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CALCULATION METHODS FOR MULTIGROUP NEUTRON CROSS SECTIONS USED IN BURNUP STUDIES

by

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ABSTRACT

Calculation of burnup of material composing a nuclear reactor is important in a feasibility study of lifetime of fuel in possible reactor systems. This work discusses (i) a basis for calculating a flux spectrum in order to obtain multigroup cross sections and (ii) a method for solving the burnup equations. Under (i) particular attention is paid to the calculation of multigroup resonance cross sections and (ii) a simple and effective analytic technique is derived. In addition, this work presents, in a consistent manner, developments in the field of reactor physics which effect the calculation of multigroup data. The physical model adopted to simplify the otherwise unmanageable equations is appropriate to a large recirculating fuel reactor operating under equilibrium conditions.

The work is divided into essentially three parts (i) the basis of multigroup data (Sections 2 and 3), (ii) the calculation of multigroup data (Sections 4, 5 and 6) and (iii) the solution of burnup and multigroup flux equations (Sections 7 and 8). Considering that neutron reactions are very dependent on neutron energy it is convenient to divide the energy range into three regions typified by completely different behaviour. These are (a) the fast region (Section 4) – neutrons are produced from fission, (b) the resonance region (Section 5) – neutrons slow down in energy and (c) the thermal region (Section 6) – neutrons scatter up and down in energy until lost.

Note: This work was first presented as a thesis for the degree of Master of Science, University of New South Wales.

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1. INTRODUCTION

The determination of multigroup cross sections used in burnup studies requires (i) the calculation of a detailed neutron flux spectrum (flux as a function of neutron energy) and (ii) the calculation of nuclide concentrations in a reactor due to evolution of the nuclides from burnup of reactor material. The multigroup data is prepared from basic nuclear reaction cross sections or resonance parameters (Hughes and Schwartz 1958), angular distribution of neutrons emitted from various reactions (Hughes and Carter 1956) and reaction mechanisms (Buckingham, et al. 1961). For thermal calculations (neutron energy less than about 1eV) molecular and crystal structure play an important role in the preparation of scattering energy exchange information (McLatchie 1962 and Macdougall 1963). The work here will not be concerned with the availability, or otherwise, of nuclear data even though this is an important consideration in a burnup study where hundreds of fission product nuclides are present in the reactor. The matter is discussed by Garrison and Roos (1962), Hansen (1961) and Cook (1967). The multigroup data is prepared for use in a space dependent calculation of neutron flux using, say, the code (computer programme) CRAM (Hassitt 1962) which solves the diffusion approximation of the Boltzmann equation for one or two dimensional geometry. The solution techniques used in diffusion space dependent codes are discussed at length by Wachspress (1966). Between the (input) basic nuclear data and the (output) multigroup data for use in reactor codes lies a programme. This programme is required to condense the basic nuclear data without too much loss of accuracy. Various programmes have been written to serve this function (GAM–Joanou and Dudek 1961, GATHER–Joanou, et al. 1963, MULGA– Clancy, et al. 1963, GALAXY–Bell, et al. 1964 and GYMEA–Pollard and Robinson 1966). Each programme has a different bias and a different extent of generality. In this work we will concentrate on studies relevant to the High Temperature Gas Cooled Reactor (H.T.G.C.R.) project of the Australian Atomic Energy Commission (A.A.E.C.).

In brief the H.T.G.C.R. project of the A.A.E.C. is a study of the feasibility of a large recirculating fuel reactor composed of one inch diameter ceramic balls of beryllia, thoria and plutonia (Ebeling and Hayes 1967). Questions which arose were numerous and covered aspects of feasibility of fabrication of a ball to retain fission products, choice of concentration of constituents, choice of fuel particle size, suitable power density, design of core structure, manner of detection of highly irradiated balls, fuel management schemes for optimum flow of fuel through the reactor, cooling of the core and its attendant safety problems, problems of recovery by chemical processing of otherwise waste material from burnt up fuel and overall economic optimization to name but a few. Many disciplines are required to work together in order to arrive at a workable design. Reactor physics calculations are required to cover both neutron and nuclide inventory for the life of fuel as part of the core design. These calculations require to account for differences in composition of balls, due to differing extents of irradiation, in different parts of the reactor. A simple model of the system operating under ultimate conditions was proposed by Bicevskis et al. (1967) and a detailed calculational tool was developed by Hesse (1967).

With a range of possible fuel compositions for the H.T.G.C.R. and extent of burnup, (expressed as fissions per initial fissile atom — FIFA) a reliable code for the preparation of multigroup data is required. This code must be capable of predicting results of a few well chosen experiments (McCulloch et al. 1965, Tattersall 1967 and Ritchie 1967) in order to give confidence in the basic nuclear data used and its manner of preparation. In this work we will investigate theoretical aspects of relevance to the design of a suitable multigroup data preparation code (implemented as GYMEA–Pollard and Robinson 1966).

2. REACTOR NEUTRON EQUATIONS

2.1 Neutron Diffusion Equation

The neutron diffusion equation (Weinberg and Wigner 1958) expressing balance of neutron process for neutrons of energy E at a point $\underset{\sim}{r}$ of the reactor at time t may be written

$$(L + \sum_m R^{(m)})\phi = -\frac{1}{v}\frac{\partial \phi}{\partial t} + S(\underset{\sim}{r},E,t), \qquad (1)$$

where $\phi(\underset{\sim}{r},E,t)d\underset{\sim}{r}\,dE\,dt$ is the flux of neutrons with energy around E (between E and E+dE) in the neighbourhood of the point $\underset{\sim}{r}$ ($d\underset{\sim}{r}$ is a volume element around $\underset{\sim}{r}$) in the time dt about t,

$S(\underset{\sim}{r},E,t)$ is an external source (not coupled with ϕ),

L is the neutron diffusion operator discussed below,

$R^{(m)}$ is the neutron reaction operator discussed below,

m is an index used to distinguish particular reactions and the summation on m extends over all neutron reactions occurring in the reactor.

The diffusion operator L is given by

$$L\phi = -\underset{\sim}{\nabla}.D(\underset{\sim}{r},E,t)\underset{\sim}{\nabla}\phi(\underset{\sim}{r},E,t), \qquad (2)$$

where $D(\underset{\sim}{r},E,t)$ is the diffusion coefficient

$$= 1/3 \sum_{\ell} N_{\ell}(\underset{\sim}{r},t)\,\sigma_{\ell}^{(tr)}(E) \;, \qquad (3)$$

σ denotes microscopic cross section with superscript indicating the reaction type (tr means transport) and subscript indicating nuclide involved,

$N_{\ell}(\underset{\sim}{r},t)$ is the concentration of nuclide ℓ,

and the summation on ℓ extends over all nuclides in the reactor (this would include fission products for a reactor operating at power).

The reaction operator $R^{(m)}$ is given by

$$R^{(m)}\phi = \sum_{\ell}(A_{\ell}^{(m)} - P_{\ell}^{(m)})\,\phi(\underset{\sim}{r},E,t) \;, \qquad (4)$$

where $A_{\ell}^{(m)}\phi$ is the neutron loss operator for reaction m with nuclide ℓ

$$= N_{\ell}(\underset{\sim}{r},t)\,\sigma_{\ell}^{(m)}(E)\,\phi(\underset{\sim}{r},E,t) \;, \qquad (5)$$

$P_{\ell}^{(m)}\phi$ is the neutron production operator

$$= N_{\ell}(\underset{\sim}{r},t)\int_0^{\infty}\sigma_{\ell}^{(m)}(E'\to E)\;\phi(\underset{\sim}{r},E',t)dE' \;, \qquad (6)$$

and $\sigma_{\ell}^{(m)}(E'\to E)$ is the cross section of nuclide ℓ for production of neutrons of energy E from an initiating neutron of energy E$'$ through reaction m. (This cross section includes the number of emitted neutrons.)

For fission (f), for example, we have

$$\sigma_{\ell}^{(m)}(E'\to E) = \nu\,\sigma_{\ell}^{(f)}(E')\,\chi(E) \;, \qquad (7)$$

where $\nu\sigma_{\ell}^{(f)}(E')$ is the cross section of nuclide ℓ for production of neutrons through fission (fission emission)

and $\chi(E)$ is the normalized fission spectrum (Cranberg et al. 1956) such that $\int_0^{\infty}\chi(E)\,dE = 1.$ (8)

In our study we will mainly be concerned with long term changes of state of the reactor with time t. These changes will be a result of long term evolution of the nuclide species composing the reactor and arise from burnup of reactor material. Unless stated otherwise in the analysis to follow, the variable t will only refer to long times (days). We are not intent on studying kinetic effects such as would follow from rapid insertion of control absorbers. We are thus only interested in the fundamental (persistent) mode of flux. For a critical reactor in the absence of an external source, Equation 1 becomes

$$(L + \sum_m R^{(m)})\ \phi = 0 \ . \tag{9}$$

Associated with Equation 9 are boundary conditions:

(i) continuity of ϕ and $\underset{\sim}{n}.D\underset{\sim}{\nabla}\phi$ at an internal boundary between different material such as the core-reflector interface ($\underset{\sim}{n}$ is a unit normal pointing out of the region concerned)

and (ii) vanishing of ϕ at an extrapolated boundary (Glasstone and Edlund 1952).

In reactor assessment studies it is convenient to imagine that even non-critical reactors correspond to a critical reactor. The idea is that we imagine a change in the number of neutrons emitted from fission such that a non-critical reactor is brought to critical (Weinberg and Wigner 1958). We thus use instead of Equation 7,

$$\sigma_\ell^{(f)}(E' \rightarrow E) = \nu\,\sigma_\ell^{(f)}(E')\chi(E)/k(t)\ , \tag{10}$$

where k(t) is the reactor multiplication.

2.2 Adjoint Diffusion Equation

From the definition of a scalar product of two reactor variables

$$(\phi, \phi^*) = \int_0^\infty \int_V \phi(\underset{\sim}{r},E,t)\ \phi^*(\underset{\sim}{r},E,t)d\underset{\sim}{r}\ dE, \tag{11}$$

where the integration over space embraces the whole reactor, the adjoint of the operator used in Equation 9, $L^* + \sum_m R^{(m)*}$, is given by

$$\left(\phi,(L^* + \sum_m R^{(m)*})\ \phi^*\right) = \left((L + \sum_m R^{(m)})\ \phi,\phi^*\right) \ . \tag{12}$$

The reactor variables ϕ and ϕ^* must be permissible for operators that act upon them which includes satisfying boundary conditions associated with these operators.

We will now derive the adjoint operator term by term.

2.2.1 Diffusion operator

Firstly

$$(L\phi,\phi^*) = -\sum_r \int_0^\infty \int_{V_r} \phi^*\ \underset{\sim}{\nabla}.D\underset{\sim}{\nabla}\phi\ d\underset{\sim}{r}\ dE\ ,$$

where V_r are volume segments of the reactor with surfaces S_r such that all discontinuities of $\underset{\sim}{\nabla}\phi$ (due to change of reactor material) lie on these surfaces. Deriving a Green's theorem appropriate to this situation we have

$$\underset{\sim}{\nabla}.(\phi^* D\underset{\sim}{\nabla}\phi - \phi D\underset{\sim}{\nabla}\phi^*) = \underset{\sim}{\nabla}\phi^*.D\underset{\sim}{\nabla}\phi + \phi^*\underset{\sim}{\nabla}.D\underset{\sim}{\nabla}\phi - \underset{\sim}{\nabla}\phi.D\underset{\sim}{\nabla}\phi^* - \phi\underset{\sim}{\nabla}.D\underset{\sim}{\nabla}\phi^*$$

then $$(L\phi,\phi^*) = -\sum_r \int_0^\infty \int_{V_r} (\phi \underset{\sim}{\nabla}.D\underset{\sim}{\nabla}\phi^* + \underset{\sim}{\nabla}.(\phi^* D\underset{\sim}{\nabla}\phi - \phi D\underset{\sim}{\nabla}\phi^*))\, d\underset{\sim}{r}\, dE$$

$$= -\sum_r \int_0^\infty \int_{V_r} \phi \underset{\sim}{\nabla}.D\underset{\sim}{\nabla}\phi^* d\underset{\sim}{r}\, dE - \sum_r \int_0^\infty \int_{S_r} \underset{\sim}{n}_r.(\phi^* D\underset{\sim}{\nabla}\phi - \phi D\underset{\sim}{\nabla}\phi^*)\, dS\, dE$$

from Gauss's theorem. The summation taken over internal surfaces vanishes (since each surface must be considered twice) provided

(i) ϕ^* and $\underset{\sim}{n}.D\underset{\sim}{\nabla}\phi^*$ are continuous across internal boundaries.

The summation taken over external surfaces vanishes provided

(ii) ϕ^* vanishes on the external (extrapolated) boundary.

The equation defining the adjoint diffusion operator L^*,

$$(\phi, L^*\phi^*) = (L\phi,\phi^*),$$

then gives $$L^*\phi^* = -\underset{\sim}{\nabla}.D\underset{\sim}{\nabla}\phi^* = L\phi^*, \tag{13}$$

hence L is symmetric.

2.2.2 Reaction loss operator

From the definition given by Equation 5, $A_\ell^{(m)}$ is symmetric.

This follows from

$$(A_\ell^{(m)}\phi,\phi^*) = \int_0^\infty \int_V N_\ell(\underset{\sim}{r},t)\sigma_\ell^{(m)}(E)\phi(\underset{\sim}{r},E,t)\,\phi^*(\underset{\sim}{r},E,t)\,d\underset{\sim}{r}\,dE.$$

Hence $$A_\ell^{(m)*}\phi^* = N_\ell(\underset{\sim}{r},t)\sigma_\ell^{(m)}(E)\phi^*(\underset{\sim}{r},E,t). \tag{14}$$

2.2.3 Reaction production operator

On the other hand the production operator $P_\ell^{(m)}$ is asymmetric.

From

$$(P_\ell^{(m)}\phi,\phi^*) = \int_0^\infty \int_0^\infty \int_V N_\ell(\underset{\sim}{r},t)\sigma_\ell^{(m)}(E'\rightarrow E)\phi(\underset{\sim}{r},E',t)\,\phi^*(\underset{\sim}{r},E,t)\,d\underset{\sim}{r}\,dE\,dE'$$

$$= \int_0^\infty \int_0^\infty \int_V N_\ell(\underset{\sim}{r},t)\sigma_\ell^{(m)}(E\rightarrow E')\phi(\underset{\sim}{r},E,t)\phi^*(\underset{\sim}{r},E',t)\,d\underset{\sim}{r}\,dE\,dE',$$

we get $$P_\ell^{(m)*}\phi^* = N_\ell(\underset{\sim}{r},t)\int_0^\infty \sigma_\ell^{(m)}(E\rightarrow E')\phi^*(\underset{\sim}{r},E',t)dE', \tag{15}$$

which is asymmetric since

$$\sigma_\ell^{(m)}(E\rightarrow E') \neq \sigma_\ell^{(m)}(E'\rightarrow E).$$

2.2.4 Adjoint equation

The adjoint diffusion equation is then given by

$$(L^* + \sum_m R^{(m)*})\phi^* = 0 \tag{16}$$

with boundary conditions (i) and (ii) of Section 2.2.1, where

$\phi^*(\underset{\sim}{r},E,t)$ is the adjoint neutron flux (sometimes called the importance – see for example Lewins 1965),

$$R^{(m)*}\phi^* = \sum_\ell (A_\ell^{(m)*} - P^{(m)*})\phi^* \tag{17}$$

and L^*, $A_\ell^{(m)*}$ and $P_\ell^{(m)*}$ are given by Equations 13, 14 and 15.

2.3 Variational Method

Variational methods of estimating quantities of interest in neutron reactor physics problems have been discussed by several authors (Selengut 1958, Parker 1962, Becker 1964 and Wachspress 1966). We introduce a functional (an operator that produces a constant) which is a measure of "goodness of fit" of an approximation to the exact solution, which, of course, is not available, but nevertheless we will find our technique does not need it. In general the functional is required to be stationary with respect to variation of its arguments (functions) about solutions of a given equation and its adjoint. Here we introduce the functional

$$F(\phi,\phi^*) = (B(\phi-\Phi),\phi^*-\Phi^*) , \tag{18}$$

where $$B = L + \sum_m R^{(m)}, \tag{19}$$

and Φ and Φ^* are solutions of Equations 9 and 16 respectively. Equation 18 obviously defines a quantity which in some sense measures "goodness of fit" of ϕ and ϕ^* to Φ and Φ^*. It remains to show that $F(\phi,\phi^*)$ is stationary.

In order to show that $F(\phi,\phi^*)$ is stationary about solutions of the diffusion equations (Φ and Φ^*) we consider

$$\phi = \Phi + \alpha U$$

$$\phi^* = \phi^* + \beta U^* ,$$

where α and β are parameters and U and U* are arbitrary permissible functions for the operator B (Equation 19) and its adjoint B* respectively. Now

$$F(\phi,\phi^*) = (B\phi,\phi^*) + (B\Phi,\Phi^*) - (B\Phi,\phi^*) - (\phi,B^*\Phi^*),$$

hence $$F(\phi,\phi^*) = (B\phi,\phi^*), \tag{20}$$

which is the form usually used. We then have

$$\frac{\partial F(\phi,\phi^*)}{\partial \alpha} = (U,B^*\phi^*) \tag{21}$$

and $$\frac{\partial F(\phi,\phi^*)}{\partial \beta} = (B\phi,U^*) , \tag{22}$$

giving $$\left.\frac{\partial F}{\partial \alpha}\right|_{\alpha,\beta=0} = 0 \tag{23}$$

and $$\left.\frac{\partial F}{\partial \beta}\right|_{\alpha,\beta=0} = 0 . \tag{24}$$

2.4 Energy Mode Approximation

We consider a number of energy mode trial functions for use with the variational method. These trial functions are given by

$$\phi(\underset{\sim}{r},E,t) = \sum_i \theta_i(\underset{\sim}{r},t) f_i(E,t) \tag{25}$$

and
$$\phi^*(\underset{\sim}{r},E,t) = \sum_i \theta_i^*(\underset{\sim}{r},t) f_i^*(E,t), \tag{26}$$

where $f_i(E,t)$ and $f_i^*(E,t)$ are suitable coordinate functions chosen by us, i and later j, range over 1,2,...,G and expressions for $\theta_i(\underset{\sim}{r},t)$ and $\theta_i^*(\underset{\sim}{r},t)$ are to be obtained. For convenience we will consider the coordinate functions to be biorthonormal, that is,

$$(f_i,f_j^*)_E = \delta_{ij} \quad , \tag{27}$$

where
$$(f_i,f_j^*)_E = \int_0^\infty f_i(E,t) f_j^*(E,t)dE$$

and δ_{ij} is the Kronecker delta.

