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LUCAS HEIGHTS

COLLISION PROBABILITY CALCULATIONS INCLUDING AXIAL LEAKAGE

by

G. DOHERTY

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ABSTRACT

Equations are presented for the calculation of collision probabilities in cylindrical geometry with axial leakage included through a complex cross section term. Numerical results are presented for two single rod, natural uranium heavy water reactor lattices. Similar calculations may be performed with modified S_n programmes and the author concludes that these are more efficient.

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Table 1 Results for System 13 (3.05 cm dia. rod on 13 cm square pitch)

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1. INTRODUCTION

Brissenden and Green (1968) have developed a formalism which allows buckling terms to be incorporated in neutron transport calculations of a single lattice cell. In cylindrical geometry, the axial buckling component is introduced by replacing the total cross section Σ of each material by the complex cross section $\Sigma + iB \cos\theta$, where B is the square root of the axial buckling and θ is the angle between the vertical axis of the cylinder and the direction of neutron travel.

If the cell calculation is performed with an S_n code, the code must be modified to compute complex angular fluxes even though the scalar flux and reaction rate at every point of the cell remain real. Use of the collision probability method, which calculates only average scalar fluxes for homogeneous sub-regions of the cell, avoids the necessity of performing complex arithmetic at the expense of complicating the integrals implicit in the definition of the collision probability matrix.

In the subsequent sections the method of calculating the collision probability matrix with complex total cross sections is developed. We have been unable to develop an approximation similar to that of Bonalumi (1961) for the complex cross section case, and the numerical integration method employed here is a little slow for routine use. We therefore conclude that the S_n codes, despite the recoding necessary to accommodate complex angular fluxes, still provide the best tool for this type of calculation in cylindrical geometry. However, in cluster geometry the numerical integration method is often employed in the evaluation of the conventional collision probabilities, and the extension to the complex cross section case using the methods developed in this paper is straightforward.

2. THE APPROXIMATION OF BRISSENDEN AND GREEN

The equation in cylindrical geometry for the angular flux $N(r,z,\underset{\sim}{\Omega})$ along a direction $\underset{\sim}{\Omega}$ can be written:

$$\eta\mu \frac{\partial N}{\partial r} - \frac{\eta\sqrt{1-\mu^2}}{r} \frac{\partial N}{\partial \psi} + \gamma \frac{\partial N}{\partial z} + \Sigma N = S(r,z,\underset{\sim}{\Omega}) \quad , \tag{2.1}$$

where

ψ = angle in the horizontal plane between the projection of $\underset{\sim}{\Omega}$ and the outward radius,

θ = angle between $\underset{\sim}{\Omega}$ and the vertical axis of the cylinder,

μ = $\cos\psi$,

γ = $\cos\theta$,

η = $\sin\theta$,

Σ = total (or transport corrected total) cross section, and

S = scattering (and possibly fission) source into the direction $\underset{\sim}{\Omega}$.

Writing

$$T_r = \eta\mu \frac{\partial}{\partial r} - \frac{\eta\sqrt{1-\mu^2}}{r} \frac{\partial}{\partial \psi} \quad , \tag{2.2}$$

Equation 2.1 can be expressed in the form

$$T_r N + \gamma \frac{\partial N}{\partial z} + \Sigma N = S \quad . \tag{2.3}$$

The object of the approximation is to remove the z dependence from Equation 2.3. We therefore assume a complex periodic solution $W(r,z,\underset{\sim}{\Omega})$ of the form

$$W(,r,z,\underset{\sim}{\Omega}) = e^{iBz}\ [W_1(r,\underset{\sim}{\Omega}) + i\, W_2\,(r,\underset{\sim}{\Omega})] \quad . \tag{2.4}$$

This enables Equation 2.3 to be written as the one dimensional form

$$T\!\!/\,(W_1 + i\,W_2) + (\Sigma + i\,B_\gamma)(W_1 + i\,W_2) = S \quad . \tag{2.5}$$

Equation 2.5 can be solved by any one dimensional transport code which can accommodate complex cross sections and angular fluxes. Our problem then is to relate the complex periodic function W with the real solution N of Equation 2.1. From consideration of the properties of W, Brissenden and Green (1961) have identified N with the real part of W.

$$N(r,z,\underset{\sim}{\Omega}) = \cos Bz\, W_1(r,\underset{\sim}{\Omega}) - \sin Bz\, W_2(r,\underset{\sim}{\Omega}) \quad . \tag{2.6}$$

The scalar flux ϕ is given by

$$\begin{aligned}\phi(r,z) &= \int N(r,z,\underset{\sim}{\Omega})\, d\underset{\sim}{\Omega} \\ &= \cos Bz \int W_1(r,\underset{\sim}{\Omega})\, d\underset{\sim}{\Omega} - \sin Bz \int W_2(r,\underset{\sim}{\Omega})\, d\underset{\sim}{\Omega}\,.\end{aligned} \tag{2.7}$$

If the finite cylinder is symmetrically located about the plane $z = 0$ we require the scalar flux to be symmetric in z. This implies

$$\int W_2\,(r,\underset{\sim}{\Omega})\, d\underset{\sim}{\Omega} = 0 \quad . \tag{2.8}$$

Equation 2.8 is most useful in assigning physical meaning to the reaction rates. In particular in the collision probability method, where only scalar fluxes are computed, it will be sufficient to evaluate the real part $W_1(r,\underset{\sim}{\Omega})$. If $B = \frac{\pi}{H}$ it leads immediately to the result

$$\phi(r, \frac{H}{2}) = \phi(r, \frac{-H}{2}) = 0 \quad . \tag{2.9}$$

For the proof of Equation 2.8 and a more detailed discussion of the approximation the reader is referred to the original paper of Brissenden and Green. In the subsequent sections we examine the solution by collision probabilities of the one dimensional problem posed in Equation 2.5. The method of solution is formally the same, whether the total cross section is complex or not, but the integrals appearing in the solution of Equation 2.5 are more difficult to compute than those of the axially infinite problem.

