference equations. We must repeat the iterations until the fluxes converge, i.e., until the relative difference in flux in each cell from one iteration to the next is very small, smaller than an accepted tolerance, typically ~10<sup>-5</sup>. A convergence criterion is also needed for  $k_{eff}$ ; typically, a difference of 0.001 or 0.01 mk from one iteration to the next is used. Once convergence has been reached, we have the sought-after solution for the flux shape, i.e., we have the unnormalized (relative) flux distribution. To find the absolute values for the flux, we can normalize the flux distribution to the total reactor fission power, for example.

#### **Energy Dependence of Neutron Flux** 7

In Section 4, we studied the spatial dependence of the neutron flux in one energy group in uniform reactors. In Sections 5 (uniform reactors) and 6 (non-uniform reactors), we studied how to determine the neutron flux both in space and in two energy groups. But what can be said about the variation of the neutron flux with energy when treated as a continuous variable (not just in two groups)? We examine this in the present section.

When we consider the range of neutron energies from  $\sim 1$  (or a few) MeV down to a fraction of 1 eV, we can subdivide the flux energy spectrum into three broad regions (note that the region boundaries cannot be considered "sharp"):

- Fission-neutron energies (>~0.5 MeV)
- Slowing-down (or moderation) range (~0.5 MeV ~0.625 eV)
- Thermal range (< ~0.625 eV)</li>

We will look at the variation of neutron flux with energy in these three regions in turn.

# 7.1 The Fission-Neutron Energy Range

This range consists of energies above ~0.5 MeV, up to several MeV, with a maximum flux magnitude around 0.7 MeV. The energy distribution ("spectrum") of neutrons in this range is determined by experimental measurement. It is found to be well approximated by:

$$\chi(E) = 0.453e^{-1.036E} \sinh \sqrt{2.29E},$$
(164)

where E is in MeV (see Figure 15). [Note: In Chapter 3, the Watt spectrum is used.]

Note that this is a distribution of the number of neutrons, but the flux can be obtained simply by multiplying by the neutron speed v (not to be confused with v, the fission neutron yield).



Figure 15 Energy distribution of fission neutrons

# 7.2 The Thermal Energy Range

Next, let us look at the thermal energy range, with neutron energies less than  $\sim$ 0.625 eV. Here, the neutrons are in thermal-equilibrium balance with the ambient medium at temperature *T*.

Analogously to the atoms in an ideal gas at thermal equilibrium, the neutron population has a Maxwellian (or approximately Maxwellian) distribution. In terms of flux:

$$\phi(E) = \frac{E}{\left(kT\right)^2} e^{-\frac{E}{kT}}.$$
(165)

Room temperature is by convention taken as  $T = 293.6 \text{ K} = 20.4^{\circ}\text{C}$ , which gives kT = 0.0253 eV. The energy value E = kT is the most probable neutron energy in a Maxwellian flux distribution, and the corresponding "thermal neutron" speed is:

$$v(kT = 0.0253 eV) = 2200 m/s.$$
 (166)

### 7.3 The Slowing-Down Energy Range

The slowing-down energy range is intermediate between the fission-energy range and the thermal-energy range. This is the most complex range because of its very broad size and the highly complex resonance scheme presented to neutrons by heavy nuclides, e.g., <sup>238</sup>U.

Therefore, especially when considering neutron absorption in the resonance range in fuel, neutron slowing-down can be very difficult to calculate and is now mostly done by numerical computation using complex lattice codes. However, under certain approximations, it is possible to derive an analytic form for the energy distribution of neutrons as they slow down in the moderator through collisions with light nuclei.

### 7.3.1 Slowing down in a hydrogen moderator

The simplest case is slowing down in hydrogen. Using analysis of the kinematics of neutron

collisions with hydrogen nuclei, the slowing-down flux  $\phi(E)$  in hydrogen can be derived. It can be shown that below the lower boundary  $E_s$  of the fission-neutron energy range and neglecting neutron absorption relative to scattering (a fairly good approximation), the slowing-down flux is inversely proportional to energy E:

$$\phi(E) = \frac{S}{E\Sigma_s},\tag{167}$$

where S is the fission source and  $\Sigma_s$  is the scattering cross section (assumed to be independent of energy).

This provides an important, simple, basic formula for the slowing-down spectrum, even if it is somewhat of an approximation. Another way of interpreting this relationship is that the product  $E\phi(E)$  is nearly constant with energy below  $E_s$ .

#### 7.3.2 Slowing down in a non-hydrogenous moderator

The analysis of the slowing-down spectrum in a non-hydrogenous moderator is more complex, but under similar approximations, the same form of the slowing-down flux can be found:

$$\phi(E) = \frac{S}{E\xi\Sigma_s},\tag{168}$$

This has the same form as in hydrogen, with an additional factor of  $\xi$  in the denominator.  $\xi$  is the average lethargy gain per collision, where the lethargy *u* is defined as:

$$u = \ln\left(\frac{E_s}{E}\right). \tag{169}$$

Refer to Chapter 3 for greater detail.

#### 7.3.3 Relaxing the no-absorption approximation

If the absorption cross section is no longer neglected, but is assumed to vary smoothly with energy (i.e., in the absence of resonances), the 1/E flux spectrum can be modified to:

$$\phi(E) = \frac{S}{E\Sigma_t(E)} \exp\left(-\int_E^{E_s} \frac{\Sigma_a(E')}{\Sigma_t(E')} \frac{dE'}{E'}\right).$$
(170)

The exponential factor in Eq. (170) represents the probability that the neutron survives slowing down to energy E; i.e., it is the resonance-escape probability to energy E, which we can denote as p(E).