We require the trial functions to form a complete set in the sense that

$$\lim_{G\to\infty} F(\phi,\phi^*) = 0 \ . \tag{28}$$

In practice we obtain approximate solutions of the diffusion equations with a finite value of G. A selective choice of coordinate functions f_i and f_i^* is thus important to keep G (and hence computational time) to a reasonable value (typically 10). We will return to this point later (Section 3).

Using the selected trial functions we require neighbouring functions to θ_i and θ_i^*. We consider

$$\theta_i = \theta_i + \alpha_i U_i$$

$$\theta_i^* = \theta_i^* + \beta_i U_i^* \ .$$

The equivalent of Equations 21 to 24 then give from our variational method the 2G equations

$$(B\sum_j \theta_j f_j, U_i^* f_i^*) = 0 \tag{29}$$

and
$$(U_i f_i, B^* \sum_j \theta_j^* f_j^*) = 0 \ . \tag{30}$$

Since the functions U_i and U_i^* are arbitrary we must have

$$(B\sum_j \theta_j f_j, f_j^*)_E = 0 \tag{31}$$

and
$$(f_i, B^* \sum_j \theta_j^* f_j^*)_E = 0 \tag{32}$$

at every point $\underset{\sim}{r}$ of the reactor. From here on we will not be particularly concerned with the adjoint energy mode equations (32).

The energy mode equations (31) are a set of equations for the unknown functions θ_i required in our estimate of the flux given by Equation 25. It should be remembered that we choose the coordinate functions, f_i. Written out more fully, Equation 31 reads

$$([L+\sum_m\sum_\ell \{A_\ell^{(m)}-P_\ell^{(m)}\}]\sum_j\theta_j f_j,f_i^*)_E = 0 \; . \tag{33}$$

We will now consider the terms one at a time.

2.4.1 Diffusion term

The diffusion term of Equation 33 is given by

$$(L\sum_j\theta_j f_j,f_i^*)_E = -\int_0^\infty \underset{\sim}{\nabla}.D(\underset{\sim}{r},E,t)\underset{\sim}{\nabla}\sum_j\{\theta_j(\underset{\sim}{r},t)f_j(E,t)\}f_i^*(E,t)dE \tag{34}$$

using the definition of L given by Equation 2. Equation 34 gives

$$(L\sum_j\theta_j f_j,f_i^*)_E = -\sum_j\underset{\sim}{\nabla}.\{\int_0^\infty D(\underset{\sim}{r},E,t)f_j(E,t)f_i^*(E,t)dE\}\underset{\sim}{\nabla}\theta_j(\underset{\sim}{r},t),$$

hence we may write

$$(L\sum_j\theta_j f_j,f_i^*)_E = -\sum_j\underset{\sim}{\nabla}.D_{ji}(\underset{\sim}{r},t)\underset{\sim}{\nabla}\theta_j(\underset{\sim}{r},t), \tag{35}$$

where $$D_{ji}(\underset{\sim}{r},t) = (Df_j,f_i^*)_E \; . \tag{36}$$

2.4.2 Reaction loss term

A typical reaction loss term of Equation 33 (using Equation 5) is

$$(A_\ell^{(m)}\sum_j\theta_j f_j,f_i^*)_E = N_\ell(\underset{\sim}{r},t)\int_0^\infty \sigma_\ell^{(m)}(E)\sum_j\{\theta_j(\underset{\sim}{r},t)f_j(E,t)\}f_i^*(E,t)dE$$

$$= N_\ell(\underset{\sim}{r},t)\sum_j\sigma_{\ell ji}^{(m)}(t)\theta_j(\underset{\sim}{r},t), \tag{37}$$

where $$\sigma_{\ell ji}^{(m)}(t) = (\sigma_\ell^{(m)}f_j,f_i^*)_E \; . \tag{38}$$

2.4.3 Reaction production term

A typical reaction production term of Equation 33 (using Equation 6) is

$$(P_\ell^{(m)}\sum_j\theta_j f_j,f_i^*)_E = N_\ell(\underset{\sim}{r},t)\int_0^\infty\int_0^\infty \sigma_\ell^{(m)}(E'\to E)\sum_j\{\theta_j(\underset{\sim}{r},t)f_j(E',t)\}f_i^*(E,t)dE'\,dE$$

$$= N_\ell(\underset{\sim}{r},t)\sum_j\sigma_{\ell j\to i}^{(m)}(t)\,\theta_j(\underset{\sim}{r},t), \tag{39}$$

where $$\sigma_{\ell j\to i}^{(m)}(t) = \int_0^\infty\int_0^\infty \sigma_\ell^{(m)}(E'\to E)f_j(E',t)f_i^*(E,t)dE'\,dE \; . \tag{40}$$

As special cases of Equations 39 and 40 we have for the fission emission term (derived from Equation 10)

$$(P_\ell^{(f)}\sum_j\theta_j f_j,f_i^*)_E = N_\ell(\underset{\sim}{r},t)\,\chi_i(t)\sum_j\nu\sigma_{\ell j}^{(f)}(t)\,\theta_j(\underset{\sim}{r},t)/k(t), \tag{41}$$

where $$\chi_i(t) = (\chi,f_i^*)_E \tag{42}$$

and $$\nu\sigma_{\ell j}^{(f)}(t) = (\nu\sigma_\ell^{(f)}f_j,1)_E \; . \tag{43}$$

2.4.4 Energy mode equations

The energy mode neutron diffusion equations are thus given by

$$\sum_j B_{ji}\theta_j(\underset{\sim}{r},t) = 0 \quad , \qquad i = 1,2,\ldots,G, \tag{44}$$

where the energy mode diffusion operator is given by

$$B_{ji}\theta_j(\underset{\sim}{r},t) = -\underset{\sim}{\nabla}.D_{ji}(\underset{\sim}{r},t)\underset{\sim}{\nabla}\theta_j(\underset{\sim}{r},t) + \sum_m\sum_\ell [N_\ell(\underset{\sim}{r},t)\{\sigma^{(m)}_{\ell ji}(t) - \sigma^{(m)}_{\ell j\to i}(t)\}]\,\theta_j(\underset{\sim}{r},t). \tag{45}$$

2.5 Multigroup Approximation

The multigroup approximation consists of dividing the energy range into G intervals $E_1(=\infty), E_2,\ldots,E_i\ldots,E_{G+1}(=0)$. We then choose the coordinate functions $f_i(E,t)$ and $f_i^*(E,t)$ in the following way:

$$f_i(E,t) = \phi_i(E,t)\,\{H(E-E_{i+1}) - H(E-E_i)\}\Big/\int_{E_{i+1}}^{E_i}\phi_i(E',t)\phi_i^*(E',t)dE' \tag{46}$$

and

$$f_i^*(E,t) = \phi_i^*(E,t)\{H(E-E_{i+1}) - H(E-E_i)\}\ , \tag{47}$$

where $H(x)$ is the Heaviside unit function

$$= 0 \ , \ x \leqslant 0$$

$$= 1 \ , \ x > 0 \ ,$$

and now $\phi_i(E,t)$ and $\phi_i^*(E,t)$ are group functions selected by us from the requirements of our problem (Section 3). (The change of notation should not cause confusion here.) Equations 46 and 47 define two biorthonormal functions since

$$(f_j, f_i^*)_E = \delta_{ji} \ .$$

This procedure amounts to the usual multigroup approach (Glasstone and Edlund 1952).

2.6 Neutron Conservation

We now demand of our multigroup constants that they have built-in neutron conservation, that is, for example, we want one neutron to be produced from an elastic scattering reaction. The number of neutrons emitted for each reaction, $\nu_\ell^{(m)}$ is given by

$$\nu_\ell^{(m)} = \int_0^\infty \sigma_\ell^{(m)}(E'\to E)dE/\sigma_\ell^{(m)}(E')\ . \tag{48}$$

whereas the multigroup approach gives

$$\nu_{\ell j}^{(m)} = \sum_i \sigma^{(m)}_{\ell j\to i}\Big/\sum_i \sigma^{(m)}_{\ell ji} = \frac{\int_{E_{j+1}}^{E_j}\left\{\sum_i\int_{E_{i+1}}^{E_i}\sigma_\ell^{(m)}(E'\to E)\phi_i^*(E,t)dE\right\}\phi_j(E',t)dE'}{\int_{E_{j+1}}^{E_j}\sigma_\ell^{(m)}(E')\phi_j(E',t)\phi_j^*(E',t)dE'}\ . \tag{49}$$

Equation 48 gives

$$\nu_\ell^{(m)} = \frac{\int_{E_{j+1}}^{E_j}\left\{\sum_i\int_{E_{i+1}}^{E_i}\sigma_\ell^{(m)}(E'\to E)dE\right\}\phi_j^*(E',t)\,\phi_j(E',t)dE'}{\int_{E_{j+1}}^{E_j}\sigma_\ell^{(m)}(E')\,\phi_j(E',t)\,\phi_j^*(E',t)dE'}$$

and since we require

$$\nu_{\ell j}^{(m)} = \nu_{\ell}^{(m)} \tag{50}$$

for all reactions for all nuclides for all groups, Equation 50 can only be satisfied, in general, by choosing

$$\phi_i^*(E,t) = 1 \quad \text{(actually a constant).} \tag{51}$$

2.7 Multigroup Constants

Using the results of previous sections the microscopic multigroup cross sections are given by

$$\sigma_{\ell i}^{(m)}(t) = \int_{E_{i+1}}^{E_i} \sigma_{\ell}^{(m)}(E)\,\phi_i(E,t)dE \Big/ \int_{E_{i+1}}^{E_i} \phi_i(E,t)dE\ , \tag{52}$$

where one index has been dropped from the symbol of Equation 38,

$$\sigma_{\ell j\to i}^{(m)}(t) = \int_{E_{j+1}}^{E_j} \left\{ \int_{E_{i+1}}^{E_i} \sigma_{\ell}^{(m)}(E'\to E)dE \right\} \phi_j(E',t)dE' \Big/ \int_{E_{j+1}}^{E_j} \phi_j(E',t)dE' \tag{53}$$

and

$$\sigma_{\ell i}^{(tr)}(\underset{\sim}{r},t) = \int_{E_{i+1}}^{E_i} \sigma_{\ell}^{(tr)}(E)D(\underset{\sim}{r},E,t)\,\phi_i(E,t)dE \Big/ \int_{E_{i+1}}^{E_i} D(\underset{\sim}{r},E,t)\,\phi_i(E,t)dE\ . \tag{54}$$

Equation 54 is obtained from the diffusion coefficient (Equation 36) now given by

$$D_i(\underset{\sim}{r},t) = \int_{E_{i+1}}^{E_i} D(\underset{\sim}{r},E,t)\,\phi_i(E,t)dE \Big/ \int_{E_{i+1}}^{E_i} \phi_i(E,t)dE, \tag{55}$$

and the requirement that an equation similar to Equation 3 may be used to produce the multigroup diffusion coefficient from the microscopic multigroup transport cross section. We obtain from Equation 54 the result

$$\frac{1}{3\sum_{\ell} N_{\ell}(\underset{\sim}{r},t)\sigma_{\ell i}^{(tr)}} = \frac{\int_{E_{i+1}}^{E_i} D(\underset{\sim}{r},E,t)\phi_i(E,t)dE}{\int_{E_{i+1}}^{E_i} 3\sum_{\ell} N_{\ell}(\underset{\sim}{r},t)\sigma_{\ell}^{(tr)}(E)D(\underset{\sim}{r},E,t)\,\phi_i(E,t)dE}\ ,$$

which when we use Equations 3 and 55 gives

$$1\Big/3\sum_{\ell} N_{\ell}(\underset{\sim}{r},t)\,\sigma_{\ell i}^{(tr)} = D_i(\underset{\sim}{r},t) \tag{56}$$

as required.

2.8 Multigroup Equations

The multigroup neutron diffusion equations are obtained from the set of equations (44) and constants of the previous section as

$$-\underset{\sim}{\nabla}.D_i(\underset{\sim}{r},t)\underset{\sim}{\nabla}\theta_i(\underset{\sim}{r},t) + \sum_{m\neq f}\sum_{\ell} N_{\ell}(\underset{\sim}{r},t)\{\sigma_{\ell i}^{(m)}(t)\theta_i(\underset{\sim}{r},t) - \sum_j \sigma_{\ell j\to i}^{(m)}(t)\theta_j(\underset{\sim}{r},t)\}$$

$$+\sum_{\ell} N_{\ell}(\underset{\sim}{r},t)\{\sigma_{\ell i}^{(f)}(t)\theta_i(\underset{\sim}{r},t) - \frac{\chi_i}{k(t)}\sum_j \nu\sigma_{\ell j}^{(f)}(t)\theta_j(\underset{\sim}{r},t)\} = 0,$$

$$i = 1,2,\ldots,G, \tag{57}$$

where $$\chi_i = \int_{E_{i+1}}^{E_i} \chi(E)dE \tag{58}$$

and $\nu\sigma_{\ell i}^{(f)}$ is given by an equation similar to Equation 52.

Several excellent computer programmes have been written for the numerical solution of the multigroup diffusion equations in one and two space dimensions (Wachspress 1957, Stone et al. 1959 and Hassitt 1962). These programmes do not solve the equations with burnup and fuel management taken into account. However it is possible to write independent programmes which can do this using the multigroup diffusion code as a basis (Hesse 1967). The theory used in the solution of the diffusion equations is presented very well by Wachspress (1966) and will not concern us here. Our main concern will be the method of calculation of multigroup data given by Equations 52 to 54 for use with these programmes. We require a "reasonable" choice for the group functions $\phi_i(E,t)$ since by this means we may be able to carry out the expensive space dependent computations with only a few groups (G=10, say). Choosing a "reasonable" set of functions is in itself not simple. This point will be discussed in the next Section.

3. A BASIS FOR SELECTING GROUP FUNCTIONS

3.1 Idealization of the Problem

In Section 2 we approximated the neutron diffusion equation using the energy multigroup approach. This approach required us to select G group functions, $\phi_i(E,t)$, i=1,2,...,G, which in some way contained detailed variation of flux with neutron energy appropriate to our study in hand but only over a limited energy range (a group). Expressions for the gross variation of the multigroup flux with group, in the form of the functions $\theta_i(\underset{\sim}{r},t)$, i=1,2,...,G, were obtained. The solution of these space dependent equations was not pursued and the dependence of the equations on t (evolution time) was hardly discussed. This Section will be concerned with a simplified reactor model which bears some resemblance to a large recirculating fuel reactor operating at equilibrium (intake of fresh fuel and discharge of spent fuel independent of time). From this model we will obtain a basis for calculating the group functions.

The selection of group functions is, in general, not unique. The argument presented here is that the functions should relate to an idealization of the actual system being studied. The reactor model resulting from this idealization should be such that results of a macroscopic nature (such as the reactor multiplication, k(t)) should also prove useful in a preliminary assessment of the merits of one system against another. In addition, it should be possible to construct experiments to help validate predictions obtained from the model.

Using the model we obtain a continuous representation of the neutron spectrum (flux as a function of energy) which we will call $\phi(E)$. The same representation then applies to each group. We are still left, however, with the problem of choosing the group boundaries.

The choice of groups should, fairly reasonably, be made on the basis of the deficiency of the model in representing the actual system, for if the model actually represented the system perfectly, one energy group would suffice. The author knows of one variational idea proposed for solving this problem (Spinks, unpublished) but it was not pursued. The problem of choosing group boundaries is a possible fruitful area for research. A rough and ready rule is to choose the number of groups G on the basis of how much computer time can be afforded for the problem being tackled. We then choose the group boundaries so that for our idealized model the total loss reaction rate is the same in each group. Another quite popular approach is to use group boundaries previously chosen by someone else.

3.2 Statement of the Model

The model consists of a large homogeneous recirculating core of fuel, without reflector, dissipating a specified power density $\underset{\sim}{P}$. Fresh fuel is added to the core, partly burnt fuel is discharged from the core and recirculated immediately and spent fuel is discharged completely after being irradiated for a time T. The whole core is assumed homogeneous so that in effect fuel is being circulated at an infinite rate. The homogeneous nature of the fuel is assumed to be complete so that individual fuel balls are assumed to be infinitely small. We also assume that the core is in equilibrium so that input and discharge of fuel is not varied. On this basis the spectrum is not dependent on time. This is the model proposed by Bicevskis et al. (1967).

For a study not concerned with burnup this model simply amounts to choosing a bare reactor core. The idea has already been used as a basis for the preparation of multigroup data (Clancy et al. 1963). In addition, experimental measurements have been made with bare fuel assemblies (McCulloch et al. 1965) which provide an important check on the validity of the multigroup data obtainable from the model and basic neutron cross sections (Cook 1966b).

