Computational methods in nuclear engineering

A3.1 Neutron diffusion computer codes

Chapters 4 and 5 presented an analytical treatment of nuclear theory. While understanding such theory provides insight into the physics of nuclear reactor calculations, it is nevertheless of only limited practical value; the nature of the assumptions that have to be made compromise the accuracy that can be achieved. These assumptions include one (or at most two) neutron energy groups and a homogeneous core.

By contrast, however, computer solutions of the steady state neutron diffusion equation (4.34) are possible, in principle, for any number of neutron energy groups. Although two group solutions usually suffice for thermal reactors, many more neutron groups (typically 30) need to be considered for fast reactors; computer solutions then become essential. Furthermore, numerical solutions allow inhomogeneity and anisotropy within the reactor core to be taken into account.

Numerical solutions of the neutron diffusion equation may be achieved by the method of finite differences. For simplicity, this is illustrated below using a one-group, one-dimensional model where, over each mesh length, the lattice parameters D and Σ_A are taken as constant.

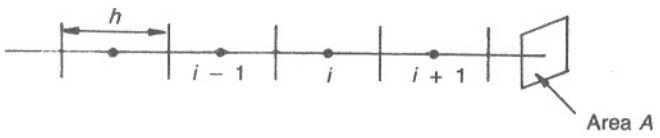

Figure A3.1. One dimensional finite-difference model of the neutron diffusion equation. Homogeneous approximations for D and Σ_a are usually employed, where the fuel element, cladding, coolant and structural material are 'smeared' over each mesh volume

Considering the volume around mesh point i, the rate of neutron absorption is given by $\Sigma_{ai}\phi_i h\mathrm{A}$ and the leakage from the volume is given by the following expressions:

$$\text{Leakage to left} = \mathrm{D_L}\left(\frac{\phi_{i-1} - \phi_i}{h}\right)\mathrm{A} \tag{A3.1}$$

$$\text{Leakage to right} = \mathrm{D_R}\left(\frac{\phi_{i+1} - \phi_i}{h}\right)\mathrm{A} \tag{A3.2}$$

where $\mathrm{D_L}$ and $\mathrm{D_R}$ are the appropriate average values for the local neutron diffusion coefficients. These are approximately given by

$$1/\mathrm{D_L} = 1/\mathrm{D}_i + 1/\mathrm{D}_{i-1} \tag{A3.3}$$

$$1/\mathrm{D_R} = 1/\mathrm{D}_i + 1/\mathrm{D}_{i+1} \tag{A3.4}$$

Hence from the neutron diffusion equation (4.34) we obtain

$$\mathrm{D_L}\left(\frac{\phi_{i-1} - \phi_i}{h}\right)\mathrm{A} + \mathrm{D_R}\left(\frac{\phi_{i+1} - \phi_i}{h}\right)\mathrm{A} - \Sigma_{ai}\phi_i h\mathrm{A} + S_i h\mathrm{A} = 0 \tag{A3.5}$$

where S_i is the neutron source per unit volume at mesh point i. From equation (4.48) we get that

$$S_i = k_\infty \Sigma_{ai}\phi_i \tag{A3.6}$$

if the volume at mesh point i contains fissile material; in non-fissile material (e.g. reflector material around the core) S_i will be zero. Hence equation (A3.5) becomes a series of n simultaneous equations where n is the number of mesh points. In matrix notation,

$$\mathbf{F}\boldsymbol{\phi} = 0 \tag{A3.7}$$

where $\mathbf{F}$ is a matrix of coefficients and $\boldsymbol{\phi}$ is a column vector of neutron fluxes. Equation (A3.7) can be solved by standard numerical techniques.

The above method is adequate provided the absorption is not too large and that we are not too near boundaries. (In these cases some inaccuracies may arise.) The method may be extended to two- or multi-group calculations by including the effects of neutron slowing-down collisions in equation (A3.5), as shown in equations (5.3) and (5.4). The method can also be readily extended to 2 or 3 dimensions by including terms describing leakage in those directions.