From the general form of the slowing-down flux, the following simplified statements about the product  $E\phi(E)$  can be deduced:

- If absorption is neglected, and under the assumption that the scattering cross section does not depend on energy,  $E\phi(E)$  is constant (flat) with E.
- If absorption is included, and assuming a smooth variation of the absorption cross section with *E*, then  $E\phi(E)$  will decrease smoothly for decreasing *E*.

These statements are shown in graphical form in Figure 16.



## Figure 16 Variation of flux with energy if absorption is smooth

### 7.3.4 Slowing down in the presence of resonances

Let us now consider absorption resonances. At a resonance energy, the neutron flux decreases significantly because of the very high absorption cross section at that energy.

As a result of the dip in flux, the absorption rate in the resonance (which is proportional to the flux) is reduced relative to the absorption rate with the "background" flux value at energies above and below the resonance, i.e., the product  $\Sigma_a \phi$  is smaller than if the flux were unaffected. This is called "resonance self-shielding".

On account of resonances, then, the slowing-down flux will be distorted relative to the smooth curve in the previous subsection, as shown in Figure 17.





### Figure 17 Variation of flux with energy in the presence of resonances

# 7.4 Neutron Flux over the Full Energy Range

With the results in the previous subsections, we are able to "piece together" the neutron flux over the energy range from fission energies to the thermal range, using:

• the fission spectrum at energies above about 500 keV;

- the slowing-down spectrum to about 0.625 eV. [Note that in the thermal energy range, neutrons can gain as well as lose energy in collisions. To be consistent with the approximation of no up-scattering in the derivation of the slowing-down spectrum, the "boundary" between thermal and epithermal energies should be selected sufficiently high to ensure negligible up-scattering from the thermal region to the epithermal region. This is one reason for the typical choice of 0.625 eV, which is about 25 times the most probable energy of 0.025 eV at room temperature, as the lower energy boundary of the epithermal range.]
- the Maxwellian spectrum at thermal energies. [Note that it is not a perfect Maxwellian, being distorted somewhat by neutron absorption].

The piecing together of the neutron-flux portions in the various energy regions is shown in the sketch in Figure 18.



Figure 18 Sketch of flux variation over full energy range

# 8 Basic Design of Standard CANDU Reactors

In this section, we look at the basic features of the standard CANDU reactor design. The CANDU design is based on the following design principles and the rationale for each:

Use natural uranium (NU) as fuel. The reason for this choice is that Canada has substantial, high-grade, domestic uranium mineral resources and, for a reactor cooled and moderated by heavy water (D<sub>2</sub>O), it is not necessary to use enriched uranium fuel. Developing a uranium-enrichment industry is extremely expensive, primarily because of the sophisticated technology involved as well as the costs associated with the stringent materials safeguards, physical security, and criticality safety requirements associated with enriched nuclear materials. Moreover, the production cost of uranium-isotope enrichment is also high using current technology, in part due to the energy requirements. Consequently, natural-uranium

fuel is much cheaper and simpler to fabricate than enriched-uranium fuel.

- Use heavy water (D<sub>2</sub>O) as neutron moderator and reactor coolant. The fission chain reaction cannot be self-sustaining with light water (H<sub>2</sub>O) as moderator and NU as fuel. The reason is that normal hydrogen (H) has a fairly large absorption cross section for thermal neutrons. Hence, light water robs neutrons from the chain reaction, and the fuel must be enriched to restore a self-sustaining balance between neutron production and capture. On the other hand, deuterium (D), or heavy hydrogen, has a very small neutron-absorption cross section and enables the use of NU fuel: heavy water provides high neutron economy. Although D<sub>2</sub>O is very expensive to produce due to the low abundance of D relative to H in nature, the large mass difference between D and H makes separation relatively easy to achieve using chemical technology processes, and, unlike enriched fuel, the D<sub>2</sub>O retains its favourable nuclear properties for the full life of the reactor.
- Use a pressure-tube rather than a pressure-vessel design. The coolant takes heat away from the fuel (to create steam and produce electricity in a turbine generator) and becomes very hot. If we want to keep the coolant liquid (or to limit boiling to a small amount), we must pressurize it (to about 100 atmospheres, ~10 MPa). Therefore, a pressure boundary must be provided. In light-water reactors (LWRs) a large, thick, steel pressure vessel is used that surrounds the entire reactor core. The first prototype CANDU reactor [Nuclear Power Demonstration (NPD), the first reactor to produce electricity in Canada (about 20 MWe)], was initially conceived with a pressure-vessel design. However, using  $D_2O$  as the moderator results in a larger vessel than for an LWR, because the smaller scattering cross section of D<sub>2</sub>O (compared to that of H<sub>2</sub>O) requires a larger moderator volume. Concerns were expressed about the huge size of the pressure vessels which would be required for larger CANDU reactors, because such vessels would be difficult to fabricate and very expensive. The design of NPD, and that of all later CANDU reactors, was therefore changed to a pressure-tube design, in which the pressure boundary occurs in a small, relatively thin, fuel channel that surrounds each fuel assembly module and its associated coolant. A pressuretube design was made possible only by emerging research on zirconium, which showed that zirconium had a very small neutron-absorption cross section and would be a very good candidate metal for the pressure tubes. Using steel, with its much larger absorption cross section, would not permit a working pressure-tube design for a reactor using natural-uranium fuel. The pressure-tube design has the additional safety feature that the break of one pressure tube is more manageable than the break of a large pressure vessel.