3.3 Reactor Neutron Equations

For a bare homogeneous system the first fundamental theorem of Weinberg and Wigner (1958) states (i) that the flux is separable in space and energy, hence

$$\Phi(\underset{\sim}{r},E) = \theta(\underset{\sim}{r})\,\phi(E) \tag{1}$$

and (ii) the spatial distribution satisfies the wave equation

$$\nabla^2\theta(\underset{\sim}{r}) + B^2\,\theta(\underset{\sim}{r}) = 0, \tag{2}$$

where B^2 is the geometric buckling of the reactor and $\theta(\underset{\sim}{r})=0$ on the extrapolated boundary. We are at liberty to normalize either $\theta(\underset{\sim}{r})$ or $\phi(E)$. Subsequent work suggests we choose

$$\int_V \theta(\underset{\sim}{r})d\underset{\sim}{r} = V. \tag{3}$$

For the model, Equations 1, 2 and the neutron diffusion equation (Equation 9 Section 2) give, after division by $\theta(\underset{\sim}{r})$,

$$D(E)B^2\phi(E) + \sum_{m\neq f}\sum_{\ell}\hat{N}_\ell\left\{\sigma_\ell^{(m)}(E)\,\phi(E) - \int_0^\infty \sigma_\ell^{(m)}(E'\rightarrow E)\phi(E')dE'\right\}$$

$$+\sum_{\ell}\hat{N}_\ell\left\{\sigma_\ell^{(f)}(E)\phi(E) - \frac{\chi(E)}{k}\int_0^\infty \nu\sigma_\ell^{(f)}(E')\phi(E')dE'\right\} = 0, \tag{4}$$

where
$$D(E) = 1/3\sum_{\ell}\hat{N}_\ell\,\sigma_\ell^{(tr)}(E), \tag{5}$$

$$\hat{N}_\ell = \frac{1}{T}\int_0^T N_\ell(t)dt, \tag{6}$$

and each other quantity is the same as in Section 2 except that we have removed emphasis of dependence on variables not applicable to this model.

Equation 4 determines the shape of the spectrum $\phi(E)$ but not the magnitude. The level of flux is chosen from the requirement that the specified power density P is to be given by

$$P = \sum_{\ell}\hat{N}_\ell\, f_\ell\, r_\ell^{(f)}, \tag{7}$$

where
$$r_\ell^{(m)} = \int_0^\infty \sigma_\ell^{(m)}(E)\phi(E)dE \tag{8}$$

and f_ℓ is the energy release per fission of nuclide ℓ. In addition, rather than specify the lifetime of fuel, T, we specify that we require a certain number of fissions per unit volume. It is convenient to normalize this quantity to FIFA (fissions per initial fissile atom); hence T is determined from the equation

$$\mathrm{FIFA} = \sum_{\ell} T\hat{N}_{\ell} r_{\ell}^{(f)} / N_o \ , \tag{9}$$

where N_o denotes the concentration of initial fissile atoms.

The set of coupled equations (4), (6), (7) and (9) may be solved provided (i) we have available all the cross section information and (ii) we can calculate the nuclide concentrations required in Equation 6. A knowledge of the cross sections $\sigma(E)$ is far from complete in a reactor containing fission products from long term irradiation (FIFA>1) (see however Cook 1966a), and in addition, the transfer cross sections $\sigma(E' \to E)$ require a detailed knowledge of the reaction mechanisms. In later Sections we will separately consider reactions typified by the following broad energy ranges (i) fast (10 MeV–0.001 MeV), (ii) resonance (10^3eV–1eV) and (iii) thermal (1eV–0.001eV). In the next section we will give the equations expressing evolution of the nuclide species in the reactor.

3.4 Reactor Nuclide Equations

Although our model for neutron reaction balance requires each fuel ball to be infinitely small, we demand that in addition a ball does exist as an entity. The average of all states of burnup of a typical ball must then be the same as the average composition in the reactor. We then have the detailed balance:

Time rate of change of N_ℓ

= loss due to n-absorption by nuclide ℓ

+ loss due to decay of nuclide ℓ

+ gain due to n-capture reactions which produce nuclide ℓ

+ gain due to decay of nuclides which produce nuclide ℓ

+ yield from fission of nuclide ℓ.

Using a dot to denote differentiation with respect to time, the actual equations may be written

$$\dot{\underset{\sim}{N}}(t) = \underset{\approx}{A}\,\underset{\sim}{N}(t), \qquad \underset{\sim}{N}(0) \text{ given}, \tag{10}$$

where $\underset{\sim}{N}(t)$ is the array of nuclide concentrations, $N_\ell(t)$, for nuclides in the reactor (ℓ=1,2,...,n),

$\underset{\approx}{A}$ is an nxn matrix with typical element,

$$a_{\ell k} = -(r_\ell^{(a)} + \lambda_\ell)\,\delta_{\ell k} + (1-\delta_{\ell k})(\sum_m y_{k\to\ell}^{(m)} r_k^{(m)} + y_{k\to\ell}\, y_k), \tag{11}$$

λ denotes radioactive decay constant, $r_\ell^{(a)}$ denotes neutron absorption reaction rate (nuclide ℓ is destroyed following the reaction) and $y_{k\to\ell}^{(m)}$ and $y_{k\to\ell}$ are yields of nuclide ℓ from nuclide k for neutron reaction m and radioactive decay respectively.

The solution of Equation 10 is deferred until Section 7. It is sufficient to note here that it may be solved analytically.

3.5 Fine Group Equations

In Section 3.3 we obtained a continuous equation for the flux $\phi(E)$ given by Equation 4. To solve the equation we again resort to a multigroup approach (g groups) however we use much finer groups than required in the broad group space dependent calculation (g>>G and we assume that the boundaries of the broad groups are a subset of the fine group boundaries). A detailed flux is again required in each fine group. Determination of this detail is postponed until Sections 4, 5 and 6. We integrate Equation 4 over each group separately and obtain the equivalent of Equation 57 of Section 2. We get

$$D_i B^2 \Phi_i + \sum_{m\neq f} \sum_{\ell} \hat{N}_\ell \{\sigma_{\ell i}^{(m)} \Phi_i - \sum_{j=1}^{g} \sigma_{\ell j\to i}^{(m)} \Phi_j\} + \sum_{\ell} \hat{N}_\ell \{\sigma_{\ell i}^{(f)} \Phi_i - \frac{\chi_i}{k} \sum_{j=1}^{g} \nu\sigma_{\ell j}^{(f)} \Phi_j\} = 0, \qquad i=1,2,\ldots,g, \tag{12}$$

$$r_\ell^{(m)} = \sum_{i=1}^{g} \sigma_{\ell i}^{(m)} \Phi_i \qquad \text{(cf. Equation 8)}; \tag{13}$$

with other quantities defined as in Section 2.7 ($\phi_i(E,t)$ replaced by $\phi(E)$) and

$$\Phi_i = \int_{E_{i+1}}^{E_i} \phi(E)\,dE\ . \tag{14}$$

The numerical method used to solve Equation 12 will be discussed in Section 8.

3.6 Group Condensation

To obtain broad group cross sections for use with space dependent calculations (required when a reflector is added, etc.) we need to condense our fine group data. We do this using the equations

$$\sigma_{\ell I}^{(m)} = \sum_{i(I)} \sigma_{\ell i}^{(m)} \Phi_i / \Phi_I\,, \tag{15}$$

$$\sigma_{\ell J\to I}^{(m)} = \sum_{j(J)} \left(\sum_{i(I)} \sigma_{\ell j\to i}^{(m)}\right) \Phi_j / \Phi_J\ , \tag{16}$$

and
$$\sigma_{\ell I}^{(tr)} = \sum_{i(I)} \sigma_{\ell i}^{(tr)} D_i \Phi_i / \sum_{i(I)} D_i \Phi_i\ , \tag{17}$$

where
$$\Phi_I = \sum_{i(I)} \Phi_i \tag{18}$$

and the summation over i extends over all fine groups which are contained in the broad group I (similarly for j and J). These equations are obtained from Equation 12 and the requirement that neutron reaction balance is to be conserved. They may also be obtained from the equations given for multigroup constants in Section 2.7.

3.7 Neutron Multiplication Constant

Neutron balance for the complete energy range gives us a simple expression for the neutron multiplication constant of the reactor. Integrating Equation 4 over the full energy range is the same as condensing Equation 12 to one group covering the whole range. Equation 12 becomes

$$D_1 B^2 \Phi_1 + \sum_{m\neq f} \sum_{\ell} \hat{N}_\ell \{\sigma_{\ell 1}^{(m)} \Phi_1 - \sigma_{\ell 1\to 1}^{(m)} \Phi_1\} + \sum_{\ell} \hat{N}_\ell \{\sigma_{\ell 1}^{(f)} \Phi_1 - \frac{\chi_1}{k} \nu\sigma_{\ell 1}^{(f)} \Phi_1\} = 0\ . \tag{19}$$

In Equation 19 the second term is zero for all scattering reactions and $\chi_1=1$ (from Equation 8 in Section 2), hence provided $\Phi\neq 0$ we have

$$k = \frac{\sum_{\ell} \hat{N}_\ell \nu\sigma_\ell^{(f)}}{\sum_{\ell} \hat{N}_\ell \sigma_\ell^{(a)} + DB^2}\ , \tag{20}$$

where we have dropped the emphasis on group dependence. If in Equation 20 we set $B^2=0$ we obtain an estimate of the infinite multiplication constant,

$$k_\infty^{\prime} = \frac{\sum_\ell \hat{N}_\ell \nu \sigma_\ell^{(f)}}{\sum_\ell \hat{N}_\ell \sigma_\ell^{(a)}} \quad . \tag{21}$$

In general this is only an estimate since the flux used in the condensation (obtained from Equation 12) depends on B^2. To achieve a critical system (k=1) we must choose B^2 as the lowest eigenvalue of Equation 12. An estimate of this critical buckling is obtained from Equation 20 as

$$B^2 = (\sum_\ell \hat{N}_\ell \nu \sigma_\ell^{(f)} - \sum_\ell \hat{N}_\ell \sigma_\ell^{(a)})/D. \tag{22}$$

Conversely if the buckling is chosen, then k becomes the eigenvalue of the homogeneous equation (12). In this case the eigenvalue must be given by Equation 20, otherwise only $\Phi=0$ is possible.

3.8 Unit Source

When using Equations 4 or 12, since the equation is homogeneous, it is frequently convenient to calculate first the flux derived from a source emitting 1 neutron per unit volume per unit time. Thus instead of using the normalization given by Equation 7 we use

$$(\sum_\ell \hat{N}_\ell \sigma_\ell^{(a)} + DB^2)\Phi = 1 \ . \tag{23}$$

Remembering that this is only an interim step we obtain the following equations in place of Equations 4 and 12:

$$D(E)B^2\phi(E) + \sum_\ell \hat{N}_\ell \sigma_\ell^{(t)}(E)\phi(E) - \sum_{m\neq f} \sum_\ell \hat{N}_\ell \int_0^\infty \sigma_\ell^{(m)}(E' \rightarrow E)\phi(E')dE' = \chi(E), \qquad 0 \leqslant E \leqslant \infty , \tag{24}$$

$$D_i B^2 \Phi_i + \sum_\ell \hat{N}_\ell \sigma_{\ell i}^{(t)} \Phi_i - \sum_{m\neq f} \sum_\ell \hat{N}_\ell \sum_{j=1}^{g} \sigma_{\ell j\rightarrow i}^{(m)} \Phi_j = \chi_i \ , \qquad i=1,2,\ldots,g, \tag{25}$$

where (t) indicates total cross section and the flux is now the flux per unit source.

In the next three Sections we investigate more closely the manner of calculation of fine group cross sections.

4. FAST REGION

4.1 Introduction

The fast energy region here will be considered to cover, roughly speaking, the range 10MeV–0.001 MeV. It is in this region that fission neutrons are emitted and threshold reactions such as $Be^9(n,2n)$ occur. Important reactions for heavy nuclides are inelastic scattering and fast fission. A consideration for most light nuclides is the highly anisotropic nature of elastic scattering (centre of mass system). As a consequence the diffusion coefficient is large and hence fast leakage is important.

In this Section we investigate properties of the so-called slowing down equation (Glasstone and Edlund 1952). Our main concern is to obtain a detailed spectrum $\phi(E)$ for use in the calculation of fine group averaged cross sections (say 30 groups covering the fast range). Several authors over the past decade have studied this problem. Amaldi (1959) presented the basic material of the subject. Rowlands (1958), Häfele (1959), Häfele and Tsagaris (1959), Hines (1959) and Duncan et al. (1961) used computers to obtain numerical estimates of $\phi(E)$, and hence various reaction rates, for fission neutrons slowing down in C^{12}, Be^9, BeO and H_2O-D_2O mixtures. Pollard (1960) and Keane (1961) developed analytic techniques for solving the slowing down equation when scattering was assumed isotropic. Later they extended their work (Keane and Pollard 1962) to include anisotropic elastic scattering. Two mechanisms were studied for the important $Be^9(n,2n)$ reaction; compound nucleus (Hines and Pollard 1962) and direct mechanism (Axford et al. 1964).

As a prelude to routine calculation of fast flux for preparation of multigroup data (later to form part of the programme MULGA – Clancy et al. 1963) Keane and Mills (1962) solved a simplified form of the slowing down equation numerically, using reaction cross sections and mechanisms given in the British barn book (Buckingham et al. 1960).

4.2 Slowing Down Equation

For an infinite system ($B^2=0$) Equation 24 of the previous Section gives

$$\sum_\ell \hat{N}_\ell \sigma_\ell^{(t)}(E)\phi(E) - \sum_{m\neq f}\sum_\ell \hat{N}_\ell \int_0^\infty \sigma_\ell^{(m)}(E'\to E)\phi(E')dE' = \chi(E), \qquad 0 \leqslant E < \infty . \tag{1}$$

For slowing down calculations a change of variable from energy E(eV) to lethargy,

$$u = \ell n(10^7/E) \quad ,$$

is found to be convenient. We will assume that there are no source neutrons with energies in excess of 10 MeV ($u<0$) and that for the energy range of interest no neutrons have their energy increased through scattering, etc. ($\sigma_\ell^{(m)}(E'\to E)=0$ for $E>E'$). For reactors at normal operating temperatures this sets a lower limit of about 1eV on the derivations to follow in this Section and the next (see however Section 6). Equation 1 then becomes

$$\sum_\ell \hat{N}_\ell \sigma_\ell^{(t)}(u)\phi(u) - \sum_{m\neq f}\sum_\ell \hat{N}_\ell \int_0^u \sigma_\ell^{(m)}(u'\to u)\,\phi(u')du' = \chi(u), \qquad 0 \leqslant u < 16 , \tag{2}$$

where the usual slowing down notation has been employed for density functions based on

$$|\phi(u)du| = |\phi(E)dE| ,$$

$$|\chi(u)du| = |\chi(E)dE|$$

and $\quad |\sigma_\ell^{(m)}(u'\to u)du| = |\sigma_\ell^{(m)}(E'\to E)dE| .$

Finally we introduce the slowing down density, F(u), through the equation

$$F(u) = \sum_\ell \hat{N}_\ell \sigma_\ell^{(t)}(u)\phi(u) \tag{3}$$

and Equation 2 becomes

$$F(u) - \sum_{m\neq f}\sum_\ell \int_0^u H_\ell^{(m)}(u'\to u)\,h_\ell^{(m)}(u')F(u')du' = \chi(u) , \tag{4}$$

with $\quad F(u)=0 , \qquad u<0 ,$

where
$$H_\ell^{(m)}(u'\to u) = \sigma_\ell^{(m)}(u'\to u)\Big/\sigma_\ell^{(m)}(u') \tag{5}$$

and
$$h_\ell^{(m)}(u') = \hat{N}_\ell \sigma_\ell^{(m)}(u')\Big/\sum_\ell \hat{N}_\ell \sigma_\ell^{(t)}(u') . \tag{6}$$

Equation 4 is the slowing down integral equation. In general we must solve the equation numerically, but we will investigate simplified versions of the equation which yield interesting analytic results. An example of the numerical method used is given by Duncan et al. (1961).

Also important in slowing down studies is the slowing down density, q(u), defined as the number of neutrons (derived from unit source) elastically scattered past a given lethargy, u. An expression for the slowing down density can be obtained by considering the difference in the number of neutrons that are elastically scattered out of du" and those that are elastically scattered into du" and then integrating. We obtain

$$q(u)=\sum_{\ell}\int_{0}^{u}\int_{0}^{u''}\{\delta(u'-u'')-H_{\ell}(u'\to u'')\}h_{\ell}(u')F(u')du'\,du'' \quad , \tag{7}$$

where the absence of superscripts denotes elastic scattering reactions and $\delta(u)$ is the Dirac delta function which is everywhere zero except in the immediate neighbourhood of u and with normalization $\int_{0}^{\infty}\delta(u)du=1$. We may reverse the order of integration in Equation 7 to give

$$q(u)=\sum_{\ell}\int_{0}^{u}\int_{u'}^{u}\{\delta(u'-u'')-H_{\ell}(u'\to u'')\}h_{\ell}(u')F(u')du''\,du'$$

$$=\sum_{\ell}\int_{0}^{u}G_{\ell}(u'\to u)h_{\ell}(u')F(u')du' \quad , \tag{8}$$

where $$G_{\ell}(u'\to u)=1-\int_{u'}^{u}H_{\ell}(u'\to u'')du''$$

$$=\int_{u}^{\infty}H_{\ell}(u'\to u'')du'' \tag{9}$$

since $$\int_{u'}^{\infty}H_{\ell}(u'\to u'')du''=1 \quad , \tag{10}$$

using Equation 48 of Section 2.

An alternative useful equation may be obtained by combining Equations 4 and 7. The equation is

$$q(u)=\int_{0}^{u}\chi(u')du'+\epsilon(u)\,, \tag{11}$$

where $\epsilon(u)$ is the neutron enhancement

$$=\sum_{\substack{m\neq f\\ m\neq s}}\sum_{\ell}\int_{0}^{u}\int_{0}^{u'}H_{\ell}^{(m)}(u'\to u'')h_{\ell}^{(m)}(u')F(u')du''\,du'$$

$$-\sum_{m\neq s}\sum_{\ell}\int_{0}^{u}h_{\ell}^{(m)}(u')F(u')du' \tag{12}$$

and (s) denotes elastic scattering.