3. MODIFICATIONS TO THE NORMAL COLLISION PROBABILITY FORMULATION

The integral transport equation, assuming isotropic scattering may be written

$$\phi(\underset{\sim}{r'}) = \int_R d\underset{\sim}{r'}\ [\Sigma_S(\underset{\sim}{r'})\ \phi(\underset{\sim}{r'}) + S(r')]\ \frac{e^{-\Sigma\,|\underset{\sim}{r} - \underset{\sim}{r'}|}}{4\pi\,|\underset{\sim}{r} - \underset{\sim}{r'}|^2} \quad . \tag{3.1}$$

Multiplication of both sides of Equation 3.1 by $\Sigma(\underset{\sim}{r})$ gives

$$\Sigma(\underset{\sim}{r})\,\phi(\underset{\sim}{r}) = \int_R d\underset{\sim}{r'}\ P(\underset{\sim}{r'},\underset{\sim}{r})\ [\Sigma_S\,(r')\,\phi\,(\underset{\sim}{r'}) + S(\underset{\sim}{r'})] \quad , \tag{3.2}$$

where

$$P(\underset{\sim}{r'},\underset{\sim}{r}) = \Sigma(\underset{\sim}{r})\ \frac{e^{-\Sigma\,|\underset{\sim}{r} - \underset{\sim}{r'}|}}{4\pi\,|\underset{\sim}{r} - \underset{\sim}{r'}|^2} \quad . \tag{3.3}$$

If the system R is divided into a number of regions R_i in which the material cross sections are constant, and the fluxes in each region are assumed uniform, the normal matrix form of the equations can easily be derived. Integrating over R_i gives

$$\int_{R_i} \Sigma(\underset{\sim}{r})\, \phi(\underset{\sim}{r})\, d\underset{\sim}{r} = \int_{R_i} d\underset{\sim}{r} \int_{R} d\underset{\sim}{r}'\, P(\underset{\sim}{r}', \underset{\sim}{r})\, \Sigma_s(\underset{\sim}{r}')\, \phi(\underset{\sim}{r}') + S(\underset{\sim}{r}')$$

$$= \underset{j}{\text{Sum}} \int_{R_i} d\underset{\sim}{r} \int_{R_j} d\underset{\sim}{r}'\, P(\underset{\sim}{r}', \underset{\sim}{r})\, [\Sigma_s(\underset{\sim}{r}')\, \phi(\underset{\sim}{r}') + S(\underset{\sim}{r}')\,] \quad . \tag{3.4}$$

Defining ϕ_i by the equation

$$V_i\, \phi_i = \int_{R_i} \phi(\underset{\sim}{r})\, d\underset{\sim}{r} \quad , \tag{3.5}$$

we may rewrite Equation 3.4 in matrix form:

$$\Sigma_i\, V_i\, \phi_i = \underset{j}{\text{Sum}}\, [\Sigma_{sj}\, \phi_j + S_j\,]\, V_j\, P_{ji} \quad , \tag{3.6}$$

where the collision probability matrix P_{ji} is given by

$$P_{ji} = \frac{1}{V_j} \int_{R_j} d\underset{\sim}{r}' \int_{R_i} d\underset{\sim}{r}\, P(\underset{\sim}{r}', \underset{\sim}{r})$$

$$= \frac{1}{V_j} \int_{R_j} d\underset{\sim}{r}' \int_{R_i} d\underset{\sim}{r}\, \frac{\Sigma(\underset{\sim}{r})\, e^{-\Sigma\, |\underset{\sim}{r}' - \underset{\sim}{r}'|}}{4\pi\, |\underset{\sim}{r} - \underset{\sim}{r}'|^2} \quad . \tag{3.7}$$

Equation 3.6 is unsuitable for our present purpose because the left hand side contains Σ_i which will be complex and angle dependent. If we carry through our analysis on Equation 3.1 instead of Equation 3.2, then equations similar to 3.6 and 3.7 can be derived:

$$V_i\, \phi_i = \underset{j}{\text{Sum}}\, [\Sigma_{sj}\, \phi_j + S_j\,]\, V_j\, Q_{ji} \quad , \quad \text{and} \tag{3.8}$$

$$Q_{ji} = \frac{1}{V_j} \int_{R_j} d\underset{\sim}{r}' \int_{R_i} d\underset{\sim}{r}\, \frac{e^{-\Sigma\, |\underset{\sim}{r} - \underset{\sim}{r}'|}}{4\pi\, |\underset{\sim}{r} - \underset{\sim}{r}'|^2} \quad . \tag{3.9}$$

If we multiply Equation 3.8 by the <u>real</u> cross section Σ_i, we get formally Equation 3.6

$$\Sigma_i V_i\, \phi_i = \underset{j}{\text{Sum}}\, [\Sigma_{sj} \phi_j + S_j\,]\, V_j\, P_{ji} \quad , \tag{3.10}$$

where now the matrix P is defined by

$$P_{ji} = \Sigma_i\, Q_{ji} \quad . \tag{3.11}$$

Thus formally the collision probability method is unaltered by the presence of the complex angle-dependent cross section, though in fact Equations 3.9 and 3.11 do involve the complex cross section in the definition of Q and hence P.