Some additional CANDU design features and some consequences of the design decisions are explored here:

- The natural-uranium lattice has low excess reactivity because the fuel is not enriched. This is a safety advantage because it limits the amount of reactivity increase available in an accident. It is also another rationale for adopting a pressure-tube design which allows on-power refuelling of the reactor to sustain the core reactivity without shutting down the reactor. Otherwise, batch refuelling of a CANDU reactor in a pressure vessel would be required every few months, which would lower its capacity factor on account of the lost operating time during refuelling and during the associated, time-consuming, shutdown/cool-down and start-up/heat-up transients.
- CANDU NU fuel achieves a discharge burnup in the ~7,500–~9,500 MW.d/Mg(U) range, depending on the specific reactor design. This is much lower than the dis-

charge burnup in LWRs (~30,000–50,000 MW.d/Mg(U)). However, considering fuel enrichment for LWRs (about 3.5%-5% <sup>235</sup>U) and the depleted-uranium tailings which are discarded, CANDU reactors are more efficient than LWRs and extract ~25% more energy per Mg of mined natural uranium.

- The pressure-tube design means that the main reactor vessel (the calandria) is not pressurized. The moderator is insulated from the hot coolant by placing a calandria tube concentric with each pressure tube, with an insulating gas in the intermediate (annulus) space. The moderator can be maintained relatively cool at ~70°C by circulating it in its own heat-exchanger circuit, which means that more of the neutrons will have lower thermal energies than in an LWR and consequently will more readily induce fission in fissile nuclides, e.g., <sup>235</sup>U and <sup>239</sup>Pu.
- CANDU reactivity devices are located interstitially between pressure tubes and are therefore in a benign (low-temperature and unpressurized) environment, which is a safety advantage. CANDU reactivity devices are not subject to being ejected from the reactor by coolant pressure.
- Heavy water is used as coolant instead of light water in all operating CANDU reactors for additional neutron economy. Light water was used as coolant in the Gentilly-1 prototype, and organic coolant was used in the Whiteshell Reactor (WR-1) engineering test unit, both of which are no longer in operation. Light water is also used as coolant in the proposed Advanced CANDU Reactor (ACR) design, to reduce capital costs associated with heavy water, and also in the Supercritical-Water-Cooled Reactor (SCWR) design.
- All operating CANDU reactors have horizontal pressure tubes (the Gentilly-1 prototype and the WR-1 had vertical pressure tubes). This orientation promotes symmetry because coolant can be circulated in opposite directions in alternate tubes (i.e., using bi-directional coolant flow), making average neutronics conditions essentially identical at the two ends of the reactor (unlike the situation in LWRs). With vertical pressure tubes, the gradient in coolant temperature and density as the coolant picks up heat and moves upward makes the neutronic and thermal-hydraulic conditions asymmetric.
- Horizontal pressure tubes also facilitate bi-directional refuelling (i.e., fuelling in opposite directions in adjacent channels), which further promotes symmetry. When the fuel is manufactured as short (~50-cm-long) fuel bundles which can easily be pushed through the pressure tube from either end, the associated fuelling machines will also be short, less cumbersome, and require less radiation shielding. With vertical tubes, the entire fuel string (consisting of a vertical stack of perhaps 12 or 13 bundles) would have to be removed from the top of the reactor, so that a very long fuel assembly would have to be used (together with a long and heavy transfer flask), or short fuel bundles would have to be connected to a common stringer.
- Whereas the loss of moderator shuts any (thermal) reactor down, the loss of coolant in a CANDU reactor does not have the same effect because the coolant is separated from the moderator. Instead, the loss of coolant in operating CANDU reactors generates a positive reactivity insertion (called the coolant void reactivity, or CVR); this is due to a number of spectral effects which change mostly the fast-fission factor and the resonance-escape probability. As a consequence, a loss-of-coolant accident in CANDU results in a positive power pulse, which must be quickly turned around by

shutdown-system action to avoid overheating the fuel. In fact, the postulated largeloss-of-coolant accident (LLOCA) scenario is the reason for the adoption of redundancy in CANDU shutdown capability design. CANDU reactors have two fast shutdown systems, which are physically and logically independent of one another and each fully capable of shutting the reactor down from any credible configuration. Shutdown system 1 consists of cadmium shut-off rods which fall under gravity (initially spring-assisted) into the reactor from above. Shutdown system 2 consists of the injection of a solution of neutron-absorbing gadolinium (a high neutron absorber) under high pressure through nozzles directly into the moderator.

- The lattice pitch (distance between the centres of neighbouring tubes) in all operating CANDU reactors is 28.575 cm. This is not the optimum value in the sense of maximizing the lattice reactivity (therefore minimizing the refuelling rate and maximizing the average fuel discharge burnup), which is closer to 34 cm or so. However, the larger volume of D<sub>2</sub>O moderator would result in a higher capital cost; the shorter pitch was selected to minimize the levellized unit-energy cost. A shorter lattice pitch of 24 cm was selected for the ACR (to reduce moderator cost, among other reasons), but the reduced moderation would not allow the chain reaction to be self-sustaining with natural-uranium fuel, and the ACR would need to use enriched fuel.
- The "workhorse" control devices in all operating CANDU reactors are "liquid" zone controllers. These control 14 compartments in which amounts of light water (used for its much higher neutron-absorption cross section than heavy water) can be varied uniformly across all compartments to control reactivity or to shape the power distribution differentially.