4.3 Special Cases

We first consider neutron slowing down in a medium for which all energy transfers are caused by scattering which is elastic and spherically symmetric in the centre of mass system. Glasstone and Edlund (1952) give the probability of scattering from u' to u for this situation. In our notation this is

$$H_{\ell}(u'\to u)=e^{u'-u}\{H(u-u')-H(u-u'-U_{\ell})\}/(1-\alpha_{\ell})\,, \tag{13}$$

where α_{ℓ} is the maximum fractional energy loss on collision $=\left(\frac{A_{\ell}-1}{A_{\ell}+1}\right)^{2}$,

A_{ℓ} is the ratio of the mass of nuclide ℓ to the mass of a neutron,

$U_{\ell}=\ln 1/\alpha_{\ell}$

and H(u) is the Heaviside unit function. Hence Equations 9 and 13 give

(i) $u-U_\ell \leqslant u' \leqslant u$

$$G_\ell(u'\to u) = \int_u^{u'+U_\ell} e^{u'-u''}du'' \Big/ (1-\alpha_\ell)$$

$$= (e^{u'-u} - \alpha_\ell)\Big/(1-\alpha_\ell) \quad ,$$

(ii) otherwise

$$G_\ell(u'\to u) = 0 \ .$$

Equations 4 and 8 are thus simply

$$F(u) - \sum_\ell \frac{1}{1-\alpha_\ell} \int_{u-U_\ell}^{u} e^{u'-u}\, h_\ell(u')F(u')du' = \chi(u) \ , \tag{14}$$

$$q(u) = \sum_\ell \frac{1}{1-\alpha_\ell} \int_{u-U_\ell}^{u} (e^{u'-u} - \alpha_\ell)\, h_\ell(u')F(u')du' \tag{15}$$

and Equation 11 becomes

$$q(u) = \int_0^u \chi(u')du' - \sum_{m\neq s} \sum_\ell \int_0^u h_\ell^{(m)}(u')F(u')du' \ . \tag{16}$$

Pollard (1960) gives an analytic solution of the above equations when absorption is absent and the scattering probabilities are constant. For the special case of a single nuclide the solution is given as

$$F(u) = \frac{1}{\xi_\ell}\left\{ \int_0^u \chi(u')du' + \zeta_2\, \xi_\ell\, \chi(u) + (\zeta_2^2 - \zeta_3)\, \xi_\ell^2 \frac{d\chi(u)}{du} + \ldots \right\} , \tag{17}$$

where ξ_ℓ is the average neutron lethargy gain per spherically symmetric elastic scattering reaction with nuclide ℓ

$$= 1 - \frac{\alpha_\ell U_\ell}{1-\alpha_\ell} \tag{18}$$

and

$$\zeta_j = \left(1 - \alpha_\ell \sum_{k=0}^{j} \frac{U_\ell^k}{k!}\right)\Big/(1-\alpha_\ell)\, \xi_\ell^j \ . \tag{19}$$

For a heavy nuclide ($A_\ell \to \infty$) Pollard (ibid.) shows that

$$\zeta_j \simeq 2^j/(j+1)!$$

and for hydrogen ($A_\ell = 1$)

$$\zeta_j = 1 \ .$$

Here we notice that Equation 17 may be written

$$F(u) = \frac{1}{\xi_\ell}\left\{ \int_0^{u+\zeta_2\xi_\ell} \chi(u')du' + (\tfrac{1}{2}\zeta_2^2 - \zeta_3)\xi_\ell^2 \frac{d\chi(u)}{du} + \ldots \right\} \tag{20}$$

which may be obtained by applying a Taylor's series expansion to the integral of the fission spectrum. Using the tables given by Pollard (ibid.) the maximum error caused by the neglect of the second term onwards amounts to less than 2 per cent. for nuclides with A_ℓ greater than 9. This maximum error occurs at 4.4 MeV. For hydrogen the error can be as much as 50 per cent and hence the truncation of Equation 20 is not recommended for extremely light nuclides ($A_\ell < 9$). Bearing in mind these considerations we obtain the approximation

$$F(u) \simeq \frac{1}{\xi_\ell}\int_0^{u+\zeta_2\xi_\ell} \chi(u')du' . \tag{21}$$

4.4 Approximate Collision Density

From the preceding work of this Section it appears that, in general, only a numerical solution of the slowing down equation (Equation 4) is possible. A direct numerical approach applied to the equation is feasible and has been tried, for slowing down in BeO, by Hines and Pollard (1962); however the method is far from routine considering the bulk of data required for the terms $H_\ell^{(m)}(u'\to u)$. Here we only require F(u) in order to calculate fine group cross sections over a narrow lethargy range and hence an approximate approach should be adequate.

Equation 21, and the observations of the previous section, suggest we should try the following expansion in Equation 8:

$$\begin{aligned} F(u') &= F(u-a(u)-\{u-a(u)-u'\}) \\ &\simeq F(u-a(u))-(u-a(u)-u')\frac{dF}{du'}(u-a(u)) , \end{aligned}$$

where a(u) is to be determined. Substituting this result into Equation 8 we obtain

$$\begin{aligned} q(u) \simeq{} & F(u-a(u))\sum_\ell \int_0^u G_\ell(u'\to u)h_\ell(u')du' \\ & - \frac{dF}{du'}(u-a(u))\sum_\ell\int_0^u G_\ell(u'\to u)h_\ell(u')(u-a(u)-u')du' . \end{aligned} \tag{22}$$

We then choose a(u) so that the second term of Equation 22 is zero, that is

$$a(u) = M_2(u)/M_1(u) , \tag{23}$$

where
$$M_j(u) = \sum_\ell \int_0^u \frac{(u-u')^{j-1}}{(j-1)!} G_\ell(u'\to u)h_\ell(u')du' . \tag{24}$$

Equation 22 is thus

$$q(u) \simeq M_1(u)F(u-a(u)) , \tag{25}$$

which when we use Equation 11 gives

$$F(u) \simeq \frac{1}{M_1(u)}\left\{\int_0^{u+a(u)} \chi(u')du' + \epsilon(u+a(u))\right\}. \tag{26}$$

This is our required approximation for the solution of the slowing down equation. In order to calculate the last term we could adopt an iterative approach using as first iterant

$$F_1(u) = \frac{1}{M_1(u)}\int_0^{u+a(u)} \chi(u')du' . \tag{27}$$

One iteration would normally suffice.

The calculation of moments given by Equation 24 is by no means trivial, but for limiting cases we can obtain reasonably simple expressions. For example, for a single nuclide as in Section 4.3 we obtain

$$M_1(u) = \int_{u-U_\ell}^{u} (e^{u'-u}-\alpha_\ell)du'/(1-\alpha_\ell)$$

$$= 1 - \frac{\alpha_\ell U_\ell}{1-\alpha_\ell} = \xi_\ell ,$$

$$M_2(u) = \int_{u-U_\ell}^{u} (u-u')(e^{u'-u} - \alpha_\ell)du' \Big/ (1-\alpha_\ell)$$

$$= \int_{o}^{U_\ell} U(e^{-U} - \alpha_\ell)dU \Big/ (1-\alpha_\ell)$$

$$= 1 - \xi_\ell - \frac{\alpha_\ell}{1-\alpha_\ell} \frac{U_\ell^2}{2} = \zeta_2 \xi_\ell^2 ,$$

hence $\quad a(u) = \zeta_2 \xi_\ell ,$

which was to be expected. As a further example following Keane and Pollard (1962) for a heavy anisotropic scatterer we obtain

$$M_1(u) = (1-\bar{\mu}_\ell)\xi_\ell$$

and $$M_2(u) = \frac{1}{2}(1-2\bar{\mu}_\ell + \overline{\mu_\ell^2})\xi_\ell^2 ,$$

where μ_ℓ is the cosine of the centre of mass scattering angle and the bar refers to the average taken over the probability distribution for obtaining particular values of μ_ℓ.

In our use of Equation 26 we could include leakage in the term $\epsilon(u + a(u))$ if required.

4.5 Fine Group Cross Sections

Having determined F(u) using Equation 26, Equation 3 gives

$$\phi(u') = F(u) \Big/ \sum_\ell \hat{N}_\ell \sigma_\ell^{(t)}(u) .$$

Our definition of multigroup cross sections given in Section 2.7 is then used in the form

$$\sigma_{\ell i}^{(m)} = \int_{u_i}^{u_{i+1}} \sigma_\ell^{(m)}(u)\phi(u)du \Big/ \int_{u_i}^{u_{i+1}} \phi(u)du \tag{28}$$

$$\sigma_{\ell j\to i}^{(m)} = \int_{u_j}^{u_{j+1}} \left\{ \int_{u_i}^{u_{i+1}} \sigma_\ell^{(m)}(u'\to u)du \right\} \phi(u')du' \Big/ \int_{u_j}^{u_{j+1}} \phi(u')du' \tag{29}$$

and $$\sigma_{\ell i}^{(tr)} = \int_{u_i}^{u_{i+1}} \sigma_\ell^{(tr)}(u)D(u)\phi(u)du \Big/ \int_{u_i}^{u_{i+1}} D(u)\phi(u)du \tag{30}$$

where $$D(u) = 1/3 \sum_\ell \hat{N}_\ell \sigma_\ell^{(tr)}(u) . \tag{31}$$

Obtaining accurate point cross sections, $\sigma(u)$, is a very important task in any reactor study; however, this is discussed elsewhere (Cook 1966a).

4.6 (n,2n) Reactions

Although the ideas presented to this stage can be directly applied to the (n,2n) reaction, for example in Be^9, multigroup computer codes do not normally expect the transfer matrix to create neutrons. We therefore need an artifice to enable the codes to handle this situation. The (n,2n) transfers can be added to the elastic scattering matrix to form a composite matrix provided we correct the total cross section which is to be such that

$$\sigma_{\ell i}^{(t)} = \sigma_{\ell i}^{(a)} + \sum_j \sigma_{\ell i \to j} \quad . \tag{32}$$

In Section 3.4, $\sigma_{\ell i}^{(a)}$ was defined as the cross section for destroying nuclide ℓ and hence it already includes the (n,2n) contribution. Firstly

$$\sum_j \sigma_{\ell i \to j}^{(n,2n)} = 2\sigma_{\ell i}^{(n,2n)} \tag{33}$$

hence we require

$$\sigma_{\ell i}^{(t)} = \sigma_{\ell i}^{(a)'} + \sum_j \sigma'_{\ell i \to j} \quad , \tag{34}$$

where $\sigma'_{\ell i \to j}$ is a pseudo scattering matrix

$$= \sigma_{\ell i \to j} + \sigma_{\ell i \to j}^{(n,2n)} \tag{35}$$

and $\sigma_{\ell i}^{(a)'}$ is a pseudo absorption cross section

$$= \sigma_{\ell i}^{(a)} - 2\sigma_{\ell i}^{(n,2n)} \quad . \tag{36}$$

Inelastic scattering could also be included in the same manner with the transfer matrix being added to Equation 35. Equation 36 does not change since $\sigma_{\ell i}^{(a)}$ does not include inelastic scattering.

The change to absorption cross section given by Equation 36 gives correct neutron balance but the nuclide balance is slightly upset. (Due to this approach, in burnup studies, Be^9 can apparently be produced in a reactor, but the amount is insignificant!)

4.7 Multigroup Equations

Including the idea of the previous section the multigroup equations of Section 3.8 become

$$D_i B^2 \Phi_i + \sum_\ell \hat{N}_\ell \sigma_{\ell i}^{(t)} \Phi_i - \sum_\ell \hat{N}_\ell \sum \sigma_{\ell j \to i} \Phi_j = \chi_i \quad , \qquad i=1,2,\ldots,g \tag{37}$$

and for convenience we have dropped the prime. Using Equation 34 this further simplifies to

$$D_i B^2 \Phi_i + \sum_\ell \hat{N}_\ell \sigma_{\ell i}^{(a)} \Phi_i - \sum_\ell \hat{N}_\ell \sum \sigma_{\ell j \to i} \Phi_j = \chi_i \quad , \qquad i=1,2,\ldots,g, \tag{38}$$

where now, and henceforth, $\sigma_{\ell i \to i}$ has the meaning

$$\sigma_{\ell i \to i} = -\sum_{j \neq i} \sigma_{\ell i \to j} \quad . \tag{39}$$

This is possible since actual self-scatter terms cancel from Equation 38.

5. RESONANCE REGION

5.1 Introduction

Broadly speaking the resonance region covers the energy range 10^3eV to 1eV. Above 10^3eV, resonances tend to be unresolved by experimental measurements. Based on level spacing of the resolved resonances, statistical prediction of unresolved resonances is possible. In this work unresolved resonances are treated as part of a background cross section (Cook 1966b). Below 1eV, thermal resonances appear, for example the 0.3eV resonance of Pu^{239}, but these resonances cannot be included in a study based on using slowing down theory which takes no account of thermalization. Even at 1eV, up-scattering of neutrons is important. In the multigroup approach we will pursue here the cross section is based on a slowing down model, but a thermalization enhancement of the flux is obtained from the neutron balance calculation (Equation 38 Section 4.7). By this means the reaction rate in the neighbourhood of 1eV includes allowance for up-scattering (see also Section 6.3). The resonance region will be covered by, say, 30 fine groups. The basic material of resonance studies is given by Weinberg and Wigner (1958) and Dresner (1960). Review articles have been presented by Nordheim (1961), Huria (1964) and Chernick and Levine (1964). In this work we will be mainly concerned with calculation of multigroup resonance data for homogeneous systems.

Calculation of absorption in resonances has been a fruitful field of research for many years. Although it is possible to solve the slowing down integral equation through each resonance using a direct numerical technique (Nordheim 1961, Collins 1963 and Pollard 1964) the machine time becomes prohibitive in routine calculation of multigroup data. The merit of the approximate analytic techniques to be discussed is that they can speed up direct numerical resonance calculations by as much as 1000 times. The importance of checking these approximate analytic techniques against the direct numerical approach cannot be overemphasized. In routine calculation of a reactor at power it is also important to make allowance for overlap of neighbouring resonances and to take into account heterogeneity of the core.

Various approximate analytic techniques have been proposed when resonances are assumed to be well separated from neighbouring resonances. With these approaches we consider each resonance in isolation. Early analytic approaches consisted of using either the narrow resonance (NR) or infinite mass (IM) approximation depending on whether the practical width of the resonance (the energy span between the two points where the resonance and potential scattering cross sections become equal) was small or large compared with the maximum loss of neutron energy on collision with the resonance absorber (Wigner et al. 1955). The rather arbitrary manner in which scattering by the absorber was included (NR) or excluded (IM) was a weakness of the approach; however, the results of using the theory were encouraging. Goldstein and Cohen (1962) suggested partial inclusion of scattering by the absorber by introducing a factor λ such that $\lambda = 1$ corresponded to the NR approximation and $\lambda=0$ corresponded to the IM approximation. The method of determining λ for this intermediate resonance (IR) approximation was based on equating absorption rates obtained from first and second iterate solutions of the slowing down equation for resonances at zero absolute temperature. McKay and Pollard (1963), using a numerical approach, showed that for practical temperatures the IR method (actually the equivalent μ-method of Goldstein and Cohen ibid.) is insensitive to a choice of parameter based on zero absolute temperature. Keane and Dyos (1966) showed that equating first and second iterate solutions in the IR approach was not always satisfactory. Pollard (1964) compared "exact" numerical estimates of absorption rate with estimates using the IR approach and dependence on the mass of the associated moderator was evident. Hill and Schaefer (1962) extended the IR method to include partial scattering by moderator nuclides as well. This method was not satisfactory until further extended by McKay (1964). McKay et al. (1965) applied further refinements to give a method which was demonstrated to give results in close agreement (2 per cent) with "exact" numerical calculations.

Calculation methods for multigroup cross sections derived from resonance absorption rates were presented by Hutchins (1964), Sumner (1964) and Nicholson (1965). Keane and Pollard (1966) and Pollard (1966) derived a method for calculating multigroup resonance cross sections which by-passed the impractical method of including flux detail in the preparation of transfer matrices, $\sigma_{\ell j \to i}$.

The emphasis in the preceding discussion was on the estimation of absorption rate of resonances in isolation. Various authors have looked at the problem of resonance overlap when the isolated resonance approach is no longer satisfactory (Rowlands 1963 and Hwang 1965). The extension of the approximate analytic techniques to handle this situation was discussed by Keane (1966) and Keane and O'Halloran (1967).

For practical reactor calculations heterogeneity of the fuel needs to be taken into account. In the H.T.G.C.R. studies, heterogeneity of fuel particles in a ball can be studied using an equivalence relation to reduce the problem to that of an equivalent homogeneous system (Keane 1964). Use of equivalence relations for heterogeneous systems was discussed by Keane and McKay (1966).

The challenge of resonance absorption studies has by no means waned over the past few years. With the increasing emphasis of fuel breeding in reactors, accurate estimates of neutron capture in resonances is important. Following increasing speed of computers more refined, although still approximate, methods which are more time consuming can be tolerated.

5.2 Resonance Integrals

In the resonance region we will consider all scattering to be elastic and spherically symmetric in the centre of mass system. Since the resonance region is well below source energies the slowing down integral equation (Equation 14 Section 4.3) becomes

$$F(u) = \sum_{\ell} \frac{1}{1-\alpha_\ell} \int_{u-U_\ell}^{u} e^{u'-u} h_\ell(u') F(u') du' . \tag{1}$$

The slowing down density is given in Section 4.3 (Equations 15 and 16) as

$$q(u) = \sum_{\ell} \frac{1}{1-\alpha_\ell} \int_{u-U_\ell}^{u} (e^{u'-u} - \alpha_\ell) h_\ell(u') F(u') du' \tag{2}$$

and
$$q(u) = 1 - \int_0^u h^{(a)}(u') F(u') du' , \tag{3}$$

where
$$h^{(a)}(u') = \sum_{m \neq s} h_\ell^{(m)}(u') . \tag{4}$$

We will consider a single resonance of a particular nuclide, designated by $\ell = 0$, assumed to be isolated from other resonances. Associated with each nuclide ℓ is a potential scattering cross section $\sigma_{s\ell}$ and an average lethargy increase on collision ξ_ℓ (Equation 18, Section 4.3). In resonance studies it is usual to eliminate direct reference to nuclide concentration from equations used by introducing

$$\sigma_{p\ell} = \hat{N}_\ell \sigma_{s\ell} / \hat{N}_o , \tag{5}$$

which is the potential scattering cross section of nuclide ℓ per resonance nuclide designated by $\ell = 0$. We then obtain an average lethargy gain on collision of

$$\bar{\xi} = \sum_{\ell} \xi_\ell \sigma_{p\ell} / \sigma_p , \tag{6}$$

where
$$\sigma_p = \sum_{\ell} \sigma_{p\ell} . \tag{7}$$

Returning to Equation 3, differentiation gives

$$\frac{dq}{du} = -h^{(a)}(u) F(u)$$

hence
$$\frac{d \, \ell n q}{du} = -h^{(a)}(u) W(u) / \bar{\xi} ,$$

where
$$W(u) = \bar{\xi} F(u) / q(u) , \tag{8}$$

which will be called here the asymptotic collision density. Proceeding we get

$$q(u) = q(u_1^*) \exp\left(- \int_{u_1^*}^{u} \sigma_p h^{(a)}(u') W(u') du' / \bar{\xi} \sigma_p \right) , \tag{9}$$

where $u_1^*(<u)$ designates the high energy cut-off of the resonance. For the full resonance range $(u>u_2^*>u_1^*)$ Equation 9 becomes

$$q(u) = pq(u_1^*) \tag{10}$$

where
$$p = e^{-I/\bar{\xi}\sigma_p} \tag{11}$$

and
$$I = \int_{u_1^*}^{u_2^*} \sigma_p h^{(a)}(u)W(u)du \ . \tag{12}$$

Equation 11 defines p , the resonance escape probability and Equation 12 defines I, the resonance integral following Pollard (1964). These are the two important quantities in resonance studies.