4. EXPLICIT FORMULAE

In the normal collision probability formulation a typical probability P_{ij} is computed from the

$$P_{ij} = \frac{2}{\pi r_1^2} \int_0^{r_1} dx \int_0^{2y_1} dy \int_0^{\pi/2} \sin\theta\, d\theta\; e^{-\Sigma_1 y/\sin\theta}\; e^{\Sigma_2 y_2/\sin\theta}$$

$$\ldots\; e^{-\Sigma_{j-1}\, y_{j-1}/\sin\theta}\; [1 - e^{-\Sigma_j y_j/\sin\theta}] \quad , \tag{4.1}$$

where $$y_i = \sqrt{r_i^2 - x^2} \tag{4.2}$$

and r_i are the outer radii of the annuli into which the cell is divided.

Instead of Σ_k we wish to use $\Sigma_k + iB\cos\theta$, so that the $(0, \pi/2)$ range of θ must be changed to $(0, \pi)$ to include both positive and negative imaginary cross section terms.

$$Q_{1j} = \frac{1}{\pi r_1^2} \int_0^{r_1} dx \int_0^{2y_1} dy \int_0^{\pi} \frac{\sin\theta}{\Sigma_j} \, d\theta \; e^{-\Sigma_1 y/\sin\theta}$$

$$e^{-\Sigma_2 y_2/\sin\theta} \cdots e^{-\Sigma_{j-1} y_{j-1}/\sin\theta} \left[1 - e^{-\Sigma_j y_j/\sin\theta}\right] . \tag{4.3}$$

Performing the integration over y we obtain

$$Q_{1j} = \frac{1}{\pi r_1^2} \int_0^{r_1} dx \int_0^{\pi} \frac{\sin^2\theta}{\Sigma_1 \Sigma_j} \, d\theta \left[1 - e^{-2\Sigma_1 y_1/\sin\theta}\right] e^{-\Sigma_2 y_2/\sin\theta} \cdots$$

$$e^{-\Sigma_{j-1} y_{j-1}/\sin\theta} \left[1 - e^{-\Sigma_j y_j/\sin\theta}\right] . \tag{4.4}$$

Replacing each Σ_k by $\Sigma_k + iB\cos\theta$ gives

$$Q_{1j} = \frac{1}{\pi r_1^2} \int_0^{r_1} dx \int_0^{\pi} \frac{\sin^2\theta \, d\theta}{(\Sigma_1 + iB\cos\theta)(\Sigma_j + iB\cos\theta)}$$

$$\left[1 - e^{-2\Sigma_1 y_1/\sin\theta} \, e^{-iB2y_1\cot\theta}\right] e^{-\Sigma_2 y_2/\sin\theta} \, e^{-iBy_2\cot\theta} \cdots$$

$$e^{-\Sigma_{y-1} y_{j-1}/\sin\theta} \, e^{iBy_{j-1}\cot\theta} \left[1 - e^{-\Sigma_j y_j/\sin\theta} \, e^{-iBy_j\cot\theta}\right] \tag{4.5}$$

$$= \frac{2}{\pi r_1^2} \int_0^{r_1} dx \; [I(X_1, Y_1, B, \Sigma_1, \Sigma_j) - I(X_2, Y_2, B, \Sigma_1, \Sigma_j)$$

$$- I(X_3, Y_3, B, \Sigma_1, \Sigma_j) + I(X_4, Y_4, B, \Sigma_1, \Sigma_j)] , \tag{4.6}$$

where

$$\begin{aligned} X_1 &= \operatorname{Sum}_{k=2}^{j-1} \Sigma_k y_k \\ X_2 &= X_1 + 2\Sigma_1 y_1 \\ X_3 &= X_1 + \Sigma_j y_j \\ X_4 &= X_2 + \Sigma_j y_j \end{aligned} \tag{4.7}$$

$$\begin{aligned} Y_1 &= \operatorname{Sum}_{k=2}^{j-1} y_k \\ Y_2 &= Y_1 + 2y_1 \\ Y_3 &= Y_1 + y_j \\ Y_4 &= Y_2 + y_j \end{aligned} \tag{4.8}$$

and

$$I(X,Y,B,\Sigma_1,\Sigma_2) = \frac{1}{2}\int_0^{\pi} d\theta \; \frac{\sin^2\theta \, e^{-X/\sin\theta} \, e^{-iBY\cot\theta}}{(\Sigma_1 + iB\cos\theta)(\Sigma_2 + iB\cos\theta)}$$

$$= \int_0^{\pi/2} d\theta \; \frac{\sin^2\theta \, e^{-X/\sin\theta}}{(\Sigma_1^2 + B^2\cos^2\theta)(\Sigma_2^2 + B^2\cos^2\theta)}$$

$$[(\Sigma_1\Sigma_2 - B^2\cos^2\theta)\cos(BY\cot\theta) - (\Sigma_1 + \Sigma_2) B\cos\theta \sin(BY\cot\theta)], \quad (4.9)$$