A3.2 Reactor kinetics computer codes

Analysis of the time behaviour of a reactor system is important during start-up conditions, power changes and under fault conditions. The simple one-group equations of reactor kinetics as given by equations (8.13) and (8.15) are normally sufficient for analysing transient behaviour of thermal reactors; however we are usually interested in spatial variation of flux (at least in one dimension) as well as variation with time. If we consider leakage in one dimension only, e.g. by considering a fuel element in the centre of a cylindrical reactor where leakage in the radial and tangential directions will

(by symmetry) be zero, then equation (8.13) can be modified to yield

$$\frac{1}{v}\frac{\delta\phi}{\delta t} = \mathrm{D}\frac{\delta^2\phi}{\delta z^2} + k_{\mathrm{eff}}(\rho - \beta)\Sigma_a\phi + \sum_{i=1}^{6}\lambda_i C_i \qquad \text{(A3.8)}$$

where z is the vertical ordinate, and equation (8.15) yields

$$\frac{\mathrm{d}C_i}{\mathrm{d}t} = k_{\mathrm{eff}}\beta_i\Sigma_a\phi - \lambda_i C_i \quad \text{(six equations)} \qquad \text{(A3.9)}$$

Here $C_i = C_i(z, t)$ and $\phi = \phi(z, t)$, ρ and hence k_{eff} are parameters, and all other terms are coefficients. Equations (A3.8) and (A3.9) may be converted, using finite-difference approximations for the leakage term $\mathrm{D}\frac{\delta^2\phi}{\delta z^2}$ as in (A3.8) to yield a matrix equation of the form

$$\mathbf{V}^{-1}\frac{\delta\psi}{\delta t} = \mathbf{F}\psi \qquad \text{(A3.10)}$$

Here **V** and **F** are coefficient matrices, and ψ is a matrix of the form

$$\begin{bmatrix} 0 \\ \phi_{r-1} \\ \phi_r \\ \phi_{r+1} \\ C_{1r} \\ \cdot \\ \cdot \\ \cdot \\ C_{6r} \\ 0 \end{bmatrix}$$

where subscript r refers to the rth out of a total of k mesh points in the z direction. Equation (A3.10) can be further arranged in this form

$$\mathbf{V}^{-1}\Delta t^{-1}(\psi_n - \psi_{n-1}) = \mathbf{F}\psi_n \qquad \text{(A3.11)}$$

where subscript n refers to time variation (Figure A3.2), and Δt is the time step size.

This set of simultaneous equations can be solved using standard techniques to yield solutions for the spatial and time variation of reactor flux for a constant value (or at most a predetermined variation) of k_{eff}. However in reactor fault studies, significant changes in fuel and coolant temperatures may occur. In those circumstances temperature feedback must be taken into account. To do this, the thermal–hydraulic equations governing the relationships between coolant flow, fuel temperature and neutron flux (as introduced in Chapter 6) must be considered, in order that the variation of temperature as a function of time and space, $T(z, t)$ can be established. The effect of such temperature variation upon reactivity may be determined

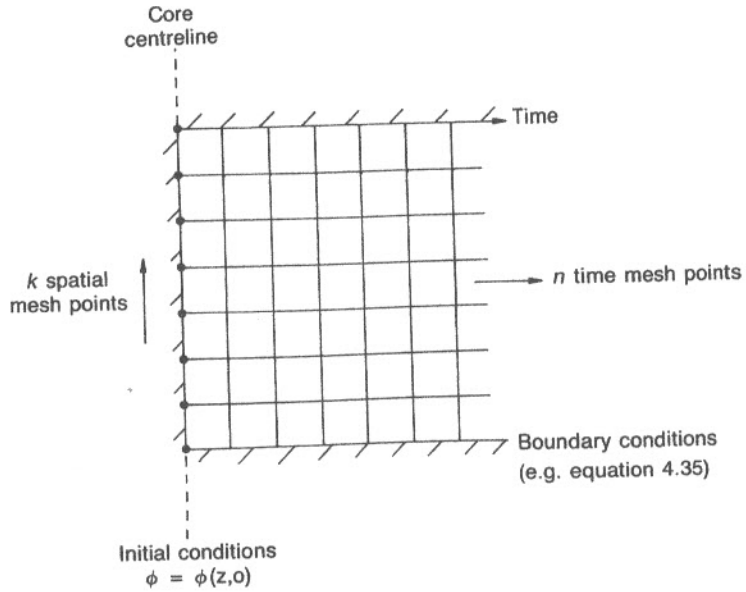

Figure A3.2. Finite-difference scheme for kinetic calculation

from previously-assessed values for the temperature coefficient of reactivity, α (equation (8.34),

$$\alpha = \frac{\delta\rho}{\delta T}$$

It is thus apparent that the neutron flux affects the temperature, which affects the reactivity, which affects the neutron flux (see Figure 8.6). We say that the differential equations governing the neutron flux and the reactor core thermal hydraulics are *coupled*. (For further discussion of methods of solution of these equations, readers are advised to read, for example, **J. Graham,** *Fast Reactor Safety*, Academic Press, 1971.)