# 9 CANDU Reactor Physics Computational Scheme

Because of the strong heterogeneity of reactor lattices (see the example of the CANDU basic lattice cell in Figure 19) and because nuclear fuel is a strong neutron absorber, the diffusion equation cannot be used in reactors based on the detailed lattice geometry. For cases where it is not desired to apply neutron transport in full-core reactor models, a two-stage or three-stage process has been developed to enable calculation of the neutron flux and the power distribution using the diffusion equation. This process is illustrated here for CANDU reactors.



### Figure 19 CANDU basic lattice cell

The computational scheme for CANDU neutronics consists of three stages. Separate computer programs have been developed to perform the calculations corresponding to each stage. The three stages are:

- lattice-cell calculation
- reactivity-device (supercell) calculation
- finite-core calculation.

# 9.1 Lattice Calculation

The first stage involves solving for the flux distribution in the basic lattice cell, which consists of the fuel, coolant, pressure and calandria tubes, and moderator, but no reactivity devices (see Figure 19). This calculation is performed using a deterministic multi-group neutron transport code such as WIMS-AECL. Then the transport code averages the nuclear properties (for absorption, moderation, fission, etc.) over the cell according to the calculated reaction rates in each sub-region of the lattice cells to determine the effective neutronic properties of the whole lattice cell (i.e., few (typically 2)-group macroscopic cross sections and diffusion coefficients). This averaging (homogenization) of the properties of the basic lattice cell dilutes the strong absorption of the fuel with the much weaker absorption in the moderator. With these homogenized properties, Fick's Law becomes a good approximation over most of the reactor model, and the diffusion equation can be used to calculate the full-core neutron-flux and power distributions. The lattice properties govern the neutron-multiplying behaviour of the reactor lattice, and therefore they must be obtained for all ages of the reactor fuel, i.e., the transport code must perform a "depletion" calculation to evolve the lattice-cell neutronic properties to reflect the changes in the nuclide composition of the fuel with irradiation/burnup. The lattice properties must also reflect any modified configurations of the lattice. For example, if the coolant is assumed "voided" in a hypothetical loss-of-coolant accident, or the temperature of the material in a sub-region is assumed to change, then the lattice properties must change accordingly.

# 9.2 Reactivity-Device Calculation

This type of calculation determines the effect of a reactivity device on the nuclear properties in its vicinity. This effect is expressed in the form of "incremental" cross sections which are added to the (unperturbed) homogenized properties of neighbouring lattice cells in a modelled volume around the device, called a "supercell"; see Figure 20.

For instance, shutoff-rod incremental cross sections dictate the local efficacy of the shutoff rods in absorbing neutrons and shutting down the fission chain reaction. The incremental cross sections of a device are obtained by calculating the differences in the supercell homogenized properties between the case when the device is inserted into the supercell and the case when it is withdrawn from it. The incremental cross sections are added to the lattice-cell cross sections in the modelled volume around the device's position in the reactor core, when that particular device is inserted.





Because the supercell also contains highly absorbing material, transport theory must again be used. CANDU reactivity devices are perpendicular to the fuel channels. Therefore, realistic supercell models are three-dimensional, and as a result supercell calculations are best done using the DRAGON transport code, which can perform calculations in three dimensions.

# 9.3 Full-Core Calculation

In the final stage, a full-core reactor model is assembled. The full-core model must incorporate, for each cell in the reactor, the homogenized unperturbed-lattice-cell cross sections which apply there, together with the incremental cross sections of nearby reactivity devices in their appropriate locations. The model therefore consists of homogenized basic-lattice cells on which are superimposed homogenized subcells representing reactivity devices. One of many such "device model areas" is shown in Figure 21; in the white subcells, the nuclear cross sections are obtained by summing the basic-cell properties and the appropriate device incremental properties.

A full, 3-D reactor model constructed in this way is used to calculate the three-dimensional flux and power distributions in the core. Because homogenized properties are used, few-group diffusion theory can be applied to the full-core reactor model.



Figure 21 Simple model with superimposed reactivity device

# **10** Evolution of Lattice Properties

When nuclear fuel is "burned" in a reactor, changes occur in the material composition of the fuel. These changes are generally called "fuel (isotopic) depletion". In this section, we look at how the properties of the CANDU lattice evolve with fuel irradiation (or burnup).

The following changes occur cumulatively in CANDU nuclear fuel with time:

- The <sup>235</sup>U depletes (i.e., its concentration, which starts at 0.72 atom% for fresh natural uranium, decreases).
- Fission products accumulate; most of these are radioactive, and many have a significant neutron-absorption cross section.
- <sup>239</sup>Pu is produced by neutron absorption in <sup>238</sup>U and two subsequent beta decays:

$$^{238}$$
U + n  $\rightarrow ^{239}$ U\*  $\rightarrow ^{239}$ Np + $\beta$   
 $^{239}$ Np  $\rightarrow ^{239}$ Pu + $\beta$ .