The result corresponding to Equation 4.6 in the normal collision probability formulation is

$$P_{1j} = \frac{2}{\pi r_1^2 \Sigma_1}\int_0^{r_1} dx \; [K_{i3}(X_1) - K_{i3}(X_2) - K_{i3}(X_3) + K_{i3}(X_4)] \quad , \quad (4.10)$$

where

$$K_{i3}(X) = \int_0^{\pi/2} d\theta \; e^{-X/\sin\theta} \sin^2\theta \quad . \quad (4.11)$$

Thus we can see that the essential form of the calculation remains unchanged, but we rely on being able to find a method of evaluating the integral of Equation 4.9 in a computer time comparable with that required for the simpler K_{i3} integral. The extension from Q_{1j} to Q_{ij} follows that already given by Doherty (1969) for the conventional probabilities. It may easily be shown from the symmetry of the integrands that

$$V_i Q_{ij} = V_j Q_{ji} \quad . \quad (4.12)$$

In our formulation

$$P_{ij} = \Sigma_j Q_{ij} \quad , \quad (4.13)$$

so that we have the normal reciprocity condition satisfied, that is,

$$V_i \Sigma_i P_{ij} = V_j \Sigma_j P_{ji} \quad . \quad (4.14)$$

5. RESULT FOR A HOMOGENEOUS SYSTEM OF INFINITE RADIUS

The leakage form of P_{11} is given by

$$P_{11} = \Sigma_1 Q_{11} \quad (5.1)$$

where

$$Q_{11} = \int_0^{\pi/2} \frac{\Sigma_1 \sin\theta \, d\theta}{\Sigma_1^2 + B^2\cos^2\theta} - \frac{1}{\pi r_1^2}\int_0^{r_1} dx \int_0^{\pi}$$

$$\frac{\sin^2\theta \, [1 - e^{-2\Sigma_1 y_1/\sin\theta} \, e^{-2iBy_1\cot\theta}] \, d\theta}{[\Sigma_1 + iB\cos\theta]^2} \quad (5.2)$$

$$= \frac{1}{B}\tan^{-1}\frac{B}{\Sigma_1} - \frac{2}{\pi r_1^2}\int_0^{r_1} dx \; \{I(0,0,B,\Sigma_1,\Sigma_1) - I(2\Sigma_1 y_1, 2y_1, B, \Sigma_1, \Sigma_1)\}. \quad (5.3)$$

Hence

$$P_{11} = \frac{\Sigma_1}{B} \tan^{-1} \frac{B}{\Sigma_1} - \frac{2\Sigma_1}{\pi r_1^2} \int_0^{r_1} dx \ \{I(0,0,B,\Sigma_1,\Sigma_1) - I(2\Sigma_1 y_1, 2y_1, B, \Sigma_1, \Sigma_1)\}. \quad (5.4)$$

In the axially infinite problem the corresponding result is

$$P_{11} = 1 - \frac{2}{\pi r_1^2 \Sigma_1} \int_0^{r_1} dx \ [Ki_3(0) - Ki_3(2\Sigma_1 y_1)] \quad . \quad (5.5)$$

If we allow r_1 to become infinitely large, Equation 5.5 reduces to

$$P_{11} = 1 \quad (5.6)$$

as we would expect, while Equation 5.4 reduces to

$$P_{11} = \frac{\Sigma_1}{B} \tan^{-1} \frac{B}{\Sigma_1} \quad . \quad (5.7)$$

It is of interest to demonstrate that this result can be obtained for a slab system with an assumed real flux distribution of sin Bz with $B = \frac{\pi}{H}$. Assuming that the system extends from $z = -\infty$ to $z = +\infty$ (the infinite reactor hypothesis) we can compute the probability of a neutron crossing the boundary $z = 0$.

$$\text{Net outflow} = \frac{1}{2}\int_0^{\infty} dz \sin Bz \int_0^{\pi/2} \sin\theta \, d\theta \ e^{-\Sigma_1 z/\cos\theta}$$

$$- \frac{1}{2}\int_{-\infty}^{0} dz \sin Bz \int_0^{\pi/2} \sin\theta \, d\theta \ e^{-\Sigma_1 z/\cos\theta} \quad (5.8)$$

$$= \int_0^{\infty} dz \sin Bz \int_0^{\pi/2} \sin\theta \, d\theta \ e^{-\Sigma_1 z/\cos\theta}$$

$$= \int_0^{\pi/2} \sin\theta \, d\theta \int_0^{\infty} \sin Bz \ e^{-\Sigma_1 z/\cos\theta}$$

$$= \int_0^{\pi/2} \sin\theta \, d\theta \ \frac{1}{B} \ \frac{B^2 \cos^2\theta}{\Sigma_1^2 + B^2 \cos^2\theta}$$

$$= \frac{1}{B}\left[1 - \frac{\Sigma_1}{B} \tan^{-1} \frac{B}{\Sigma_1}\right] \quad . \quad (5.9)$$

From symmetry the net outflow through $z = H$ is identical so that the total outflow may be written:

$$\text{Total outflow} = \frac{2}{B}\left[1 - \frac{\Sigma_1}{B} \tan^{-1} \frac{B}{\Sigma_1}\right] \quad . \quad (5.10)$$

If we assume that the total outflow from the two faces of the slab [0,H] arises from within the slab then

$$P_{11} = 1 - \frac{\text{total outflow}}{\text{source}}$$

$$= 1 - \frac{\frac{2}{B}\left[1 - \frac{\Sigma_1}{B}\tan^{-1}\frac{B}{\Sigma_1}\right]}{\int_0^H \sin Bz\,dz}$$

$$= \frac{\Sigma_1}{B}\tan^{-1}\frac{B}{\Sigma_1} \quad . \tag{5.11}$$

Thus the result (5.7) can be obtained by considerations other than the complex cross section method. It is an important result because we shall see in the next section that the boundary condition is chosen to retain this form of P_{11}.