If in a fine group i we partition the lethargy ranges $u_1^* < u_2^* < \ldots < u_{m+1}^*$ around m individual (isolated) resonances with resonance escape probabilities $p_1, p_2, \ldots, p_m$, then Equation 10 becomes

$$q(u) = pq(u_1^*) \ , \qquad u > u_{m+1}^* \tag{13}$$

where
$$p = \prod_{k=1}^{m} p_k \ , \tag{14}$$

that is
$$p = e^{-I/\bar{\xi}\sigma_p} \ , \tag{15}$$

where
$$I = \sum_{k=1}^{m} I_k \ , \tag{16}$$

which is the sum of the individual resonance integrals expressed per nuclide $\ell = 0$. We are thus in a position to calculate resonance integrals provided (i) the resonance cross sections are known (required as $h^{(a)}(u)$) and (ii) we can calculate the asymptotic collision density, W(u).

5.3 Resonance Cross Sections

We will assume the cross sections (of one resonance) to be represented by single level Doppler broadened Breit-Wigner resonance contours (Dresner 1960)

$$\sigma^{(t)}(u) = \sigma_p + \sigma_o \psi(\theta, x) \ , \tag{17}$$

$$\sigma_o^{(s)}(u) = \sigma_{po} + \frac{\Gamma_n}{\Gamma} \sigma_o \psi(\theta, x) \ , \tag{18}$$

and
$$\sigma_o^{(a)}(u) = \frac{\Gamma_a}{\Gamma} \sigma_o \psi(\theta, x) \ , \tag{19}$$

where σ_o is the peak resonance cross section (at an energy of E_reV)

$$= 2.608 \times 10^6 g_j \Gamma_n / E_r \Gamma \ ,$$

g_j is the resonance spin factor,

Γ_n is the resonance neutron width (eV),

Γ_a is the resonance absorption width (eV),

$\Gamma = \Gamma_n + \Gamma_a$,

$$\psi(\theta, x) = \frac{\theta}{2\sqrt{\pi}} \int_{-\infty}^{\infty} e^{-\frac{1}{4}\theta^2 (x-y)^2} dy \Big/ (1+y^2) \tag{20}$$

(the profile function of Voigt 1912),

$$\theta = \frac{\Gamma}{2}\sqrt{\left(\frac{A}{E_r T}\right)} ,$$

T is the temperature of the medium (eV),

A is the atomic mass of the absorber,

$$x = 2(E - E_r)/\Gamma , \tag{21}$$

$$E = 10^7 e^{-u} (\text{eV}) \tag{22}$$

and the total cross section given by Equation 17 includes scattering due to all nuclides but is given per nuclide $\ell = 0$.

The definition of $h^{(a)}(u)$ is

$$h^{(a)}(u) = \sigma_o^{(a)}(u)/\sigma^{(t)}(u) ,$$

hence
$$\sigma_p h^{(a)}(u) = \frac{\Gamma_a}{\Gamma}\,\sigma_o\,\beta\,\frac{\psi(\theta,x)}{\psi(\theta,x) + \beta} , \tag{23}$$

where
$$\beta = \sigma_p/\sigma_o \tag{24}$$

and in addition we have

$$\frac{du}{dx} = -\Gamma/2E .$$

Equation 12 then becomes

$$I = \frac{\Gamma_a \sigma_o}{E_r}\, g(\theta,\beta;W) , \tag{25}$$

where
$$g(\theta,\beta;W) = \frac{\beta}{2}\int_{-\infty}^{\infty} \frac{\psi(\theta,x)}{\psi(\theta,x) + \beta}\, W(u)dx , \tag{26}$$

which is obtained using the two usual assumptions of resonance studies (Dresner 1960)

(i) that $\frac{du}{dx} \simeq -\Gamma/2E_r$ (27)

and (ii) that the finite range $(x(u_1^*), x(u_2^*))$ may be replaced by an infinite range.

5.4 Asymptotic Collision Density

5.4.1 Narrow resonance approximation

Let us consider $u < u_1^*$ and we will assume that we are in a region of no absorption. Equation 1 (following Glasstone and Edlund 1952) gives

$$F(u) = c \tag{28}$$

where c is a constant. Equations 2 and 3 show that

$$c = q(u_1^*)/\bar{\xi} , \tag{29}$$

hence for this region

$$W(u) = 1 . \tag{30}$$

If in addition we have a region of no absorption for $u >> u_2^*$ Equation 28 still holds but with c given by

$$c = q(u_2^*)/\bar{\xi} ,$$

hence Equation 30 is again obtained. For a single nuclide with resonance properties of the resonance under consideration but otherwise hydrogen-like it may be shown that Equation 30 again holds, but here inside the range of the resonance as well ($u_1^* \leqslant u \leqslant u_2^*$) (Weinberg and Wigner 1958). Also for a resonance absorber satisfying the condition of Spinney (1957)

$$\frac{\sigma_{po}}{\sigma_p} = \frac{\Gamma_n}{\Gamma} , \tag{31}$$

and for which the absorption is small and the resonance is narrow compared with collision ranges of moderator, Equation 30 is again obtained. These qualitative discussions indicate the range of applicability of the NR approximation which corresponds to using Equation 30 for the full resonance range.

In the notation of this work the NR integral is given by

$$I_{NR} = \frac{\Gamma_a \sigma_o}{E_r} g(\theta,\beta;1) \tag{32}$$

and $\quad g(\theta,\beta;1) = \beta J(\theta,\beta)$,

where $\quad J(\theta,\beta) = \int_0^\infty \frac{\psi(\theta,x)}{\psi(\theta,x)+\beta} dx$, (33)

which is the widely used resonance function tabulated by Bell et al. (1963) and approximated by Doherty (1963) for rapid resonance calculations. The well known limits (Dresner ibid.)

$$g(\theta,\infty;1) = \pi/2$$

and $\quad g(\infty,\beta;1) = \pi/2 \sqrt{(1+1/\beta)}$

follow from the definition of the resonance profile function (Equation 20).

We now pursue a simplified version of the method of McKay et al. (1965) to illustrate the method. From Equation 8, W(u) is composed of two lethargy dependent components (i) q(u) and (ii) F(u). The second can vary considerably more than the first as u covers the resonance. Also the first is a monotonically decreasing function varying from $q(u_1^*)$ for $u \leqslant u_1^*$ to $q(u_2^*)$ for $u \geqslant u_2^*$.

5.4.2 Approximate slowing down density

Since the absorption in the neighbourhood of the resonance peak (x=0) is the greatest contributor to the resonance integral it is here that q(u) is most important in $W(u) = \bar{\xi}F(u)/q(u)$. This suggests we choose an average slowing down density, say

$$q(u) = \frac{1}{2}(q(u_1^*) + q(u_2^*))$$

or

$$q(u) = \frac{1}{2}(1+p)q(u_1^*) . \tag{34}$$

5.4.3 Approximate collision density

The collision density in the absence of the resonance is

$$F(u) = q(u_1^*)/\bar{\xi} \tag{35}$$

hence using this as first iterant, Equation 1 becomes

$$F(u) = \frac{q(u_1^*)}{\bar{\xi}} \sum_\ell \frac{1}{1-\alpha_\ell} \int_{u-U_\ell}^{u} e^{u'-u} h_\ell(u')du'$$

giving $$F(u) = \frac{q(u_1^*)}{\bar{\xi}} \sum_\ell \frac{1}{1-\alpha_\ell} \frac{\Gamma}{2E_r} \int_x^{(x+x_\ell)/\alpha_\ell} \frac{\sigma_{p\ell} + \delta_{\ell o}\sigma_o \psi(\theta,x')\Gamma_n/\Gamma}{\sigma_p + \sigma_o \psi(\theta,x')} dx' \tag{36}$$

using the approximation given by Equation 27 and setting $e^{u'-u} = 1$,

where $x_\ell = 2E_r(1-\alpha_\ell)/\Gamma$.

For the resonance absorber we have $\alpha_o \to 1$ and for moderator nuclides $\alpha_\ell \to 0$. Hence if we write

$$F(u) = \frac{q(u_1^*)}{\bar{\xi}} \sum_\ell \frac{1}{x_\ell^*} \int_x^{x+x_\ell^*} \frac{\sigma_{p\ell} + \delta_{\ell o}\sigma_o \psi(\theta,x')\Gamma_n/\Gamma}{\sigma_p + \sigma_o \psi(\theta,x')} dx' \quad , \tag{37}$$

where $$x_\ell^* = 2E_r(1-\alpha_\ell)/\Gamma\alpha_\ell \quad , \tag{38}$$

then we maintain a mean value of F(u) in some sense and Equation 35 is reproduced in the absence of the resonance. The change from Equation 36 to Equation 37 is obviously greatest for moderator nuclides and since the moderator term is largely dominated by off-resonance conditions the change appears reasonable. Equation 37 then reduces to

$$F(u) = \frac{q(u_1^*)}{\bar{\xi}} \left\{ 1 - \sum_\ell \frac{a_\ell}{x_\ell^*} \int_x^{x+x_\ell^*} \frac{\psi(\theta,x')}{\psi(\theta,x')+\beta} dx' \right\}, \tag{39}$$

where $$a_\ell = \frac{\sigma_{p\ell}}{\sigma_p} - \sigma_{\ell o}\frac{\Gamma_n}{\Gamma} \quad , \tag{40}$$

which should be compared with the Spinney condition given as Equation 31.

5.4.4 Approximate resonance integral

Combining the results of Sections 5.4.2 and 5.4.3 we have

$$W(u) = \frac{2}{1+p} \left\{ 1 - \sum_\ell \frac{a_\ell}{x_\ell^*} \int_x^{x+x_\ell^*} \frac{\psi(\theta,x')}{\psi(\theta,x')+\beta} dx' \right\} \tag{41}$$

and then Equation 26 becomes

$$g(\theta,\beta;W) = \frac{2}{1+p} \beta \left\{ J(\theta,\beta) - \frac{1}{2} \sum_\ell \frac{a_\ell}{x_\ell^*} K(\theta,\beta,\beta,x_\ell^*) \right\} \quad , \tag{42}$$

where $$K(\theta,\beta,\gamma,\delta) = \int_{-\infty}^{\infty} \int_x^{x+\delta} \frac{\psi(\theta,x)}{\psi(\theta,x)+\beta} \frac{\psi(\theta,x')}{\psi(\theta,x')+\gamma} dx'\, dx \quad , \tag{43}$$

which has been studied by McKay and Pollard (1965). From their work

$$K(\theta,\beta,\gamma,\delta) \simeq \frac{4}{\pi} J(\theta,\beta)\, J(\theta,\gamma) \tan^{-1} \left\{ \frac{\delta\sqrt{(\beta\gamma)}}{\beta\sqrt{(1+1/\gamma)}+\gamma\sqrt{(1+1/\beta)}} \right\} , \tag{44}$$

so that Equation 42 becomes

$$g(\theta,\beta;W) \simeq \frac{2}{1+p} \beta J(\theta,\beta) \left[1 - \frac{2}{\pi} J(\theta,\beta) \sum_\ell \frac{a_\ell}{x_\ell^*} \tan^{-1} \frac{x_\ell^*}{2\sqrt{(1+1/\beta)}} \right] . \tag{45}$$

The procedure of McKay et al. (1965) for calculating resonance integrals follows the lines of the preceding arguments except that the λ method of Hill and Schaefer (1962) is used. This method requires the first iterant for F(u) (and the cross sections) to nuclide free parameters, λ_ℓ , one for each nuclide. We then choose the parameters (non-uniquely) so that our first and second iterants give the same resonance integral. We will not pursue the method further.

5.5 Multigroup Resonance Cross Sections

Having calculated resonance integrals and resonance escape probabilities for the m resonances in a fine group i of lethargy width δu_i we require a method for calculation of multigroup resonance cross sections. Having determined flux detail in the form of W(u) (say Equation 41) then to be consistent this same detail should be included in the calculation of transfer matrices $\sigma_{\ell j\to i}$ (Equation 29 of Section 4.5). This approach is not feasible in general as we would be faced with continual recalculation of the matrices prior to each use in a multigroup calculation. We are in an unusual position in the resonance region, as distinct from the other regions, as we know the final reaction rates we require. For the group under consideration the reaction rate is simply $(1-p)q(u_1^*)$, where p is given by Equation 14. Rather than put detail into the calculation of transfer matrices, which are normally based on a flat flux approximation, we modify the multigroup resonance cross sections so that we obtain the known reaction rate. This is the method suggested by Keane and Pollard (1966) and Pollard (1966).

In the absence of leakage ($B^2 = 0$) and below source energies ($\chi_i = 0$) Equation 38 of Section 4.7 becomes

$$\left\{ \sum_{k=1}^{m} \hat{N}_{\ell(k)} \sigma^{(a)}_{\ell(k)i} + \sum_{\ell} \hat{N}_\ell \left|\sigma_{\ell i\to i}\right| \right\} \Phi_i = \sum_{\ell} \hat{N}_\ell \sum_{j<i} \sigma_{\ell j\to i} \Phi_j \quad , \tag{46}$$

where $\ell(k)$ designates the nuclide which corresponds to the k^{th} resonance of the group. Now

$$\sum_{\ell} \hat{N}_\ell \sum_{j<i} \sigma_{\ell j\to i} \Phi_j = f_i \, q(u_1^*) \quad , \tag{47}$$

where f_i is the probability of a neutron entering group i, since $f_i \, q(u_1^*)$ is the rate of entry of neutrons to the group. It may be shown (Joanou and Dudek 1961) that

$$f_i = \sum_{\ell} \hat{N}_\ell \, \sigma_{s\ell} \, \xi_\ell f_{\ell i} / \bar{\xi} \sum \hat{N}_\ell \sigma_{s\ell} \tag{48}$$

where

$$\begin{aligned} f_{\ell i} &= (1-e^{-\delta u_i} - \alpha_\ell \, \delta u_i)/\xi_\ell (1-\alpha_\ell) \;, & \delta u_i &< U_\ell \\ &= 1 \;, & \delta u_i &\geqslant U_\ell \;. \end{aligned} \tag{49}$$

In the absence of absorption (and with $W(u) = 1$) we have

$$F(u) = q(u_1^*)/\bar{\xi} \quad ,$$

hence Equation 3 of Section 4.2 becomes

$$\phi(u) = q(u_1^*)/\bar{\xi} \sum_{\ell} \hat{N}_\ell \, \sigma_{s\ell}$$

and the definition $\Phi_i = \int_{u_i}^{u_{i+1}} \phi(u) \, du$,

gives

$$\Phi_i = q(u_1^*) \; \delta u_i / \bar{\xi} \sum_{\ell} \hat{N}_\ell \sigma_{s\ell} \quad . \tag{50}$$

Hence we must have (from Equations 46, 47 and 50)

$$\sum_{\ell} \hat{N}_\ell \left|\sigma_{\ell i\to i}\right| = \bar{\xi} \sum_{\ell} \hat{N}_\ell \sigma_{s\ell} f_i / \delta u_i \quad . \tag{51}$$

The discussion at the beginning of the section indicated that we choose our multigroup cross sections so that we reproduce the known reaction rate. We thus have

$$\sum_{k=1}^{m} \hat{N}_{\ell(k)} \, \sigma^{(a)}_{\ell(k)i} \, \Phi_i = (1 - \prod_{k=1}^{m} p_k) \, q(u_1^*) \quad . \tag{52}$$

Equations 46, 47, 51 and 52 when put together give

$$\Phi_i = (\prod_{k=1}^{m} p_k + f_i - 1)\, q(u_i^*)\, \delta u_i / f_i\, \bar{\xi} \sum_{\ell} \hat{N}_\ell \sigma_{s\ell} \tag{53}$$

and

$$\sum_{k=1}^{m} \hat{N}_{\ell(k)} \sigma^{(a)}_{\ell(k)i} = (1 - \prod_{k=1}^{m} p_k) f_i\, \bar{\xi} \sum_{\ell} \hat{N}_\ell \sigma_{s\ell} \Big/ (\prod_{k=1}^{m} p_k + f_i - 1)\, \delta u_i \quad . \tag{54}$$

We now define the major part of the cross section

$$\sigma^{(a)*}_{\ell(k)i} = (1 - p_k)\, \bar{\xi} \sum_{\ell} \hat{N}_\ell \sigma_{s\ell} / p_k \hat{N}_{\ell(k)}\, \delta u_i \ , \tag{55}$$

that is

$$\sigma^{(a)*}_{\ell(k)i} = (1 - p_k)\, \bar{\xi}\, \sigma_p / p_k\, \delta u_i \ , \tag{56}$$

then

$$\sigma^{(a)}_{\ell(k)i} = \sigma^{(a)*}_{\ell(k)i}\, C_k \ , \tag{57}$$

where

$$C_k = \prod_{h=1}^{k} p_h \Big/ \left\{ 1 - (1 - \prod_{h=1}^{m} p_h) / f_i \right\} , \tag{58}$$

which we will call a gross flux correction factor. Equation 58 is to be simplified.