- <sup>235</sup>Pu participates strongly in the fission chain reaction (because it is fissile, like <sup>235</sup>U), but while it continues to be created at about the same rate from <sup>238</sup>U, its net rate of increase slows.
- Further neutron absorptions lead from <sup>239</sup>Pu to <sup>240</sup>Pu (non-fissile), and then to <sup>241</sup>Pu (fissile).
- Other higher actinides are also formed (e.g., curium, americium).
- The total fissile fraction in the fuel ( $^{235}U + {}^{239}Pu + {}^{241}Pu$ ) decreases monotonically. The evolution of the concentration of these three nuclides is shown in Figure 22.

A typical graph of reactivity  $\rho_{\infty}$  of the infinite CANDU lattice versus fuel irradiation, obtained from a cell calculation using a transport code, is shown in Figure 23. The following points are of note:

- The fresh-fuel infinite lattice (where the fuel has not yet received any irradiation) has a high reactivity (~78 mk when the <sup>135</sup>Xe and other saturating fission products have built up). To achieve a steady state in the infinite lattice with fresh fuel, a corresponding amount of negative reactivity must be added to the lattice [e.g., by dissolving a neutron poison (i.e., a material with a large neutron absorption cross section) in the moderator] to suppress the initial supercriticality.
- The reactivity starts to decrease immediately on account of <sup>235</sup>U depletion.
- It then starts to increase for a while, on account of production of <sup>239</sup>Pu, which is slightly more effective than <sup>235</sup>U. Note the slight delay due to the <sup>239</sup>Np ~2-day half-life.
- However the rate of increase of reactivity slows (because the net rate of plutonium production decreases), and the reactivity proceeds through a maximum, called the plutonium peak, with increasing burnup (note that this is not a peak in <sup>239</sup>Pu concentration, but in lattice-cell reactivity!).
- Following the plutonium peak, the reactivity decreases monotonically on account of the continuing depletion of <sup>235</sup>U and the continuing accumulation of fission products.
- The infinite lattice reaches zero reactivity at an irradiation corresponding to a burnup of ~6,700 MW.d/Mg(U).



• A <u>homogeneous</u> infinite lattice with fuel beyond that burnup would be subcritical.

### Figure 22 Evolution of fuel isotopic densities



#### Figure 23 Infinite-lattice reactivity vs. irradiation

However, remember that the infinite lattice does not experience reactivity losses due to neutron leakage; moreover, it does not account for neutron absorption in all the reactivity devices within the core. Consequently, a homogeneous reactor with all fuel at the same irradiation would reach zero reactivity at a much lower burnup than the infinite lattice.

In the CANDU-6 reactor, leakage is about -30 mk, and the average in-core reactivity-device load is ~-18 mk. Therefore, an estimate of the reactivity  $\rho_{eff}$  of a finite homogeneous CANDU-6 reactor can be obtained by subtracting 48 mk from the reactivity of the infinite lattice; see Figure 24.



#### Figure 24 Finite-reactor reactivity vs. irradiation

In a homogeneous reactor, a significant amount of additional negative reactivity (~30 mk) is required to suppress the initial supercriticality. A homogeneous CANDU-6 would reach zero reactivity at an irradiation corresponding to a burnup of ~4,000 MW.d/Mg(U). A homogeneous CANDU-6 with fuel beyond that burnup would be subcritical [note that the argument is hypothetical in any case because a homogeneous finite reactor would not remain homogeneous with burnup]. Therefore, if the CANDU-6 were to be batch-refuelled, the discharge burnup would be only ~4,000 MW.d/Mg(U).

However, CANDU reactors are refuelled on-power, and therefore there is always (except near start of life) a mixture of fresh fuel and fuel with high irradiation. The fuel with high irradiation has negative "local reactivity", but this is compensated for by the positive local reactivity of low-irradiation fuel. The proper mixture of fuel in this inhomogeneous reactor (obtained by the proper rate of daily refuelling) maintains the reactor critical day-to-day. Physically, the older fuel does the job of reducing the high reactivity of the young fuel, a job which moderator poison does in the batch-refuelled reactor. The difference is that whereas the poison is just a "parasitic" absorber, the older fuel does provide fissions and therefore additional energy.

The mixture of new and old fuel makes it possible to drive the discharge burnup to a much higher value than that deduced from the "homogeneous" reactivity curve. We can guess (or calculate) approximately how far we can drive the exit burnup by determining what value gives equal "positive" and "negative" areas "under" the reactivity curve [this tells us where the average  $\rho_{eff}$  would be 0]; see Figure 25.

From the figure, we can see that positive and negative areas are equal when the average exit (or discharge) burnup to which we can take the fuel with daily refuelling is ~7,500 MW.d/Mg(U). This is almost twice the discharge-to-burnup value attainable in the "batch-refuelled" reactor and represents quite a benefit provided by on-power refuelling!



Figure 25 Averaging reactivity with daily refuelling

# **11** Summary of Relationship to Other Chapters

- The Neutron Physics chapter explains the interactions that neutrons have with matter and defines all the basic quantities needed in the study of the fission chain reaction and the analysis of reactors.
- The present chapter covers mostly the time-independent neutron-diffusion equation and the analysis of steady-state (time-independent) neutron distributions, either in the presence of external sources or in fission reactors. It has not covered time-dependent phenomena, which are left for the following chapter.
- The Reactor Kinetics chapter covers the time-dependent neutron-diffusion equations and

studies the phenomena of fast-neutron kinetics, fission-product poisoning, reactivity coefficients, and others in reactors.