6. BOUNDARY CONDITIONS

The usual assumption employed in the calculation of cylindrical geometry with a reflecting outer boundary is that returning neutrons have a distribution $\sin\theta\cos\psi$. Use of this distribution leads without difficulty to the surface/volume reciprocity relation

$$P_{Bi} = \frac{2}{\pi R} V_i \Sigma_i P_{iB} \quad . \tag{6.1}$$

If we examine for a moment a one region cell infinite in the z direction and with a radial reflecting boundary, then

$$P_{11} = \frac{2}{\pi r_1^2 \Sigma_1}\int_0^{r_1} dx \; [K_{i3}(0) - K_{i3}(2\Sigma\, y_1)] \tag{6.2}$$

$$P_{1B} = \frac{2}{\pi r_1^2 \Sigma_1}\int_0^{r_1} dx \; [K_{i3}(0) - K_{i3}(2\Sigma_1 y_1)] \tag{6.3}$$

$$P_{B1} = \frac{2}{\pi r_1} V_1 \Sigma_1 P_{1B}$$

$$= \frac{4}{\pi r_1}\int_0^{r_1} dx \; [K_{i3}(0) - K_{i3}(2\Sigma_1 y_1)] \tag{6.4}$$

$$P_{BB} = 1 - \frac{4}{\pi r_1}\int_0^{r_1} dx\, K_{i3}(2\Sigma_1 y_1) \tag{6.5}$$

$$1 - P_{BB} = 1 - \frac{4}{\pi r_1}\int_0^{r_1} dx\, K_{i3}(2\Sigma_1 y_1)$$

$$= \frac{4}{\pi r_1}\int_0^{r_1} dx \; [K_{i3}(0) - K_{i3}(2\Sigma_1 y_1)] \quad . \tag{6.6}$$

Hence $$P_{11} + \frac{P_{1B} P_{B1}}{1 - P_{BB}} = 1 \quad . \tag{6.7}$$

Thus neutrons are conserved by the boundary condition, independently of the radius r_1 of the single region cell. Evidently we require a similar conservation condition for a one region system with axial leakage. The result corresponding to 6.7 we have seen in the previous section to be

$$P_{11} + \frac{P_{1B}\,P_{B1}}{1 - P_{BB}} = \frac{\Sigma_1}{B}\tan^{-1}\frac{B}{\Sigma_1} \quad . \tag{6.8}$$

Now in the leakage situation we have the following results:

$$P_{11} = \frac{\Sigma_1}{B}\tan^{-1}\frac{B}{\Sigma_1} - \frac{2\Sigma_1}{\pi r_1^2}\int dx\,\left[\,I(0,0,B,\Sigma_1,\Sigma_1) - I(2y_1\Sigma_1,2y_1,B,\Sigma_1,\Sigma_1)\right] \tag{6.9}$$

and

$$P_{1B} = \frac{2}{\pi r_1^2}\int_0^{r_1} dx\,\left[J(0,0,B,\Sigma_1) - J(2\Sigma_1 y_1,2y_1,B,\Sigma_1)\right] \quad , \tag{6.10}$$

where the function J is defined by

$$J(x,y,b,\Sigma) = \int_0^{\pi/2} d\theta\,\sin^2\theta\, e^{-x/\sin\theta}\,\frac{\left[\Sigma\cos(By\cot\theta) - B\cos\theta\sin(By\cot\theta)\right]}{\Sigma^2 + B^2\cos^2\theta} \quad . \tag{6.11}$$

If we choose to employ the $\sin\theta\cos\psi$ distribution at the radial boundary then:

$$P_{B1} = \frac{4\Sigma_1}{\pi r_1}\int_0^{r_1} dx\,\left[J(0,0,B,\Sigma_1) - J(2\Sigma_1 y_1,2y_1,B,\Sigma_1)\right] \tag{6.12}$$

$$P_{BB} = \frac{4}{\pi r_1}\int_0^{r_1} K(2\Sigma_1 y_1,2y_1,B) \tag{6.13}$$

where the function K is defined by:

$$K(x,y,B) = \int_0^{\pi/2} d\theta\,\sin^2\theta\, e^{-x/\sin\theta}\cos(By\cot\theta) \quad . \tag{6.14}$$