An approximation to C_k is required which will preserve neutron balance given by Equation 46 but which does not distinguish between the actual ordering of resonances in the group. We assume that

$$C_k = 1 + a(\sum_{h=1}^{m} \epsilon_h - \epsilon_k) + b\epsilon_k \ , \tag{59}$$

where $\epsilon_k = 1 - p_k$. Equation 46 reduces to

$$\sum_{k=1}^{m} \epsilon_k \left\{ 1 - a(\sum_{h=1}^{m} \epsilon_h - \epsilon_k) + b\epsilon_k \right\} \Big/ f_i (1 - \epsilon_k) = \left[1 - \left\{ 1 - \prod_{k=1}^{m} (1 - \epsilon_k) \right\} \Big/ f_i \right]^{-1} - 1 \ , \tag{60}$$

and we require this to be accurate to terms $\epsilon_k\, \epsilon_h$. The expression on the right of Equation 60 simplifies considerably, to the order of accuracy specified, since

$$\prod_{k=1}^{m} (1 - \epsilon_k) = 1 - \sum_{k=1}^{m} \epsilon_k + \sum_{k=1}^{m-1} \epsilon_k \sum_{h>k}^{m} \epsilon_h \ . \tag{61}$$

Equation 60 then becomes

$$\sum_{k=1}^{m} \epsilon_k + a(\sum_{k=1}^{m} \epsilon_k)^2 + (b + 1 - a) \sum_{k=1}^{m} \epsilon_k^2 = \sum_{k=1}^{m} \epsilon_k - \sum_{k=1}^{m-1} \epsilon_k \sum_{h>k}^{m} \epsilon_h + \frac{1}{f_i} (\sum_{k=1}^{m} \epsilon_k)^2 \tag{62}$$

and using the equation

$$(\sum_{k=1}^{m} \epsilon_k)^2 = \sum_{k=1}^{m} \epsilon_k^2 + 2 \sum_{k=1}^{m-1} \epsilon_k \sum_{h>k}^{m} \epsilon_h \ , \tag{63}$$

this further simplifies to

$$2a \sum_{k=1}^{m-1} \epsilon_k \sum_{h>k}^{m} \epsilon_h + (b+1) \sum_{k=1}^{m} \epsilon_k^2 = (\frac{2}{f_i} - 1) \sum_{k=1}^{m-1} \epsilon_k \sum_{h>k}^{m} \epsilon_h + \frac{1}{f_i} \sum_{k=1}^{m} \epsilon_k^2 \ . \tag{64}$$

Hence we must have

$$a = \frac{1}{f_i} - \frac{1}{2} \tag{65}$$

and

$$b = \frac{1}{f_i} - 1 \ . \tag{66}$$

The gross flux correction factor is then given by

$$C_k = 1 + (\frac{1}{f_i} - \frac{1}{2}) \sum_{h=1}^{m} \epsilon_h - \frac{1}{2\epsilon_k}$$

and finally

$$C_k = 1 + \left\{(\frac{2}{f_i} - 1) \sum_{h=1}^{m} \hat{N}_{\ell(h)} \sigma^{(a)*}_{\ell(h)i} - \hat{N}_{\ell(k)} \sigma^{(a)*}_{\ell(k)i}\right\} \delta u_i / 2\bar{\xi} \sum_{\ell} \hat{N}_\ell \sigma_{s\ell} , \qquad (67)$$

using Equation 55.

5.6 Implementation

The code GYMEA (Pollard and Robinson 1966) uses the McKay et al. (1965) resonance theory and multigroup resonance cross sections defined in the previous section. Calculations of resonance absorption rates using resonance theory direct and using the multigroup cross sections in a calculation of neutron balance (Equation 38, Section 4.7) are found to be in close agreement, as expected. These reaction rates also compare favourably (within about 3 per cent) with "exact" numerical results obtained from PEAS (Pollard 1964). Comparison of results obtained using different resonance theories are given by Keane and Kletzmayr (1966) using the code LUBRA (Kletzmayr 1966).

6. THERMAL REGION

6.1 Introduction

For reactor studies, the thermal region, roughly speaking, covers the energy range 1eV to 0.001 eV. In this region, absorption cross sections for some nuclides are approximated by a 1/v variation with neutron velocity v. Other nuclides have low energy resonances which are important, for example U^{233} and Pu^{239}. These resonances are usually so wide that within each group of our fine group set, say 50 groups covering the thermal region, the variation is not excessive. In the fast and resonance region, neutron scattering mechanisms, $\sigma_\ell(E' \rightarrow E)$, were obtained from simple (billiard ball) collision studies. This approach is no longer applicable to the thermal region, as thermal motion of the scatterers, and chemical bonds between them, change the nature of the scattering mechanisms. Thus in a system of BeO we no longer think of scattering of neutrons with Be and O as separate nuclides, but rather we think of scattering with BeO as an entity. The study of the mechanisms of scattering by crystals is complicated by interference effects since the neutron wavelength is comparable with atomic dimensions.

In this section we will consider some aspects of thermal neutron scattering in so far as the calculation of flux spectra is affected (neutron thermalization). Considering that a large number of fine groups is to be used to cover the thermal region, the assumption that the flux, $\phi(u)$, is flat across a group is possibly adequate, however, it is felt that the study being undertaken here would not be complete without mention of thermal reactions. The essentials of thermalization studies are given by Amaldi (1959) and Beckurts and Wirtz (1964). Reviews have been presented by Nelkin (1961), Honeck (1963) and Lawande (1965).

For many years the study of thermalization has preoccupied research workers. The first commercial reactors depended on thermal reactions for maintaining criticality and this prompted considerable interest in the thermal region. Major developments for the ten years after World War II included the proposal of the basic flux equation for an ideal gas by Wigner and Wilkins (1944) and the calculation of thermal neutron spectra in D_2O by Brown and St. John (1954). The integral equation for the flux spectrum was reduced by Wilkins (1944) to give a second order differential equation. In the last ten years or so Hurwitz, Nelkin and Habetler (1956), using a different approach, produced the same equation (the so-called heavy gas equation). In the limit as the ratio of absorption to scattering tends to zero the solution of the thermalization equation tends to a Maxwellian; $\phi(E) \propto M(E)$ ($= \frac{E}{T^2} e^{-E/T}$, T the temperature in eV). Coveyou et al. (1956) showed that even for non-limiting absorption, the flux spectrum, $\phi(E)$, is approximated by a Maxwellian, but at a temperature T (the effective neutron temperature) increased above the actual material temperature to simulate the effect of absorption (spectrum hardening). Westcott (1957) used a representation of the flux as a composite of $1/E$, a Maxwellian $M(E)$ and a joining function coupling the two together, as a basis for producing a two group cross section convention. The use of a heavy gas equation was later rejuvenated by Horowitz (1962) who suggested that an arbitrary function $f(E)$ should be introduced into the equation. The function $f(E)$ was used by several authors to include chemical binding effects (Corngold 1962, Leslie 1962 and Schaefer and Allsopp 1962). The disadvantage of this approach is the sensitivity of $f(E)$ to materials other than major scatterers (Pu^{239}, for example). A modified heavy gas equation was used by Clancy et al. (1963) in the MULGA programme for routine calculation of neutron spectra required in the calculation of multigroup data.

The detailed scattering mechanisms are usually expressed in terms of a scattering law $S(\alpha,\beta)$, where α and β are respectively the dimensionless momentum and dimensionless energy transferred to the neutron. Computer codes have been written, (i) to produce $S(\alpha,\beta)$ from results of detailed scattering studies (LEAP – McLatchie 1962) and (ii) to produce point and multigroup transfer representations $\sigma_L(E'\to E)$ and $\sigma_{Lj\to i}$ (PIXSE – Macdougall 1963) – here L refers to molecules rather than nuclides.

Just as measurements on bare fuel assemblies provide an important check for our overall multigroup data, so neutron chopper spectrum measurements and pulsed neutron experiments highlight gross detail of our thermal transfer matrices, $\sigma_{Lj\to i}$. Interpretation of results of reactor physics measurements is by no means straightforward, nevertheless, the effort spent in analysing the experiments pays handsome dividends in the form of understanding of the essentials of neutron interaction phenomena. For the H.T.G.C.R. studies the bare fuel work of McCulloch et al. (1965) has already been mentioned. Tattersall (1967) has measured thermal neutron spectra for fuelled stacks placed in the MOATA reactor and Ritchie (1967) has measured the persistent decay mode following neutron pulses in BeO stacks. Comparison of these experiments with theoretical predictions is being undertaken (Robinson 1966 and Maher 1966).

6.2 Thermalization Operator

For the thermal region Equation 24 of Section 3.7 becomes

$$S\phi(E) = A(E)\phi(E) - \chi(E) \ , \tag{1}$$

where S is the thermalization operator given by

$$S\phi(E) = \sum_L \hat{N}_L \left\{ \int_0^\infty \sigma_L(E'\to E)\phi(E')dE' - \sigma_L(E)\phi(E) \right\}, \tag{2}$$

L is an index used to denote associated nuclides (for example BeO),

$$A(E) = \sum_\ell \hat{N}_\ell \sigma_\ell^{(a)}(E) + D(E)B^2 \ , \tag{3}$$

and $\phi(E)$ is the neutron flux per unit energy normalized to unit loss rate,

$$\int_0^\infty A(E)\phi(E)dE = 1 \ . \tag{4}$$

The slowing down density defined in Section 4.2 here becomes

$$q(E) = \sum_L \hat{N}_L \int_E^\infty \int_0^\infty \{\sigma_L(E''\to E')\phi(E'') - \sigma_L(E'\to E'')\phi(E')\} dE'\, dE'' \ , \tag{5}$$

hence

$$q(E) = \sum_L \hat{N}_L \int_0^E \int_0^\infty \{\sigma_L(E'\to E'')\phi(E') - \sigma_L(E''\to E')\phi(E'')\} dE'\, dE'' \ , \tag{6}$$

since

$$q(O) = 0 \ . \tag{7}$$

Equation 7 follows from Equations 11 and 12 of Section 4.2 (which may be shown to still hold) as the effect of fast reactions is absent and we have

$$q(E) = \int_E^\infty \{\chi(E') - A(E')\,\phi(E')\}\,dE' \ ,$$

hence
$$q(E) = \int_0^E \{A(E')\phi(E') - \chi(E')\}\,dE' \ . \tag{8}$$

If we integrate Equation 1 we obtain

$$\int_0^E S\phi(E'')dE'' = q(E) \, , \tag{9}$$

using Equation 8. Equation 9 is simply Equation 6 in alternate guise. For all thermal studies the source spectrum $\chi(E)$ may be dropped from the preceding equations.

Two important properties of the thermalization operator are

$$\text{(i)} \quad SM(E) = 0 \ , \tag{10}$$

where $M(E) = \frac{E}{T^2}\, e^{-E/T}$ (Maxwellian spectrum) and T is the temperature of (11)

the material, and

$$\text{(ii)} \quad \int_0^\infty S\phi(E) = 0 \ . \tag{12}$$

Properties (i) and (ii) follow from the detailed balance condition (Beckurts and Wirtz 1964)

$$M(E')\sigma_L(E' \to E) = M(E)\sigma_L(E \to E') \ , \tag{13}$$

and the neutron balance condition

$$q(\infty) = 0 \ . \tag{14}$$

Equations 1 and 10 show that

$$\phi(E) \propto M(E) \quad \text{as} \quad A(E) \to 0 \ , \tag{15}$$

hence the change of variable

$$\mu(E) = \phi(E)/M(E) \tag{16}$$

appears appropriate. With this change, Equation 1 becomes

$$S'\mu(E) = A(E)\mu(E) \tag{17}$$

where
$$S'\mu(E) = \sum_L N_L \left\{ \int_0^\infty \sigma_L(E \to E')\mu(E')dE' - \sigma_L(E)\mu(E) \right\} , \tag{18}$$

using the detailed balance condition, Equation 13.

6.3 Heavy Gas Equation

In Equation 18 we expand $\mu(E')$ in a Taylor's series

$$\mu(E') = \mu(E-(E-E')) = \sum_{k=0}^{\infty} \frac{(-1)^k}{k!} \frac{d^k\mu}{dE^k} (E-E')^k \ , \tag{19}$$

and we obtain

$$S'\mu(E) = \sum_L \hat{N}_L \sum_{k=0}^{\infty} \frac{(-1)^k}{k!} \frac{d^k\mu}{dE^k} \sigma_{L(k)}(E) - \sigma_L(E)\,\mu(E) \ , \tag{20}$$

where the scattering moments are given by

$$\sigma_{L(k)}(E)=\int_0^\infty \sigma_L(E\rightarrow E')(E-E')^k dE' \quad , \tag{21}$$

with the obvious special case

$$\sigma_{L(0)}(E)=\sigma_L(E) \quad .$$

Considering a dissociated nuclide ℓ with average slowing down lethargy gain on isotropic elastic scattering of ξ_ℓ then for a heavy nuclide ($\xi_\ell\rightarrow 0$) Beckurts and Wirtz (ibid.) give

$$\sigma_{\ell(1)}(E)=\xi_\ell \sigma_{s\ell}(E-2T) \quad , \tag{22}$$

and

$$\sigma_{\ell(2)}(E)=2\xi_\ell \sigma_{s\ell} ET \quad , \tag{23}$$

where $\sigma_{s\ell}$ is the free atom cross section of nuclide ℓ. The remaining moments are of higher order than ξ_ℓ. Equations 22 and 23 also require the condition

$$E >> \xi_\ell T/2 \tag{24}$$

to be satisfied. Using these results Equation 20 becomes

$$S'\mu(E) \simeq \sum_\ell \hat{N}_\ell \xi_\ell \sigma_{s\ell} \{-(E-2T)\frac{d\mu}{dE} + ET\frac{d^2\mu}{dE^2}\} \quad . \tag{25}$$

The heavy gas equation is then

$$\sum_\ell \hat{N}_\ell \xi_\ell \sigma_{s\ell} \{-(E-2T)M(E)\frac{d\mu}{dE} + M(E)\, ET\frac{d^2\mu}{dE^2}\} = A(E)M(E)\,\mu(E) \quad ,$$

which simplifies to

$$\frac{d}{dE}\sum_\ell \hat{N}_\ell \xi_\ell \sigma_{s\ell} \{(E-T)\phi(E) + ET\frac{d\phi(E)}{dE}\} = A(E)\phi(E) \quad . \tag{26}$$

Using Equations 8 and 26 we have the result

$$q(E) = \hat{\sum_\ell} N_\ell \xi_\ell \sigma_{s\ell} \{(E-T)\phi(E) + ET\frac{d\phi(E)}{dE}\} \quad , \tag{27}$$

and a partial change back to lethargy u gives

$$q(u) = \sum_\ell \hat{N}_\ell \xi_\ell \sigma_{s\ell} \{(1-2\frac{T}{E})\phi(u) + \frac{T}{E}\frac{d\phi(u)}{du}\} \quad . \tag{28}$$

Equation 28 is trivial to solve numerically using a computer (Clancy et al. 1963) and therefore we will not pursue approximate analytic solutions for the complete thermal range. We are content to consider thermalization at energies corresponding to the join between our resonance and thermal regions (about 1eV).

In the absence of absorption and for $E \geqslant 1eV (T/E \leqslant 0.025$ at room temperature) Equation 28 gives

$$\phi(u) \simeq (1+2\frac{T}{E})\, q(u)\Big/\sum_\ell \hat{N}_\ell \xi_\ell \sigma_{s\ell}$$

$$\simeq (1+2\frac{T}{E})\phi_{T=0}(u) \quad , \tag{29}$$

where $\phi_{T=0}(u)$ is the normal slowing down flux (Section 5). In Section 4 we stated that we would extend slowing down theory to 1eV (just below the important Pu^{240} resonance). Equation 29 suggests that at room temperature the incident flux on the 1eV Pu^{240} resonance will be increased by 5 per cent due to upscattering of neutrons. As a consequence, the reaction rate will be increased by the same amount. This result is in agreement with the observations of Griggs (1965) and the calculations of Pollard (unpublished) using the code GYMEA (Pollard and Robinson 1966) but with more realistic scattering models than discussed here.

6.4 Pulsed Neutron Studies

Without going into the important question of existence of discrete decay modes (Corngold 1965) we assume that a suitable time after a neutron pulse has been admitted to a bare moderator assembly the flux may be represented by

$$\phi(E,t) = \phi(E)e^{-\lambda t} \quad , \tag{30}$$

where λ is the decay constant of the fundamental mode. Using Equation 30, the multigroup equations 38 of Section 4.7, modified to be consistent with Equation 1 of Section 2, become

$$D_i B^2 \Phi_i + \sum_\ell \hat{N}_\ell \sigma^{(a)}_\ell \Phi_i - \sum_L \hat{N}_L \sum_j \sigma_{Lj\to i} \Phi_j = \frac{\lambda}{v_i} \Phi_i \quad , \qquad i=1,2,\ldots,g, \tag{31}$$

where
$$v_i = \int_{u_i}^{u_{i+1}} \phi(u)du \Bigg/ \int_{u_i}^{u_{i+1}} \frac{\phi(u)}{v} du \quad . \tag{32}$$

We adopt an iterative procedure for solving Equation 31. The multigroup approach has been used by other authors (for example Ghatak and Honeck 1965).