# **12 Problems**

# Problem 1

There is an infinite homogeneous non-multiplying medium with diffusion length 8 cm and diffusion coefficient 2 cm. There are four isotropic point sources of neutrons on the *x*-*y* plane:

- Source  $S_1 = 10^8 \text{ s}^{-1}$  at (x, y) = (10 cm, 0)
- Source  $S_2 = 10^8 \text{ s}^{-1}$  at (x, y) = (-10 cm, 0)
- Source  $S_3 = 10^{10} \text{ s}^{-1}$  at (x, y) = (0, 20 cm)
- Source  $S_4 = 10^{10} \text{ s}^{-1}$  at (x, y) = (0, -20 cm)
- (a) Find the total flux at (x, y) = (0, 0)
- (b) Find the magnitude and direction of the total current at (x, y) = (0, 0)
- (c) Find the value and the direction of the total current at (x, y) = (0, -10 cm).

# Problem 2

An isotropic point source of strength S n.s<sup>-1</sup> is located at the origin of axes in a homogeneous non-multiplying material. The material is characterized by an absorption cross section  $\Sigma_a$  and a diffusion constant D.

- (a) Imagine a sphere of arbitrary radius *R* centred at the origin of axes. Calculate the integrated absorption rate of neutrons (per s) within the sphere.
- (b) What is happening to the remaining neutrons (the difference between the number emitted and the number absorbed per s)? Prove this by calculation.

# Problem 3

Suppose that you have an infinite plane source of neutrons in the y-z plane (i.e., at x = 0), which emits a total of N neutrons per cm<sup>2</sup> per s (half in the positive and half in the negative x-direction).

Of course, we can think of the plane source as an infinite number of point sources, one at each point of the plane. Let us take the emission from each point source as isotropic. If the point source actually has differential area dA (which can be as small as we want), then the point-source strength will be *NdA* neutrons per s.

Calculate the flux at any point x in space by integrating the flux from all point sources (by symmetry, this will of course be the same for any values of y and z). Show that you get the formula for the flux from the infinite plane source.

# Problem 4

This is an exercise on the quantitative aspects of the neutron cycle.

Refer to the figure below which pertains to a critical reactor. Refer also to the notes in the figure. You are asked to calculate how many **thermal** neutrons escape from the reactor per unit time.

Remember that the two main things that can happen when a neutron is absorbed in the fuel

are capture (when the neutron is absorbed and a gamma ray is emitted) and fission (when the neutron is absorbed and fission is induced). Therefore, the ratio of capture to fission,  $\sigma_{\gamma}/\sigma_{f}$ , is an important parameter. To solve the problem, use the data given and find the right sequence (up and/or down) for filling numbers into the boxes.

Note that numbers need not be exact integers. In each box, retain non-integer numbers to 3 decimal places.



### Problem 5

A homogeneous, bare cylindrical reactor with extrapolated axial length 5.8 m is critical. It is operated at a fission power of 900 MW. In one energy group, the reactor material is known to have v = 2.38,  $\Sigma_f = 0.0042$  cm<sup>-1</sup>, and D = 1.14 cm  $\Sigma_a = 0.0099$  cm<sup>-1</sup>.

The leakage is 9.6 mk. [Note: neglect the extrapolation distance.]

- (a) Calculate the reactor buckling and the material's absorption cross section.
- (b) Determine the reactor's extrapolated diameter.
- (c) What is the average flux in the reactor?
- (d) What is the ratio of the flux on the cylindrical reactor axis at 50 cm from the reactor face to the maximum flux in the reactor?

Design the proportions of a cylindrical reactor which minimize leakage [neglect the extrapolation distance].

## Problem 7

A research reactor is in the shape of a parallelepiped with a square base of side 5.2 m and a height of 6.8 m. The reactor is filled uniformly with a fuel of one-group properties  $v\Sigma_f = 0.0072$  cm<sup>-1</sup> (and v = 2.45) and  $\Sigma_a = 0.0070$  cm<sup>-1</sup>. The reactor operates steadily at a fission power of 15 MW. The average value of energy per fission  $E_f = 200$  MeV, and 1 eV =1.6\*10<sup>-19</sup> J. [Neglect the extrapolation distance.]

(a) What is the value of the diffusion coefficient?

(b) What is the average value of the neutron flux?

(c) What is the maximum value of the neutron flux?

(d) At what rate is the fuel consumed in the entire reactor (in nuclides.s<sup>-1</sup>) **and** at the centre of the reactor (in nuclides.cm<sup>-3</sup>.s<sup>-1</sup>)?

## Problem 8

A critical homogeneous reactor in the shape of a cube loses 4% of produced neutrons through leakage.

- a) Calculate  $k_{\infty}$  for an infinite reactor made of the same material.
- b) The initial reactor is re-shaped into a sphere. Calculate the new  $k_{\rm eff}$  .

NOTE: Use one-group diffusion theory and ignore the extrapolation length.

### Problem 9

A reactor is made in the shape of a cone, with the base radius equal to the height and both equal to 3 m. The reactor is homogeneous, with the following properties:

$$v\Sigma_f = 0.002 \text{ cm}^{-1}$$
  
 $\Sigma_a = 0.0018 \text{ cm}^{-1}$ 

Calculate the number of neutrons leaking out of the reactor per second knowing that the reactor is critical and that the average flux in the reactor is  $10^{13}$  n/cm<sup>2</sup>/s.