Using Equations 6.9 and 6.13 we obtain

$$P_{11} + \frac{P_{1B}\,P_{B1}}{1 - P_{BB}} = \frac{\Sigma_1}{B}\tan^{-1}\frac{B}{\Sigma_1} - \frac{2\Sigma_1}{\pi r_1^2}\int_0^{r_1} dx\,\left[I(0,0,B,\Sigma_1,\Sigma_1) - I(2\Sigma_1 y_1,2y_1,B,\Sigma_1,\Sigma_1)\right] + \frac{2\Sigma_1}{\pi r_1^2}\,\frac{\left\{\int_0^{r_1} dx\,\left[J(0,0,B,\Sigma_1) - J(2\Sigma_1 y_1,2y_1,B,\Sigma_1)\right]\right\}^2}{\int_0^{r_1} dx\,\left[K(0,0,B) - K(2\Sigma_1 y_1,2y_1,B)\right]} \quad . \tag{6.15}$$

Clearly this result is unacceptable, but it suggests the modification which must be made in order to obtain the result of Equation 6.8. If we associate with the neutrons reflecting from the outer radial boundary the distribution

$$\frac{\Sigma_1}{\Sigma_1 + i\,B\cos\theta}\,\sin\theta\cos\psi \quad ,$$

rather than the $\sin\theta\cos\psi$ distribution of the axially infinite problem, then

$$P_{B1} = \frac{\Sigma_1}{r_1 J(0,0,B,\Sigma_1)} \int_0^{r_1} I(0,0,B,\Sigma_1\ \Sigma_1) - I(2\Sigma_1 y_1, 2y_1, B, \Sigma_1, \Sigma_1)\ dx \qquad (6.16)$$

and

$$P_{BB} = \frac{1}{r_1 J(0,0,B,\Sigma_1)} \int_0^{r_1} [J(2\Sigma_1 y_1, 2y_1, B, \Sigma_1)]\ dx\ . \qquad (6.17$$

Hence

$$P_{BB} = \frac{1}{r_1 J(0,0,B,\Sigma_1)} \int_0^{r_1} [J(,0,0,B,\Sigma_1) - J(2\Sigma_1 y_1, 2y_1, B, \Sigma_1)]\ dx \qquad (6.18)$$

and Equation 6.8 is immediately satisfied.

The extension of this boundary condition to multi-region cells is quite straightforward. For each region i from which neutrons start we compute the probability P_{iB} . With these neutrons reflected at the boundary we associate the distribution

$$\frac{\Sigma_i}{\Sigma_i + i\,B\cos\theta} \quad \sin\theta\cos\psi \quad ,$$

and compute P_{Bj} for each such starting distribution of neutrons. If we denote by P_{iBj} and P_{iBB} the probabilities P_{Bj} and P_{BB} for neutrons arising in region i and reflected at the boundary then

$$P_{ij} = P_{ij} + \frac{P_{iB}\,P_{iBj}}{1 - P_{iBB}} \quad . \qquad (6.19)$$

7. NUMERICAL ASPECTS OF THE CALCULATION

The calculation is essentially the same as for the axially infinite case except for the following points. Instead of the function

$$K_{i3}(x) = \int_0^{\pi/2} e^{-x/\sin\theta} \sin^2\theta\, d\theta \quad , \qquad (7.1)$$

we have to evaluate the integrals

$$J(x,y,b,\Sigma) = \int_0^{\pi/2} d\theta\, e^{-x/\sin\theta} \sin^2\theta\ \frac{[\Sigma\cos(By\cot\theta) - B\cos\theta\sin(By\cot\theta)]}{\Sigma^2 + B^2\cos^2\theta} \qquad (7.2)$$

and

$$I(x,y,B,\Sigma_1,\Sigma_2) = \int_0^{\pi/2} d\theta\ e^{-x/\sin\theta} \sin^2\theta\ \frac{[(\Sigma_1\Sigma_2 - B^2\cos^2\theta)\cos(By\cot\theta) - (\Sigma_1+\Sigma_2)B\cos\theta\sin(By\cot\theta)]}{(\Sigma_1^2 + B^2\cos^2\theta)(\Sigma_2^2 + B^2\cos^2\theta)} . \qquad (7.3)$$

Numerical experimentation showed that 16–point Gauss Legendre quadrature in θ gave adequate accuracy over the range of interest of the variables. The running times with the integrals evaluated by quadrature are prohibitively long and we have investigated expansions in B^2 for I and J. The expansions to order B^4 retain sufficient accuracy for the normal range of B^2 and are considerably faster than the quadrature method. The expansion for J is

$$J(x,y,B,\Sigma) = \frac{1}{\Sigma} K_{i3}(x) + \frac{B^2}{\Sigma}\left\{K_{i3}(x)\left[\frac{3y}{\Sigma x} - \frac{3y^2}{x^2} - \frac{1}{\Sigma^2}\right] - K_{i4}(x)\,\frac{y^2}{2x} + K_{i5}(x)\left[\frac{1}{\Sigma^2} - \frac{4y}{\Sigma x} + \frac{4y^2}{x^2}\right]\right\}$$

$$+ \frac{B^4}{\Sigma}\left\{K_{i3}(x)\left[\frac{-3y^4}{8x^2} + y^3\left(\frac{2}{3\Sigma x} - \frac{1}{\Sigma x^3}\right) + y^2\left(\frac{3}{\Sigma^2 x^2} - \frac{1}{2\Sigma^2}\right)\right.\right.$$

$$\left. + y\left(\frac{x}{5\Sigma^3} - \frac{3}{x\Sigma^3}\right) + \left(\frac{1}{\Sigma^4} - \frac{x^2}{30\Sigma^4}\right)\right]$$