Starting with the guess $\Phi_i^{(0)}$ we set

$$\chi_i^{(k)} = \frac{\lambda}{v_i} \Phi_i^{(k)} \quad , \qquad k=0,1,\ldots, \tag{33}$$

which is re-normalized to be consistent with

$$\sum_i \chi_i^{(k)} = 1 \quad , \tag{34}$$

where k is an iteration index and $\chi_i^{(k)}$ is a pseudo source. Equation 31 is then

$$D_i B^2 \Phi_i^{(k)} + \sum_\ell \hat{N}_\ell \sigma_i^{(a)} \Phi_i^{(k)} - \sum_L \hat{N}_L \sum_j \sigma_{Lj\to i} \Phi_j^{(k)} = \chi_i^{(k-1)}, \qquad k=1,2,\ldots \tag{35}$$

A solution procedure for the basic Equation 35 is given in Section 8. The same procedure may be used here but with an outer loop forcing convergence until

$$|\chi_i^{(k)} - \chi_i^{(k-1)}| < \epsilon \quad , \tag{36}$$

where ϵ is a suitable tolerance parameter. When convergence is achieved

$$\lambda = 1 \Bigg/ \sum_i \frac{1}{v_i} \Phi_i^{(k)} \quad . \tag{37}$$

The code GYMEA has been used (Maher 1966) to calculate fundamental decay modes of pulsed neutrons in BeO stacks of different buckling for comparison with the measurements of Ritchie (1967). In this work the compatibility of D(E) with the scattering model is important. The method is by no means completely satisfactory, but the advantage of in-situ calculation in a code used for everyday multigroup data preparation is not to be overlooked, as this provides a valuable check on both the data and its manner of preparation. Maher (1967) is pursuing other approaches which should prove to be more worthwhile than the simple method given here.

7. SOLUTION OF BURNUP EQUATIONS

7.1 Introduction

From Section 3.4 (Equation 10) the reactor nuclide equations may be written as a coupled set of first order linear differential equations in the form

$$\dot{\underset{\sim}{N}}(t) = \underset{\approx}{A}\,\underset{\sim}{N}(t) \quad , \quad \underset{\sim}{N}(0) \text{ given}, \tag{1}$$

where $\underset{\sim}{N}(t)$ is the array of nuclide concentrations, $N_\ell(t)$, for nuclides in the reactor ($\ell = 1,2,\ldots,n$),

and $\underset{\approx}{A}$ is an nxn matrix with typical element

$$a_{\ell k} = -(r^{(a)}_\ell + \lambda_\ell)\,\delta_{\ell k} + (1-\delta_{\ell k})\,(\sum_m y^{(m)}_{k\to\ell}\, r^{(m)}_k + y_{k\to\ell}\,\lambda_k) \,, \tag{2}$$

using the notation of that section. The off-diagonal elements of $\underset{\approx}{A}$ given above are non-negative and the diagonal elements are negative, except for some elements which are dominated by the (n,2n) reaction as mentioned in Section 4.6, and are distinct.

Denoting a typical nuclide ℓ by $(\ell)^A_Z$, where A is the mass number and Z is the isotope number, the six main processes which cause evolution of the nuclide species in a reactor are specified below:

(i) (n,f)-reactions, $(k)^{A'}_{Z'} \to (\ell)^A_Z$ ($y^{(f)}_{k\to\ell}$ given by Walker 1964),

(ii) (n,γ)-reactions, $(k)^{A-1}_Z \to (\ell)^A_Z$,

(iii) β-decay, $(k)^A_{Z-1} \to (\ell)^A_Z$,

(iv) (n,2n)-reactions, $(k)^{A+1}_Z \to (\ell)^A_Z$

(v) (n,α)-reactions, $(k)^{A+3}_{Z+2} \to (\ell)^A_Z$,

and (vi) (n,p)-reactions, $(k)^A_{Z+1} \to (\ell)^A_Z$.

If we arrange the nuclides in order, an isotope at a time, lightest first, except that fission products follow the fissile nuclides, then the matrix $\underset{\approx}{A}$ is nearly lower triangular since the first three mechanisms are by far the most important. A few rearrangements may make the array more nearly triangular, but a few isolated elements will remain above the diagonal (these are a result of so-called loop reactions). In practice some of these elements are significant. For example, the $Be^9(n,\alpha)$ reaction sets up a loop in the following way:

(i) $Be^9_4 + n^1_0 \to He^6_2 + He^4_2$,

(ii) $He^6_2 \to Li^6_3 + \beta^0_{-1}$,

(iii) $Li^6_3 + n^1_0 \to H^3_1 + He^4_2$,

(iv) $H^3_1 \to He^3_2 + \beta^0_{-1}$,

(v) $He^3_2 + n^1_0 \to H^3_1 + H^1_1$.

To some extent the above reactions negate the neutron enhancement obtained from the $Be^9(n,2n)$ reaction. For a typical H.T.G.C.R. equilibrium calculation (Gemmell et al. 1967) the enhancement in the absence of the reactions (ii) to (v) (about 4 per cent) is halved when the reactions are considered.

In burnup studies based on constant power output for a fixed core, $\underset{\approx}{A}$ is a function of time through (i) the level of flux necessary to maintain a constant power and (ii) the spectrum of the reactor which changes as the burnup proceeds. For this situation it is usual to solve the set of equations (1) using a numerical integration technique (Hoffman 1956, Alexander et al. 1961, Arai et al. 1961 and Todt 1962). For the equilibrium model studied here an analytic technique is desirable as $\underset{\approx}{A}$ is independent of time. Even for studies when $\underset{\approx}{A}$ is time dependent, an analytic technique has advantages provided we may consider $\underset{\approx}{A}$ to be step-wise time-independent (Cannon et al. 1961, Benson and Collins 1962 and England 1962). An interesting method has been proposed by Joanou et al. (1964) which approximates the time dependence of $\underset{\approx}{A}$ by a polynomial representation in an analytic method. The step procedure of the normal analytic method is replaced by an iterative procedure, but the number of time consuming spectrum calculations is considerably reduced. Recently Pollard and Robinson (1966) proposed a simple analytic technique which relies on the fact that in most burnup calculations the matrix $\underset{\approx}{A}$ is nearly triangular (or by rearrangement can be made nearly triangular). This is the method which we will pursue.

7.2 Elementary Transformations

We will assume that the order of the nuclides is chosen so that A is lower triangular except for a few elements. For these instances we will assume that (i) the elements are just off the diagonal and (ii) no two such elements neighbour each other. We thus have

$$a_{\ell k} = 0 \quad , \quad k > \ell \qquad \text{for } \ell = 1,2,\ldots,n \tag{3}$$

except for (i) $a_{k-1,k} \neq 0, \quad k = i_1, i_2, \ldots, i_m \quad ,$ (4)

with (ii) $i_{h+1} - i_h > 1, \quad h = 1,2,\ldots,m-1 \quad .$ (5)

As mentioned in the previous section this is not a serious restriction in reactor burnup calculations.

Elementary transformations are required to reduce $\underset{\approx}{A}$ to triangular form. Introducing the matrix

$$\underset{\approx}{I}_j(x) = (\delta_{\ell k} + x\,\delta_{\ell,j-1}\,\delta_{jk}), \tag{6}$$

then by direct multiplication we may verify that

$$\underset{\approx}{I}_j(x)\,\underset{\approx}{I}_j(y) = \underset{\approx}{I}_j(x+y) \quad ,$$

hence $\underset{\approx}{I}_j(x)\,\underset{\approx}{I}_j(-x) = \underset{\approx}{I}_j(0)$ (the unit matrix) . (7)

We thus obtain

$$\underset{\approx}{I}_j^{-1}(x) = \underset{\approx}{I}_j(-x). \tag{8}$$

Let us consider the transformed matrix

$$\underset{\approx}{A}' = \underset{\approx}{I}_j(x_j)\,\underset{\approx}{A}\,\underset{\approx}{I}_j(-x_j) \quad . \tag{9}$$

The elements of this matrix are given by

$$a'_{\ell k} = \sum_g \sum_h (\delta_{\ell g} + x_j\,\delta_{\ell,j-1}\,\delta_{jg})\,a_{gh}(\delta_{hk} - x_j\,\delta_{h,j-1}\,\delta_{jk}) \quad , \tag{10}$$

which simplifies to

$$a'_{\ell k} = a_{\ell k} \quad , \quad \ell \neq j-1 \ , \quad k \neq j \ , \tag{11}$$

$$a'_{\ell j} = a_{\ell j} - x_j \, a_{\ell, j-1} \quad , \quad \ell \neq j-1 \ , \tag{12}$$

$$a'_{j-1,k} = a_{j-1,k} + x_j \, a_{jk} \quad , \quad k \neq j \ , \tag{13}$$

$$a'_{j-1,j} = a_{j-1,j} + x_j (a_{jj} - a_{j-1,j-1}) - x_j^2 \, a_{j,j-1} \quad . \tag{14}$$

If we choose $\quad j = i_h \qquad (15)$

and $\quad a'_{j-1,j} = 0 \ ,$

that is $\quad a_{j,j-1} x_j^2 - (a_{jj} - a_{j-1,j-1}) x_j - a_{j-1,j} = 0 \ , \qquad (16)$

then $\underset{\approx}{A}'$ has one less non-zero element above the leading diagonal than $\underset{\approx}{A}$. This follows from the restriction given by Equations 3, 4 and 5 and Equation 16. Repeated application of Equations 11 to 16 for $h = 1,2,\ldots,m-1$ thus results in a matrix $\underset{\approx}{A}'$ which is lower triangular.

The roots of Equation 16 are always real since the off-diagonal elements of $\underset{\approx}{A}$ are non-negative. If $a_{j,j-1} \neq 0$, then two choices are generally available for a root of Equation 16. Since the solution of Equation 1 is independent of whether we apply elementary transformations or not (we only introduced them to simplify the analysis) the choice of root is immaterial.

Starting with Equation 1 we may obtain

$$\{\prod_{h=m-1}^{1} \underset{\approx}{I}_{i_h}(x_{i_h})\} \dot{\underset{\sim}{N}}(t) = \{\prod_{h=m-1}^{1} \underset{\approx}{I}_{i_h}(x_{i_h})\} \underset{\approx}{A} \{\prod_{h=1}^{m-1} \underset{\approx}{I}_{i_h}(-x_{i_h})\}\{\prod_{h=m-1}^{1} \underset{\approx}{I}_{i_h}(x_{i_h})\} \underset{\sim}{N}(t), \tag{17}$$

using Equation 8, where Π denotes a product over the range indicated (perhaps backwards). In terms of our lower triangular matrix $\underset{\approx}{A}'$, Equation 17 becomes

$$\dot{\underset{\sim}{N}}'(t) = \underset{\approx}{A}' \, \underset{\sim}{N}'(t) \quad , \tag{18}$$

where $\quad \underset{\sim}{N}'(t) = \prod_{h=m-1}^{1} \underset{\approx}{I}_{i_h}(x_{i_h}) \underset{\sim}{N}(t) \quad , \qquad (19)$

hence $\quad \underset{\sim}{N}(t) = \prod_{h=1}^{m-1} \underset{\approx}{I}_{i_h}(-x_{i_h}) \underset{\sim}{N}'(t) \quad , \qquad (20)$

which has elements given by

$$N_\ell(t) = N'_\ell(t) - x_{i_h} \, \delta_{\ell, i_h - 1} N'_{i_h}(t) \quad , \qquad \ell = 1,2,\ldots,n \ . \tag{21}$$

We will now develop an analytic method for solving Equation 18. The required initial conditions may be obtained from Equation 19 in the form

$$N'_\ell(0) = N_\ell(0) + x_{i_h} \, \delta_{\ell, i_h - 1} \, N_{i_h}(0) \quad , \quad \ell = 1,2,\ldots,n \ . \tag{22}$$

When we have solved Equation 18, Equation 21 will enable us to calculate the required concentrations.

7.3 Analytic Method

The set of equations (18) may be written

$$\dot{N}_\ell(t) = \sum_{g \leq \ell} a_{\ell g} N_g(t) \quad , \tag{23}$$

where, for the moment, we have discarded the prime and ℓ ranges over $1,2,\ldots,n$. Hence taking the Laplace transform of Equation 23 we have

$$p\overline{N}_\ell(p)-N_\ell(0)=\sum_{g\leqslant\ell} a_{\ell g}\overline{N}_g(p) \tag{24}$$

where $\overline{N}_\ell(p)=\int_0^\infty e^{-pt}N_\ell(t)dt.$

Equation 24 then simplifies to

$$\overline{N}_\ell(p)=\{N_\ell(0)+\sum_{g<\ell} a_{\ell g}\overline{N}_g(p)\}\Big/(p-a_{\ell\ell}) \ . \tag{25}$$

The usual approach adopted for reducing the above equation is the following:

$$\overline{N}_1(p)=N_1(0)\Big/(p-a_{11})$$

$$\overline{N}_2(p)=\{N_2(0)+a_{21}\overline{N}_1(p)\}\Big/(p-a_{22})$$

$$=\frac{N_2(0)}{p-a_{22}}+\frac{a_{21}N_1(0)}{(p-a_{11})(p-a_{22})}$$

$$=\frac{N_2(0)}{p-a_{22}}+\frac{a_{21}N_1(0)}{a_{11}-a_{22}}\left(\frac{1}{p-a_{11}}-\frac{1}{p-a_{22}}\right) ,$$

etc., using partial fractions. Rather than use this approach directly, here we will pursue a method which produces a simple recurrence relation for use with a computer.

We notice that

$$\overline{N}_\ell(p)=\sum_{k\leqslant\ell} b_{\ell k}\Big/(p-a_{kk}) , \tag{26}$$

where the coefficients $b_{\ell k}$ are to be determined. Equation 25 is thus equivalent to

$$\sum_{k\leqslant\ell} b_{\ell k}\Big/(p-a_{kk})=\{N_\ell(0)+\sum_{g<\ell} a_{\ell g}\sum_{k\leqslant g} b_{gk}\Big/(p-a_{kk})\}\Big/(p-a_{\ell\ell})$$

$$=\frac{N_\ell(0)}{p-a_{\ell\ell}}+\sum_{g<\ell} a_{\ell g}\sum_{k\leqslant g}\frac{b_{gk}}{a_{kk}-a_{\ell\ell}}\left(\frac{1}{p-a_{kk}}-\frac{1}{p-a_{\ell\ell}}\right) .$$

Comparing coefficients of $1/(p-a_{kk})$ we get

$$b_{\ell k}=\sum_{k\leqslant g<\ell} a_{\ell g}\, b_{gk}\Big/(a_{kk}-a_{\ell\ell}), \qquad k=1,2,\ldots,\ell-1; \quad \ell=2,3,\ldots,n \tag{27}$$

and $$b_{\ell\ell}=N_\ell(0)-\sum_{g<\ell} a_{\ell g}\sum_{k\leqslant g}\frac{b_{gk}}{a_{kk}-a_{\ell\ell}} ,$$

hence $$b_{\ell\ell}=N_\ell(0)-\sum_{k<\ell} b_{\ell k} , \quad \ell=1,2,\ldots,n . \tag{28}$$

Equations 27 and 28 express a simple recurrence relation which enables all the required coefficients in Equation 26 to be determined provided the indices (ℓ,k) are varied in the following way:

$$(1,1);\ (2,1),\ (2,2);\ (3,1),(3,2),(3,3);\ldots,(n,n).$$

This method is thus ideally suited for use with a computer.

Returning to Equation 26 we readily obtain

$$N'_\ell(t) = \sum_{k\leq\ell} b_{\ell k}\, e^{a'_{kk} t} \quad , \tag{29}$$

using standard Laplace transform results (the prime has been restored). Equation 21 finally gives the required solution of the burnup equations.

7.4 Average Concentrations

The average concentrations given by Equation 6 of Section 3.3 may be obtained directly from Equations 29 and 21 as

$$\hat{N}'_\ell(T) = \sum_{k\leq\ell} b_{\ell k} (e^{a'_{kk}T} - 1)/a'_{kk} T \ , \tag{30}$$

and

$$\hat{N}_\ell(T) = \hat{N}'_\ell(T) - x_{i_h}\, \delta_{\ell, i_{h-1}}\, \hat{N}'_{i_h}(T) \ . \tag{31}$$

For small arguments the exponential is best expanded to give

$$(e^{a'_{kk}T} - 1)/a'_{kk} T = 1 + \frac{1}{2} a'_{kk} T + \frac{1}{6} a'^{2}_{kk} T^2 + \ldots, \tag{32}$$

which is numerically superior to the direct evaluation method for this situation.

7.5 Inner Iteration

Using Equations 30 and 31 we need to choose T so that a given FIFA is achieved (Equation 9, Section 3.3). We do this using a simple regula-falsi iterative scheme. This iteration will be referred to as the inner iteration to distinguish it from the outer iteration required to adjust the spectrum (Section 8). Note here the advantage of having the analytic solution available (Equation 30).

7.6 Implementation

The techniques discussed in this Section have been implemented in the computer code GYMEA (Pollard and Robinson 1966). In this code the burnup mechanisms are supplied along with the nuclear data from a library tape. This is a great advantage over having built-in burnup mechanisms in a programme, as particular reactions can be studied separately and with different degrees of precision (say the production of U^{232} from Th^{232}, which is not of direct interest in neutronics calculations). Experience with the method in GYMEA has shown that single precision floating point arithmetic (36 bits) is adequate for normal calculations.

8. SOLUTION OF FLUX EQUATIONS

8.1 Introduction

The multigroup flux equations required to be solved (Section 4.7) may be written

$$\underset{\approx}{W}\, \underset{\sim}{\Phi} = \underset{\sim}{\chi} \quad , \tag{1}$$

where elements of $\underset{\approx}{W}$ are given by

$$w_{ij} = (\sum_\ell \hat{N}_\ell \sigma^{(a)}_{\ell i} + D_i B^2)\, \delta_{ij} - \sum_\ell \hat{N}_\ell \sigma_{\ell j \to i} \tag{2}$$

where i and j range over 1,2,...,g, and Φ_j and χ_i are respectively elements of $\underset{\sim}{\Phi}$ and $\underset{\sim}{\chi}$. In practice g is usually 100 or more and hence direct solution using, say, the Gauss-Jordan method

(Ralston and Wilf 1960) is too time consuming on a computer. For this problem an iterative solution technique is both feasible and worthwhile. The basic ideas behind these methods are given by Faddeeva (1959), Householder (1964) and Wachspress (1966). Here we are content to investigate a simple technique in order to understand the essentials of any iterative procedure.