Problem 10

Imagine we have nuclear material with the following properties in two energy groups:

$$\Sigma_{a1} = 0.0011 \text{ cm}^{-1}, \Sigma_{1\to 2} = 0.0068 \text{ cm}^{-1}, \Sigma_{a2} = 0.0043 \text{ cm}^{-1}, v\Sigma_{f2} = 0.00528 \text{ cm}^{-1}$$

 $D_1 = 1.07 \text{ cm}, D_2 = 0.92 \text{ cm}.$ 

(a) Calculate the reactivity of an infinite lattice made of this material.

- (b) In this infinite lattice, what fraction of neutrons is captured in resonances?
- (c) We are asked to make a critical homogeneous reactor with this material, cylindrical in shape, with a diameter 10% greater than the axial dimension [neglect the extrapolation distance]. What will be this reactor's dimensions?
- (d) Calculate the fast and thermal non-leakage probabilities for this reactor. Also, what is the total leakage in mk?
- (e) What is the ratio of the group-1 flux to the group-2 flux in the reactor?

# **13** Appendix A: Reactor Statics

In this Appendix, we derive Fick's Law.

We copy here the angle-integrated version of the time-independent neutron-transport equation:

$$S(\vec{r}, E) + \chi(E) \int_{E'} v \Sigma_f(\vec{r}, E') \phi(\vec{r}, E') dE' + \int_{E'} \Sigma_s(\vec{r}, E' \to E) \phi(\vec{r}, E') dE' - \Sigma_t(\vec{r}, E) \phi(\vec{r}, E) - \vec{\nabla} \cdot \vec{J}(\vec{r}, E) = 0$$

(presented earlier as Eq. (16)). Our overall objective is to rewrite the last term (the leakage term) in terms of the total flux  $\phi(\vec{r}, E)$  only.

We first try to obtain an equation for the total current  $\vec{J}(\vec{r}, E)$  by multiplying the transport equation (7), which depends on angle, by  $\hat{\Omega}$  and integrating over it, yielding Eq. (A.1):

$$\frac{1}{4\pi} S(\vec{r}, E) \int_{\hat{\Omega}} \hat{\Omega} d\hat{\Omega} + \frac{\chi(E)}{4\pi} \int_{E'\hat{\Omega}'} \nabla \Sigma_{f}(\vec{r}, E') \phi(\vec{r}, \hat{\Omega}', E') d\hat{\Omega}' dE' \int_{\hat{\Omega}} \hat{\Omega} d\hat{\Omega} + 
\int_{\hat{\Omega}\hat{\Omega}'E'} \sum_{s} (\vec{r}, E' \to E, \hat{\Omega}' \to \hat{\Omega}) \phi(\vec{r}, \hat{\Omega}', E') \hat{\Omega} dE' d\hat{\Omega}' d\hat{\Omega} - 
\Sigma_{t}(\vec{r}, E) \int_{\hat{\Omega}} \phi(\vec{r}, \hat{\Omega}, E) \hat{\Omega} d\hat{\Omega} - \int_{\hat{\Omega}} \vec{\nabla} \cdot \vec{J}(\vec{r}, \hat{\Omega}, E) \hat{\Omega} d\hat{\Omega} = 0$$
(A.1)

In the first two terms, which we can call  $T_1$  and  $T_2$ , we used the assumption of isotropy in the external and fission sources, so that these terms are proportional to the integral  $\int_{\hat{\Omega}} \hat{\Omega} d\hat{\Omega}$ . This is a vector quantity; for instance, the *x* component is  $\int_{\hat{\Omega}} \hat{\Omega}_x d\hat{\Omega}$ . It is clear that this integral (and similarly for the other components) must have a zero value because there are as many positive  $\hat{\Omega}_x$ 's as there are negative. Therefore, the first two terms drop out of the equation:

$$T_1 = T_2 = 0. (A.2)$$

Let us jump to the fourth term, which by definition is:

$$\int_{\hat{\Omega}} \phi\left(\vec{r},\hat{\Omega},E\right) \hat{\Omega} d\hat{\Omega} = \int_{\hat{\Omega}} \vec{J}\left(\vec{r},\hat{\Omega},E\right) d\hat{\Omega} = \vec{J}\left(\vec{r},E\right) d\hat{\Omega}$$

Therefore, the fourth term, which we call  $T_4$ , becomes:

$$T_4 = -\Sigma_t \left( \vec{r}, E \right) \vec{J} \left( \vec{r}, E \right)$$
(A.3)

Let us look at the third term,  $T_3$ :

$$\begin{split} T_{3} &= \int_{E'\hat{\Omega}'\hat{\Omega}} \sum_{\hat{\Omega}'\hat{\Omega}} \Sigma_{s} \left( \vec{r}, E' \to E, \hat{\Omega}' \to \hat{\Omega} \right) \hat{\Omega} d\hat{\Omega} \phi \left( \vec{r}, \hat{\Omega}', E' \right) d\hat{\Omega}' dE' \\ &= \int_{E'\hat{\Omega}'\hat{\Omega}} \sum_{\hat{\Omega}} \sum_{\hat{\Omega}'\hat{\Omega}} \Sigma_{s} \left( \vec{r}, E' \to E, \hat{\Omega}' \to \hat{\Omega} \right) \hat{\Omega} \hat{\Omega}' \cdot \hat{\Omega}' d\hat{\Omega} \phi \left( \vec{r}, \hat{\Omega}', E' \right) d\hat{\Omega}' dE'. \end{split}$$

where we have introduced into the integral the unity factor  $\hat{\Omega} \cdot \hat{\Omega}' \equiv 1$ . Also, recall that  $\Sigma_s$  is not

a function of absolute angles, but only of the cosine  $\hat{\Omega} \cdot \hat{\Omega}'$ .