$$+ K_{i4}(x)\left[\frac{-y^3}{6\Sigma x^2} + \frac{y^2}{2\Sigma^2 x} - \frac{y}{5\Sigma^3} + \frac{x}{30\Sigma^4}\right]$$

$$\left. + K_{i5}(x)\left[\frac{y^4}{2x^2} + y^3\left(\frac{4}{3\Sigma x^3} - \frac{2}{3\Sigma x}\right) + y^2\left(\frac{1}{2\Sigma^2} - \frac{4}{\Sigma^2 x^2}\right) + y\left(\frac{4}{x\Sigma^3} - \frac{x}{5\Sigma^3}\right) + \left(\frac{x^2}{30\Sigma^4} - \frac{7}{6\Sigma^4}\right)\right]\right\}$$

(7.4)

A similar expansion for I can be obtained from the relation:

$$I(x,y,B,\Sigma_1,\Sigma_2) = \frac{1}{\Sigma_1 - \Sigma_2}\left[J(x,y,B,\Sigma_2) - J(x,y,B,\Sigma_1)\right] \quad . \qquad (7.5)$$

For the argument values, $x = y = 0$, which are required for normalisation purposes:

$$J(0,0,B,\Sigma) = \frac{1}{\Sigma}\left[\frac{\pi}{4} - \frac{\pi}{16}\,\frac{B^2}{\Sigma^2} + \frac{\pi}{32}\,\frac{B^4}{\Sigma^4}\right] \qquad (7.6)$$

$$I(0,0,B,\Sigma_1,\Sigma_2) = \frac{1}{\Sigma_1\Sigma_2}\left[\frac{\pi}{4} - \frac{\pi B^2}{16}\left(\frac{1}{\Sigma_1^2} + \frac{1}{\Sigma_1\Sigma_2} + \frac{1}{\Sigma_2^2}\right)\right. \qquad (7.7)$$

$$\left. + \frac{\pi B^4}{32}\left(\frac{1}{\Sigma_1^4} + \frac{1}{\Sigma_1^3\Sigma_2} + \frac{1}{\Sigma_1^2\Sigma_2^2} + \frac{1}{\Sigma_1\Sigma_2^3} + \frac{1}{\Sigma_2^4}\right)\right] \quad .$$

The K_{in} functions appearing in Equation 7.4 and the corresponding form for I have been programmed from rational approximations due to Anderson (1970 – private communication) and Makino (1967).

The other minor computational difficulty arises because in the leakage formulation, probability is not conserved. Probability conservation in the axially infinite problem allows us to renormalise the probabilities so that they automatically satisfy the relation

$$\underset{j}{\text{Sum}}\ P_{ij} = 1 \quad . \qquad (7.8)$$

In the leakage case we cannot use this property to renormalise and must therefore pay more attention to the behaviour of the functions for large x which are often truncated in the axially infinite problem.

8. CALCULATION OF AN AXIAL DIFFUSION COEFFICIENT D_z

We define β_i by the relation

$$\beta_i = 1 - \underset{j}{\text{Sum}}\ P_{ij} \quad . \qquad (8.1)$$

The equations for the fluxes in one group can be written

$$V_i \Sigma_i^T \phi_i = \mathop{Sum}_j V_j [T_j + \Sigma_j^S \phi_j] P_{ji} \quad . \tag{8.2}$$

Summing 8.2 over all regions we obtain

$$\mathop{Sum}_i V_i \Sigma_i^T \phi_i = \mathop{Sum}_j V_j [T_j + \Sigma_j^S \phi_j] - \mathop{Sum}_j \beta_j V_j [T_j + \Sigma_j^S \phi_j] . \tag{8.3}$$

The corresponding one group homogenised axial diffusion equation can be written

$$\Sigma^T \phi = S + \Sigma^S \phi - DB^2 \phi \quad . \tag{8.4}$$

This allows us to define an axial diffusion coefficient D_z from the relation

$$D_z = \frac{\mathop{Sum}_j \beta_j V_j [T_j + \Sigma_j^S \phi_j]}{B^2 \, Sum \, V_j \phi_j} \quad . \tag{8.5}$$

In Equation 8.5 the term $T_j = \Sigma_j^S \phi_j$ represents the total neutron production rate in the group in region j. T_j contains inelastic scattering from other groups together with the fission neutron source if appropriate.

9. RESULTS AND CONCLUSIONS

In the previous sections we have developed the collision probability method for a cylindrical cell with the axial buckling term explicitly included. Despite the fact that it is unnecessary to introduce complex arithmetic into the collision probability calculation, the S_n method is computationally more efficient for this problem. The difficulties of the collision probability approach are that the integrals I and J discussed in Section 7 cannot be evaluated to sufficient accuracy by a rapid approximation, and that the application of the boundary condition derived in Section 6 includes considerably more computation than the reciprocity conditions which apply to the axially infinite problem. The results derived here will carry over unchanged to cluster geometry but the calculation will be too slow to allow routine use of this approximation.

Having established the superiority of the S_n formulation of this approximation we restricted the calculations with the collision probability code to a check of the leakage method previously used in calculations for some single rod, natural uranium, heavy water lattices (Doherty 1968). These calculations consisted of a 127 group homogeneous calculation using GYMEA (Pollard and Robinson 1969) followed by a 16 group main transport calculation using WDSN (Green 1967). The leakage was included previously by subtracting DB^2 from the self-scattering cross section Σ_{gg} of each material, where the diffusion coefficient D was calculated by GYMEA for the homogenised cell.