A3.3 Monte Carlo computer codes

On some occasions we are only interested in determining a value for k_{eff} for a given system; for example, it might be required to demonstrate that in a storage pond containing irradiated fuel, k_{eff} was very much less than unity for all conceivable fuel configurations (i.e. that a criticality was not possible – see also Chapter 12). The most suitable method of solving such a problem is to use a so-called 'Monte Carlo' code.

The Monte Carlo method goes right back to the statistical nature of the neutron transport problem. The technique consists of tracing in detail the path followed by individual neutrons drawn at random from the population

in the reactor. Monte Carlo trials typically proceed as follows:

1. Take one neutron produced by a fission and assign it a randomly determined position and velocity, consistent with Figure 2.6.
2. Depending upon its speed and direction, the neutron will either collide with a moderator atom and slow down, or collide with a fuel atom and cause a further fission, or be captured without fission, or escape from the system (Figure A3.3).
3. If the neutron is moderated, assign it an appropriate new direction and speed (equations (2.19) to (2.21)) and continue the trial.
4. If the neutron causes fission, assign an appropriate number of fission neutrons to the event (Table 3.2), and assign the fission neutrons randomly determined speeds and directions. Continue the trial following each fission neutron.
5. Continue the trial until the original neutron and any subsequent neutrons generated have escaped from the system. (If this does not happen then it suggests $k_{\text{eff}} > 1{\cdot}0$.)
6. Repeat the trial many times. On a computer, this is easy to do. Hand calculation would, however, be impossibly tedious.

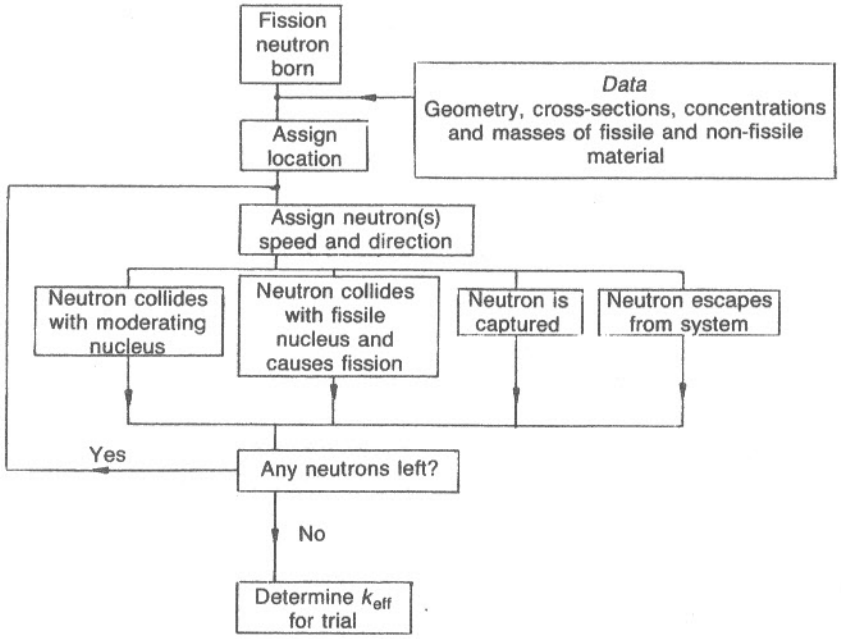

Figure A3.3. A single Monte Carlo trial for determining k_{eff} for a system which is believed to be sub-critical. Some thousands of such trials are required to yield accurate results

7. The average ratio of (number of first generation neutrons):(number of second generation neutrons) is then equivalent to k_{eff}.

The Monte Carlo method is a statistical method. The results can therefore have confidence limits assigned to their accuracy. The method was developed largely by von Neumann and Ulam during the Second World War, although full development of the technique awaited the advent of large digital computers. The method can deal with any inhomogeneity or anisotropy in a potentially critical array of fissile material.