$$\therefore T_3 = \int_{E'\hat{\Omega}'} \hat{\Omega}' \left[ \int_{\hat{\Omega}} \Sigma_s \left( \vec{r}, E' \to E, \hat{\Omega} \cdot \hat{\Omega}' \right) \hat{\Omega} \cdot \hat{\Omega}' d\hat{\Omega} \right] \phi \left( \vec{r}, \hat{\Omega}', E' \right) d\hat{\Omega}' dE'.$$

The integral over  $\hat{\Omega}$  can be written as

$$\Sigma_{sa}\left(\vec{r}, E' \to E\right) = 2\pi \int_{-1}^{1} \Sigma_{s}\left(\vec{r}, E' \to E, \mu\right) \mu d\mu, \tag{A.4}$$

and

$$: T_{3} = \int_{E'} \Sigma_{sa} \left( \vec{r}, E' \to E \right) \int_{\hat{\Omega}'} \phi \left( \vec{r}, \hat{\Omega}', E' \right) \hat{\Omega}' d\bar{\Omega}' dE' = \int_{E} \Sigma_{sa} \left( \vec{r}, E' \to E \right) \vec{J} \left( \vec{r}, E' \right) dE'.$$
(A.5)

Note that if the scattering cross section were isotropic,  $\Sigma_s$  would not depend on  $\mu$ , and therefore  $\Sigma_{sa}$  would be 0. Although this is not a good approximation, one that is more reasonable is to neglect the energy change in anisotropic scattering, i.e., to assume that  $\Sigma_{sa}(\vec{r}, E' \rightarrow E)$  is a delta function =  $\delta(E' - E)\Sigma_{sa}(\vec{r}, E)$ , which leads to

$$T_{3} = \Sigma_{sa}\left(\vec{r}, E\right) J\left(\vec{r}, E\right),\tag{A.6}$$

where

$$\Sigma_{sa}(\vec{r}, E) = 2\pi \int_{-1}^{1} \Sigma_{s}(\vec{r}, E, \mu) \, \mu d \, \mu \equiv \overline{\mu} \Sigma_{s}(\vec{r}, E)$$
(A.7)

and  $\mu$  is the average cosine of the scattering angle.

Moving on to the fifth term,  $T_5$ :

$$T_{5} = -\int_{\hat{\Omega}} \vec{\nabla} \cdot \vec{J} \left( \vec{r}, \hat{\Omega}, E \right) \hat{\Omega} d\hat{\Omega} = -\int_{\hat{\Omega}} \vec{\nabla} \cdot \phi \left( \vec{r}, \hat{\Omega}, E \right) \hat{\Omega} \hat{\Omega} d\hat{\Omega}.$$
(A.8)

To calculate the integral, we adopt again the assumption of weak angular dependence of the angular flux, which leads to the following approximate expression [Eq. (27)] for the angular flux in terms of the total flux and the total current expression; see derivation in Section 2.3:

$$\phi\left(\hat{\Omega}\right) = \frac{\phi}{4\pi} + \frac{3\tilde{J}\cdot\hat{\Omega}}{4\pi}.$$
(27)

Substituting this expression into Eq. (A.8), we get

$$T_{5} = -\int_{\hat{\Omega}} \vec{\nabla} \cdot \left[ \frac{\phi(\vec{r}, E)}{4\pi} + \frac{3}{4\pi} \vec{J} \cdot \hat{\Omega} \right] \hat{\Omega} \hat{\Omega} d\hat{\Omega}.$$
(A.9)

Now it can be shown (a reasonable result) that the integral of the product of two components of  $\hat{\Omega}$ , e.g.,  $\Omega_i \Omega_j$ , is equal to  $4\pi/3$  if i = j, but 0 if  $i \neq j$ . Similarly, the integral of the product of three components is 0.

Using these two results, Eq. (A.9) becomes

$$T_5 = -\frac{1}{3}\nabla\phi(\vec{r}, E). \tag{A.10}$$

Incorporating all these results for the various terms [Eqs. (A.2), (A.3), (A.6), (A.10)], Eq. (A.1) becomes:

$$0 + 0 + \Sigma_{sa}(\vec{r}, E)\vec{J}(\vec{r}, E) - \Sigma_{t}(\vec{r}, E)\vec{J}(\vec{r}, E) - \frac{1}{3}\nabla\phi(\vec{r}) = 0,$$
(A.11)

which yields the final approximation for the total current:

$$\vec{J}(\vec{r},E) = -\frac{1}{3\left(\Sigma_t(\vec{r},E) - \Sigma_{sa}(\vec{r},E)\right)} \nabla \phi(\vec{r},E),$$
(A.12)

which is Fick's Law, giving for the diffusion coefficient,

$$D(\vec{r}, E) = \frac{1}{3\left(\Sigma_t(\vec{r}, E) - \Sigma_{sa}(\vec{r}, E)\right)}.$$
(A.13)

The quantity in parentheses in Eq. (A.13) is defined as the transport cross section,  $\Sigma_{tr}(\vec{r})$ .

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