Since these calculations were performed, a few region condensation calculation in 69 groups, described by Doherty (1970), has been inserted between the GYMEA and WDSN steps. There have also been some changes in the basic nuclear data for these isotopes. Neither of these alterations has significantly reduced the 1 percent discrepancy between theory and experiment which was previously reported. If anything the changes in the data have made the agreement a little worse. We selected for comparison two of the lattices listed by Doherty (1968); numbers 13 and 12 of Table 3 of that reference. The first set of runs were performed for system 13; a 3.05 cm diameter rod on a 13 cm square pitch. The results of these runs are presented in Table 1.

The first run shown is reproduced from Doherty (1968). Comparison with run 2 shows the effect of data changes and the few region condensation calculation. Unfortunately the changes in data tend to worsen the agreement for all the systems considered. Run 3 is identical with run 2 except that the collision probability code ICPP replaces WDSN in the main transport calculation. The 0.33 percent discrepancy prompted further investigation in runs 4, 5, 6, 7. Run 4 shows that changing the order of integration in the ICPP calculation does not influence the result. By contrast run 5 shows that changing from S_4 to S_8 in the WDSN calculation results in a 0.09 percent increase in k. Doubling the number of moderator mesh intervals in WDSN for run 6 shows a negligible 0.01 percent increase in k. However doubling the number of moderator mesh intervals for the ICPP calculations of run 7 gives a 0.12 percent reduction in k.

Both the dependence on angle in WDSN and the dependence on moderator mesh intervals in ICPP vary, with the moderator pitch, becoming worse for the larger pitches. Table 2 shows that the difference between S_4 WDSN, and ICPP with 8 mesh intervals in the moderator is 1.2 percent for a 2.53 cm diameter rod on a 25.4 cm triangular pitch. This demonstrates that for larger pitches S_4 is inadequate in WDSN while the mesh interval in the moderator for an ICPP calculation must be chosen conservatively at 0.5 cm in D_2O. The error in the collision probability calculation is due to the flat flux assumption which becomes a poorer approximation in both the very high and very low energy groups for large pitches. The error in using S_4 in WDSN is simply that the number of angles is inadequate to represent a flux which becomes less isotropic for large pitches.

Run 8 of Table 1 repeats run 3 with the new leakage approximation giving a small increase in k of 0.2 percent. This difference is due to the use, in the DB^2 representation of leakage, of a D calculated in GYMEA for the homogenised cell. Use of the normal flux volume weighted D would largely remove the discrepancy. It was not expected that the new leakage calculation would effect a dramatic improvement in the agreement in k, and we ran these calculations merely to appraise the leakage representation previously employed.

Run 9 of Table 1 shows the sensitivity of the estimate of k to the assumed concentration of ^{235}U in natural uranium. An increase from 0.716 to 0.72 atoms percent results in an increase in k of 0.21 percent. The final k figure of 0.9997 is misleading in that the problem was run with 5 mesh regions in the moderator so that k is high by 0.1 to 0.2 percent. The final k figure of Table 2 is also based on an inadequate number of mesh points and is high by 0.4 to 0.6 percent.

Calculations on some of the other lattices confirmed the trends evident in Tables 1 and 2, and these may be summarised as follows:

(a) The use of the leakage collision probability method is worth roughly 0.2 percent in k out of a total leakage of about 14 percent. Alteration of the old method of computing D to the usual flux-volume weighted one would result in a similar improvement.

(b) An increase in the ^{235}U concentration from 0.716 to 0.72 atoms percent increases k by roughly 0.25 percent. The value of 0.72 percent is in common use and there seems little point in retaining the lower value.

(c) To ensure adequate accuracy in collision probability calculations for this type of cell, a moderator mesh interval of 0.5 cm in D_2O should suffice.

(d) S_8 should be standard for WDSN calculations on large pitches, though for clusters occupying a larger volume at the centre of the cell the error in S_4 should be smaller.

(e) The changes in data made since the previous set of calculations were performed have offset any improvement in the calculation and the results for this system remain roughly 1 percent low.

10. REFERENCES

Bonalumi, R. (1961). – Neutron fast collision probabilities in reactor physics. Energia Nucleare, 8(5): 326.

Brissenden, R.J. and Green, C. (1968). – The superposition of buckling modes on to cell calculations and applications in the computer programme WDSN. AEEW-M809.

Doherty, G. (1968). – Theoretical analysis of some heavy water natural uranium lattices. AAEC/TM461.

Doherty, G. (1969). – Some methods of calculating fast flight collision probabilities in slab and cylindrical lattices. AAEC/TM489.

Doherty, G. (1970). – Few group condensation calculations for lattice cells. AAEC/TM532.

Green, C. (1967). – The Winfrith DSN Programme, Mark 2. AEEW-R498.

Makino, K. (1967). – Some rational approximations for the Bickley function K_{in}. Nucleonik 9:351.

Pollard, J.P. and Robinson, G.S. (1969). – 360–GYMEA. A nuclide depletion, space independent, multigroup neutron diffusion data preparation code (an unpublished extension of the 7040 version AAEC/E147).