8.2 Solution of Slowing Down Equations

Bearing in mind the restriction on up-scatters derived from the scattering matrix (Section 4.2), $\underset{\approx}{W}$ may be partitioned thus

$$\underset{\approx}{W} = \left(\begin{array}{c|c} \underset{\approx}{W}'' & 0 \\ \hline \underset{\approx}{W}''' & \underset{\approx}{W}' \end{array}\right) \quad , \tag{3}$$

where $\underset{\approx}{W}'$ is a matrix $(g-h+1)x(g-h+1)$

$\underset{\approx}{W}''$ is a lower triangular matrix $(h-1)x(h-1)$

and $\underset{\approx}{W}'''$ is a matrix $(g-h+1)x(h-1)$.

Equation 1 may then be written

$$\left(\begin{array}{c|c} \underset{\approx}{W}'' & 0 \\ \hline \underset{\approx}{W}''' & \underset{\approx}{W}' \end{array}\right) \left(\begin{array}{c} \underset{\sim}{\Phi}'' \\ \hline \underset{\sim}{\Phi}' \end{array}\right) = \left(\begin{array}{c} \underset{\sim}{\chi}'' \\ \hline \underset{\sim}{\chi}''' \end{array}\right) , \tag{4}$$

using an obvious notation.

We therefore obtain

$$\underset{\approx}{W}'' \underset{\sim}{\Phi}'' = \underset{\sim}{\chi}'' \tag{5}$$

and

$$\underset{\approx}{W}' \underset{\sim}{\Phi}' = \underset{\sim}{\chi}' , \tag{6}$$

where

$$\underset{\sim}{\chi}' = \underset{\sim}{\chi}''' - \underset{\approx}{W}''' \underset{\sim}{\Phi}'' . \tag{7}$$

Firstly, Equation 5 may be readily solved since $\underset{\approx}{W}''$ is triangular. Written out in terms of elements, Equation 5 is the set of slowing down equations

$$\sum_{i \leqslant j} w_{ij} \Phi_j = \chi_i \quad , \quad i=1,2,\ldots,h-1 \quad , \tag{8}$$

and the solution is immediately

$$\Phi_i = (\chi_i - \sum_{i<j} w_{ij} \Phi_j)/w_{ii} \quad , \quad i=1,2,\ldots,h-1 \quad , \tag{9}$$

since $w_{ii} \neq 0$.

Equation 7 defines a vector for which all elements are known, as the slowing down flux, $\underset{\sim}{\Phi}''$, is available from Equation 9. The vector $\underset{\sim}{\chi}'$ is thus essentially a slowing down source. We now require a method for obtaining the thermal flux given as the solution of Equation 6.

8.3 Solution of Thermal Equations

The set of equations (6) may be written

$$(\underset{\approx}{A} - \underset{\approx}{C}) \underset{\sim}{\Phi}' = \underset{\sim}{\chi}' , \tag{10}$$

where $\underset{\approx}{A}$ is a matrix $(g-h+1) \times (g-h+1)$ with elements

$$a_{ij} = \{\sum_{\ell} \hat{N}_{\ell} (\sigma_{\ell i}^{(a)} - \sigma_{\ell i \to i}) + D_i B^2\} \delta_{ij} \quad ,$$

C is a matrix $(g-h+1)\times(g-h+1)$ with elements $c_{ij} = \sum_{\ell} \hat{N}_{\ell}\sigma_{\ell j\to i}(1-\delta_{ij})$ and now i and j range over the values $h, h+1, \ldots, g$.

Equation 10 becomes

$$\underset{\sim}{\Phi}' = \underset{\approx}{A}^{-1}\underset{\sim}{\chi}' + \underset{\approx}{A}^{-1}\underset{\approx}{C}\,\underset{\sim}{\Phi}' \;, \tag{11}$$

which we will solve using the direct recurrence relation

$$\underset{\sim}{\Phi}'^{(k)} = \underset{\approx}{A}^{-1}\underset{\sim}{\chi}' + \underset{\approx}{A}^{-1}\underset{\approx}{C}\,\underset{\sim}{\Phi}'^{(k-1)} \;, \quad k=1,2,\ldots, \tag{12}$$

given a guess, $\underset{\sim}{\Phi}'^{(0)}$, for the solution. It is required to show that the method will converge. The form of Equation 12 is the simplest iterative scheme. Other much more complicated schemes are normally used (Section 8.3.4), however the simple scheme illustrates the general requirements.

8.3.1 Norms

A norm of a vector $\underset{\sim}{x}$ (Faddeva 1959) is a non-negative number $||\underset{\sim}{x}||$ satisfying the conditions

(i) $||\underset{\sim}{x}|| \geqslant 0$ with equality being satisfied only if $\underset{\sim}{x} \equiv 0$,

(ii) $||b\underset{\sim}{x}|| = |b|\,||\underset{\sim}{x}||$ (b a constant) ,

and (iii) $||\underset{\sim}{x}+\underset{\sim}{y}|| \leqslant ||\underset{\sim}{x}|| + ||\underset{\sim}{y}||$.

In this work we will use a vector norm given by

$$||\underset{\sim}{x}|| = \sum_i \mu_i |x_i| \;, \tag{13}$$

where μ_i is a set of positive numbers. First we must show that the number obtained from Equation 13 is a norm. Properties (i) and (ii) follow immediately and (iii) follows from the simple inequality

$$|x_i + y_i| \leqslant |x_i| + |y_i| \;.$$

A norm of a matrix P is a non-negative number $||\underset{\approx}{P}||$ satisfying

(i) $||\underset{\approx}{P}|| \geqslant 0$ with equality being satisfied only if $\underset{\approx}{P} \equiv 0$,

(ii) $||b\underset{\approx}{P}|| = |b|\;||\underset{\approx}{P}||$ (b a constant) ,

(iii) $||\underset{\approx}{P}+\underset{\approx}{Q}|| \leqslant ||\underset{\approx}{P}|| + ||\underset{\approx}{Q}||$,

and (iv) $||\underset{\approx}{P}\underset{\approx}{Q}|| \leqslant ||\underset{\approx}{P}||\;||\underset{\approx}{Q}||$.

We also require this norm to be consistent with the definition of vector norm in the following way;

(v) $||\underset{\approx}{P}\underset{\sim}{x}|| \leqslant ||\underset{\approx}{P}||\;||\underset{\sim}{x}||$.

Here we will use the matrix norm

$$||\underset{\approx}{P}|| = \max_j \left(||\underset{\sim}{P}_j|| / \mu_j \right) , \tag{14}$$

$$= \max_j \left(\sum_i \mu_i |p_{ij}| / \mu_j \right) ,$$

(which means we choose j to maximize the quantity indicated), where $\underset{\sim}{P}_j$ is the j^{th} column of $\underset{\approx}{P}$ and

p_{ij} are elements of $\underset{\approx}{P}$. Again properties (i) and (ii) are obvious. We now check on the remaining properties.

(iii) For the j^{th} column of $\underset{\approx}{P}$ and $\underset{\approx}{Q}$, using an obvious notation, we have

$$\frac{\|\underset{\sim}{P}_j + \underset{\sim}{Q}_j\|}{\mu_j} \leqslant \frac{\|\underset{\sim}{P}_j\|}{\mu_j} + \frac{\|\underset{\sim}{Q}_j\|}{\mu_j} \quad ,$$

$$\leqslant \max_j \left(\|\underset{\sim}{P}_j\|/\mu_j\right) + \max_j \left(\|\underset{\sim}{Q}_j\|/\mu_j\right) \quad ,$$

therefore
$$\max_j \left(\|\underset{\sim}{P}_j + \underset{\sim}{Q}_j\|/\mu_j\right) \leqslant \max_j \left(\|\underset{\sim}{P}_j\|/\mu_j\right) + \max_j \left(\|\underset{\sim}{Q}_j\|/\mu_j\right) \quad ,$$

hence
$$\|\underset{\approx}{P} + \underset{\approx}{Q}\| \leqslant \|\underset{\approx}{P}\| + \|\underset{\approx}{Q}\| \quad .$$

(iv) Here we have

$$\|\underset{\approx}{P}\,\underset{\approx}{Q}\| = \max_j \left(\sum_i \mu_i \left|\sum_k p_{ik}\, q_{kj}\right| / \mu_j\right) \quad ,$$

$$\leqslant \max_j \left(\sum_i \mu_i \sum_k |p_{ik}|\,|q_{kj}| / \mu_j\right) \quad ,$$

$$\leqslant \max_j \left(\sum_k \sum_i \mu_i \frac{|p_{ik}|}{\mu_k}\, \mu_k \frac{|q_{kj}|}{\mu_j}\right) \quad ,$$

$$\leqslant \max_k \left(\sum_i \mu_i |p_{ik}|/\mu_k\right) \max_j \left(\sum_k \mu_k |q_{kj}|\, \mu_j\right) \quad ,$$

$$\leqslant \|\underset{\approx}{P}\|\ \|\underset{\approx}{Q}\| \quad .$$

(v) <u>Finally</u>

$$\|\underset{\approx}{P}\,\underset{\sim}{x}\| = \sum_i \mu_i \left|\sum_k p_{ik}\, x_k\right| \quad ,$$

$$\leqslant \sum_i \mu_i \sum_k |p_{ik}|\,|x_k| \quad ,$$

$$\leqslant \max_k \left(\sum_i \mu_i |p_{ik}|/\mu_k\right) \sum_k \mu_k |x_k|$$

$$\leqslant \|\underset{\approx}{P}\|\ \|\underset{\sim}{x}\| \quad .$$

8.3.2 <u>Convergence</u>

Returning to Equation 12 and introducing a vector which is the deviation of our k^{th} iterant from the solution of Equation 11 we have

$$\underset{\sim}{y}^{(k)} = \underset{\approx}{A}^{-1}\,\underset{\approx}{C}\ \underset{\sim}{y}^{(k-1)} \quad , \tag{15}$$

where
$$\underset{\sim}{y}^{(k)} = \underset{\sim}{\Phi}' - \underset{\sim}{\Phi}'^{(k)} \quad . \tag{16}$$

From Equation 15 we have

$$\underset{\sim}{y}^{(k)} = (\underset{\approx}{A}^{-1}\underset{\approx}{C})^k\, \underset{\sim}{y}^{(0)} \quad , \tag{17}$$

then
$$\|\underset{\sim}{y}^{(k)}\| \leqslant \|\underset{\approx}{A}^{-1}\underset{\approx}{C}\|^k\, \|\underset{\sim}{y}^{(0)}\| \quad . \tag{18}$$

Hence if we have

$$\|\underset{\approx}{A}^{-1}\underset{\approx}{C}\| < 1 \tag{19}$$

then $$\lim_{k\to\infty} \|\underset{\sim}{y}^{(k)}\| = 0 \quad ,$$

which from property (i) of our norm gives

$$\lim_{k\to\infty} \underset{\sim}{y}^{(k)} = 0 \quad ,$$

that is $$\underset{\sim}{\Phi}' = \lim_{k\to\infty} \underset{\sim}{\Phi}'^{(k)} \quad . \tag{20}$$

Convergence is thus assured if the inequality (19) is satisfied.

From the definitions of Section 8.3 we have

$$\|\underset{\approx}{A}^{-1}\underset{\approx}{C}\| = \max_j \left(\sum_i \mu_i \; |c_{ij}| / a_{ii}\mu_j\right) \quad . \tag{21}$$

If we choose $\mu_i = a_{ii}$ (22)

then $$\|\underset{\approx}{A}^{-1}\underset{\approx}{C}\| = \max_j \left(\sum_i |c_{ij}| / a_{jj}\right)$$

and $$\sum_i |c_{ij}| = \sum_\ell \hat{N}_\ell \, |\sigma_{\ell j\to j}| ,$$

using the definition of outscatter term given by Equation 39 of Section 4.7. Hence we have

$$\|\underset{\approx}{A}^{-1}\underset{\approx}{C}\| < 1$$

since $$\sum_\ell \hat{N}_\ell \, |\sigma_{\ell j\to j}| \Big/ \left(\sum_\ell \hat{N}_\ell (\sigma_{\ell j}^{(a)} + |\sigma_{\ell j\to j}|) + D_j B^2\right) < 1 \quad .$$

The method will thus always converge.

8.3.3 Termination

Rather than use the parameters μ_i given by Equation 22, if we choose instead

$$\mu_i = \sum_\ell \hat{N}_\ell \sigma_{\ell i}^{(a)} + D_i B^2 \quad , \tag{23}$$

then the norm becomes more meaningful. From Equation 10, and Equation 39 of Section 4.7,we have

$$\|\underset{\sim}{\Phi}'\| = p \quad , \tag{24}$$

where p is the known probability of a neutron slowing down

$$= \sum_{i=h}^{g} \chi_i' \quad , \tag{25}$$

In addition if we terminate the calculation when

$$\|\underset{\sim}{y}^{(k)}\| \leqslant \epsilon \quad , \tag{26}$$

where ϵ is a prescribed error limit, then reaction rates per source neutron will be in error by no more than ϵ.

In order to estimate $\|y^{(k)}\|$ required for termination of the calculation (inequality (26)) we proceed as follows. From Equation 15 we obtain

$$\underset{\sim}{y}^{(k)} - \underset{\sim}{y}^{(k+1)} = (\underset{\approx}{I} - \underset{\approx}{A}^{-1}\underset{\approx}{C})\underset{\sim}{y}^{(k)} \quad ,$$

where $\underset{\approx}{I}$ is the unit matrix. Hence

$$\underset{\sim}{y}^{(k)} = (\underset{\approx}{I} - \underset{\approx}{A}^{-1}\underset{\approx}{C})^{-1} (\underset{\sim}{y}^{(k)} - \underset{\sim}{y}^{(k+1)})$$

$$= (\underset{\approx}{I} - \underset{\approx}{A}^{-1}\underset{\approx}{C})^{-1}\underset{\approx}{A}^{-1}\underset{\approx}{C}\,(\underset{\sim}{y}^{(k-1)} - \underset{\sim}{y}^{(k)})$$

$$= (\underset{\approx}{I} - \underset{\approx}{A}^{-1}\underset{\approx}{C})^{-1}\underset{\approx}{A}^{-1}\underset{\approx}{C}\,(\underset{\sim}{\Phi}'^{(k)} - \underset{\sim}{\Phi}'^{(k-1)}),$$

therefore $$\|\underset{\sim}{y}^{(k)}\| \leqslant \|\underset{\approx}{A}^{-1}\underset{\approx}{C}\| \; \|\underset{\sim}{\Phi}'^{(k)} - \underset{\sim}{\Phi}'^{(k-1)}\| / (1 - \|\underset{\approx}{A}^{-1}\underset{\approx}{C}\|) \quad . \tag{27}$$

Equation 21 is used to calculate the matrix norm $\|\underset{\approx}{A}^{-1}\underset{\approx}{C}\|$.

A useful check at the termination of the procedure is to compare $\|\Phi'^{(k)}\|$ with p (Equation 24). Also at the beginning of the calculation the guess should be normalized so that

$$\|\underset{\sim}{\Phi}'^{(0)}\| = p \quad .$$

8.3.4 Acceleration

In practice it is necessary to apply techniques that accelerate the convergence of the simple scheme presented here (Householder 1964). A procedure proposed by Robinson (1964) and used in the code GYMEA (Pollard and Robinson 1966) is recommended.

8.4 Outer Iteration

For equilibrium calculations (Section 3), on completion of a spectrum calculation, the power density obtained is calculated thus

$$P = \sum_{\ell} \hat{N}_{\ell} f_{\ell} r_{\ell}^{(f)} \; , \tag{28}$$

where $$r_{\ell}^{(m)} = \sum_{i=1}^{g} \sigma_{\ell i}^{(m)} \Phi_i \; , \tag{29}$$

and here the normalization of the flux is chosen to be the same as during the burnup calculation

$$\sum_{i=1}^{g} \Phi_i = \Phi \quad . \tag{30}$$

Should the power obtained not agree with the power specified, to within a certain prescribed limit, then a further burnup (inner) iteration is carried out. This procedure is described more fully in Bicevskis et al. (1967).

For criticality calculations, a suitable spectrum-determining parameter, perhaps buckling, is adjusted using a simple regula-falsi iterative scheme to achieve a specified multiplication (usually 1).

9. CONCLUSION

Various methods have been discussed for the calculation of multigroup data for use in nuclear studies. These methods were biased towards detailed calculation of the neutron spectrum in a bare homogeneous recirculating core of a reactor operating at power and in equilibrium. Particular attention was given to calculating multigroup data for the important resonance region and to a simple method for solving the burnup equations. Analytic techniques were employed in both cases. Considering the needs of a variety of people engaged in reactor physics calculations, from assessment studies

(Bicevskis et al. 1967), to comparison of predictions with experiments (Robinson 1966 and Maher 1966), a versatile computational aid is required. Out of these needs came GYMEA (Pollard and Robinson 1966).

Little mention was made of the problems of obtaining the basic nuclear data (Cook 1966a) and of using multigroup data in reactor calculations (Hesse 1967). No mention was made of choosing pseudo fission products. These pseudo fission products are chosen so that hundreds of fission products may be effectively replaced by a few nuclides that have the same reactivity effect and similar burnup characteristics. Using pseudo fission products is important in extensive space dependent burnup calculations in order to keep computational time within reason. A simple basis for obtaining pseudo fission products is given by Pollard and Robertson (1966).

The checking out of the computational aid by comparison with experiments has been mentioned (Section 6). The checking of approximate theories used is an important step and this requires designing other codes which, in a limited sense, enable comparison to be made between approximate theories and "exact" theories (for example PEAS–Pollard 1964 and LUBRA–Kletzmayr 1966). The checking of coding is the first step, but is this step ever completed?

Many important problems were only touched upon, such as (i) the calculation of resonance overlap, (ii) the calculation of decay modes in pulsed neutron assemblies and (iii) the choosing of group boundaries. As nuclear reactors become more and more competitive with fossil fuel reactors as a means of producing electrical power so more and more emphasis is going to be placed on reliable calculations. The day will come when reactor physics is a branch of well understood engineering, but not in the foreseeable future.

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